

Accurate relativistic Gaussian basis sets for H through Lr determined
by atomic SCF calculations with the third-order Douglas-Kroll approximation

Takashi Tsuchiya, Minori Abe, Takahito Nakajima, and Kimihiko Hirao

Department of Applied Chemistry, Graduate School of Engineering,

The University of Tokyo, Tokyo, Japan, 113-8656

HYDROGEN 1S(1), 2S
CHARGE = 1.000000
SYMMETRY SPECIES S
NUMBER OF BASIS FUNCTIONS 6
NUMBER OF CLOSED SHELLS 0
NUMBER OF OPEN SHELLS 1
OPEN SHELL OCCUPATION NUMBER 1

*** FINAL SCF RESULTS ***

E = -0.499952177

ORBITAL ENERGIES AND EXPANSION COEFFICIENTS

	S	1S
BASIS/ORB.ENERGY		-0.4999522
S	8.2932759D+01	0.0020043
S	1.2452437D+01	0.0152888
S	2.8330596D+00	0.0753169
S	8.0001038D-01	0.2563345
S	2.5859498D-01	0.4976187
S	8.9969184D-02	0.2967561

HELIUM 1S(2), 1S
CHARGE = 2.000000
SYMMETRY SPECIES S
NUMBER OF BASIS FUNCTIONS 6
NUMBER OF CLOSED SHELLS 1
NUMBER OF OPEN SHELLS 0
OPEN SHELL OCCUPATION NUMBER 0

*** FINAL SCF RESULTS ***

E = -2.861253228

ORBITAL ENERGIES AND EXPANSION COEFFICIENTS

	S	1S
BASIS/ORB.ENERGY		-0.9176327
S	2.3423121D+02	0.0026101
S	3.5178392D+01	0.0195509
S	7.9910313D+00	0.0910179

S 2.2124420D+00 0.2720138
S 6.6706612D-01 0.4780090
S 2.0894799D-01 0.3078198

LITHIUM 1S(2)2S(1), 2S

CHARGE = 3.000000

SYMMETRY SPECIES S

NUMBER OF BASIS FUNCTIONS 12

NUMBER OF CLOSED SHELLS 1

NUMBER OF OPEN SHELLS 1

OPEN SHELL OCCUPATION NUMBER 1

*** FINAL SCF RESULTS ***

E = -7.433370144

ORBITAL ENERGIES AND EXPANSION COEFFICIENTS

	S	1S	2S
BASIS/ORB.ENERGY		-2.4778426	-0.1963357
S 7.2374275D+03	0.0001294		-0.0000202
S 1.0797167D+03	0.0008446		-0.0001320
S 2.4550191D+02	0.0043113		-0.0006759
S 6.9535877D+01	0.0176301		-0.0027740
S 2.2661995D+01	0.0592836		-0.0094992
S 8.1311063D+00	0.1587099		-0.0263036
S 3.1001323D+00	0.3159007		-0.0572085
S 1.2283838D+00	0.4011539		-0.0951622
S 4.9395016D-01	0.1992589		-0.1215708
S 9.3077167D-02	0.0096482		0.3011788
S 4.5958947D-02	-0.0052404		0.5511039
S 2.1498396D-02	0.0017083		0.2512361

BERYLLIUM 1S(2)2S(2), 1S

CHARGE = 4.000000

SYMMETRY SPECIES S

NUMBER OF BASIS FUNCTIONS 12

NUMBER OF CLOSED SHELLS 2

NUMBER OF OPEN SHELLS 0

OPEN SHELL OCCUPATION NUMBER 0

*** FINAL SCF RESULTS ***

E = -14.575483926

ORBITAL ENERGIES AND EXPANSION COEFFICIENTS

	S	1S	2S
BASIS/ORB.ENERGY		-4.7331763	-0.3093051
S 1.4682369D+04	0.0001303		-0.0000237
S 2.1819292D+03	0.0007660		-0.0001401
S 4.9572119D+02	0.0038229		-0.0006959
S 1.4041641D+02	0.0156043		-0.0028835
S 4.5765949D+01	0.0530626		-0.0098524
S 1.6453927D+01	0.1457940		-0.0286399
S 6.3169932D+00	0.3026836		-0.0637870
S 2.5345931D+00	0.4046899		-0.1171951
S 1.0353655D+00	0.2222588		-0.1210940
S 2.5279254D-01	0.0129795		0.2535158
S 1.0516439D-01	-0.0046937		0.5818290
S 4.2606883D-02	0.0012437		0.2916449

BORON 1S(2)2S(2)2P(1), 2P

CHARGE = 5.000000

SYMMETRY SPECIES	S	P
NUMBER OF BASIS FUNCTIONS	12	8
NUMBER OF CLOSED SHELLS	2	0
NUMBER OF OPEN SHELLS	0	1
OPEN SHELL OCCUPATION NUMBER	0	1

*** FINAL SCF RESULTS ***

E = -24.535564106

ORBITAL ENERGIES AND EXPANSION COEFFICIENTS

	S	1S	2S
BASIS/ORB.ENERGY		-7.6968967	-0.4948840
S 1.3480560D+06	0.0000090		-0.0000018
S 1.2257850D+04	0.0002792		-0.0000565
S 1.8066410D+03	0.0017150		-0.0003464
S 4.0647600D+02	0.0086796		-0.0017674

S	1.1399080D+02	0.0351532	-0.0072045
S	3.6850240D+01	0.1132335	-0.0242221
S	1.3110910D+01	0.2730690	-0.0627779
S	4.9649870D+00	0.4259671	-0.1269257
S	1.9365210D+00	0.2803800	-0.1458062
S	5.0377510D-01	0.0232095	0.2137488
S	2.0607320D-01	-0.0065852	0.5870210
S	7.8884860D-02	0.0017840	0.3344241
	P	2P	
BASIS/ORB.ENERGY			
P	1.0414650D+04	0.0000010	
P	3.4853960D+01	0.0024720	
P	8.1604000D+00	0.0169461	
P	2.4504900D+00	0.0720362	
P	8.4564540D-01	0.2133820	
P	3.1535330D-01	0.4032403	
P	1.1731410D-01	0.4175701	
P	4.3559860D-02	0.1106621	

CARBON 1S(2)2S(2)2P(2), 3P

CHARGE = 6.000000

SYMMETRY SPECIES	S	P
NUMBER OF BASIS FUNCTIONS	12	8
NUMBER OF CLOSED SHELLS	2	0
NUMBER OF OPEN SHELLS	0	1
OPEN SHELL OCCUPATION NUMBER	0	2

*** FINAL SCF RESULTS ***

E = -37.703411795

ORBITAL ENERGIES AND EXPANSION COEFFICIENTS

	S	1S	2S
BASIS/ORB.ENERGY		-11.3295160	-0.7061062
S	4.5124820D+04	0.0001294	-0.0000276
S	6.1961920D+03	0.0006718	-0.0001438
S	1.3782820D+03	0.0031441	-0.0006692
S	3.8407490D+02	0.0129638	-0.0028043

S	1.2253810D+02	0.0459682	-0.0099760
S	4.3028190D+01	0.1335709	-0.0307888
S	1.6267920D+01	0.2937170	-0.0731027
S	6.4817410D+00	0.4118032	-0.1404628
S	2.6444920D+00	0.2389097	-0.1281762
S	7.3803660D-01	0.0180750	0.2734604
S	2.9059560D-01	-0.0039175	0.5831421
S	1.1263710D-01	0.0012194	0.2880620
	P	2P	
BASIS/ORB.ENERGY			-0.4330986
P	2.4525670D+05	0.0000000	
P	5.8932910D+01	0.0022559	
P	1.3755350D+01	0.0164414	
P	4.2164940D+00	0.0692941	
P	1.4937720D+00	0.2050245	
P	5.6387880D-01	0.3783243	
P	2.1711960D-01	0.4103445	
P	8.0478260D-02	0.1616921	

NITROGEN 1S(2)2S(2)2P(3), 4S

CHARGE = 7.000000

SYMMETRY SPECIES	S	P
NUMBER OF BASIS FUNCTIONS	12	8
NUMBER OF CLOSED SHELLS	2	0
NUMBER OF OPEN SHELLS	0	1
OPEN SHELL OCCUPATION NUMBER	0	3

*** FINAL SCF RESULTS ***

E = -54.429980222

ORBITAL ENERGIES AND EXPANSION COEFFICIENTS

	S	1S	2S
BASIS/ORB.ENERGY		-15.6370550	-0.9462512
S	4.8826840D+04	0.0001741	-0.0000384
S	7.2247520D+03	0.0008232	-0.0001823
S	1.6347500D+03	0.0037639	-0.0008296
S	4.6257430D+02	0.0149745	-0.0033556

S	1.5111380D+02	0.0508005	-0.0114498
S	5.4494730D+01	0.1416139	-0.0340499
S	2.1114050D+01	0.2997938	-0.0785096
S	8.6208790D+00	0.4020946	-0.1459149
S	3.5983780D+00	0.2257692	-0.1212977
S	1.0772050D+00	0.0181184	0.2682677
S	4.2258370D-01	-0.0029319	0.5829653
S	1.5943640D-01	0.0010056	0.2982498
	P	2P	
BASIS/ORB.ENERGY			-0.5672261
P	5.6295490D+02	0.0001355	
P	7.9426320D+01	0.0023242	
P	2.0132560D+01	0.0160947	
P	6.3655350D+00	0.0684727	
P	2.2806870D+00	0.2016746	
P	8.6447220D-01	0.3739485	
P	3.2919430D-01	0.4093448	
P	1.2069820D-01	0.1759819	

OXYGEN 1S(2)2S(2)2P(4), 3P

CHARGE = 8.000000

SYMMETRY SPECIES	S	P
NUMBER OF BASIS FUNCTIONS	12	8
NUMBER OF CLOSED SHELLS	2	0
NUMBER OF OPEN SHELLS	0	1
OPEN SHELL OCCUPATION NUMBER	0	4

*** FINAL SCF RESULTS ***

E = -74.861352001

ORBITAL ENERGIES AND EXPANSION COEFFICIENTS

	S	1S	2S
BASIS/ORB.ENERGY		-20.6833120	-1.2461006
S	1.0923490D+05	0.0001217	-0.0000276
S	1.5421330D+04	0.0005400	-0.0001231
S	3.2728280D+03	0.0024511	-0.0005555
S	8.7010720D+02	0.0102669	-0.0023660

S	2.6827060D+02	0.0377960	-0.0087062
S	9.1492820D+01	0.1166062	-0.0285008
S	3.3617400D+01	0.2773524	-0.0728022
S	1.3046480D+01	0.4218986	-0.1491252
S	5.2035230D+00	0.2677807	-0.1395426
S	1.4774290D+00	0.0241023	0.2652784
S	5.7775210D-01	-0.0044785	0.5898264
S	2.1267430D-01	0.0014688	0.2955465
	P	2P	
BASIS/ORB.ENERGY			
P	3.6640670D+02	0.0003957	
P	6.6279560D+01	0.0047148	
P	1.8745580D+01	0.0263073	
P	6.4268600D+00	0.0963098	
P	2.4445130D+00	0.2384549	
P	9.5771700D-01	0.3777412	
P	3.6884010D-01	0.3689625	
P	1.3644960D-01	0.1495526	

FLUORINE 1S(2)2S(2)2P(5), 2P

CHARGE = 9.000000

SYMMETRY SPECIES	S	P
NUMBER OF BASIS FUNCTIONS	12	8
NUMBER OF CLOSED SHELLS	2	0
NUMBER OF OPEN SHELLS	0	1
OPEN SHELL OCCUPATION NUMBER	0	5

*** FINAL SCF RESULTS ***

E = -99.496033584

ORBITAL ENERGIES AND EXPANSION COEFFICIENTS

	S	1S	2S
BASIS/ORB.ENERGY		-26.4073140	-1.5755631
S	1.1049550D+05	0.0001633	-0.0000378
S	1.5883580D+04	0.0006918	-0.0001611
S	3.5492390D+03	0.0029074	-0.0006727
S	9.8969550D+02	0.0113741	-0.0026796

S	3.1932050D+02	0.0393741	-0.0092684
S	1.1337070D+02	0.1157825	-0.0289983
S	4.2968910D+01	0.2708393	-0.0727212
S	1.6933990D+01	0.4178100	-0.1504609
S	6.7785120D+00	0.2738892	-0.1421046
S	1.9343030D+00	0.0262721	0.2671760
S	7.5047140D-01	-0.0047615	0.5926633
S	2.7320820D-01	0.0016021	0.2927879
	P	2P	
BASIS/ORB.ENERGY			-0.7293400
P	3.4519790D+02	0.0006124	
P	7.4125440D+01	0.0056268	
P	2.2561850D+01	0.0288925	
P	7.9804130D+00	0.1031980	
P	3.0727400D+00	0.2457403	
P	1.2100660D+00	0.3742403	
P	4.6432470D-01	0.3603010	
P	1.6923000D-01	0.1512699	

NEON 1S(2)2S(2)2P(6), 1S

CHARGE = 10.000000

SYMMETRY SPECIES	S	P
NUMBER OF BASIS FUNCTIONS	12	8
NUMBER OF CLOSED SHELLS	2	1
NUMBER OF OPEN SHELLS	0	0
OPEN SHELL OCCUPATION NUMBER	0	0

*** FINAL SCF RESULTS ***

E = -128.684089534

ORBITAL ENERGIES AND EXPANSION COEFFICIENTS

	S	1S	2S
BASIS/ORB.ENERGY		-32.8115270	-1.9354010
S	1.0027703D+05	0.0002301	-0.0000541
S	1.5024777D+04	0.0009442	-0.0002231
S	3.4194243D+03	0.0039169	-0.0009214
S	9.6833099D+02	0.0150440	-0.0036033

S	3.1576162D+02	0.0506811	-0.0122007
S	1.1381543D+02	0.1415561	-0.0365407
S	4.4142643D+01	0.3015704	-0.0851788
S	1.8081932D+01	0.4014370	-0.1581241
S	7.5854437D+00	0.2227955	-0.1160160
S	2.3503864D+00	0.0191502	0.2965008
S	9.0552447D-01	-0.0022686	0.5861880
S	3.3151899D-01	0.0009763	0.2735738
	P	2P	
BASIS/ORB.ENERGY			-0.8496043
P	2.9874009D+02	0.0010899	
P	7.0702612D+01	0.0084663	
P	2.2515939D+01	0.0396798	
P	8.2802704D+00	0.1273139	
P	3.2879672D+00	0.2691812	
P	1.3221027D+00	0.3712341	
P	5.1743659D-01	0.3298036	
P	1.9198390D-01	0.1281071	

SODIUM K(2)L(8)3S(1), 2S

CHARGE = 11.000000

SYMMETRY SPECIES	S	P
NUMBER OF BASIS FUNCTIONS	16	11
NUMBER OF CLOSED SHELLS	2	1
NUMBER OF OPEN SHELLS	1	0
OPEN SHELL OCCUPATION NUMBER	1	0

*** FINAL SCF RESULTS ***

E = -162.068053304

ORBITAL ENERGIES AND EXPANSION COEFFICIENTS

	S	1S	2S	3S
BASIS/ORB.ENERGY		-40.5371590	-2.8048964	-0.1823184
S	5.0537790D+08	0.0000009	-0.0000002	0.0000000
S	3.5490950D+05	0.0001046	-0.0000256	-0.0000039
S	4.9559050D+04	0.0003971	-0.0000972	-0.0000146
S	1.0648830D+04	0.0014924	-0.0003672	-0.0000551

S	2.8641880D+03	0.0055392	-0.0013582	-0.0002050
S	8.9995120D+02	0.0193017	-0.0048217	-0.0007233
S	3.1521240D+02	0.0598792	-0.0151217	-0.0022910
S	1.1999330D+02	0.1549282	-0.0420946	-0.0063303
S	4.8706540D+01	0.3074808	-0.0927452	-0.0142569
S	2.0732000D+01	0.3840697	-0.1621367	-0.0248682
S	8.9898210D+00	0.2049141	-0.1112899	-0.0184020
S	3.0107970D+00	0.0189263	0.2849907	0.0520755
S	1.2157860D+00	-0.0020099	0.5849984	0.1147950
S	4.8074890D-01	0.0010174	0.2825873	0.1674811
S	5.9497170D-02	-0.0001671	0.0051616	-0.6326926
S	2.3714950D-02	0.0000841	-0.0017567	-0.4660395

P 2P

BASIS/ORB. ENERGY -1.5169595

P	1.2039210D+03	0.0001697
P	2.7918010D+02	0.0013579
P	8.9503960D+01	0.0073022
P	3.3513740D+01	0.0288675
P	1.3784940D+01	0.0874884
P	6.0591920D+00	0.1928101
P	2.7675380D+00	0.2966548
P	1.2969130D+00	0.3158156
P	6.4171030D-01	0.2174861
P	3.3142390D-01	0.0928687
P	1.5156870D-01	0.0131758

MAGNESIUM K(2)L(8)3S(2), 1S

CHARGE = 12.000000

SYMMETRY SPECIES S P

NUMBER OF BASIS FUNCTIONS 16 11

NUMBER OF CLOSED SHELLS 3 1

NUMBER OF OPEN SHELLS 0 0

OPEN SHELL OCCUPATION NUMBER 0 0

*** FINAL SCF RESULTS ***

E = -199.921720023

ORBITAL ENERGIES AND EXPANSION COEFFICIENTS

	S	1S	2S	3S
BASIS/ORB. ENERGY		-49.1164370	-3.7795254	-0.2533505
S 1.6940680D+06		0.0000409	-0.0000104	-0.0000020
S 1.9233690D+05		0.0001624	-0.0000412	-0.0000079
S 3.9966580D+04		0.0005057	-0.0001282	-0.0000247
S 1.0658150D+04		0.0016602	-0.0004227	-0.0000815
S 3.2031780D+03		0.0056951	-0.0014490	-0.0002786
S 1.0644670D+03		0.0189089	-0.0048813	-0.0009435
S 3.8524090D+02		0.0569286	-0.0149340	-0.0028729
S 1.4966940D+02		0.1464135	-0.0409087	-0.0079635
S 6.1396250D+01		0.2948228	-0.0920185	-0.0178703
S 2.6307710D+01		0.3833976	-0.1614845	-0.0325137
S 1.1481140D+01		0.2232379	-0.1314242	-0.0264202
S 4.1640140D+00		0.0252294	0.2187985	0.0477700
S 1.7538990D+00		-0.0021028	0.5828543	0.1612811
S 7.1374240D-01		0.0011183	0.3494029	0.2017332
S 1.1313050D-01		-0.0001740	0.0100994	-0.5961927
S 4.0721010D-02		0.0000771	-0.0031912	-0.5327349
	P	2P		
BASIS/ORB. ENERGY		-2.2804445		
P 1.2134440D+03		-0.0002479		
P 2.7466330D+02		-0.0020541		
P 8.7111880D+01		-0.0108897		
P 3.2753450D+01		-0.0411937		
P 1.3630200D+01		-0.1169983		
P 6.0397180D+00		-0.2373102		
P 2.7455230D+00		-0.3388711		
P 1.2383500D+00		-0.3441383		
P 9.0131990D-01		0.0369074		
P 5.8515990D-01		-0.1675183		
P 2.3001770D-01		-0.0184309		

ALUMINUM K(2)L(8)3S(2)3P(1), 2P
 CHARGE = 13.000000

SYMMETRY SPECIES	S	P
NUMBER OF BASIS FUNCTIONS	16	11
NUMBER OF CLOSED SHELLS	3	1
NUMBER OF OPEN SHELLS	0	1
OPEN SHELL OCCUPATION NUMBER	0	1

*** FINAL SCF RESULTS ***

E = -242.313123200

ORBITAL ENERGIES AND EXPANSION COEFFICIENTS

	S	1S	2S	3S
BASIS/ORB.ENERGY		-58.6202430	-4.9282867	-0.3941824
S 1.4629480D+06	0.0000535	-0.0000140	-0.0000032	
S 1.9152620D+05	0.0001987	-0.0000519	-0.0000120	
S 3.7762870D+04	0.0006852	-0.0001789	-0.0000412	
S 9.8457790D+03	0.0021881	-0.0005737	-0.0001329	
S 3.0711180D+03	0.0070158	-0.0018399	-0.0004227	
S 1.0708940D+03	0.0218383	-0.0058192	-0.0013542	
S 4.0689400D+02	0.0612084	-0.0166029	-0.0038102	
S 1.6595320D+02	0.1477088	-0.0427940	-0.0100643	
S 7.0830320D+01	0.2882614	-0.0932823	-0.0215774	
S 3.1078560D+01	0.3763509	-0.1636461	-0.0401129	
S 1.3714470D+01	0.2246346	-0.1356255	-0.0320189	
S 5.1101110D+00	0.0269217	0.2083737	0.0523983	
S 2.2218860D+00	-0.0021837	0.5781054	0.2066897	
S 9.3876970D-01	0.0011545	0.3623572	0.2317678	
S 1.8217580D-01	-0.0001952	0.0131123	-0.6262596	
S 6.5149610D-02	0.0000763	-0.0033545	-0.5316555	
	P	2P	3P	
BASIS/ORB.ENERGY		-3.2162687	-0.2094584	
P 1.3478230D+03	0.0002880	-0.0000519		
P 3.1320780D+02	0.0023009	-0.0004135		
P 9.7617320D+01	0.0129228	-0.0023392		
P 3.5127490D+01	0.0529030	-0.0096323		
P 1.3850100D+01	0.1572720	-0.0293251		
P 5.7392250D+00	0.3157161	-0.0595749		
P 2.4003200D+00	0.4036788	-0.0808808		

P	9.9561500D-01	0.2551224	-0.0496639
P	3.3667850D-01	0.0327197	0.1963935
P	1.2119170D-01	-0.0032202	0.5530354
P	4.2488240D-02	0.0012276	0.3990669

SILICON K(2)L(8)3S(2)3P(2), 3P

CHARGE = 14.000000

SYMMETRY SPECIES	S	P
NUMBER OF BASIS FUNCTIONS	16	11
NUMBER OF CLOSED SHELLS	3	1
NUMBER OF OPEN SHELLS	0	1
OPEN SHELL OCCUPATION NUMBER	0	2

*** FINAL SCF RESULTS ***

E = -289.458522579

ORBITAL ENERGIES AND EXPANSION COEFFICIENTS

	S	1S	2S	3S
BASIS/ORB. ENERGY		-68.9763470	-6.1821790	-0.5413992
S	1.4532050D+06	0.0000667	-0.0000178	-0.0000046
S	1.8302460D+05	0.0002489	-0.0000666	-0.0000171
S	3.7505200D+04	0.0008177	-0.0002188	-0.0000559
S	9.8992510D+03	0.0026394	-0.0007092	-0.0001825
S	3.0673790D+03	0.0085157	-0.0022918	-0.0005837
S	1.0688040D+03	0.0261926	-0.0071705	-0.0018557
S	4.0615850D+02	0.0729649	-0.0204393	-0.0051983
S	1.6487680D+02	0.1725112	-0.0520887	-0.0136655
S	7.0465290D+01	0.3148181	-0.1086411	-0.0278661
S	3.1359840D+01	0.3599734	-0.1729309	-0.0480449
S	1.4240230D+01	0.1792547	-0.1073098	-0.0267738
S	5.5168310D+00	0.0184579	0.2679652	0.0747961
S	2.4571510D+00	-0.0011922	0.5748153	0.2582519
S	1.0999210D+00	0.0007870	0.3080514	0.2123543
S	2.5729500D-01	-0.0001432	0.0117947	-0.6487283
S	9.1532160D-02	0.0000455	-0.0022364	-0.5312266
	P	2P	3P	
BASIS/ORB. ENERGY		-4.2541900	-0.2964965	

P	1.7614500D+03	0.0002832	-0.0000608
P	3.5227440D+02	0.0027537	-0.0005865
P	1.0383810D+02	0.0160379	-0.0034693
P	3.6926340D+01	0.0642406	-0.0139080
P	1.4694410D+01	0.1792795	-0.0403209
P	6.2293350D+00	0.3313769	-0.0744519
P	2.7058220D+00	0.3887278	-0.0976293
P	1.1769120D+00	0.2173788	-0.0326605
P	4.1866660D-01	0.0246143	0.2718293
P	1.6047890D-01	-0.0020769	0.5526579
P	5.9297820D-02	0.0008805	0.3192874

PHOSPHORUS K(2)L(8)3S(2)3P(3), 4S

CHARGE = 15.000000

SYMMETRY SPECIES	S	P
NUMBER OF BASIS FUNCTIONS	16	11
NUMBER OF CLOSED SHELLS	3	1
NUMBER OF OPEN SHELLS	0	1
OPEN SHELL OCCUPATION NUMBER	0	3

*** FINAL SCF RESULTS ***

E = -341.536165018

ORBITAL ENERGIES AND EXPANSION COEFFICIENTS

	S	1S	2S	3S
BASIS/ORB. ENERGY		-80.1898310	-7.5471161	-0.6990913
S	1.4602470D+06	0.0000799	-0.0000218	-0.0000060
S	1.8357460D+05	0.0002983	-0.0000815	-0.0000224
S	3.7467910D+04	0.0009823	-0.0002683	-0.0000736
S	9.8733730D+03	0.0031603	-0.0008676	-0.0002394
S	3.0623380D+03	0.0101486	-0.0027913	-0.0007634
S	1.0676600D+03	0.0310082	-0.0086988	-0.0024129
S	4.0618090D+02	0.0851386	-0.0245254	-0.0067078
S	1.6496500D+02	0.1963054	-0.0616759	-0.0173632
S	7.0411130D+01	0.3396839	-0.1245954	-0.0345378
S	3.1296320D+01	0.3436426	-0.1832001	-0.0551420
S	1.4259500D+01	0.1354679	-0.0655892	-0.0162065

S	5.5701620D+00	0.0100754	0.3728315	0.1199906
S	2.4627800D+00	-0.0002121	0.5731492	0.3242153
S	1.1410240D+00	0.0003356	0.2005328	0.1337547
S	3.3118200D-01	-0.0000816	0.0070642	-0.6805545
S	1.1800560D-01	0.0000157	-0.0006752	-0.5112161
	P	2P	3P	
BASIS/ORB.ENERGY		-5.3994972	-0.3909960	
P	2.0882410D+03	0.0002742	-0.0000656	
P	4.4994810D+02	0.0023603	-0.0005583	
P	1.3483760D+02	0.0138646	-0.0033418	
P	4.7843450D+01	0.0572872	-0.0137795	
P	1.8974450D+01	0.1670816	-0.0419335	
P	7.9999640D+00	0.3275287	-0.0822622	
P	3.4517080D+00	0.4007563	-0.1127047	
P	1.4990910D+00	0.2246035	-0.0327455	
P	5.4416330D-01	0.0250935	0.3047042	
P	2.1177930D-01	-0.0020020	0.5516408	
P	7.9410370D-02	0.0007155	0.2866630	

SULFUR K(2)L(8)3S(2)3P(4), 3P

CHARGE = 16.000000

SYMMETRY SPECIES S P

NUMBER OF BASIS FUNCTIONS 16 11

NUMBER OF CLOSED SHELLS 3 1

NUMBER OF OPEN SHELLS 0 1

OPEN SHELL OCCUPATION NUMBER 0 4

*** FINAL SCF RESULTS ***

E = -398.589026149

ORBITAL ENERGIES AND EXPANSION COEFFICIENTS

	S	1S	2S	3S
BASIS/ORB.ENERGY		-92.2943170	-9.0535284	-0.8837449
S	1.4624900D+06	0.0000949	-0.0000264	-0.0000077
S	1.8318600D+05	0.0003547	-0.0000986	-0.0000287
S	3.7362930D+04	0.0011669	-0.0003246	-0.0000942
S	9.8356230D+03	0.0037462	-0.0010473	-0.0003048

S	3.0561810D+03	0.0119436	-0.0033512	-0.0009715
S	1.0666020D+03	0.0363168	-0.0104018	-0.0030393
S	4.0570210D+02	0.0982349	-0.0290825	-0.0084563
S	1.6515130D+02	0.2193767	-0.0714582	-0.0211813
S	7.0536460D+01	0.3597905	-0.1406737	-0.0418334
S	3.1093080D+01	0.3249012	-0.1895865	-0.0601227
S	1.3786740D+01	0.0962670	-0.0132518	-0.0017705
S	5.6284700D+00	0.0030813	0.4727353	0.1783915
S	2.4316130D+00	0.0011935	0.5593349	0.3805907
S	1.0160220D+00	-0.0003571	0.1013694	0.0126380
S	3.8879040D-01	0.0001159	-0.0012976	-0.7170143
S	1.4182360D-01	-0.0000422	0.0010433	-0.4553098
	P	2P	3P	
BASIS/ORB. ENERGY		-6.6817980	-0.4365443	
P	2.0282170D+03	0.0003641	0.0000935	
P	4.6207420D+02	0.0027823	0.0007043	
P	1.4752100D+02	0.0145342	0.0037663	
P	5.5026120D+01	0.0565753	0.0145733	
P	2.2478250D+01	0.1623156	0.0438971	
P	9.6724070D+00	0.3204720	0.0864364	
P	4.2437700D+00	0.4003962	0.1223351	
P	1.8672210D+00	0.2301640	0.0295494	
P	6.8571640D-01	0.0268264	-0.3270710	
P	2.6217470D-01	-0.0016492	-0.5439183	
P	9.5072720D-02	0.0009415	-0.2792492	

CHLORINE K(2)L(8)3S(2)3P(5), 2P

CHARGE = 17.000000

SYMMETRY SPECIES S P

NUMBER OF BASIS FUNCTIONS 16 11

NUMBER OF CLOSED SHELLS 3 1

NUMBER OF OPEN SHELLS 0 1

OPEN SHELL OCCUPATION NUMBER 0 5

*** FINAL SCF RESULTS ***

E = -460.895255882

ORBITAL ENERGIES AND EXPANSION COEFFICIENTS

	S	1S	2S	3S
BASIS/ORB. ENERGY		-105.2598300	-10.6733940	-1.0791419
S 1.4681380D+06		0.0001118	-0.0000316	-0.0000095
S 1.8161420D+05		0.0004211	-0.0001189	-0.0000360
S 3.7093820D+04		0.0013699	-0.0003874	-0.0001173
S 9.8301760D+03		0.0043731	-0.0012414	-0.0003757
S 3.0535910D+03		0.0139379	-0.0039839	-0.0012082
S 1.0656650D+03		0.0420525	-0.0122576	-0.0037167
S 4.0523290D+02		0.1122642	-0.0341506	-0.0104256
S 1.6511050D+02		0.2422433	-0.0815492	-0.0250499
S 7.0764460D+01		0.3728166	-0.1559381	-0.0492284
S 3.0964810D+01		0.3018821	-0.1875583	-0.0612376
S 1.2781670D+01		0.0660723	0.0556172	0.0189292
S 5.6325000D+00		-0.0029390	0.5440752	0.2415652
S 2.4608260D+00		0.0023649	0.4968049	0.3763121
S 8.3277000D-01		-0.0009642	0.0558749	-0.1971496
S 3.8426000D-01		0.0004972	-0.0094582	-0.6925665
S 1.5207480D-01		-0.0001359	0.0024678	-0.3284964
	P	2P	3P	
BASIS/ORB. ENERGY		-8.0728397	-0.5055126	
P 2.1826550D+03		0.0004305	0.0001166	
P 4.6749890D+02		0.0035851	0.0009634	
P 1.4475210D+02		0.0190612	0.0052175	
P 5.3805760D+01		0.0709965	0.0195011	
P 2.2302900D+01		0.1890280	0.0543788	
P 9.7571330D+00		0.3433744	0.0994406	
P 4.3889950D+00		0.3816835	0.1259261	
P 1.9935790D+00		0.1833206	-0.0059708	
P 7.8229290D-01		0.0183511	-0.3638986	
P 3.0360500D-01		0.0001605	-0.5226703	
P 1.1144440D-01		0.0006800	-0.2519793	

 ARGON 1S(2)2S(2)2P(6)3S(2)3P(6), 1S
 CHARGE = 18.000000

SYMMETRY SPECIES	S	P
NUMBER OF BASIS FUNCTIONS	16	11
NUMBER OF CLOSED SHELLS	3	2
NUMBER OF OPEN SHELLS	0	0
OPEN SHELL OCCUPATION NUMBER	0	0

*** FINAL SCF RESULTS ***

E = -528.631401375

ORBITAL ENERGIES AND EXPANSION COEFFICIENTS

	S	1S	2S	3S
BASIS/ORB.ENERGY		-119.0893400	-12.4087510	-1.2862042
S 9.0594654D+05	0.0001793	-0.0000513	-0.0000160	
S 1.3567833D+05	0.0005718	-0.0001637	-0.0000512	
S 3.0875153D+04	0.0017862	-0.0005126	-0.0001604	
S 8.7435747D+03	0.0054639	-0.0015731	-0.0004915	
S 2.8515182D+03	0.0167481	-0.0048709	-0.0015280	
S 1.0287890D+03	0.0487578	-0.0144591	-0.0045253	
S 4.0062368D+02	0.1256297	-0.0392332	-0.0124104	
S 1.6543793D+02	0.2622661	-0.0912103	-0.0289542	
S 7.1440876D+01	0.3769579	-0.1679430	-0.0553033	
S 3.1593420D+01	0.2705108	-0.1751224	-0.0591078	
S 1.2909758D+01	0.0496431	0.1088562	0.0384730	
S 5.9392494D+00	-0.0035105	0.5631311	0.2772990	
S 2.6826989D+00	0.0021569	0.4455695	0.3586965	
S 9.4345618D-01	-0.0008537	0.0446656	-0.2783291	
S 4.2511714D-01	0.0004017	-0.0057314	-0.6808338	
S 1.7179354D-01	-0.0001151	0.0017962	-0.2806506	
	P	2P	3P	
BASIS/ORB.ENERGY		-9.5741318	-0.5901651	
P 1.8688067D+03	0.0006458	0.0001809		
P 4.4294722D+02	0.0046354	0.0012970		
P 1.4319547D+02	0.0233101	0.0066077		
P 5.4013866D+01	0.0848159	0.0243936		
P 2.2378905D+01	0.2185501	0.0653639		
P 9.7396561D+00	0.3739721	0.1152319		
P 4.3610083D+00	0.3643618	0.1227584		

P	1.9585564D+00	0.1284126	-0.0660230
P	8.2555522D-01	0.0069578	-0.4036956
P	3.2961519D-01	0.0008114	-0.4897753
P	1.2421539D-01	-0.0001458	-0.2085800

POTASSIUM K(2)L(8)3S(2)3P(6)4S(1), 2S

CHARGE = 19.000000

SYMMETRY SPECIES	S	P
NUMBER OF BASIS FUNCTIONS	20	15
NUMBER OF CLOSED SHELLS	3	2
NUMBER OF OPEN SHELLS	1	0
OPEN SHELL OCCUPATION NUMBER	1	0

*** FINAL SCF RESULTS ***

E = -601.464033940

ORBITAL ENERGIES AND EXPANSION COEFFICIENTS

	S	1S	2S	3S	4S
BASIS/ORB. ENERGY		-134.1355200	-14.6011590	-1.7608667	-0.1475703
S	1.4612300D+07	0.0000266	-0.0000077	-0.0000025	-0.0000005
S	1.7414610D+06	0.0000961	-0.0000278	-0.0000092	-0.0000018
S	3.3617610D+05	0.0002874	-0.0000833	-0.0000274	-0.0000053
S	8.4319950D+04	0.0007870	-0.0002284	-0.0000754	-0.0000146
S	2.5264470D+04	0.0020805	-0.0006044	-0.0001989	-0.0000381
S	8.6259150D+03	0.0055200	-0.0016136	-0.0005337	-0.0001039
S	3.2209340D+03	0.0149213	-0.0043847	-0.0014420	-0.0002746
S	1.2857860D+03	0.0392041	-0.0117771	-0.0039145	-0.0007676
S	5.4360000D+02	0.0945382	-0.0293776	-0.0096949	-0.0018319
S	2.4031470D+02	0.1975968	-0.0671203	-0.0226560	-0.0044908
S	1.0970850D+02	0.3215846	-0.1283417	-0.0433140	-0.0080798
S	5.1441940D+01	0.3244053	-0.1822897	-0.0656580	-0.0134905
S	2.4486550D+01	0.1422935	-0.0812799	-0.0278299	-0.0039308
S	1.0391780D+01	0.0138401	0.3222522	0.1326497	0.0226153
S	4.9151520D+00	-0.0005783	0.5770640	0.3830288	0.0883167
S	2.3731580D+00	0.0004626	0.2501091	0.2030631	0.0279982
S	8.7295440D-01	-0.0002111	0.0168898	-0.5681065	-0.1100322
S	3.7526360D-01	0.0000700	-0.0016616	-0.5939107	-0.2832183

S	1.6715900D-01	-0.0000301	0.0008655	-0.0910756	-0.0372829
S	2.7677640D-02	0.0000033	-0.0000840	-0.0010192	1.0759191
	P	2P	3P		
BASIS/ORB.ENERGY		-11.5242390	-0.9530912		
P	1.1082040D+05	0.0000059	-0.0000018		
P	1.4565150D+04	0.0000416	-0.0000127		
P	3.3308110D+03	0.0002462	-0.0000749		
P	1.0190310D+03	0.0013023	-0.0003987		
P	3.6797120D+02	0.0059467	-0.0018189		
P	1.4780250D+02	0.0226199	-0.0070091		
P	6.4062590D+01	0.0701561	-0.0220302		
P	2.9418030D+01	0.1698291	-0.0552435		
P	1.3980790D+01	0.3025259	-0.1009779		
P	6.7780980D+00	0.3624998	-0.1313478		
P	3.3199720D+00	0.2241502	-0.0482041		
P	1.5460510D+00	0.0437275	0.2292632		
P	7.1067870D-01	0.0001945	0.4599655		
P	3.1792930D-01	0.0006921	0.3791873		
P	1.3372930D-01	-0.0001575	0.0896727		

CALCIUM K(2)L(8)3S(2)3P(6)4S(2), 1S

CHARGE = 20.000000

SYMMETRY SPECIES S P

NUMBER OF BASIS FUNCTIONS 20 15

NUMBER OF CLOSED SHELLS 4 2

NUMBER OF OPEN SHELLS 0 0

OPEN SHELL OCCUPATION NUMBER 0 0

*** FINAL SCF RESULTS ***

E = -679.636932919

ORBITAL ENERGIES AND EXPANSION COEFFICIENTS

	S	1S	2S	3S	4S
BASIS/ORB.ENERGY		-150.1121800	-16.9634810	-2.2616005	-0.1962555
S	1.5429060D+07	0.0000301	-0.0000088	-0.0000030	-0.0000007
S	1.7177660D+06	0.0001145	-0.0000335	-0.0000116	-0.0000028
S	3.2529080D+05	0.0003372	-0.0000988	-0.0000341	-0.0000081

S	8.3104290D+04	0.0009008	-0.0002645	-0.0000913	-0.0000218
S	2.5219110D+04	0.0023628	-0.0006946	-0.0002394	-0.0000572
S	8.6628000D+03	0.0062755	-0.0018570	-0.0006423	-0.0001537
S	3.2209670D+03	0.0170451	-0.0050761	-0.0017494	-0.0004176
S	1.2837380D+03	0.0443690	-0.0135341	-0.0047028	-0.0011264
S	5.4345920D+02	0.1053518	-0.0333900	-0.0115647	-0.0027619
S	2.4083900D+02	0.2148118	-0.0750735	-0.0265217	-0.0063676
S	1.0996770D+02	0.3356527	-0.1403827	-0.0499914	-0.0119729
S	5.1344530D+01	0.3098439	-0.1865678	-0.0707038	-0.0171470
S	2.4284190D+01	0.1121979	-0.0437062	-0.0151920	-0.0035388
S	1.0500930D+01	0.0076599	0.4006365	0.1845486	0.0455655
S	4.9229230D+00	0.0003493	0.5694037	0.4374290	0.1163776
S	2.3406070D+00	-0.0000342	0.1761242	0.1071278	0.0248393
S	9.2145250D-01	-0.0000417	0.0079433	-0.7090708	-0.2298038
S	3.8267100D-01	-0.0000153	0.0004690	-0.5241506	-0.3351936
S	6.5332900D-02	0.0000009	0.0000715	-0.0146731	0.6714642
S	2.6184550D-02	-0.0000005	-0.0000301	0.0046132	0.4919800

P

2P

3P

BASIS/ORB. ENERGY	-13.6371450	-1.3388309			
P	5.1912480D+04	0.0000146	-0.0000047		
P	8.8878330D+03	0.0000849	-0.0000277		
P	2.4233700D+03	0.0004355	-0.0001419		
P	8.3383440D+02	0.0019901	-0.0006511		
P	3.2965730D+02	0.0078672	-0.0025796		
P	1.4247560D+02	0.0265166	-0.0087995		
P	6.5465540D+01	0.0752583	-0.0254087		
P	3.1433170D+01	0.1713689	-0.0597992		
P	1.5494100D+01	0.2944578	-0.1059786		
P	7.7651150D+00	0.3493499	-0.1353237		
P	3.9249850D+00	0.2223632	-0.0549790		
P	1.9243700D+00	0.0498780	0.2133267		
P	9.1383950D-01	0.0015917	0.4657830		
P	4.2021050D-01	0.0004597	0.3898355		
P	1.7575970D-01	-0.0001154	0.0852798		

SCANDIUM K(2)L(8)3S(2)3P(6)4S(2)3D(1), 2D

CHARGE = 21.000000

SYMMETRY SPECIES	S	P	D
NUMBER OF BASIS FUNCTIONS	20	15	9
NUMBER OF CLOSED SHELLS	4	2	0
NUMBER OF OPEN SHELLS	0	0	1
OPEN SHELL OCCUPATION NUMBER	0	0	1

*** FINAL SCF RESULTS ***

E = -763.292507304

ORBITAL ENERGIES AND EXPANSION COEFFICIENTS

	S	1S	2S	3S	4S
BASIS/ORB.ENERGY		-166.8243700	-19.2610690	-2.5910906	-0.2113551
S	1.2809350D+07	0.0000387	-0.0000114	-0.0000040	-0.0000010
S	1.5431980D+06	0.0001370	-0.0000406	-0.0000143	-0.0000034
S	3.0974160D+05	0.0003861	-0.0001144	-0.0000403	-0.0000096
S	8.2804010D+04	0.0010020	-0.0002974	-0.0001048	-0.0000249
S	2.5477230D+04	0.0026732	-0.0007946	-0.0002801	-0.0000666
S	8.6623970D+03	0.0071683	-0.0021448	-0.0007568	-0.0001800
S	3.2094240D+03	0.0193904	-0.0058491	-0.0020650	-0.0004916
S	1.2778540D+03	0.0498876	-0.0154348	-0.0054673	-0.0012997
S	5.4418700D+02	0.1158760	-0.0374524	-0.0133198	-0.0031768
S	2.4156850D+02	0.2325375	-0.0835185	-0.0300810	-0.0071584
S	1.1006900D+02	0.3467476	-0.1523048	-0.0560996	-0.0134610
S	5.1222490D+01	0.2914675	-0.1863312	-0.0720061	-0.0172160
S	2.3850440D+01	0.0865039	-0.0008152	0.0000968	-0.0002343
S	1.0651950D+01	0.0029663	0.4671566	0.2380429	0.0601117
S	4.9512770D+00	0.0011623	0.5487909	0.4576474	0.1203099
S	2.2012840D+00	-0.0004857	0.1182131	0.0013824	-0.0021951
S	9.9520890D-01	0.0001635	-0.0007764	-0.7278829	-0.2475604
S	4.2603180D-01	-0.0000761	0.0019534	-0.4718296	-0.3059261
S	7.6349140D-02	0.0000146	-0.0002146	-0.0131891	0.6550520
S	2.9666690D-02	-0.0000065	0.0000958	0.0039087	0.5102173
	P	2P	3P		
BASIS/ORB.ENERGY		-15.6843960	-1.5747796		
P	5.2100920D+04	0.0000177	-0.0000059		

P	8.8783560D+03	0.0001035	-0.0000348
P	2.4202830D+03	0.0005280	-0.0001774
P	8.3395720D+02	0.0023998	-0.0008107
P	3.2971210D+02	0.0094288	-0.0031911
P	1.4248480D+02	0.0314558	-0.0108029
P	6.5473930D+01	0.0876841	-0.0306824
P	3.1440280D+01	0.1930508	-0.0700754
P	1.5489910D+01	0.3163978	-0.1188175
P	7.7698220D+00	0.3423856	-0.1386523
P	3.9262920D+00	0.1839043	-0.0117785
P	1.9039380D+00	0.0316476	0.2883732
P	9.0668620D-01	0.0005783	0.4788257
P	4.2230460D-01	0.0003884	0.3167219
P	1.7530430D-01	-0.0000695	0.0520694
	D	3D	
BASIS/ORB. ENERGY			-0.3357116
D	1.2598350D+02	0.0007795	
D	3.6094410D+01	0.0068256	
D	1.3193220D+01	0.0308203	
D	5.2908960D+00	0.0960128	
D	2.2767190D+00	0.2112964	
D	9.9784630D-01	0.3183156	
D	4.3224480D-01	0.3535379	
D	1.8104010D-01	0.2624935	
D	7.0556810D-02	0.0872456	

TITANIUM K(2)L(8)3S(2)3P(6)4S(2)3D(2), 3F

CHARGE = 22.000000

SYMMETRY SPECIES	S	P	D
NUMBER OF BASIS FUNCTIONS	20	15	9
NUMBER OF CLOSED SHELLS	4	2	0
NUMBER OF OPEN SHELLS	0	0	1
OPEN SHELL OCCUPATION NUMBER	0	0	2

*** FINAL SCF RESULTS ***

E = -852.754544452

ORBITAL ENERGIES AND EXPANSION COEFFICIENTS

	S	1S	2S	3S	4S
BASIS/ORB. ENERGY		-184.4021600	-21.6494830	-2.9050549	-0.2223638
S 1.6528400D+07		0.0000371	-0.0000111	-0.0000040	-0.0000009
S 1.8552430D+06		0.0001406	-0.0000420	-0.0000150	-0.0000035
S 3.4234070D+05		0.0004316	-0.0001291	-0.0000462	-0.0000108
S 8.3105730D+04		0.0012053	-0.0003611	-0.0001293	-0.0000301
S 2.4246960D+04		0.0032488	-0.0009758	-0.0003490	-0.0000813
S 8.1300170D+03		0.0086461	-0.0026141	-0.0009378	-0.0002186
S 3.0479930D+03		0.0224573	-0.0068627	-0.0024556	-0.0005722
S 1.2499940D+03		0.0551190	-0.0172924	-0.0062393	-0.0014550
S 5.4615680D+02		0.1235688	-0.0407097	-0.0146619	-0.0034211
S 2.4848620D+02		0.2367399	-0.0869193	-0.0319972	-0.0074756
S 1.1629540D+02		0.3378931	-0.1526179	-0.0568428	-0.0133342
S 5.5604170D+01		0.2777385	-0.1798181	-0.0717673	-0.0168980
S 2.6720930D+01		0.0858563	-0.0074375	-0.0003558	-0.0001554
S 1.2459630D+01		0.0041656	0.4191964	0.2085994	0.0511645
S 6.0568740D+00		0.0009928	0.5457253	0.4523185	0.1168876
S 2.9410320D+00		-0.0003155	0.1691505	0.0758409	0.0174153
S 1.1928670D+00		0.0000486	0.0077006	-0.7209540	-0.2362647
S 4.9985810D-01		-0.0000427	0.0007043	-0.5097614	-0.3087522
S 8.3406730D-02		0.0000070	0.0000264	-0.0152885	0.6512874
S 3.2001670D-02		-0.0000032	-0.0000080	0.0048179	0.5057323
	P	2P	3P		
BASIS/ORB. ENERGY		-17.8167780	-1.7970785		
P 4.7945460D+04		0.0000232	-0.0000080		
P 8.2685230D+03		0.0001361	-0.0000468		
P 2.2666380D+03		0.0006985	-0.0002404		
P 7.8283370D+02		0.0031642	-0.0010910		
P 3.1041640D+02		0.0122564	-0.0042569		
P 1.3454730D+02		0.0399646	-0.0140538		
P 6.2287110D+01		0.1059475	-0.0382778		
P 3.0404530D+01		0.2139843	-0.0798632		
P 1.5575050D+01		0.3065133	-0.1197820		
P 8.4317700D+00		0.2956651	-0.1209521		

P	4.6479770D+00	0.1748290	-0.0245235
P	2.4502470D+00	0.0426941	0.2279613
P	1.2018010D+00	0.0023536	0.4639247
P	5.5920010D-01	0.0004186	0.3746872
P	2.3479650D-01	-0.0000211	0.0810830
	D	3D	
BASIS/ORB.ENERGY		-0.4315287	
D	1.7127790D+02	0.0005985	
D	4.7911700D+01	0.0056921	
D	1.7369540D+01	0.0277346	
D	6.9694200D+00	0.0895359	
D	3.0103480D+00	0.2055925	
D	1.3292270D+00	0.3206007	
D	5.7895860D-01	0.3577158	
D	2.4441550D-01	0.2615004	
D	9.5591120D-02	0.0867170	

VANADIUM K(2)L(8)3S(2)3P(6)4S(2)3D(3), 4F

CHARGE = 23.000000

SYMMETRY SPECIES	S	P	D
NUMBER OF BASIS FUNCTIONS	20	15	9
NUMBER OF CLOSED SHELLS	4	2	0
NUMBER OF OPEN SHELLS	0	0	1
OPEN SHELL OCCUPATION NUMBER	0	0	3

*** FINAL SCF RESULTS ***

E = -948.151500025

ORBITAL ENERGIES AND EXPANSION COEFFICIENTS

	S	1S	2S	3S	4S
BASIS/ORB.ENERGY		-202.8700000	-24.1553880	-3.2240909	-0.2325207
S	1.6668050D+07	0.0000418	-0.0000126	-0.0000046	-0.0000010
S	1.8566050D+06	0.0001594	-0.0000480	-0.0000174	-0.0000040
S	3.4119260D+05	0.0004899	-0.0001478	-0.0000535	-0.0000122
S	8.2515820D+04	0.0013690	-0.0004137	-0.0001498	-0.0000342
S	2.4055780D+04	0.0036798	-0.0011157	-0.0004040	-0.0000922
S	8.0762020D+03	0.0097392	-0.0029726	-0.0010779	-0.0002457

S	3.0381510D+03	0.0250587	-0.0077459	-0.0028104	-0.0006417
S	1.2503670D+03	0.0609312	-0.0193560	-0.0070536	-0.0016075
S	5.4660870D+02	0.1353298	-0.0454386	-0.0166354	-0.0038072
S	2.4855880D+02	0.2525971	-0.0952526	-0.0354279	-0.0080823
S	1.1641900D+02	0.3432888	-0.1626924	-0.0620462	-0.0143104
S	5.5484730D+01	0.2578247	-0.1746810	-0.0703745	-0.0161036
S	2.6329490D+01	0.0654135	0.0381122	0.0176346	0.0037342
S	1.2524240D+01	0.0017880	0.4771784	0.2596946	0.0635251
S	6.0680070D+00	0.0009462	0.5144969	0.4544696	0.1144341
S	2.8832020D+00	-0.0003295	0.1189687	-0.0204359	-0.0074736
S	1.2633840D+00	0.0000593	0.0037531	-0.7344339	-0.2433100
S	5.3766090D-01	-0.0000396	0.0010423	-0.4614115	-0.2816020
S	9.2506740D-02	0.0000062	-0.0000320	-0.0124333	0.6364815
S	3.4681180D-02	-0.0000027	0.0000165	0.0036809	0.5197961

P

2P

3P

BASIS/ORB. ENERGY -20.0597740 -2.0233704

P	4.7689830D+04	0.0000279	-0.0000098		
P	8.2183390D+03	0.0001635	-0.0000572		
P	2.2637380D+03	0.0008272	-0.0002895		
P	7.8402370D+02	0.0037432	-0.0013151		
P	3.1013700D+02	0.0144323	-0.0051036		
P	1.3458010D+02	0.0463206	-0.0166424		
P	6.2327460D+01	0.1206682	-0.0445623		
P	3.0361920D+01	0.2359684	-0.0904782		
P	1.5547650D+01	0.3193817	-0.1282587		
P	8.4769040D+00	0.2767760	-0.1148570		
P	4.7216180D+00	0.1474524	0.0147233		
P	2.4319990D+00	0.0305124	0.2849909		
P	1.1963690D+00	0.0007844	0.4666819		
P	5.6242860D-01	0.0005794	0.3187568		
P	2.3621200D-01	-0.0000538	0.0566002		

D

3D

BASIS/ORB. ENERGY -0.4993303

D	1.8217040D+02	0.0006917			
D	5.2710580D+01	0.0061575			

D	1.9604460D+01	0.0288287
D	8.0720930D+00	0.0910181
D	3.5509370D+00	0.2064715
D	1.5942780D+00	0.3182954
D	7.0512720D-01	0.3523154
D	3.0065250D-01	0.2597313
D	1.1757850D-01	0.0893638

CHROMIUM K(2)L(8)3S(2)3P(6)4S(1)3D(5), 7S

CHARGE = 24.000000

SYMMETRY SPECIES	S	P	D
NUMBER OF BASIS FUNCTIONS	20	15	9
NUMBER OF CLOSED SHELLS	3	2	0
NUMBER OF OPEN SHELLS	1	0	1
OPEN SHELL OCCUPATION NUMBER	1	0	5

*** FINAL SCF RESULTS ***

E = -1049.674679861

ORBITAL ENERGIES AND EXPANSION COEFFICIENTS

	S	1S	2S	3S	4S
BASIS/ORB. ENERGY		-222.0334900	-26.5595630	-3.3411327	-0.2261321
S 1.6720450D+07	0.0000471	-0.0000143	-0.0000052	-0.0000011	
S 1.8562330D+06	0.0001798	-0.0000546	-0.0000198	-0.0000042	
S 3.4011640D+05	0.0005523	-0.0001679	-0.0000609	-0.0000130	
S 8.2251290D+04	0.0015394	-0.0004690	-0.0001701	-0.0000363	
S 2.3952950D+04	0.0041428	-0.0012671	-0.0004599	-0.0000982	
S 8.0388140D+03	0.0108897	-0.0033532	-0.0012176	-0.0002599	
S 3.0359990D+03	0.0277808	-0.0086807	-0.0031590	-0.0006755	
S 1.2503650D+03	0.0672240	-0.0216151	-0.0078864	-0.0016821	
S 5.4681130D+02	0.1471773	-0.0503509	-0.0185210	-0.0039717	
S 2.4851830D+02	0.2683300	-0.1039462	-0.0387592	-0.0082744	
S 1.1646040D+02	0.3443893	-0.1714009	-0.0660755	-0.0142974	
S 5.5596390D+01	0.2361835	-0.1642448	-0.0663939	-0.0141777	
S 2.5628230D+01	0.0503842	0.0903173	0.0405094	0.0083708	
S 1.2574520D+01	-0.0010548	0.5162264	0.3013920	0.0696024	
S 6.1323280D+00	0.0015199	0.4740258	0.4329847	0.1021426	

S	2.7638940D+00	-0.0006303	0.0852951	-0.1336415	-0.0360796
S	1.2698890D+00	0.0002138	-0.0009271	-0.7323157	-0.2387455
S	5.4046700D-01	-0.0000798	0.0016023	-0.3925467	-0.2259877
S	9.1330410D-02	0.0000148	-0.0000439	-0.0101224	0.6048813
S	3.4052700D-02	-0.0000064	0.0001671	0.0033090	0.5363814
	P	2P	3P		
BASIS/ORB. ENERGY		-22.1973740	-2.0621509		
P	4.5934300D+04	0.0000339	-0.0000119		
P	8.1994210D+03	0.0001915	-0.0000672		
P	2.2710960D+03	0.0009735	-0.0003419		
P	7.8380960D+02	0.0044058	-0.0015544		
P	3.0984540D+02	0.0168371	-0.0059818		
P	1.3463880D+02	0.0532146	-0.0192524		
P	6.2371660D+01	0.1362602	-0.0507549		
P	3.0305360D+01	0.2574451	-0.0999046		
P	1.5543660D+01	0.3271364	-0.1332469		
P	8.5085540D+00	0.2574515	-0.1030230		
P	4.7615840D+00	0.1204867	0.0548031		
P	2.4401090D+00	0.0213257	0.3250315		
P	1.1984680D+00	0.0005605	0.4515668		
P	5.6275310D-01	0.0005455	0.2795294		
P	2.3645220D-01	0.0000088	0.0488011		
	D	3D			
BASIS/ORB. ENERGY		-0.3666886			
D	2.3690590D+02	0.0005346			
D	6.1089050D+01	0.0059125			
D	2.1340960D+01	0.0308068			
D	8.3996820D+00	0.1010658			
D	3.5756720D+00	0.2233451			
D	1.5447120D+00	0.3259470			
D	6.5044710D-01	0.3419610			
D	2.6032020D-01	0.2604911			
D	9.6010580D-02	0.1046237			

MANGANESE K(2)L(8)3S(2)3P(6)4S(2)3D(5), 6S

CHARGE = 25.000000

SYMMETRY SPECIES	S	P	D
NUMBER OF BASIS FUNCTIONS	20	15	9
NUMBER OF CLOSED SHELLS	4	2	0
NUMBER OF OPEN SHELLS	0	0	1
OPEN SHELL OCCUPATION NUMBER	0	0	5

*** FINAL SCF RESULTS ***

E = -1157.404894686

ORBITAL ENERGIES AND EXPANSION COEFFICIENTS

	S	1S	2S	3S	4S
BASIS/ORB. ENERGY		-242.4888700	-29.5262170	-3.8806242	-0.2505905
S 1.6703496D+07		0.0000527	-0.0000161	-0.0000059	-0.0000013
S 1.8690115D+06		0.0002007	-0.0000614	-0.0000226	-0.0000049
S 3.3922763D+05		0.0006239	-0.0001911	-0.0000704	-0.0000153
S 8.1300736D+04		0.0017425	-0.0005349	-0.0001970	-0.0000429
S 2.3685419D+04		0.0046478	-0.0014326	-0.0005281	-0.0001152
S 7.9841759D+03		0.0121429	-0.0037724	-0.0013908	-0.0003028
S 3.0263726D+03		0.0306614	-0.0096711	-0.0035768	-0.0007819
S 1.2520832D+03		0.0734987	-0.0239377	-0.0088695	-0.0019284
S 5.4709397D+02		0.1597448	-0.0555700	-0.0208055	-0.0045656
S 2.4825246D+02		0.2830528	-0.1129559	-0.0428541	-0.0093168
S 1.1646300D+02		0.3425709	-0.1781535	-0.0703090	-0.0156202
S 5.5811828D+01		0.2120555	-0.1515363	-0.0624158	-0.0134322
S 2.5818830D+01		0.0383719	0.1439716	0.0665615	0.0140057
S 1.2574694D+01		-0.0007349	0.5543673	0.3512377	0.0845202
S 6.1616307D+00		0.0010021	0.4161343	0.3987954	0.0939752
S 2.7822694D+00		-0.0004399	0.0610282	-0.2341294	-0.0608959
S 1.3119202D+00		0.0001433	-0.0004735	-0.7150115	-0.2500138
S 5.8899907D-01		-0.0000580	0.0012518	-0.3393328	-0.2156474
S 1.0974191D-01		0.0000099	-0.0000984	-0.0078411	0.6153530
S 3.9630428D-02		-0.0000040	0.0000413	0.0021158	0.5383739
	P	2P	3P		
BASIS/ORB. ENERGY		-24.8811370	-2.4893003		
P 4.8651154D+04		0.0000381	-0.0000136		
P 8.3673813D+03		0.0002223	-0.0000798		

P	2.2852910D+03	0.0011356	-0.0004083
P	7.8635173D+02	0.0051049	-0.0018421
P	3.1087259D+02	0.0193966	-0.0070642
P	1.3469393D+02	0.0609988	-0.0226325
P	6.2347613D+01	0.1518874	-0.0582640
P	3.0315353D+01	0.2779307	-0.1110371
P	1.5400319D+01	0.3424719	-0.1450598
P	8.2292547D+00	0.2369864	-0.0827353
P	4.6458324D+00	0.0831312	0.0956998
P	2.5983347D+00	0.0153381	0.3040468
P	2.8611961D-01	0.0000044	0.0507142
P	6.6928457D-01	0.0004670	0.2848719
P	1.3704745D+00	0.0009170	0.4277392
	D	3D	
BASIS/ORB. ENERGY		-0.6256591	
D	2.0113773D+02	0.0009339	
D	5.9697767D+01	0.0077492	
D	2.2712206D+01	0.0345769	
D	9.5508116D+00	0.1052406	
D	4.2791942D+00	0.2245933	
D	1.9492770D+00	0.3259549	
D	8.7236600D-01	0.3400561	
D	3.7511423D-01	0.2363987	
D	1.4742170D-01	0.0762480	

IRON K(2)L(8)3S(2)3P(6)4S(2)3D(6), 5D

CHARGE = 26.000000

SYMMETRY SPECIES	S	P	D
NUMBER OF BASIS FUNCTIONS	20	15	9
NUMBER OF CLOSED SHELLS	4	2	0
NUMBER OF OPEN SHELLS	0	0	1
OPEN SHELL OCCUPATION NUMBER	0	0	6

*** FINAL SCF RESULTS ***

E = -1271.365568577

ORBITAL ENERGIES AND EXPANSION COEFFICIENTS

	S	1S	2S	3S	4S
BASIS/ORB. ENERGY		-263.6856100	-32.4360450	-4.2478340	-0.2614428
S 6.7207850D+07		0.0000212	-0.0000065	-0.0000024	-0.0000005
S 7.3135460D+06		0.0000811	-0.0000250	-0.0000093	-0.0000020
S 1.2898560D+06		0.0002492	-0.0000768	-0.0000285	-0.0000061
S 2.9729780D+05		0.0006823	-0.0002106	-0.0000782	-0.0000168
S 8.2030030D+04		0.0017707	-0.0005472	-0.0002030	-0.0000437
S 2.5799180D+04		0.0045453	-0.0014121	-0.0005257	-0.0001133
S 8.9567480D+03		0.0118420	-0.0036992	-0.0013713	-0.0002949
S 3.3595960D+03		0.0310291	-0.0098732	-0.0036935	-0.0007968
S 1.3419500D+03		0.0781768	-0.0256089	-0.0095256	-0.0020494
S 5.6458810D+02		0.1743636	-0.0616896	-0.0234362	-0.0050658
S 2.4837920D+02		0.3072753	-0.1255276	-0.0477819	-0.0103101
S 1.1350840D+02		0.3482206	-0.1939528	-0.0787509	-0.0171721
S 5.3094010D+01		0.1812587	-0.1192633	-0.0478459	-0.0103718
S 2.2315200D+01		0.0215933	0.3033789	0.1471075	0.0327267
S 1.0716860D+01		-0.0018977	0.5961314	0.4670941	0.1111345
S 5.1957180D+00		0.0008404	0.2615257	0.1804353	0.0413527
S 1.9301770D+00		-0.0003050	0.0173232	-0.7192310	-0.2155730
S 7.7996100D-01		0.0000722	-0.0006059	-0.5390794	-0.2859161
S 1.1510950D-01		-0.0000177	0.0002930	-0.0161011	0.6204468
S 4.1661070D-02		0.0000080	-0.0001272	0.0052602	0.5204731
	P	2P	3P		
BASIS/ORB. ENERGY		-27.5024580	-2.7557083		
P 4.8583310D+04		0.0000445	0.0000162		
P 8.3660940D+03		0.0002591	0.0000941		
P 2.2846350D+03		0.0013228	0.0004813		
P 7.8575470D+02		0.0059077	0.0021599		
P 3.1094600D+02		0.0222610	0.0082166		
P 1.3469170D+02		0.0692127	0.0260953		
P 6.2344850D+01		0.1682640	0.0656717		
P 3.0292930D+01		0.2969947	0.1212407		
P 1.5392230D+01		0.3425795	0.1475305		
P 8.2282760D+00		0.2120654	0.0601550		
P 4.6525990D+00		0.0648653	-0.1366533		

P	2.5794920D+00	0.0105493	-0.3371165
P	1.3636890D+00	0.0006646	-0.4110363
P	6.7283420D-01	0.0004086	-0.2407737
P	2.8677540D-01	0.0000116	-0.0367959
D		3D	
BASIS/ORB.ENERGY -0.6323776			
D	2.7306550D+02	0.0006256	
D	8.0264000D+01	0.0055040	
D	3.0241020D+01	0.0269166	
D	1.2616500D+01	0.0877541	
D	5.6043950D+00	0.2031762	
D	2.5257040D+00	0.3190862	
D	1.1050130D+00	0.3538002	
D	4.5984990D-01	0.2644092	
D	1.7386000D-01	0.0971127	

COBALT K(2)L(8)3S(2)3P(6)4S(2)3D(7), 4F

CHARGE = 27.000000

SYMMETRY SPECIES	S	P	D
NUMBER OF BASIS FUNCTIONS	20	15	9
NUMBER OF CLOSED SHELLS	4	2	0
NUMBER OF OPEN SHELLS	0	0	1
OPEN SHELL OCCUPATION NUMBER	0	0	7

*** FINAL SCF RESULTS ***

E = -1391.904434026

ORBITAL ENERGIES AND EXPANSION COEFFICIENTS

	S	1S	2S	3S	4S
BASIS/ORB.ENERGY		-285.7828200	-35.4648350	-4.6193961	-0.2712766
S	6.8378190D+07	0.0000234	-0.0000072	-0.0000027	-0.0000006
S	7.3692460D+06	0.0000901	-0.0000279	-0.0000104	-0.0000022
S	1.2954280D+06	0.0002766	-0.0000858	-0.0000320	-0.0000068
S	2.9810610D+05	0.0007561	-0.0002349	-0.0000878	-0.0000186
S	8.2220140D+04	0.0019598	-0.0006096	-0.0002277	-0.0000483
S	2.5822900D+04	0.0050265	-0.0015728	-0.0005889	-0.0001250
S	8.9631840D+03	0.0130394	-0.0041037	-0.0015331	-0.0003251

S	3.3621020D+03	0.0340491	-0.0109331	-0.0041117	-0.0008732
S	1.3422380D+03	0.0851231	-0.0281973	-0.0105839	-0.0022461
S	5.6471420D+02	0.1871078	-0.0673725	-0.0257373	-0.0054746
S	2.4826660D+02	0.3202972	-0.1345936	-0.0519108	-0.0110614
S	1.1346470D+02	0.3403569	-0.1986845	-0.0813167	-0.0174320
S	5.3267650D+01	0.1574473	-0.0943239	-0.0386373	-0.0083555
S	2.2577000D+01	0.0155645	0.3627159	0.1873755	0.0416633
S	1.0727370D+01	-0.0010697	0.5953226	0.4897285	0.1148265
S	5.1267590D+00	0.0004862	0.2054382	0.1051071	0.0228290
S	2.0454520D+00	-0.0002124	0.0105819	-0.7365269	-0.2206909
S	8.3355690D-01	0.0000414	0.0005241	-0.5084853	-0.2704069
S	1.2595560D-01	-0.0000104	0.0000789	-0.0146631	0.6032216
S	4.4890640D-02	0.0000046	-0.0000305	0.0046416	0.5374524

P

2P

3P

BASIS/ORB. ENERGY -30.2329510 -3.0242976

P	4.8963140D+04	0.0000515	0.0000189		
P	8.3456870D+03	0.0003023	0.0001109		
P	2.2799360D+03	0.0015284	0.0005618		
P	7.8583140D+02	0.0067934	0.0025110		
P	3.1081170D+02	0.0254084	0.0094856		
P	1.3474590D+02	0.0778774	0.0297760		
P	6.2332250D+01	0.1853264	0.0734359		
P	3.0247970D+01	0.3145500	0.1309698		
P	1.5390230D+01	0.3374085	0.1464179		
P	8.2376440D+00	0.1872314	0.0337383		
P	4.6587240D+00	0.0501796	-0.1746327		
P	2.5684760D+00	0.0072871	-0.3623207		
P	1.3572820D+00	0.0006082	-0.3895492		
P	6.7620240D-01	0.0003356	-0.2014964		
P	2.8847480D-01	0.0000196	-0.0272786		

D

3D

BASIS/ORB. ENERGY -0.6594306

D	2.7537830D+02	0.0007648			
D	8.0658160D+01	0.0067231			
D	3.0232990D+01	0.0323261			

D	1.2611280D+01	0.1021545
D	5.6161100D+00	0.2235739
D	2.5253840D+00	0.3288198
D	1.1052020D+00	0.3420104
D	4.6148340D-01	0.2422901
D	1.7550980D-01	0.0843201

NICKEL K(2)L(8)3S(2)3P(6)4S(2)3D(8), 3F

CHARGE = 28.000000

SYMMETRY SPECIES	S	P	D
NUMBER OF BASIS FUNCTIONS	20	15	9
NUMBER OF CLOSED SHELLS	4	2	0
NUMBER OF OPEN SHELLS	0	0	1
OPEN SHELL OCCUPATION NUMBER	0	0	8

*** FINAL SCF RESULTS ***

E = -1519.130128039

ORBITAL ENERGIES AND EXPANSION COEFFICIENTS

	S	1S	2S	3S	4S
BASIS/ORB. ENERGY		-308.7933600	-38.6234370	-5.0019802	-0.2807395
S 6.8573180D+07	0.0000260	-0.0000081	-0.0000030	-0.0000006	
S 7.3712920D+06	0.0000998	-0.0000311	-0.0000117	-0.0000024	
S 1.3017820D+06	0.0003054	-0.0000953	-0.0000358	-0.0000075	
S 2.9870850D+05	0.0008369	-0.0002615	-0.0000983	-0.0000205	
S 8.2337350D+04	0.0021606	-0.0006764	-0.0002542	-0.0000531	
S 2.5855370D+04	0.0055379	-0.0017444	-0.0006563	-0.0001371	
S 8.9647770D+03	0.0143243	-0.0045411	-0.0017083	-0.0003571	
S 3.3641940D+03	0.0371909	-0.0120448	-0.0045487	-0.0009504	
S 1.3425840D+03	0.0924011	-0.0309554	-0.0117184	-0.0024534	
S 5.6456870D+02	0.1998761	-0.0732205	-0.0280904	-0.0058750	
S 2.4827240D+02	0.3316830	-0.1434797	-0.0560716	-0.0118066	
S 1.1330310D+02	0.3316712	-0.2023988	-0.0832634	-0.0175098	
S 5.3056160D+01	0.1346983	-0.0661230	-0.0280622	-0.0061809	
S 2.2811340D+01	0.0102959	0.4213734	0.2314643	0.0514351	
S 1.0677930D+01	-0.0001755	0.5882660	0.5031054	0.1157802	
S 4.8803330D+00	0.0000809	0.1533045	0.0146660	0.0015061	

S	2.1078690D+00	-0.0000776	0.0029894	-0.7533037	-0.2287379
S	8.6988690D-01	0.0000019	0.0016054	-0.4606874	-0.2485098
S	1.3673590D-01	-0.0000018	-0.0001215	-0.0119143	0.5921330
S	4.7892400D-02	0.0000008	0.0000556	0.0035431	0.5491593
	P	2P	3P		
BASIS/ORB. ENERGY		-33.0825750	-3.3010617		
P	5.1568330D+04	0.0000561	0.0000207		
P	8.8048630D+03	0.0003258	0.0001206		
P	2.3754010D+03	0.0016749	0.0006212		
P	8.0317640D+02	0.0076613	0.0028577		
P	3.1153830D+02	0.0292808	0.0110487		
P	1.3346270D+02	0.0889327	0.0344343		
P	6.1712680D+01	0.2032733	0.0817895		
P	3.0027180D+01	0.3314573	0.1404709		
P	1.5147230D+01	0.3367252	0.1458349		
P	7.8246240D+00	0.1626821	-0.0173033		
P	4.1428990D+00	0.0284992	-0.2668994		
P	2.3196840D+00	0.0031770	-0.3315429		
P	1.3814930D+00	0.0003639	-0.3109615		
P	7.3143950D-01	0.0003603	-0.1899092		
P	3.1313330D-01	0.0000238	-0.0267312		
	D	3D			
BASIS/ORB. ENERGY		-0.6893488			
D	2.8345150D+02	0.0009097			
D	8.0785470D+01	0.0082087			
D	3.0181000D+01	0.0382133			
D	1.2622230D+01	0.1172322			
D	5.6207420D+00	0.2426282			
D	2.5242870D+00	0.3348851			
D	1.1048470D+00	0.3298841			
D	4.6236340D-01	0.2218121			
D	1.7701300D-01	0.0728789			

COPPER K(2)L(8)3S(2)3P(6)4S(1)3D(10), 2S
 CHARGE = 29.000000

SYMMETRY SPECIES	S	P	D
NUMBER OF BASIS FUNCTIONS	20	15	9
NUMBER OF CLOSED SHELLS	3	2	1
NUMBER OF OPEN SHELLS	1	0	0
OPEN SHELL OCCUPATION NUMBER	1	0	0

*** FINAL SCF RESULTS ***

E = -1653.194993352

ORBITAL ENERGIES AND EXPANSION COEFFICIENTS

	S	1S	2S	3S	4S
BASIS/ORB. ENERGY		-332.4893700	-41.6565580	-5.1539998	-0.2445242
S 6.7793730D+07	0.0000289	-0.0000091	-0.0000034	-0.0000034	-0.0000006
S 7.4022270D+06	0.0001098	-0.0000344	-0.0000129	-0.0000129	-0.0000023
S 1.3080110D+06	0.0003355	-0.0001053	-0.0000395	-0.0000395	-0.0000070
S 3.0053580D+05	0.0009223	-0.0002899	-0.0001088	-0.0001088	-0.0000192
S 8.2258000D+04	0.0023856	-0.0007514	-0.0002822	-0.0002822	-0.0000499
S 2.5879870D+04	0.0060631	-0.0019217	-0.0007222	-0.0007222	-0.0001277
S 8.9765310D+03	0.0156728	-0.0050048	-0.0018831	-0.0018831	-0.0003329
S 3.3675650D+03	0.0404938	-0.0132201	-0.0049858	-0.0049858	-0.0008820
S 1.3428960D+03	0.0999706	-0.0338814	-0.0128436	-0.0128436	-0.0022732
S 5.6418310D+02	0.2127992	-0.0792731	-0.0303890	-0.0303890	-0.0053832
S 2.4811230D+02	0.3417635	-0.1524140	-0.0598883	-0.0598883	-0.0106563
S 1.1300260D+02	0.3211710	-0.2040535	-0.0840489	-0.0840489	-0.0149903
S 5.2547730D+01	0.1134427	-0.0351352	-0.0153095	-0.0153095	-0.0028645
S 2.3161700D+01	0.0060441	0.4686598	0.2687147	0.2687147	0.0503923
S 1.0756720D+01	0.0005586	0.5704648	0.4994813	0.4994813	0.0975406
S 4.6423960D+00	-0.0002549	0.1175133	-0.0901180	-0.0901180	-0.0227210
S 2.0779930D+00	0.0000671	-0.0025749	-0.7635495	-0.7635495	-0.1952527
S 8.5188350D-01	-0.0000355	0.0022232	-0.3895842	-0.3895842	-0.1882508
S 1.1547540D-01	0.0000056	-0.0002272	-0.0085037	-0.0085037	0.5523084
S 4.0529830D-02	-0.0000025	0.0001032	0.0025687	0.0025687	0.5635438
	P	2P	3P		
BASIS/ORB. ENERGY		-35.7998020	-3.3612464		
P 5.1547640D+04	0.0000644	0.0000238			
P 8.8521460D+03	0.0003704	0.0001372			
P 2.3887210D+03	0.0019015	0.0007056			

P	8.0480520D+02	0.0087293	0.0032611
P	3.1098980D+02	0.0331796	0.0125471
P	1.3335420D+02	0.0987677	0.0384250
P	6.1725930D+01	0.2203937	0.0891831
P	3.0004980D+01	0.3449769	0.1477044
P	1.5137720D+01	0.3240481	0.1361566
P	7.7766310D+00	0.1388239	-0.0546252
P	4.1183440D+00	0.0192957	-0.2957214
P	2.3086330D+00	0.0032639	-0.3283406
P	1.3821200D+00	-0.0000682	-0.2845808
P	7.3677900D-01	0.0004799	-0.1707545
P	3.1498890D-01	0.0000374	-0.0249183
	D	3D	
BASIS/ORB. ENERGY			
D	3.1281730D+02	0.0008629	
D	8.8135560D+01	0.0081044	
D	3.2228440D+01	0.0394674	
D	1.3186590D+01	0.1239251	
D	5.7295240D+00	0.2527732	
D	2.5019170D+00	0.3353050	
D	1.0550470D+00	0.3237648	
D	4.1568650D-01	0.2296603	
D	1.4785470D-01	0.0883465	

ZINC K(2)L(8)3S(2)3P(6)4S(2)3D(10), 1S

CHARGE = 30.000000

SYMMETRY SPECIES	S	P	D
NUMBER OF BASIS FUNCTIONS	20	15	9
NUMBER OF CLOSED SHELLS	4	2	1
NUMBER OF OPEN SHELLS	0	0	0
OPEN SHELL OCCUPATION NUMBER	0	0	0

*** FINAL SCF RESULTS ***

E = -1794.319828742

ORBITAL ENERGIES AND EXPANSION COEFFICIENTS

S	1S	2S	3S	4S
---	----	----	----	----

BASIS/ORB. ENERGY	-357.5658300	-45.3292120	-5.7974096	-0.2983234
S 7.0817880D+07	0.0000311	-0.0000098	-0.0000037	-0.0000008
S 7.5722940D+06	0.0001201	-0.0000379	-0.0000144	-0.0000029
S 1.3230680D+06	0.0003685	-0.0001163	-0.0000441	-0.0000089
S 3.0250570D+05	0.0010086	-0.0003188	-0.0001208	-0.0000245
S 8.2854280D+04	0.0026082	-0.0008264	-0.0003134	-0.0000635
S 2.5950900D+04	0.0066416	-0.0021169	-0.0008031	-0.0001626
S 8.9847100D+03	0.0171211	-0.0055080	-0.0020936	-0.0004245
S 3.3685880D+03	0.0438715	-0.0144271	-0.0054928	-0.0011111
S 1.3487580D+03	0.1067060	-0.0365962	-0.0140266	-0.0028510
S 5.6724390D+02	0.2250443	-0.0850773	-0.0329533	-0.0066689
S 2.4830630D+02	0.3530036	-0.1625881	-0.0648274	-0.0132795
S 1.1190550D+02	0.3117775	-0.2047861	-0.0855795	-0.0173624
S 5.0426170D+01	0.0920051	0.0043418	0.0022380	-0.0000383
S 2.3428200D+01	0.0005655	0.5003875	0.3009365	0.0660256
S 1.1091260D+01	0.0019547	0.5318787	0.4805957	0.1063703
S 4.8970560D+00	-0.0009019	0.1039594	-0.1224633	-0.0301646
S 2.2538020D+00	0.0003646	-0.0017929	-0.7432134	-0.2303864
S 9.6126800D-01	-0.0001234	0.0020197	-0.3929689	-0.2125037
S 1.5577700D-01	0.0000221	-0.0001972	-0.0095537	0.5814411
S 5.3135660D-02	-0.0000092	0.0000844	0.0027377	0.5576236

	P	2P	3P
BASIS/ORB. ENERGY	-39.1350460	-3.8756757	
P 5.7518010D+04	0.0000667	0.0000250	
P 9.3627720D+03	0.0004060	0.0001525	
P 2.4180840D+03	0.0021837	0.0008217	
P 8.0005350D+02	0.0100024	0.0037920	
P 3.1005840D+02	0.0371862	0.0142838	
P 1.3337250D+02	0.1090604	0.0431944	
P 6.1701480D+01	0.2377502	0.0980853	
P 2.9958730D+01	0.3563779	0.1561060	
P 1.5108250D+01	0.3077951	0.1248294	
P 7.7517470D+00	0.1163305	-0.0943042	
P 4.0851060D+00	0.0139180	-0.3276858	
P 2.2820190D+00	0.0024292	-0.3336600	

P	1.3707160D+00	0.0000095	-0.2566183
P	7.4767650D-01	0.0003635	-0.1355919
P	3.1878770D-01	0.0000108	-0.0164130
	D	3D	
BASIS/ORB.ENERGY		-0.7609888	
D	2.9980320D+02	0.0011200	
D	9.1795170D+01	0.0087260	
D	3.5637370D+01	0.0389156	
D	1.5216270D+01	0.1180247	
D	6.8536920D+00	0.2421966	
D	3.0972170D+00	0.3325770	
D	1.3578490D+00	0.3269336	
D	5.6523940D-01	0.2245023	
D	2.1251050D-01	0.0777623	

GALLIUM K(2)L(8)M(18)4S(2)4P(1), 2P

CHARGE = 31.000000

SYMMETRY SPECIES	S	P	D
NUMBER OF BASIS FUNCTIONS	20	15	9
NUMBER OF CLOSED SHELLS	4	2	1
NUMBER OF OPEN SHELLS	0	1	0
OPEN SHELL OCCUPATION NUMBER	0	1	0

*** FINAL SCF RESULTS ***

E = -1942.234245329

ORBITAL ENERGIES AND EXPANSION COEFFICIENTS

	S	1S	2S	3S	4S
BASIS/ORB.ENERGY		-383.7120900	-49.2844420	-6.5784987	-0.4336555
S	7.0959040D+07	0.0000342	-0.0000108	-0.0000041	-0.0000010
S	7.6033240D+06	0.0001322	-0.0000419	-0.0000160	-0.0000038
S	1.3192400D+06	0.0004065	-0.0001289	-0.0000494	-0.0000116
S	3.0267050D+05	0.0010998	-0.0003494	-0.0001338	-0.0000314
S	8.3251810D+04	0.0028477	-0.0009073	-0.0003476	-0.0000816
S	2.5933120D+04	0.0072891	-0.0023366	-0.0008952	-0.0002097
S	8.9765470D+03	0.0185878	-0.0060205	-0.0023125	-0.0005434
S	3.3720960D+03	0.0474969	-0.0157396	-0.0060516	-0.0014160

S	1.3486200D+03	0.1145311	-0.0397271	-0.0154025	-0.0036299
S	5.6755490D+02	0.2374832	-0.0912870	-0.0357422	-0.0083649
S	2.4818870D+02	0.3603580	-0.1711823	-0.0693059	-0.0164880
S	1.1167490D+02	0.2970835	-0.2010901	-0.0851883	-0.0199359
S	4.9241650D+01	0.0762254	0.0484820	0.0230473	0.0046788
S	2.3275170D+01	-0.0024658	0.5419210	0.3456394	0.0891668
S	1.1081480D+01	0.0026103	0.4849909	0.4541423	0.1156672
S	4.8993520D+00	-0.0012799	0.0798118	-0.2071498	-0.0567444
S	2.3008210D+00	0.0005840	-0.0013594	-0.7301112	-0.2832209
S	1.0265820D+00	-0.0002025	0.0016337	-0.3481188	-0.2282127
S	2.0922290D-01	0.0000412	-0.0001700	-0.0084651	0.6370489
S	7.3485840D-02	-0.0000158	0.0000634	0.0019023	0.5336434
	P	2P	3P	4P	
BASIS/ORB. ENERGY	-42.7397690	-4.5228043	-0.2068067		
P	4.9597560D+04	0.0000873	0.0000332	0.0000054	
P	8.5216950D+03	0.0005049	0.0001927	0.0000314	
P	2.3038990D+03	0.0025748	0.0009825	0.0001613	
P	7.8303950D+02	0.0114701	0.0044247	0.0007193	
P	3.0554940D+02	0.0423837	0.0165364	0.0027250	
P	1.3116530D+02	0.1232749	0.0498933	0.0081366	
P	6.0060420D+01	0.2659932	0.1119355	0.0186542	
P	2.8478480D+01	0.3855091	0.1743345	0.0285383	
P	1.3712750D+01	0.2885151	0.0911038	0.0151787	
P	6.3599160D+00	0.0700693	-0.2546504	-0.0525519	
P	2.9038490D+00	0.0019047	-0.5163409	-0.0983409	
P	1.2702450D+00	0.0013936	-0.3459267	-0.0917331	
P	4.8107990D-01	-0.0002126	-0.0474342	0.1194578	
P	1.5285910D-01	0.0000956	0.0014855	0.5446110	
P	4.8563430D-02	-0.0000310	-0.0007428	0.4960748	
	D	3D			
BASIS/ORB. ENERGY	-1.1646013				
D	4.5791230D+02	0.0006287			
D	1.2854330D+02	0.0058931			
D	4.8135830D+01	0.0297590			
D	2.0161900D+01	0.0985940			

D	9.0373380D+00	0.2209937
D	4.1220690D+00	0.3290663
D	1.8356450D+00	0.3444087
D	7.7932260D-01	0.2400633
D	2.9996760D-01	0.0768475

GERMANIUM K(2)L(8)M(18)4S(2)4P(2), 3P

CHARGE = 32.000000

SYMMETRY SPECIES	S	P	D
NUMBER OF BASIS FUNCTIONS	20	15	9
NUMBER OF CLOSED SHELLS	4	2	1
NUMBER OF OPEN SHELLS	0	1	0
OPEN SHELL OCCUPATION NUMBER	0	2	0

*** FINAL SCF RESULTS ***

E = -2097.120773585

ORBITAL ENERGIES AND EXPANSION COEFFICIENTS

	S	1S	2S	3S	4S
BASIS/ORB. ENERGY		-410.8402000	-53.4325170	-7.4033724	-0.5662276
S 6.7849860D+07	0.0000387	-0.0000123	-0.0000048	-0.0000012	
S 7.4520550D+06	0.0001445	-0.0000460	-0.0000178	-0.0000046	
S 1.3367880D+06	0.0004372	-0.0001394	-0.0000539	-0.0000139	
S 3.0503260D+05	0.0012103	-0.0003864	-0.0001495	-0.0000385	
S 8.2939380D+04	0.0031219	-0.0010004	-0.0003874	-0.0001000	
S 2.5960830D+04	0.0078979	-0.0025444	-0.0009848	-0.0002537	
S 8.9797630D+03	0.0202452	-0.0066067	-0.0025658	-0.0006635	
S 3.3672560D+03	0.0512871	-0.0171051	-0.0066443	-0.0017094	
S 1.3496470D+03	0.1222908	-0.0429681	-0.0168611	-0.0043754	
S 5.6790310D+02	0.2498246	-0.0974301	-0.0385779	-0.0099256	
S 2.4835020D+02	0.3654560	-0.1797143	-0.0739334	-0.0193927	
S 1.1141580D+02	0.2826319	-0.1934535	-0.0830442	-0.0213212	
S 4.7105710D+01	0.0624646	0.1005312	0.0492472	0.0118306	
S 2.3205140D+01	-0.0058625	0.5574112	0.3786626	0.1091274	
S 1.1240890D+01	0.0034078	0.4455335	0.4169292	0.1157160	
S 4.7209460D+00	-0.0016749	0.0661812	-0.3046729	-0.0924257	
S 2.2969380D+00	0.0009060	-0.0057513	-0.6993179	-0.3315730	

S	1.0856240D+00	-0.0003320	0.0026758	-0.2920474	-0.2114942
S	2.6056570D-01	0.0000706	-0.0004194	-0.0081450	0.6771368
S	9.3193650D-02	-0.0000247	0.0001397	0.0015246	0.5174561
	P	2P	3P	4P	
BASIS/ORB. ENERGY		-46.5226340	-5.2076300	-0.2858951	
P	4.9291810D+04	0.0000990	0.0000382	0.0000075	
P	8.5900400D+03	0.0005622	0.0002179	0.0000430	
P	2.3201620D+03	0.0028921	0.0011210	0.0002205	
P	7.8229940D+02	0.0129416	0.0050738	0.0010033	
P	3.0499730D+02	0.0471290	0.0187119	0.0036878	
P	1.3120960D+02	0.1345923	0.0555458	0.0110546	
P	6.0064460D+01	0.2829517	0.1216379	0.0241479	
P	2.8512470D+01	0.3879632	0.1792240	0.0363297	
P	1.3781060D+01	0.2648325	0.0670821	0.0109963	
P	6.3840140D+00	0.0570073	-0.2982686	-0.0702257	
P	2.9060420D+00	0.0012356	-0.5269968	-0.1344008	
P	1.2712070D+00	0.0011185	-0.3027407	-0.0782871	
P	4.2229260D-01	-0.0001992	-0.0280137	0.2441517	
P	1.6033300D-01	0.0001038	0.0033497	0.5699116	
P	5.8016510D-02	-0.0000346	-0.0010976	0.3424374	
	D	3D			
BASIS/ORB. ENERGY		-1.5983597			
D	4.4965610D+02	0.0007634			
D	1.3221530D+02	0.0066579			
D	5.0118460D+01	0.0327622			
D	2.1242420D+01	0.1057855			
D	9.6266770D+00	0.2307292			
D	4.4519600D+00	0.3341099			
D	2.0279210D+00	0.3388280			
D	8.9021290D-01	0.2196249			
D	3.5348260D-01	0.0601296			

ARSENIC K(2)L(8)M(18)4S(2)4P(3), 4S

CHARGE = 33.000000

SYMMETRY SPECIES

S P D

NUMBER OF BASIS FUNCTIONS	20	15	9
NUMBER OF CLOSED SHELLS	4	2	1
NUMBER OF OPEN SHELLS	0	1	0
OPEN SHELL OCCUPATION NUMBER	0	3	0

*** FINAL SCF RESULTS ***

E = -2259.095511826

ORBITAL ENERGIES AND EXPANSION COEFFICIENTS

	S	1S	2S	3S	4S
BASIS/ORB. ENERGY		-438.9577400	-57.7759910	-8.2740835	-0.7027929
S 7.2421890D+07	0.000408	-0.0000131	-0.0000051	-0.0000014	
S 7.7040750D+06	0.0001575	-0.0000504	-0.0000197	-0.0000054	
S 1.3365730D+06	0.0004840	-0.0001550	-0.0000606	-0.0000168	
S 3.0394350D+05	0.0013170	-0.0004225	-0.0001651	-0.0000457	
S 8.3289250D+04	0.0033816	-0.0010894	-0.0004263	-0.0001181	
S 2.5994450D+04	0.0086027	-0.0027863	-0.0010898	-0.0003012	
S 8.9795770D+03	0.0218944	-0.0071922	-0.0028237	-0.0007834	
S 3.3667950D+03	0.0553655	-0.0186023	-0.0073028	-0.0020162	
S 1.3464700D+03	0.1308397	-0.0465134	-0.0184686	-0.0051420	
S 5.6774580D+02	0.2607128	-0.1033889	-0.0414234	-0.0114418	
S 2.4923080D+02	0.3673427	-0.1861924	-0.0777822	-0.0219019	
S 1.1199520D+02	0.2665249	-0.1844035	-0.0802660	-0.0221396	
S 4.6328140D+01	0.0515716	0.1583685	0.0810341	0.0219824	
S 2.2611220D+01	-0.0062117	0.5924934	0.4311878	0.1342824	
S 1.0910110D+01	0.0032639	0.3817974	0.3577699	0.1061374	
S 4.5498340D+00	-0.0016351	0.0430589	-0.4529038	-0.1560591	
S 2.1494630D+00	0.0009331	-0.0030621	-0.6795838	-0.4009016	
S 1.0337510D+00	-0.0003923	0.0016736	-0.1811291	-0.1328504	
S 3.0892460D-01	0.0001001	-0.0003318	-0.0047624	0.7170595	
S 1.1206710D-01	-0.0000306	0.0000878	0.0005291	0.4949176	
	P	2P	3P	4P	
BASIS/ORB. ENERGY		-50.4853970	-5.9328692	-0.3680265	
P 4.9515580D+04	0.0001124	0.0000441	0.0000098		
P 8.4637830D+03	0.0006493	0.0002553	0.0000569		
P 2.2908560D+03	0.0032876	0.0012953	0.0002874		
P 7.7965970D+02	0.0143992	0.0057321	0.0012807		

P	3.0545690D+02	0.0520421	0.0210459	0.0046790
P	1.3097990D+02	0.1477822	0.0621095	0.0139804
P	5.9698960D+01	0.3012652	0.1326249	0.0297125
P	2.8408790D+01	0.3855789	0.1807578	0.0416023
P	1.3883000D+01	0.2377668	0.0428504	0.0057380
P	6.6102210D+00	0.0475902	-0.3159446	-0.0838241
P	3.0821260D+00	0.0016841	-0.5170709	-0.1548983
P	1.3919830D+00	0.0007929	-0.2858490	-0.0779075
P	4.8254700D-01	-0.0001076	-0.0262492	0.2924507
P	1.9228260D-01	0.0000567	0.0032250	0.5668626
P	7.2849660D-02	-0.0000193	-0.0009048	0.2963080
	D	3D		
BASIS/ORB.ENERGY		-2.0668833		
D	7.1896480D+02	0.0003604		
D	2.0798400D+02	0.0032671		
D	7.9590850D+01	0.0171524		
D	3.4514110D+01	0.0610645		
D	1.5730540D+01	0.1637904		
D	7.2805600D+00	0.2993089		
D	3.3000700D+00	0.3734579		
D	1.4173160D+00	0.2979159		
D	5.4472730D-01	0.0987108		

SELENIUM K(2)L(8)M(18)4S(2)4P(4), 3P

CHARGE = 34.000000

SYMMETRY SPECIES S P D

NUMBER OF BASIS FUNCTIONS 20 15 9

NUMBER OF CLOSED SHELLS 4 2 1

NUMBER OF OPEN SHELLS 0 1 0

OPEN SHELL OCCUPATION NUMBER 0 4 0

*** FINAL SCF RESULTS ***

E = -2428.152510218

ORBITAL ENERGIES AND EXPANSION COEFFICIENTS

	S	1S	2S	3S	4S
BASIS/ORB.ENERGY		-468.0955200	-62.3400410	-9.2139048	-0.8594298

S	7.0126910D+07	0.0000455	-0.0000146	-0.0000058	0.0000017
S	7.6150590D+06	0.0001720	-0.0000553	-0.0000218	0.0000064
S	1.3399940D+06	0.0005250	-0.0001690	-0.0000667	0.0000196
S	3.0471930D+05	0.0014348	-0.0004625	-0.0001826	0.0000536
S	8.3264650D+04	0.0036792	-0.0011914	-0.0004711	0.0001383
S	2.6000940D+04	0.0093087	-0.0030304	-0.0011976	0.0003512
S	8.9882070D+03	0.0236359	-0.0078166	-0.0031012	0.0009120
S	3.3653010D+03	0.0595865	-0.0201619	-0.0080003	0.0023449
S	1.3451580D+03	0.1392622	-0.0501091	-0.0201220	0.0059360
S	5.6764000D+02	0.2720451	-0.1096483	-0.0444719	0.0130548
S	2.4958650D+02	0.3681746	-0.1927128	-0.0816961	0.0243645
S	1.1248470D+02	0.2487526	-0.1716823	-0.0758312	0.0223162
S	4.5767340D+01	0.0423622	0.2159933	0.1154886	-0.0344583
S	2.2295360D+01	-0.0060175	0.6045286	0.4680331	-0.1549340
S	1.0805420D+01	0.0029552	0.3284367	0.2949448	-0.0936134
S	4.4801370D+00	-0.0014150	0.0308140	-0.5680517	0.2230363
S	2.0468810D+00	0.0007512	-0.0018359	-0.6601805	0.4660577
S	8.6721290D-01	-0.0003509	0.0011453	-0.0908048	0.0205492
S	3.4341860D-01	0.0001378	-0.0004107	0.0020027	-0.7603858
S	1.2788100D-01	-0.0000354	0.0000881	-0.0007787	-0.4419573
	P	2P	3P	4P	
BASIS/ORB. ENERGY	-54.6523630	-6.7217922	-0.4015045		
P	4.8566150D+04	0.0001281	-0.0000510	0.0000123	
P	8.4316000D+03	0.0007292	-0.0002909	0.0000704	
P	2.2946350D+03	0.0036497	-0.0014596	0.0003514	
P	7.8377970D+02	0.0159025	-0.0064280	0.0015592	
P	3.0586350D+02	0.0576126	-0.0236966	0.0057192	
P	1.3060430D+02	0.1612046	-0.0690313	0.0168844	
P	5.9465130D+01	0.3173664	-0.1427410	0.0347406	
P	2.8363770D+01	0.3820681	-0.1815842	0.0455140	
P	1.3896050D+01	0.2142798	-0.0129188	-0.0026085	
P	6.6186080D+00	0.0378358	0.3539924	-0.1025645	
P	3.1194380D+00	0.0012333	0.5075141	-0.1732423	
P	1.4491170D+00	0.0006472	0.2450714	-0.0583369	
P	5.3959100D-01	-0.0000986	0.0206208	0.3416771	

P	2.1459710D-01	0.0000390	-0.0013050	0.5526237
P	8.0700040D-02	-0.0000162	0.0006320	0.2671357
	D	3D		
BASIS/ORB.ENERGY		-2.5943733		
D	6.5851230D+02	0.0004987		
D	2.0180170D+02	0.0039484		
D	8.0065640D+01	0.0195765		
D	3.4777660D+01	0.0705180		
D	1.5742740D+01	0.1842938		
D	7.2754480D+00	0.3192682		
D	3.3192220D+00	0.3711756		
D	1.4637820D+00	0.2624861		
D	5.8195150D-01	0.0732443		

BROMINE K(2)L(8)M(18)4S(2)4P(5), 2P

CHARGE = 35.000000

SYMMETRY SPECIES	S	P	D
NUMBER OF BASIS FUNCTIONS	20	15	9
NUMBER OF CLOSED SHELLS	4	2	1
NUMBER OF OPEN SHELLS	0	1	0
OPEN SHELL OCCUPATION NUMBER	0	5	0

*** FINAL SCF RESULTS ***

E = -2604.510642926

ORBITAL ENERGIES AND EXPANSION COEFFICIENTS

	S	1S	2S	3S	4S
BASIS/ORB.ENERGY		-498.2301400	-67.0973680	-10.1956580	-1.0205306
S	7.2009610D+07	0.0000490	-0.0000158	-0.0000063	-0.0000019
S	7.6859820D+06	0.0001880	-0.0000607	-0.0000242	-0.0000074
S	1.3348240D+06	0.0005753	-0.0001860	-0.0000742	-0.0000228
S	3.0371420D+05	0.0015592	-0.0005049	-0.0002014	-0.0000619
S	8.3266680D+04	0.0039816	-0.0012959	-0.0005174	-0.0001591
S	2.6029000D+04	0.0100560	-0.0032906	-0.0013141	-0.0004040
S	8.9968490D+03	0.0254451	-0.0084688	-0.0033923	-0.0010439
S	3.3665500D+03	0.0639202	-0.0217871	-0.0087431	-0.0026890
S	1.3428090D+03	0.1483477	-0.0540081	-0.0219022	-0.0067548

S	5.6636340D+02	0.2831689	-0.1161416	-0.0477539	-0.0147362
S	2.4983410D+02	0.3665730	-0.1979735	-0.0849360	-0.0264385
S	1.1312160D+02	0.2308156	-0.1574597	-0.0710172	-0.0221857
S	4.5638330D+01	0.0345092	0.2739301	0.1543222	0.0498337
S	2.1857130D+01	-0.0050767	0.6198061	0.5052885	0.1745145
S	1.0444100D+01	0.0024969	0.2687683	0.2265300	0.0782616
S	4.5552250D+00	-0.0012093	0.0180460	-0.6464489	-0.2856510
S	2.0469360D+00	0.0005256	0.0008541	-0.6252017	-0.4891268
S	6.7755470D-01	-0.0002627	-0.0000086	-0.0548315	0.1776828
S	3.3353780D-01	0.0001575	-0.0000213	0.0109053	0.7321830
S	1.3402780D-01	-0.0000375	-0.0000111	-0.0022389	0.3318115

	P	2P	3P	4P
BASIS/ORB. ENERGY		-58.9953300	-7.5476821	-0.4558501
P	5.0578350D+04	0.0001396	-0.0000563	0.0000145
P	8.5101240D+03	0.0008152	-0.0003297	0.0000853
P	2.2986400D+03	0.0040684	-0.0016510	0.0004260
P	7.8319730D+02	0.0176870	-0.0072528	0.0018824
P	3.0553480D+02	0.0632662	-0.0264633	0.0068494
P	1.3064040D+02	0.1739055	-0.0757764	0.0198405
P	5.9330130D+01	0.3344684	-0.1537503	0.0402128
P	2.8140710D+01	0.3805509	-0.1815594	0.0485645
P	1.3662560D+01	0.1886755	0.0253744	-0.0144115
P	6.5349470D+00	0.0269871	0.3952890	-0.1248075
P	3.1114500D+00	0.0015490	0.4922540	-0.1875382
P	1.4723140D+00	0.0001911	0.1996686	-0.0286651
P	5.9142640D-01	0.0000330	0.0145744	0.3833991
P	2.3702630D-01	-0.0000301	0.0004082	0.5387650
P	9.0022450D-02	0.0000013	0.0004073	0.2349508

	D	3D
BASIS/ORB. ENERGY		-3.1542587
D	6.9176450D+02	0.0005516
D	2.0306310D+02	0.0048200
D	7.7678530D+01	0.0247205
D	3.3603410D+01	0.0831302
D	1.5641360D+01	0.1967458

D	7.4681440D+00	0.3205218
D	3.5128360D+00	0.3613886
D	1.5923600D+00	0.2427944
D	6.4640880D-01	0.0617789

KRYPTON K(2)L(8)M(18)4S(2)4P(6), 1S

CHARGE = 36.000000

SYMMETRY SPECIES	S	P	D
NUMBER OF BASIS FUNCTIONS	20	15	9
NUMBER OF CLOSED SHELLS	4	3	1
NUMBER OF OPEN SHELLS	0	0	0
OPEN SHELL OCCUPATION NUMBER	0	0	0

*** FINAL SCF RESULTS ***

E = -2788.288402229

ORBITAL ENERGIES AND EXPANSION COEFFICIENTS

	S	1S	2S	3S	4S
BASIS/ORB. ENERGY		-529.3673100	-72.0496940	-11.2202690	-1.1872838
S 1.1707591D+07		0.0001848	-0.0000599	-0.0000241	-0.0000077
S 1.7530660D+06		0.0005158	-0.0001674	-0.0000674	-0.0000215
S 3.9894461D+05		0.0013452	-0.0004376	-0.0001763	-0.0000563
S 1.1299920D+05		0.0032266	-0.0010526	-0.0004240	-0.0001354
S 3.6864908D+04		0.0076118	-0.0025019	-0.0010094	-0.0003222
S 1.3308700D+04		0.0179222	-0.0059416	-0.0023974	-0.0007663
S 5.1908150D+03		0.0422144	-0.0143343	-0.0058115	-0.0018555
S 2.1530297D+03		0.0959657	-0.0337622	-0.0137207	-0.0043939
S 9.3903602D+02		0.1950124	-0.0749972	-0.0309445	-0.0098969
S 4.2714550D+02		0.3134614	-0.1407301	-0.0590826	-0.0190480
S 2.0138050D+02		0.3220157	-0.1981092	-0.0877514	-0.0282864
S 9.7253536D+01		0.1514621	-0.0851767	-0.0384832	-0.0128845
S 4.3055680D+01		0.0165270	0.3587693	0.2126948	0.0732258
S 2.1209810D+01		-0.0012774	0.5794191	0.5100083	0.1824824
S 1.0445680D+01		0.0006035	0.2230721	0.1442917	0.0551778
S 4.5907630D+00		-0.0003153	0.0140867	-0.6913240	-0.3402020
S 2.1202840D+00		0.0001124	0.0007041	-0.5669544	-0.4775457
S 7.0817700D-01		-0.0000547	-0.0000745	-0.0443528	0.2879455

S	3.5037800D-01	0.0000341	-0.0000011	0.0087594	0.7008992
S	1.4518900D-01	-0.0000080	-0.0000176	-0.0019840	0.2812249
	P	2P	3P	4P	
BASIS/ORB. ENERGY		-63.5149410	-8.4114712	-0.5230651	
P	2.0288003D+04	0.0003759	-0.0001539	0.0000417	
P	4.8044380D+03	0.0016306	-0.0006693	0.0001820	
P	1.5600440D+03	0.0071353	-0.0029455	0.0007988	
P	5.9601679D+02	0.0266102	-0.0111169	0.0030324	
P	2.5221070D+02	0.0831922	-0.0356531	0.0097116	
P	1.1453100D+02	0.2012831	-0.0899443	0.0247838	
P	5.4473227D+01	0.3454078	-0.1634655	0.0450724	
P	2.6767730D+01	0.3506776	-0.1645502	0.0460083	
P	1.3294320D+01	0.1548339	0.0715364	-0.0300014	
P	6.4650530D+00	0.0194493	0.4272661	-0.1447404	
P	3.1176790D+00	0.0013726	0.4724415	-0.1964716	
P	1.4886490D+00	0.0000493	0.1603049	0.0099577	
P	6.3560500D-01	0.0000608	0.0093504	0.4144721	
P	2.6124400D-01	-0.0000302	0.0004632	0.5167957	
P	1.0160800D-01	0.0000082	-0.0000272	0.2105994	
	D	3D			
BASIS/ORB. ENERGY		-3.7474975			
D	6.6548530D+02	0.0006914			
D	2.0021573D+02	0.0057282			
D	7.7557880D+01	0.0283544			
D	3.3683689D+01	0.0941139			
D	1.5627280D+01	0.2173091			
D	7.4430590D+00	0.3359993			
D	3.5330890D+00	0.3511054			
D	1.6359300D+00	0.2097290			
D	6.7822592D-01	0.0463290			

RUBIDIUM K(2)L(8)M(18)4S(2)4P(6)5S(1), 2S

CHARGE = 37.000000

SYMMETRY SPECIES	S	P	D
NUMBER OF BASIS FUNCTIONS	23	19	12

NUMBER OF CLOSED SHELLS	4	3	1
NUMBER OF OPEN SHELLS	1	0	0
OPEN SHELL OCCUPATION NUMBER	1	0	0

*** FINAL SCF RESULTS ***

E = -2979.175011378

ORBITAL ENERGIES AND EXPANSION COEFFICIENTS

	S	1S	2S	3S	4S	5S
BASIS/ORB. ENERGY	-561.7888100	-77.4685020	-12.5551940	-1.5655343	-0.1396307	
S 9.6419450D+08	0.0000090	-0.0000029	-0.0000012	0.0000004	0.0000001	
S 9.4152760D+07	0.0000366	-0.0000119	-0.0000048	0.0000016	0.0000003	
S 1.6096160D+07	0.0001031	-0.0000336	-0.0000136	0.0000046	0.0000010	
S 4.0773590D+06	0.0002309	-0.0000753	-0.0000306	0.0000103	0.0000022	
S 1.2029040D+06	0.0005565	-0.0001815	-0.0000738	0.0000250	0.0000053	
S 3.6321620D+05	0.0013558	-0.0004432	-0.0001802	0.0000609	0.0000128	
S 1.1626510D+05	0.0031895	-0.0010453	-0.0004252	0.0001439	0.0000304	
S 3.9689800D+04	0.0075389	-0.0024885	-0.0010128	0.0003421	0.0000720	
S 1.4386300D+04	0.0180383	-0.0060096	-0.0024497	0.0008308	0.0001756	
S 5.5227670D+03	0.0434531	-0.0148159	-0.0060554	0.0020433	0.0004295	
S 2.2374380D+03	0.1009253	-0.0357732	-0.0147058	0.0050043	0.0010591	
S 9.5428940D+02	0.2070477	-0.0803952	-0.0334353	0.0112824	0.0023687	
S 4.2600190D+02	0.3284056	-0.1511867	-0.0645009	0.0221831	0.0047091	
S 1.9740500D+02	0.3193986	-0.2031776	-0.0908360	0.0306818	0.0064098	
S 9.3442640D+01	0.1280047	-0.0544134	-0.0255377	0.0101036	0.0022894	
S 4.2379330D+01	0.0088123	0.4262205	0.2689121	-0.1009523	-0.0218142	
S 2.0273620D+01	0.0005895	0.5810368	0.5354327	-0.2004933	-0.0421075	
S 9.3055640D+00	-0.0003813	0.1583085	0.0214346	-0.0202196	-0.0061392	
S 4.5116560D+00	0.0001671	-0.0008749	-0.7424419	0.4376313	0.1013433	
S 2.1245760D+00	-0.0000878	0.0030727	-0.4885728	0.4295429	0.0975661	
S 6.1373000D-01	0.0000259	-0.0006682	-0.0247603	-0.7192467	-0.1996055	
S 2.4796410D-01	-0.0000087	0.0001993	0.0036955	-0.5659526	-0.2984207	
S 2.5207380D-02	0.0000010	-0.0000226	-0.0003609	-0.0073427	1.0908182	
	P	2P	3P	4P		
BASIS/ORB. ENERGY	-68.4812550	-9.5782834	-0.8077124			
P 1.5571320D+06	0.0000078	-0.0000032	0.0000010			
P 2.0550960D+05	0.0000339	-0.0000140	0.0000042			

P	4.5124010D+04	0.0001244	-0.0000515	0.0000154
P	1.3056110D+04	0.0004467	-0.0001851	0.0000553
P	4.5189830D+03	0.0016065	-0.0006686	0.0001992
P	1.7640670D+03	0.0056561	-0.0023611	0.0007061
P	7.5317060D+02	0.0186371	-0.0078706	0.0023485
P	3.4306240D+02	0.0547836	-0.0235318	0.0070681
P	1.6432690D+02	0.1355488	-0.0603664	0.0181408
P	8.1786960D+01	0.2591242	-0.1204579	0.0366437
P	4.2025020D+01	0.3469479	-0.1713338	0.0522010
P	2.1976940D+01	0.2697906	-0.0998153	0.0289924
P	1.1388510D+01	0.0895664	0.1717960	-0.0692299
P	5.9798220D+00	0.0080734	0.4211716	-0.1601828
P	3.1947780D+00	0.0016348	0.3941653	-0.1915277
P	1.6744850D+00	-0.0001677	0.1525024	0.0201305
P	7.4110260D-01	0.0001139	0.0130960	0.4301552
P	3.2259000D-01	-0.0000487	-0.0002346	0.5258165
P	1.3191520D-01	0.0000128	0.0001189	0.1743094

D 3D

BASIS/ORB. ENERGY -4.6401200

D	1.4068430D+03	0.0001857
D	4.0520410D+02	0.0016697
D	1.5342070D+02	0.0095807
D	6.6641910D+01	0.0376638
D	3.1222630D+01	0.1074684
D	1.5429480D+01	0.2196622
D	7.8202200D+00	0.3138988
D	4.0047120D+00	0.3174262
D	2.0561940D+00	0.2016254
D	1.0359800D+00	0.0649056
D	5.3515490D-01	0.0070359
D	3.3548550D-01	0.0016445

 STRONTIUM K(2)L(8)M(18)4S(2)4P(6)5S(2), 1S

CHARGE = 38.000000

SYMMETRY SPECIES

S P D

NUMBER OF BASIS FUNCTIONS	23	19	12
NUMBER OF CLOSED SHELLS	5	3	1
NUMBER OF OPEN SHELLS	0	0	0
OPEN SHELL OCCUPATION NUMBER	0	0	0

*** FINAL SCF RESULTS ***

E = -3177.382280253

ORBITAL ENERGIES AND EXPANSION COEFFICIENTS

	S	1S	2S	3S	4S	5S
BASIS/ORB. ENERGY		-595.2516600	-83.1089750	-13.9542110	-1.9481785	-0.1811716
S 1.3569260D+09	0.0000074	-0.0000024	-0.0000010	-0.0000004	0.0000001	
S 1.4189280D+08	0.0000297	-0.0000097	-0.0000040	-0.0000014	0.0000004	
S 2.2561580D+07	0.0000948	-0.0000310	-0.0000127	-0.0000045	0.0000012	
S 4.7991920D+06	0.0002561	-0.0000838	-0.0000344	-0.0000122	0.0000032	
S 1.2197830D+06	0.0006395	-0.0002094	-0.0000859	-0.0000306	0.0000079	
S 3.5352680D+05	0.0015110	-0.0004963	-0.0002033	-0.0000723	0.0000188	
S 1.1362200D+05	0.0034466	-0.0011345	-0.0004664	-0.0001659	0.0000430	
S 3.9972540D+04	0.0077781	-0.0025821	-0.0010573	-0.0003763	0.0000977	
S 1.5034940D+04	0.0179113	-0.0059895	-0.0024743	-0.0008803	0.0002278	
S 5.9266800D+03	0.0425452	-0.0145926	-0.0059843	-0.0021318	0.0005539	
S 2.4070210D+03	0.1008176	-0.0358188	-0.0149587	-0.0053275	0.0013776	
S 1.0067110D+03	0.2147401	-0.0839745	-0.0349523	-0.0124933	0.0032499	
S 4.3308840D+02	0.3523205	-0.1646744	-0.0718754	-0.0257507	0.0066556	
S 1.9028210D+02	0.3279753	-0.2181262	-0.0969938	-0.0352012	0.0092113	
S 8.3268830D+01	0.0973278	0.0208659	0.0067974	0.0028140	-0.0009003	
S 3.7216830D+01	-0.0003634	0.5714902	0.4144295	0.1609886	-0.0418369	
S 1.6956880D+01	0.0017269	0.5002813	0.4660454	0.1958660	-0.0525950	
S 6.0329330D+00	-0.0007816	0.0577506	-0.5756631	-0.3165904	0.0887992	
S 2.7319180D+00	0.0003487	-0.0083390	-0.7053800	-0.6109543	0.1762030	
S 7.2816780D-01	-0.0001334	0.0026036	-0.0515307	0.6500724	-0.2325881	
S 3.2427680D-01	0.0000705	-0.0013476	0.0128202	0.6296460	-0.4046882	
S 5.5514810D-02	-0.0000194	0.0003590	-0.0029422	0.0226566	0.6812188	
S 2.3200240D-02	0.0000094	-0.0001732	0.0013848	-0.0076556	0.4945594	
	P	2P	3P	4P		
BASIS/ORB. ENERGY		-73.6485160	-10.8029390	-1.0948752		
P 1.3547070D+06	0.0000094	-0.0000039	0.0000013			

P	2.0027480D+05	0.0000372	-0.0000156	0.0000050
P	4.5452310D+04	0.0001358	-0.0000569	0.0000182
P	1.3185880D+04	0.0004934	-0.0002071	0.0000664
P	4.5326570D+03	0.0017727	-0.0007463	0.0002394
P	1.7696120D+03	0.0062289	-0.0026345	0.0008457
P	7.5334270D+02	0.0204821	-0.0087577	0.0028156
P	3.4327860D+02	0.0595431	-0.0259643	0.0083726
P	1.6456650D+02	0.1451033	-0.0655884	0.0212614
P	8.1886080D+01	0.2721056	-0.1288934	0.0420972
P	4.1990790D+01	0.3501402	-0.1750366	0.0577369
P	2.1998290D+01	0.2509339	-0.0825197	0.0239004
P	1.1534090D+01	0.0767138	0.2023480	-0.0854409
P	5.9852400D+00	0.0070937	0.4569545	-0.1968151
P	3.1154600D+00	0.0009205	0.3781131	-0.1951264
P	1.5911500D+00	-0.0000352	0.1058710	0.0888551
P	7.6550800D-01	0.0000434	0.0061842	0.4767814
P	3.5261350D-01	-0.0000215	0.0005135	0.4866807
P	1.4713900D-01	0.0000058	-0.0001255	0.1203276

D 3D

BASIS/ORB. ENERGY -5.5866894

D	1.4603780D+03	0.0002075
D	4.0820880D+02	0.0019411
D	1.5361230D+02	0.0110615
D	6.6613940D+01	0.0428881
D	3.1205520D+01	0.1199402
D	1.5425240D+01	0.2370597
D	7.8089830D+00	0.3262234
D	4.0017030D+00	0.3102675
D	2.0494720D+00	0.1767317
D	1.0104080D+00	0.0470073
D	4.2661020D-01	0.0031847
D	3.6121430D-01	-0.0000796

 YTTRIUM K(2)L(8)M(18)4S(2)4P(6)5S(2)4D(1), 2D

CHARGE = 39.000000

SYMMETRY SPECIES	S	P	D
NUMBER OF BASIS FUNCTIONS	23	19	12
NUMBER OF CLOSED SHELLS	5	3	1
NUMBER OF OPEN SHELLS	0	0	1
OPEN SHELL OCCUPATION NUMBER	0	0	1

*** FINAL SCF RESULTS ***

E = -3382.990463061

ORBITAL ENERGIES AND EXPANSION COEFFICIENTS

	S	1S	2S	3S	4S	5S
BASIS/ORB. ENERGY		-629.6654800	-88.8661390	-15.3112860	-2.2380356	-0.2010215
S	1.3196340D+09	0.0000083	-0.0000027	-0.0000011	-0.0000004	0.0000001
S	1.3889770D+08	0.0000321	-0.0000105	-0.0000044	-0.0000016	0.0000004
S	2.2983740D+07	0.0001003	-0.0000329	-0.0000136	-0.0000050	0.0000013
S	4.8916790D+06	0.0002755	-0.0000905	-0.0000374	-0.0000138	0.0000037
S	1.2262860D+06	0.0006960	-0.0002289	-0.0000947	-0.0000349	0.0000094
S	3.5242810D+05	0.0016368	-0.0005398	-0.0002231	-0.0000821	0.0000221
S	1.1327720D+05	0.0037265	-0.0012329	-0.0005110	-0.0001881	0.0000505
S	3.9821710D+04	0.0083540	-0.0027847	-0.0011503	-0.0004238	0.0001140
S	1.5100880D+04	0.0189233	-0.0063699	-0.0026524	-0.0009763	0.0002619
S	5.9816070D+03	0.0449573	-0.0154937	-0.0064137	-0.0023659	0.0006367
S	2.4221700D+03	0.1066983	-0.0382945	-0.0161205	-0.0059397	0.0015926
S	1.0085020D+03	0.2249774	-0.0889150	-0.0374124	-0.0138540	0.0037320
S	4.3341100D+02	0.3582431	-0.1717402	-0.0757125	-0.0280686	0.0075252
S	1.9035410D+02	0.3173585	-0.2140590	-0.0966208	-0.0364154	0.0098645
S	8.1634850D+01	0.0845873	0.0531447	0.0247206	0.0100664	-0.0028796
S	3.7844500D+01	-0.0031755	0.5811950	0.4344509	0.1753141	-0.0473596
S	1.7520390D+01	0.0024094	0.4719773	0.4454078	0.1962596	-0.0546883
S	6.4452590D+00	-0.0010644	0.0538374	-0.5845313	-0.3391271	0.0987608
S	2.9570450D+00	0.0004883	-0.0072603	-0.7012463	-0.6367584	0.1932723
S	8.3322300D-01	-0.0001886	0.0022888	-0.0534250	0.6590798	-0.2553395
S	3.7482750D-01	0.0000975	-0.0011762	0.0123849	0.6409500	-0.4137482
S	6.8104270D-02	-0.0000265	0.0003052	-0.0027900	0.0242766	0.6545485
S	2.7801650D-02	0.0000123	-0.0001414	0.0012559	-0.0075188	0.5303467
	P	2P	3P	4P		
BASIS/ORB. ENERGY		-78.9121730	-11.9806460	-1.3038283		

P	1.2990600D+06	0.0000106	-0.0000045	0.0000015
P	2.0314360D+05	0.0000404	-0.0000171	0.0000057
P	4.5573760D+04	0.0001523	-0.0000646	0.0000217
P	1.3150260D+04	0.0005443	-0.0002310	0.0000776
P	4.5470330D+03	0.0019523	-0.0008314	0.0002795
P	1.7686180D+03	0.0068714	-0.0029408	0.0009888
P	7.5340070D+02	0.0223982	-0.0096969	0.0032678
P	3.4332350D+02	0.0646471	-0.0285781	0.0096561
P	1.6460610D+02	0.1552282	-0.0712342	0.0242235
P	8.1856200D+01	0.2845640	-0.1371007	0.0469615
P	4.1993430D+01	0.3499966	-0.1770821	0.0613236
P	2.2021000D+01	0.2342487	-0.0622274	0.0166404
P	1.1512510D+01	0.0650990	0.2379834	-0.1049455
P	5.9864180D+00	0.0049788	0.4727289	-0.2207332
P	3.1247030D+00	0.0009088	0.3477943	-0.1866633
P	1.5857970D+00	-0.0001352	0.0812267	0.1627134
P	7.6734540D-01	0.0000691	0.0032659	0.5273205
P	3.5810260D-01	-0.0000331	0.0005282	0.4218219
P	1.4807130D-01	0.0000077	-0.0001251	0.0781874
	D	3D	4D	
BASIS/ORB. ENERGY		-6.4841473	-0.2313219	
D	1.5437870D+03	0.0002139	-0.0000442	
D	4.3594020D+02	0.0019608	-0.0004197	
D	1.6469150D+02	0.0110726	-0.0023069	
D	7.1474800D+01	0.0435198	-0.0093672	
D	3.3083220D+01	0.1267697	-0.0268197	
D	1.5905370D+01	0.2613201	-0.0570067	
D	7.6937620D+00	0.3641172	-0.0722388	
D	3.6991070D+00	0.3190825	-0.0592964	
D	1.7065470D+00	0.1310821	0.0954787	
D	6.4638210D-01	0.0122719	0.3648919	
D	2.3255920D-01	-0.0006797	0.4966035	
D	7.6305080D-02	0.0002463	0.3066013	

 ZIRCONIUM K(2)L(8)M(18)4S(2)4P(6)5S(2)4D(2), 3F

CHARGE = 40.000000

SYMMETRY SPECIES	S	P	D
NUMBER OF BASIS FUNCTIONS	23	19	12
NUMBER OF CLOSED SHELLS	5	3	1
NUMBER OF OPEN SHELLS	0	0	1
OPEN SHELL OCCUPATION NUMBER	0	0	2

*** FINAL SCF RESULTS ***

E = -3596.257826079

ORBITAL ENERGIES AND EXPANSION COEFFICIENTS

	S	1S	2S	3S	4S	5S
BASIS/ORB. ENERGY		-665.0901800	-94.7992050	-16.6864400	-2.5055860	-0.2134876
S	1.3409480D+09	0.0000089	-0.0000029	-0.0000012	-0.0000005	0.0000001
S	1.3986370D+08	0.0000343	-0.0000113	-0.0000047	-0.0000018	0.0000005
S	2.4062260D+07	0.0001028	-0.0000339	-0.0000141	-0.0000053	0.0000014
S	5.1674850D+06	0.0002902	-0.0000957	-0.0000399	-0.0000151	0.0000041
S	1.2477940D+06	0.0007661	-0.0002531	-0.0001055	-0.0000399	0.0000107
S	3.4595500D+05	0.0018248	-0.0006042	-0.0002517	-0.0000952	0.0000257
S	1.1069580D+05	0.0040286	-0.0013398	-0.0005595	-0.0002115	0.0000569
S	3.9814830D+04	0.0087602	-0.0029319	-0.0012211	-0.0004622	0.0001246
S	1.5286390D+04	0.0199602	-0.0067627	-0.0028369	-0.0010720	0.0002884
S	6.0352230D+03	0.0477383	-0.0165297	-0.0069044	-0.0026173	0.0007062
S	2.4339590D+03	0.1125554	-0.0408134	-0.0173095	-0.0065475	0.0017611
S	1.0105550D+03	0.2352732	-0.0939707	-0.0399568	-0.0152129	0.0041087
S	4.3316720D+02	0.3637196	-0.1789831	-0.0796548	-0.0303195	0.0081565
S	1.9046440D+02	0.3045314	-0.2072086	-0.0949148	-0.0368883	0.0100199
S	8.0050680D+01	0.0738679	0.0877980	0.0452695	0.0189032	-0.0052909
S	3.8418340D+01	-0.0056816	0.5843074	0.4500725	0.1870384	-0.0507684
S	1.8113770D+01	0.0031057	0.4450687	0.4245901	0.1950418	-0.0546407
S	6.8791370D+00	-0.0013586	0.0505975	-0.5916747	-0.3598981	0.1054613
S	3.1906480D+00	0.0006275	-0.0063209	-0.6989954	-0.6562195	0.2016554
S	9.3450750D-01	-0.0002384	0.0019575	-0.0541657	0.6779563	-0.2712878
S	4.1915020D-01	0.0001189	-0.0009861	0.0115494	0.6409380	-0.4051507
S	7.6307310D-02	-0.0000311	0.0002443	-0.0025244	0.0234814	0.6581110
S	3.0220390D-02	0.0000141	-0.0001105	0.0011070	-0.0069928	0.5274843
P		2P	3P	4P		

BASIS/ORB. ENERGY	-84.3294520	-13.1706510	-1.4948716
P 1.3873920D+06	0.0000113	-0.0000048	0.0000017
P 2.0533990D+05	0.0000449	-0.0000192	0.0000067
P 4.6117600D+04	0.0001656	-0.0000709	0.0000247
P 1.3285410D+04	0.0005982	-0.0002566	0.0000892
P 4.5629230D+03	0.0021430	-0.0009224	0.0003212
P 1.7769700D+03	0.0074810	-0.0032376	0.0011267
P 7.5621980D+02	0.0243950	-0.0106850	0.0037315
P 3.4352750D+02	0.0702251	-0.0314533	0.0110045
P 1.6445350D+02	0.1655945	-0.0770966	0.0271940
P 8.1916590D+01	0.2951617	-0.1445414	0.0513015
P 4.2050510D+01	0.3495433	-0.1783246	0.0640948
P 2.1953340D+01	0.2187185	-0.0388566	0.0069313
P 1.1350420D+01	0.0535311	0.2832752	-0.1291721
P 5.8758880D+00	0.0031228	0.4865547	-0.2455300
P 3.0823000D+00	0.0008357	0.3014031	-0.1571040
P 1.5989270D+00	-0.0002039	0.0589577	0.2243260
P 7.9890740D-01	0.0000842	0.0028778	0.5283008
P 3.8326360D-01	-0.0000404	0.0002724	0.3803323
P 1.6045860D-01	0.0000082	-0.0000472	0.0662426
D	3D	4D	
BASIS/ORB. ENERGY	-7.3906182	-0.3159060	
D 1.4472630D+03	0.0002717	-0.0000649	
D 4.2789390D+02	0.0022748	-0.0005508	
D 1.6486610D+02	0.0124985	-0.0030050	
D 7.1796700D+01	0.0485566	-0.0118519	
D 3.3226150D+01	0.1394210	-0.0341040	
D 1.5940230D+01	0.2788830	-0.0686324	
D 7.6873630D+00	0.3740700	-0.0860415	
D 3.6833530D+00	0.3004638	-0.0513398	
D 1.6994100D+00	0.1022262	0.1363830	
D 6.9344320D-01	0.0073209	0.4005676	
D 2.6663750D-01	0.0001440	0.4705723	
D 9.3592730D-02	0.0000255	0.2379564	

NIOBIUM K(2)L(8)M(18)4S(2)4P(6)5S(1)4D(4), 6D

CHARGE = 41.000000

SYMMETRY SPECIES	S	P	D
NUMBER OF BASIS FUNCTIONS	23	19	12
NUMBER OF CLOSED SHELLS	4	3	1
NUMBER OF OPEN SHELLS	1	0	1
OPEN SHELL OCCUPATION NUMBER	1	0	4

*** FINAL SCF RESULTS ***

E = -3817.318350874

ORBITAL ENERGIES AND EXPANSION COEFFICIENTS

	S	1S	2S	3S	4S	5S
BASIS/ORB.ENERGY	-701.4346100	-100.8062300	-17.9759400	-2.6511616	-0.2286285	
S 1.2048890D+09	0.0000103	-0.0000034	-0.0000014	-0.0000005	0.0000001	
S 1.3309570D+08	0.0000381	-0.0000126	-0.0000053	-0.0000020	0.0000005	
S 2.2693030D+07	0.0001180	-0.0000391	-0.0000164	-0.0000063	0.0000017	
S 4.8440320D+06	0.0003220	-0.0001067	-0.0000448	-0.0000172	0.0000046	
S 1.2317800D+06	0.0007995	-0.0002652	-0.0001114	-0.0000428	0.0000114	
S 3.5754560D+05	0.0018588	-0.0006182	-0.0002594	-0.0000998	0.0000266	
S 1.1603900D+05	0.0042034	-0.0014032	-0.0005903	-0.0002271	0.0000604	
S 4.0530320D+04	0.0095864	-0.0032259	-0.0013535	-0.0005214	0.0001389	
S 1.5164950D+04	0.0216875	-0.0073806	-0.0031199	-0.0011997	0.0003187	
S 6.0233870D+03	0.0498635	-0.0174058	-0.0073210	-0.0028257	0.0007536	
S 2.4807450D+03	0.1137268	-0.0414644	-0.0177419	-0.0068274	0.0018127	
S 1.0537180D+03	0.2308734	-0.0930386	-0.0398107	-0.0154392	0.0041235	
S 4.6135570D+02	0.3542491	-0.1736606	-0.0779936	-0.0301920	0.0080128	
S 2.0609060D+02	0.3044534	-0.2079312	-0.0954635	-0.0378158	0.0101733	
S 8.9853290D+01	0.0803038	0.0637362	0.0314245	0.0136893	-0.0038841	
S 4.2087470D+01	-0.0027308	0.5773702	0.4426930	0.1869833	-0.0500378	
S 1.9679130D+01	0.0022033	0.4681418	0.4482152	0.2101270	-0.0583825	
S 7.3422450D+00	-0.0010046	0.0556035	-0.5874338	-0.3700996	0.1081814	
S 3.4436180D+00	0.0004756	-0.0080525	-0.7019429	-0.6713734	0.2033611	
S 1.0401380D+00	-0.0001833	0.0024869	-0.0552092	0.6839687	-0.2691888	
S 4.5959150D-01	0.0000918	-0.0012322	0.0110075	0.6472812	-0.4087981	
S 9.1934610D-02	-0.0000259	0.0003295	-0.0026278	0.0268167	0.5326394	
S 3.6757290D-02	0.0000114	-0.0001487	0.0011451	-0.0111054	0.6525443	

	P	2P	3P	4P
BASIS/ORB. ENERGY		-89.7981740	-14.2699970	-1.5778651
P 1.4010550D+06	0.0000125	0.0000125	-0.0000054	0.0000019
P 2.0685950D+05	0.0000494	0.0000494	-0.0000213	0.0000076
P 4.6261660D+04	0.0001828	0.0001828	-0.0000790	0.0000281
P 1.3279500D+04	0.0006603	0.0006603	-0.0002861	0.0001015
P 4.5630500D+03	0.0023512	0.0023512	-0.0010222	0.0003632
P 1.7788680D+03	0.0081777	0.0081777	-0.0035765	0.0012701
P 7.5647780D+02	0.0265835	0.0265835	-0.0117731	0.0041963
P 3.4351450D+02	0.0758214	0.0758214	-0.0343871	0.0122823
P 1.6444320D+02	0.1761122	0.1761122	-0.0831245	0.0299470
P 8.1906870D+01	0.3059313	0.3059313	-0.1521900	0.0552024
P 4.2071980D+01	0.3464351	0.3464351	-0.1774008	0.0650302
P 2.1935600D+01	0.2021291	0.2021291	-0.0140217	-0.0038638
P 1.1307980D+01	0.0440888	0.0440888	0.3195870	-0.1496052
P 5.8706910D+00	0.0023055	0.0023055	0.4888065	-0.2606992
P 3.0900680D+00	0.0006043	0.0006043	0.2662510	-0.1228204
P 1.5989740D+00	-0.0001432	-0.0001432	0.0437496	0.2907393
P 8.0008940D-01	0.0000394	0.0000394	0.0019304	0.5279468
P 3.8372200D-01	-0.0000266	-0.0000266	0.0002934	0.3289007
P 1.6163000D-01	0.0000030	0.0000030	0.0000076	0.0534895
	D	3D	4D	
BASIS/ORB. ENERGY		-8.2038968	-0.2867945	
D 4.1075270D+03	0.0000746	0.0000746	-0.0000180	
D 6.3423290D+02	0.0015112	0.0015112	-0.0003641	
D 2.0007400D+02	0.0113339	0.0113339	-0.0027537	
D 7.8968190D+01	0.0507897	0.0507897	-0.0123618	
D 3.4695890D+01	0.1522684	0.1522684	-0.0377206	
D 1.6146580D+01	0.3035331	0.3035331	-0.0741269	
D 7.5898300D+00	0.3929090	0.3929090	-0.0917375	
D 3.5362290D+00	0.2791686	0.2791686	-0.0261409	
D 1.5431620D+00	0.0685678	0.0685678	0.1996844	
D 6.3185980D-01	0.0010686	0.0010686	0.4184928	
D 2.3968880D-01	0.0008485	0.0008485	0.4290008	
D 8.3414910D-02	-0.0001996	-0.0001996	0.2123339	

MOLYBDENUM K(2)L(8)M(18)4S(2)4P(6)5S(1)4D(5), 7S

CHARGE = 42.000000

SYMMETRY SPECIES	S	P	D
NUMBER OF BASIS FUNCTIONS	23	19	12
NUMBER OF CLOSED SHELLS	4	3	1
NUMBER OF OPEN SHELLS	1	0	1
OPEN SHELL OCCUPATION NUMBER	1	0	5

*** FINAL SCF RESULTS ***

E = -4046.292011494

ORBITAL ENERGIES AND EXPANSION COEFFICIENTS

	S	1S	2S	3S	4S	5S
BASIS/ORB. ENERGY		-738.9189700	-107.1150400	-19.4078570	-2.8956597	-0.2370909
S 1.4423010D+09	0.0000102	-0.0000034	-0.0000014	-0.0000006	0.0000001	
S 1.3850920D+08	0.0000422	-0.0000140	-0.0000059	-0.0000023	0.0000006	
S 2.2330600D+07	0.0001289	-0.0000429	-0.0000181	-0.0000071	0.0000019	
S 4.8760050D+06	0.0003411	-0.0001135	-0.0000479	-0.0000188	0.0000050	
S 1.2466860D+06	0.0008535	-0.0002843	-0.0001202	-0.0000471	0.0000125	
S 3.5922570D+05	0.0020179	-0.0006739	-0.0002848	-0.0001117	0.0000296	
S 1.1456530D+05	0.0045932	-0.0015407	-0.0006526	-0.0002557	0.0000678	
S 4.0226950D+04	0.0101563	-0.0034329	-0.0014509	-0.0005696	0.0001512	
S 1.5261270D+04	0.0228096	-0.0078091	-0.0033233	-0.0013017	0.0003447	
S 6.0670310D+03	0.0526862	-0.0184900	-0.0078394	-0.0030840	0.0008194	
S 2.4900560D+03	0.1199842	-0.0441690	-0.0190277	-0.0074585	0.0019739	
S 1.0531300D+03	0.2408190	-0.0981967	-0.0424197	-0.0167761	0.0044641	
S 4.6145170D+02	0.3567087	-0.1790484	-0.0811358	-0.0319941	0.0084640	
S 2.0721980D+02	0.2913603	-0.2008403	-0.0933453	-0.0378199	0.0101429	
S 9.0051400D+01	0.0712773	0.0902098	0.0475938	0.0209931	-0.0058375	
S 4.3063020D+01	-0.0035553	0.5804685	0.4556318	0.1965333	-0.0524777	
S 2.0396970D+01	0.0022988	0.4473644	0.4333044	0.2096913	-0.0582177	
S 7.8512320D+00	-0.0010417	0.0526349	-0.5873321	-0.3831555	0.1119486	
S 3.7185010D+00	0.0004841	-0.0068239	-0.7060291	-0.6870366	0.2086032	
S 1.1453490D+00	-0.0001827	0.0020440	-0.0580356	0.6942597	-0.2774364	
S 5.0537080D-01	0.0000904	-0.0010129	0.0113983	0.6482264	-0.4026790	
S 1.0456460D-01	-0.0000252	0.0002638	-0.0027393	0.0269224	0.4980573	

S	4.0524980D-02	0.0000107	-0.0001173	0.0011492	-0.0112202	0.6871143
	P	2P	3P	4P		
BASIS/ORB. ENERGY	-95.5423090	-15.5041140	-1.7488269			
P	1.4176790D+06	0.0000136	-0.0000059	0.0000022		
P	2.0865440D+05	0.0000543	-0.0000237	0.0000086		
P	4.6272250D+04	0.0002023	-0.0000883	0.0000321		
P	1.3257510D+04	0.0007254	-0.0003173	0.0001152		
P	4.5679090D+03	0.0025731	-0.0011294	0.0004107		
P	1.7793670D+03	0.0089335	-0.0039466	0.0014353		
P	7.5673640D+02	0.0288640	-0.0129178	0.0047140		
P	3.4351670D+02	0.0816992	-0.0375038	0.0137250		
P	1.6440970D+02	0.1866685	-0.0892650	0.0329482		
P	8.1916810D+01	0.3159408	-0.1595899	0.0593857		
P	4.2078780D+01	0.3420744	-0.1748539	0.0654411		
P	2.1905730D+01	0.1854156	0.0125188	-0.0158812		
P	1.1282450D+01	0.0359765	0.3538921	-0.1714666		
P	5.8690470D+00	0.0018212	0.4868715	-0.2745045		
P	3.0850870D+00	0.0003711	0.2311728	-0.0800295		
P	1.5987470D+00	-0.0000775	0.0312378	0.3531786		
P	8.0073240D-01	-0.0000023	0.0017118	0.5210330		
P	3.8552660D-01	-0.0000122	0.0001608	0.2789365		
P	1.6187280D-01	-0.0000006	0.0000355	0.0385143		
	D	3D	4D			
BASIS/ORB. ENERGY	-9.1464741	-0.3409629				
D	2.5824030D+03	0.0001263	-0.0000324			
D	6.9301570D+02	0.0011848	-0.0003123			
D	2.5547700D+02	0.0072595	-0.0018789			
D	1.0751770D+02	0.0323236	-0.0085619			
D	4.8475040D+01	0.1054893	-0.0277891			
D	2.2831430D+01	0.2432203	-0.0656039			
D	1.0889790D+01	0.3741045	-0.0945962			
D	5.1458410D+00	0.3491265	-0.0762204			
D	2.3426160D+00	0.1347105	0.1214173			
D	9.4059410D-01	0.0103911	0.4094502			
D	3.5013850D-01	0.0000834	0.4712928			

D 1.1727850D-01 -0.0000165 0.2554680

TECHNETIUM K(2)L(8)M(18)4S(2)4P(6)5S(2)4D(5), 6S

CHARGE = 43.000000

SYMMETRY SPECIES	S	P	D
NUMBER OF BASIS FUNCTIONS	23	19	12
NUMBER OF CLOSED SHELLS	5	3	1
NUMBER OF OPEN SHELLS	0	0	1
OPEN SHELL OCCUPATION NUMBER	0	0	5

*** FINAL SCF RESULTS ***

E = -4283.158588404

ORBITAL ENERGIES AND EXPANSION COEFFICIENTS

	S	1S	2S	3S	4S	5S
BASIS/ORB. ENERGY		-777.6166800	-113.7948000	-21.0493840	-3.2987900	-0.2406757
S 1.2434930D+09	0.0000118	-0.0000039	-0.0000017	0.0000007	0.0000002	
S 1.3811110D+08	0.0000430	-0.0000143	-0.0000061	0.0000024	0.0000006	
S 2.4017470D+07	0.0001308	-0.0000437	-0.0000186	0.0000074	0.0000019	
S 5.1186040D+06	0.0003639	-0.0001215	-0.0000517	0.0000207	0.0000054	
S 1.2642730D+06	0.0009301	-0.0003111	-0.0001324	0.0000530	0.0000138	
S 3.5501440D+05	0.0022146	-0.0007427	-0.0003160	0.0001265	0.0000331	
S 1.1281890D+05	0.0049451	-0.0016666	-0.0007106	0.0002841	0.0000742	
S 4.0070800D+04	0.0107512	-0.0036503	-0.0015537	0.0006225	0.0001630	
S 1.5361320D+04	0.0239161	-0.0082353	-0.0035279	0.0014098	0.0003681	
S 6.1232190D+03	0.0555747	-0.0196128	-0.0083783	0.0033643	0.0008814	
S 2.4964180D+03	0.1267012	-0.0470814	-0.0204211	0.0081676	0.0021323	
S 1.0533090D+03	0.2495556	-0.1030063	-0.0448965	0.0181332	0.0047570	
S 4.6270880D+02	0.3580080	-0.1837619	-0.0840213	0.0338086	0.0088265	
S 2.0861440D+02	0.2793057	-0.1934275	-0.0909221	0.0377270	0.0099717	
S 8.9548210D+01	0.0633370	0.1229453	0.0682062	-0.0305643	-0.0082712	
S 4.3508730D+01	-0.0048350	0.5854568	0.4737453	-0.2093124	-0.0552561	
S 2.0912250D+01	0.0026327	0.4190239	0.4062270	-0.2037793	-0.0558888	
S 8.2327740D+00	-0.0011958	0.0484274	-0.6103444	0.4153879	0.1199622	
S 3.9356300D+00	0.0005614	-0.0061482	-0.6883410	0.6926790	0.2088598	
S 1.2646690D+00	-0.0002063	0.0017925	-0.0556342	-0.7128742	-0.2859848	
S 5.5784720D-01	0.0000936	-0.0008348	0.0091459	-0.6510532	-0.3808720	

S	9.8231430D-02	-0.0000226	0.0001884	-0.0019290	-0.0226165	0.6277876
S	3.7194760D-02	0.0000100	-0.0000833	0.0008245	0.0066220	0.5484166
	P	2P	3P	4P		
BASIS/ORB. ENERGY	-101.6294800	-16.9398480	-2.0638575			
P	1.4890350D+06	0.0000146	-0.0000064	0.0000024		
P	2.0890460D+05	0.0000606	-0.0000266	0.0000100		
P	4.6094990D+04	0.0002223	-0.0000979	0.0000366		
P	1.3270960D+04	0.0007942	-0.0003505	0.0001310		
P	4.5677710D+03	0.0028166	-0.0012474	0.0004666		
P	1.7801040D+03	0.0097227	-0.0043370	0.0016238		
P	7.5707620D+02	0.0312818	-0.0141408	0.0053087		
P	3.4347160D+02	0.0878198	-0.0407882	0.0153770		
P	1.6437730D+02	0.1972232	-0.0955035	0.0362852		
P	8.1935420D+01	0.3252208	-0.1667169	0.0640119		
P	4.2071990D+01	0.3363534	-0.1705522	0.0652775		
P	2.1870090D+01	0.1689046	0.0405095	-0.0291628		
P	1.1268760D+01	0.0291391	0.3860589	-0.1957541		
P	5.8655530D+00	0.0014947	0.4813312	-0.2860627		
P	3.0540780D+00	0.0001860	0.1971021	-0.0284656		
P	1.5960470D+00	-0.0000329	0.0201630	0.4111579		
P	8.0384180D-01	-0.0000282	0.0021216	0.5088366		
P	3.9140030D-01	-0.0000018	-0.0001629	0.2261542		
P	1.6008010D-01	-0.0000016	0.0000581	0.0234292		
	D	3D	4D			
BASIS/ORB. ENERGY	-10.2844600	-0.5149400				
D	2.4862630D+03	0.0001472	-0.0000429			
D	6.9915450D+02	0.0013143	-0.0003855			
D	2.5762490D+02	0.0080949	-0.0023745			
D	1.0821340D+02	0.0358015	-0.0105917			
D	4.8710460D+01	0.1152207	-0.0344193			
D	2.2919570D+01	0.2592855	-0.0779582			
D	1.0901540D+01	0.3845457	-0.1102091			
D	5.1600500D+00	0.3317924	-0.0691403			
D	2.3518510D+00	0.1115021	0.1636513			
D	1.0005040D+00	0.0064763	0.4387158			

D	4.017000D-01	0.0006754	0.4418038
D	1.4688780D-01	-0.0001740	0.1839687

RUTHENIUM K(2)L(8)M(18)4S(2)4P(6)5S(1)4D(7), 5F

CHARGE = 44.000000

SYMMETRY SPECIES	S	P	D
NUMBER OF BASIS FUNCTIONS	23	19	12
NUMBER OF CLOSED SHELLS	4	3	1
NUMBER OF OPEN SHELLS	1	0	1
OPEN SHELL OCCUPATION NUMBER	1	0	7

*** FINAL SCF RESULTS ***

E = -4528.110876216

ORBITAL ENERGIES AND EXPANSION COEFFICIENTS

	S	1S	2S	3S	4S	5S
BASIS/ORB. ENERGY	-817.1161100	-120.4066800	-22.4578470	-3.4378843	-0.2380346	
S	2.2913010D+09	0.0000088	-0.0000029	-0.0000013	0.0000005	0.0000001
S	1.9771230D+08	0.0000398	-0.0000133	-0.0000057	0.0000023	0.0000006
S	2.8318070D+07	0.0001378	-0.0000462	-0.0000198	0.0000080	0.0000020
S	5.2667880D+06	0.0004106	-0.0001377	-0.0000589	0.0000238	0.0000059
S	1.2103250D+06	0.0010627	-0.0003570	-0.0001529	0.0000618	0.0000154
S	3.3568960D+05	0.0024542	-0.0008265	-0.0003538	0.0001430	0.0000357
S	1.0982600D+05	0.0051949	-0.0017592	-0.0007548	0.0003047	0.0000760
S	4.0551990D+04	0.0110451	-0.0037661	-0.0016131	0.0006530	0.0001632
S	1.5648690D+04	0.0252391	-0.0087392	-0.0037660	0.0015194	0.0003788
S	6.1658910D+03	0.0589563	-0.0209234	-0.0090006	0.0036521	0.0009134
S	2.5036550D+03	0.1328573	-0.0498363	-0.0217531	0.0087826	0.0021893
S	1.0546390D+03	0.2586989	-0.1080699	-0.0474981	0.0193995	0.0048587
S	4.6289790D+02	0.3599103	-0.1890604	-0.0871842	0.0354006	0.0088251
S	2.0938660D+02	0.2654100	-0.1840298	-0.0873927	0.0368527	0.0093057
S	8.9720430D+01	0.0555239	0.1539396	0.0885450	-0.0403033	-0.0103687
S	4.4210660D+01	-0.0049298	0.5838543	0.4853852	-0.2166216	-0.0546435
S	2.1566910D+01	0.0025118	0.3967117	0.3838066	-0.1984296	-0.0520863
S	8.6659190D+00	-0.0011282	0.0455261	-0.6236389	0.4396616	0.1214628
S	4.1780060D+00	0.0005170	-0.0055579	-0.6791884	0.6864663	0.1978416
S	1.3606990D+00	-0.0001819	0.0015454	-0.0541669	-0.7367139	-0.2842595

S	5.8893690D-01	0.0000796	-0.0007053	0.0082532	-0.6363664	-0.3492328
S	1.0086070D-01	-0.0000192	0.0001556	-0.0017994	-0.0226991	0.5779252
S	3.8257260D-02	0.0000086	-0.0000732	0.0007914	0.0083693	0.5843892
	P	2P	3P	4P		
BASIS/ORB. ENERGY	-107.6232400	-18.1377260	-2.1405108			
P	1.4433300D+06	0.0000163	-0.0000072	0.0000027		
P	2.1323560D+05	0.0000640	-0.0000284	0.0000107		
P	4.7725040D+04	0.0002346	-0.0001041	0.0000394		
P	1.3679820D+04	0.0008432	-0.0003753	0.0001419		
P	4.6660900D+03	0.0030141	-0.0013460	0.0005093		
P	1.8021720D+03	0.0104794	-0.0047166	0.0017868		
P	7.6156340D+02	0.0337251	-0.0153885	0.0058445		
P	3.4443780D+02	0.0940594	-0.0441712	0.0168570		
P	1.6431970D+02	0.2090568	-0.1024579	0.0394085		
P	8.1639640D+01	0.3353205	-0.1743568	0.0678544		
P	4.1899800D+01	0.3276741	-0.1632946	0.0627468		
P	2.1801870D+01	0.1520022	0.0701082	-0.0435286		
P	1.1271930D+01	0.0233813	0.4135309	-0.2152338		
P	5.8951390D+00	0.0013057	0.4671858	-0.2872105		
P	3.0621530D+00	0.0000332	0.1692535	0.0327604		
P	1.5467710D+00	0.0000000	0.0140806	0.4826458		
P	7.4958480D-01	-0.0000467	0.0013728	0.4834627		
P	3.4819360D-01	0.0000036	-0.0000179	0.1609363		
P	1.3161250D-01	-0.0000033	0.0000527	0.0109377		
	D	3D	4D			
BASIS/ORB. ENERGY	-11.1824660	-0.3925127				
D	2.4767220D+03	0.0001671	-0.0000484			
D	7.0406480D+02	0.0014639	-0.0004220			
D	2.5924870D+02	0.0090505	-0.0026327			
D	1.0835570D+02	0.0399059	-0.0116297			
D	4.8746220D+01	0.1255915	-0.0372476			
D	2.2967270D+01	0.2747649	-0.0811534			
D	1.0909350D+01	0.3927231	-0.1113734			
D	5.1754750D+00	0.3119032	-0.0515340			
D	2.3616410D+00	0.0914891	0.1918384			

D	1.0098370D+00	0.0043347	0.4310590
D	3.9065710D-01	0.0008399	0.4272681
D	1.3326060D-01	-0.0000448	0.2038036

RHODIUM K(2)L(8)M(18)4S(2)4P(6)5S(1)4D(8), 4F

CHARGE = 45.000000

SYMMETRY SPECIES	S	P	D
NUMBER OF BASIS FUNCTIONS	23	19	12
NUMBER OF CLOSED SHELLS	4	3	1
NUMBER OF OPEN SHELLS	1	0	1
OPEN SHELL OCCUPATION NUMBER	1	0	8

*** FINAL SCF RESULTS ***

E = -4781.326572973

ORBITAL ENERGIES AND EXPANSION COEFFICIENTS

	S	1S	2S	3S	4S	5S
BASIS/ORB. ENERGY		-857.8155000	-127.3637100	-24.0481010	-3.7108469	-0.2355330
S	9.2937800D+08	0.0000167	-0.0000056	-0.0000024	0.0000010	0.0000002
S	1.1100870D+08	0.0000560	-0.0000188	-0.0000081	0.0000033	0.0000008
S	2.1009460D+07	0.0001598	-0.0000538	-0.0000231	0.0000095	0.0000023
S	4.7417420D+06	0.0004314	-0.0001453	-0.0000625	0.0000256	0.0000061
S	1.2170830D+06	0.0010730	-0.0003619	-0.0001559	0.0000638	0.0000152
S	3.5311060D+05	0.0024893	-0.0008420	-0.0003627	0.0001483	0.0000355
S	1.1424040D+05	0.0055722	-0.0018936	-0.0008166	0.0003343	0.0000798
S	4.0087940D+04	0.0124902	-0.0042839	-0.0018483	0.0007555	0.0001809
S	1.5046750D+04	0.0278531	-0.0096914	-0.0041955	0.0017204	0.0004094
S	6.0281360D+03	0.0614958	-0.0220281	-0.0095562	0.0039048	0.0009388
S	2.5388120D+03	0.1312310	-0.0494887	-0.0216905	0.0089302	0.0021153
S	1.1153500D+03	0.2442045	-0.1026733	-0.0455415	0.0186469	0.0045168
S	5.0996930D+02	0.3394139	-0.1746018	-0.0804033	0.0335462	0.0078657
S	2.3963150D+02	0.2718749	-0.1893696	-0.0910466	0.0374593	0.0093978
S	1.1199460D+02	0.0753634	0.0613703	0.0360227	-0.0140920	-0.0044441
S	5.4147270D+01	0.0000704	0.5332685	0.4058718	-0.1892265	-0.0435868
S	2.6319690D+01	0.0015841	0.4878491	0.5057443	-0.2406957	-0.0641136
S	1.1329400D+01	-0.0009675	0.0871509	-0.3138844	0.1703849	0.0563350
S	5.8670960D+00	0.0006228	-0.0111825	-0.7881131	0.7849564	0.1875468

S	2.9761080D+00	-0.0003078	0.0048020	-0.2289982	0.1210296	0.0710004
S	1.2411080D+00	0.0001088	-0.0015311	-0.0111752	-0.9078466	-0.4152194
S	5.3092230D-01	-0.0000297	0.0003610	0.0000485	-0.4343824	-0.1570193
S	6.2886270D-02	0.0000027	-0.0000366	-0.0000788	-0.0039786	1.0827857
	P	2P	3P	4P		
BASIS/ORB. ENERGY						
		-113.9311000	-19.5085740	-2.3373279		
P	1.4491960D+06	0.0000178	-0.0000079	0.0000030		
P	2.1390440D+05	0.0000700	-0.0000313	0.0000120		
P	4.7865170D+04	0.0002562	-0.0001146	0.0000440		
P	1.3702280D+04	0.0009205	-0.0004129	0.0001587		
P	4.6692180D+03	0.0032829	-0.0014780	0.0005682		
P	1.8030640D+03	0.0113647	-0.0051590	0.0019872		
P	7.6182740D+02	0.0363946	-0.0167611	0.0064686		
P	3.4443200D+02	0.1005794	-0.0477361	0.0185352		
P	1.6428620D+02	0.2198423	-0.1090267	0.0426353		
P	8.1623130D+01	0.3429039	-0.1805899	0.0716168		
P	4.1887000D+01	0.3187781	-0.1550832	0.0597986		
P	2.1782800D+01	0.1370317	0.0999361	-0.0584588		
P	1.1270260D+01	0.0187091	0.4402503	-0.2378542		
P	5.9078050D+00	0.0011125	0.4490647	-0.2823979		
P	3.0532760D+00	-0.0000639	0.1418117	0.0943105		
P	1.5414790D+00	0.0000150	0.0093452	0.5146472		
P	7.4778050D-01	-0.0000554	0.0014239	0.4477211		
P	3.4790060D-01	0.0000064	-0.0000665	0.1295643		
P	1.2790300D-01	-0.0000037	0.0000566	0.0075843		
	D	3D	4D			
BASIS/ORB. ENERGY						
		-12.2467930	-0.4267308			
D	2.7333870D+03	0.0001698	-0.0000513			
D	7.1971690D+02	0.0016166	-0.0004839			
D	2.6281470D+02	0.0099434	-0.0030190			
D	1.0905680D+02	0.0441627	-0.0133833			
D	4.8689940D+01	0.1379858	-0.0427781			
D	2.2909960D+01	0.2891763	-0.0885297			
D	1.0963730D+01	0.3935077	-0.1161494			
D	5.2380870D+00	0.2934214	-0.0356418			

D	2.3729900D+00	0.0763509	0.2298086
D	1.0239690D+00	0.0023954	0.4374173
D	4.0469550D-01	0.0010801	0.3988519
D	1.4147220D-01	-0.0000477	0.1799559

PALLADIUM K(2)L(8)M(18)4S(2)4P(6)5S(0)4D(10), 1S

CHARGE = 46.000000

SYMMETRY SPECIES	S	P	D
NUMBER OF BASIS FUNCTIONS	23	19	12
NUMBER OF CLOSED SHELLS	4	3	2
NUMBER OF OPEN SHELLS	0	0	0
OPEN SHELL OCCUPATION NUMBER	0	0	0

*** FINAL SCF RESULTS ***

E = -5042.907433628

ORBITAL ENERGIES AND EXPANSION COEFFICIENTS

	S	1S	2S	3S	4S
BASIS/ORB. ENERGY		-899.4492100	-134.3806500	-25.5307030	-3.8387510
S	1.0514600D+09	0.0000166	-0.0000056	-0.0000024	-0.0000010
S	1.2177690D+08	0.0000583	-0.0000197	-0.0000085	-0.0000035
S	2.1652850D+07	0.0001725	-0.0000583	-0.0000252	-0.0000104
S	4.7998030D+06	0.0004610	-0.0001559	-0.0000675	-0.0000278
S	1.2237080D+06	0.0011518	-0.0003900	-0.0001689	-0.0000696
S	3.5235040D+05	0.0026789	-0.0009097	-0.0003941	-0.0001623
S	1.1369570D+05	0.0059609	-0.0020353	-0.0008826	-0.0003637
S	4.0045200D+04	0.0132276	-0.0045561	-0.0019769	-0.0008144
S	1.5077210D+04	0.0294800	-0.0103208	-0.0044933	-0.0018533
S	6.0255250D+03	0.0650587	-0.0234333	-0.0102274	-0.0042165
S	2.5375220D+03	0.1371261	-0.0522571	-0.0230458	-0.0095335
S	1.1158770D+03	0.2522242	-0.1071991	-0.0478967	-0.0198254
S	5.0951880D+02	0.3421690	-0.1803799	-0.0837571	-0.0350345
S	2.3924080D+02	0.2604681	-0.1811533	-0.0879413	-0.0368890
S	1.1051610D+02	0.0660920	0.0865154	0.0517755	0.0221629
S	5.5782290D+01	-0.0020031	0.5185694	0.4016263	0.1871081
S	2.8003580D+01	0.0023391	0.4719975	0.4922282	0.2404980
S	1.2744070D+01	-0.0015245	0.0984229	-0.2089400	-0.1176528

S	6.9481750D+00	0.0011011	-0.0116697	-0.7653720	-0.6814720
S	3.6695430D+00	-0.0006237	0.0062988	-0.3329198	-0.3907801
S	1.7771000D+00	0.0002802	-0.0024850	-0.0251142	0.6306690
S	8.4223930D-01	-0.0001026	0.0007796	-0.0010788	0.6995733
S	3.6214420D-01	0.0000228	-0.0001836	-0.0003669	0.1273981
	P	2P	3P	4P	
BASIS/ORB. ENERGY	-120.2687200	-20.7648610	-2.4005444		
P	1.4515300D+06	0.0000195	-0.0000087	0.0000034	
P	2.1430360D+05	0.0000765	-0.0000344	0.0000133	
P	4.7983560D+04	0.0002794	-0.0001259	0.0000488	
P	1.3714470D+04	0.0010044	-0.0004540	0.0001761	
P	4.6695630D+03	0.0035682	-0.0016190	0.0006276	
P	1.8041900D+03	0.0122993	-0.0056284	0.0021881	
P	7.6189240D+02	0.0392203	-0.0182252	0.0070941	
P	3.4442840D+02	0.1072383	-0.0514112	0.0201601	
P	1.6427330D+02	0.2306614	-0.1157232	0.0456645	
P	8.1599440D+01	0.3494390	-0.1861692	0.0746767	
P	4.1887370D+01	0.3086503	-0.1450918	0.0554092	
P	2.1763920D+01	0.1231813	0.1304914	-0.0736895	
P	1.1271320D+01	0.0146890	0.4636370	-0.2587405	
P	5.9225490D+00	0.0010691	0.4273483	-0.2677076	
P	3.0323550D+00	-0.0002012	0.1177340	0.1560711	
P	1.5370540D+00	0.0000604	0.0054436	0.5269151	
P	7.4601760D-01	-0.0000783	0.0017171	0.4111985	
P	3.4394500D-01	0.0000132	-0.0001443	0.1122677	
P	1.2756040D-01	-0.0000060	0.0000976	0.0064308	
	D	3D	4D		
BASIS/ORB. ENERGY	-13.1922810	-0.3264560			
D	2.6648900D+03	0.0001891	-0.0000569		
D	7.4702560D+02	0.0016548	-0.0004873		
D	2.7679020D+02	0.0099111	-0.0029902		
D	1.1633710D+02	0.0433137	-0.0129370		
D	5.2053150D+01	0.1380823	-0.0425185		
D	2.4191290D+01	0.2997793	-0.0904497		
D	1.1336250D+01	0.4084288	-0.1198077		

D	5.3113190D+00	0.2832844	-0.0162420
D	2.3214210D+00	0.0612437	0.2716317
D	9.7178560D-01	0.0000542	0.4401549
D	3.6940300D-01	0.0008487	0.3732542
D	1.2267130D-01	-0.0002206	0.1769291

SILVER K(2)L(8)M(18)4S(2)4P(6)5S(1)4D(10), 2S

CHARGE = 47.000000

SYMMETRY SPECIES	S	P	D
NUMBER OF BASIS FUNCTIONS	23	19	12
NUMBER OF CLOSED SHELLS	4	3	2
NUMBER OF OPEN SHELLS	1	0	0
OPEN SHELL OCCUPATION NUMBER	1	0	0

*** FINAL SCF RESULTS ***

E = -5312.999006338

ORBITAL ENERGIES AND EXPANSION COEFFICIENTS

	S	1S	2S	3S	4S	5S
BASIS/ORB. ENERGY		-942.4683300	-141.9220200	-27.3730520	-4.2717899	-0.2366372
S	1.4242040D+09	0.0000153	-0.0000052	-0.0000023	0.0000009	0.0000002
S	1.3434240D+08	0.0000623	-0.0000211	-0.0000092	0.0000038	0.0000009
S	2.2221430D+07	0.0001869	-0.0000634	-0.0000276	0.0000115	0.0000026
S	4.7612140D+06	0.0005053	-0.0001715	-0.0000746	0.0000312	0.0000070
S	1.2029560D+06	0.0012431	-0.0004227	-0.0001841	0.0000769	0.0000172
S	3.4977170D+05	0.0028606	-0.0009755	-0.0004247	0.0001775	0.0000396
S	1.1258530D+05	0.0064553	-0.0022139	-0.0009659	0.0004031	0.0000899
S	3.9349020D+04	0.0143028	-0.0049514	-0.0021578	0.0009032	0.0002020
S	1.4864230D+04	0.0313663	-0.0110434	-0.0048439	0.0020198	0.0004500
S	5.9870730D+03	0.0683030	-0.0247786	-0.0108482	0.0045568	0.0010208
S	2.5477870D+03	0.1405159	-0.0539951	-0.0240510	0.0100254	0.0022306
S	1.1354020D+03	0.2537077	-0.1089366	-0.0487315	0.0206459	0.0046379
S	5.1999390D+02	0.3449688	-0.1840954	-0.0867558	0.0363274	0.0080711
S	2.4107010D+02	0.2573953	-0.1796239	-0.0863794	0.0379634	0.0086398
S	1.0712390D+02	0.0568075	0.1421237	0.0828044	-0.0397403	-0.0093068
S	5.2477240D+01	-0.0031204	0.5804607	0.4898863	-0.2260943	-0.0507464
S	2.5543550D+01	0.0018585	0.4099637	0.4038373	-0.2193534	-0.0521317

S	1.0282920D+01	-0.0008598	0.0481616	-0.6329905	0.4815603	0.1212264
S	5.0324640D+00	0.0003937	-0.0062478	-0.6776925	0.7027467	0.1784810
S	1.7024590D+00	-0.0001325	0.0015938	-0.0540199	-0.7812054	-0.2656006
S	7.2072090D-01	0.0000533	-0.0006672	0.0065837	-0.6211321	-0.2982036
S	1.0485820D-01	-0.0000112	0.0001302	-0.0013350	-0.0187343	0.5708721
S	3.8060620D-02	0.0000051	-0.0000594	0.0005970	0.0057605	0.5679551
	P	2P	3P	4P		
BASIS/ORB. ENERGY	-127.0952400	-22.3703790	-2.7427266			
P	1.4890430D+06	0.0000209	-0.0000095	0.0000037		
P	2.1738320D+05	0.0000831	-0.0000377	0.0000149		
P	4.8066390D+04	0.0003060	-0.0001389	0.0000548		
P	1.3707480D+04	0.0010921	-0.0004971	0.0001964		
P	4.6788940D+03	0.0038587	-0.0017637	0.0006962		
P	1.8063970D+03	0.0133006	-0.0061345	0.0024298		
P	7.6182950D+02	0.0421850	-0.0197703	0.0078380		
P	3.4442310D+02	0.1140851	-0.0552383	0.0220828		
P	1.6425420D+02	0.2414019	-0.1224509	0.0492430		
P	8.1556610D+01	0.3553378	-0.1913998	0.0783694		
P	4.1824890D+01	0.2979061	-0.1330903	0.0504796		
P	2.1705110D+01	0.1095220	0.1620281	-0.0909453		
P	1.1276060D+01	0.0114240	0.4830379	-0.2812356		
P	5.9409340D+00	0.0009688	0.4013388	-0.2495791		
P	3.0334390D+00	-0.0002574	0.0972790	0.2176983		
P	1.5312680D+00	0.0000662	0.0038034	0.5441408		
P	7.4570420D-01	-0.0000786	0.0014362	0.3739508		
P	3.4430970D-01	0.0000141	-0.0001152	0.0834603		
P	1.1692110D-01	-0.0000046	0.0000540	0.0033903		
	D	3D	4D			
BASIS/ORB. ENERGY	-14.4784070	-0.5106044				
D	4.1870490D+03	0.0001076	-0.0000345			
D	9.3414040D+02	0.0013743	-0.0004360			
D	3.0365240D+02	0.0102006	-0.0032877			
D	1.1914120D+02	0.0483751	-0.0155624			
D	5.1770470D+01	0.1532828	-0.0505944			
D	2.3949640D+01	0.3150444	-0.1020851			

D	1.1350170D+01	0.4016895	-0.1243925
D	5.4371820D+00	0.2583463	-0.0019151
D	2.4745750D+00	0.0546641	0.2875060
D	1.0762690D+00	0.0008448	0.4419797
D	4.3477530D-01	0.0005790	0.3546122
D	1.5732580D-01	-0.0001443	0.1411457

CADMIUM K(2)L(8)M(18)4S(2)4P(6)5S(2)4D(10), 1S

CHARGE = 48.000000

SYMMETRY SPECIES	S	P	D
NUMBER OF BASIS FUNCTIONS	23	19	12
NUMBER OF CLOSED SHELLS	5	3	2
NUMBER OF OPEN SHELLS	0	0	0
OPEN SHELL OCCUPATION NUMBER	0	0	0

*** FINAL SCF RESULTS ***

E = -5591.533823244

ORBITAL ENERGIES AND EXPANSION COEFFICIENTS

	S	1S	2S	3S	4S	5S
BASIS/ORB. ENERGY		-986.6305700	-149.7287100	-29.3096660	-4.7441304	-0.2809024
S	1.2809250D+09	0.0000172	-0.0000058	-0.0000026	0.0000011	0.0000003
S	1.3386140D+08	0.0000659	-0.0000224	-0.0000098	0.0000042	0.0000010
S	2.2228700D+07	0.0002013	-0.0000685	-0.0000300	0.0000127	0.0000031
S	4.7661420D+06	0.0005382	-0.0001834	-0.0000802	0.0000340	0.0000084
S	1.2108270D+06	0.0013235	-0.0004518	-0.0001978	0.0000838	0.0000207
S	3.4978940D+05	0.0030712	-0.0010517	-0.0004603	0.0001951	0.0000483
S	1.1215930D+05	0.0068892	-0.0023730	-0.0010406	0.0004406	0.0001090
S	3.9264130D+04	0.0151804	-0.0052806	-0.0023143	0.0009826	0.0002435
S	1.4832470D+04	0.0332648	-0.0117764	-0.0051908	0.0021964	0.0005430
S	5.9712030D+03	0.0719663	-0.0262875	-0.0115827	0.0049348	0.0012246
S	2.5429580D+03	0.1468296	-0.0569398	-0.0254910	0.0107859	0.0026644
S	1.1337150D+03	0.2606717	-0.1134658	-0.0511704	0.0219957	0.0054711
S	5.2254220D+02	0.3407651	-0.1850543	-0.0877869	0.0373137	0.0092119
S	2.4584200D+02	0.2445751	-0.1711474	-0.0830371	0.0371233	0.0093376
S	1.1178690D+02	0.0538808	0.1459929	0.0868299	-0.0422172	-0.0108449
S	5.5120140D+01	-0.0023958	0.5759510	0.4870052	-0.2285949	-0.0572220

S	2.6937380D+01	0.0016083	0.4104478	0.4145323	-0.2287465	-0.0599327
S	1.1171210D+01	-0.0007660	0.0491037	-0.6008825	0.4621074	0.1285334
S	5.4914430D+00	0.0003385	-0.0051971	-0.7104983	0.7436354	0.2130613
S	1.8634490D+00	-0.0001155	0.0012938	-0.0628190	-0.7527122	-0.2930243
S	8.0990950D-01	0.0000487	-0.0005780	0.0085576	-0.6518128	-0.3454764
S	1.3249900D-01	-0.0000105	0.0001125	-0.0017309	-0.0208725	0.6134399
S	4.7262450D-02	0.0000046	-0.0000489	0.0007278	0.0061662	0.5500042
	P	2P	3P	4P		
BASIS/ORB. ENERGY	-134.1515500	-24.0605630	-3.1168322			
P	1.5304840D+06	0.0000224	-0.0000102	0.0000041		
P	2.1947190D+05	0.0000904	-0.0000412	0.0000166		
P	4.8278480D+04	0.0003334	-0.0001523	0.0000612		
P	1.3669230D+04	0.0011949	-0.0005478	0.0002204		
P	4.6798230D+03	0.0041453	-0.0019078	0.0007671		
P	1.8190400D+03	0.0141747	-0.0065876	0.0026579		
P	7.6529890D+02	0.0452743	-0.0213876	0.0086399		
P	3.4395300D+02	0.1221488	-0.0597293	0.0243357		
P	1.6361800D+02	0.2525727	-0.1294939	0.0531078		
P	8.1452670D+01	0.3581835	-0.1950211	0.0814366		
P	4.1792720D+01	0.2876217	-0.1191984	0.0445295		
P	2.1451780D+01	0.0972669	0.2000297	-0.1133245		
P	1.1152850D+01	0.0073527	0.5010406	-0.3038065		
P	5.9224060D+00	0.0014134	0.3624991	-0.2220071		
P	3.1043460D+00	-0.0005839	0.0801416	0.2630757		
P	1.5588140D+00	0.0001872	0.0046003	0.5624144		
P	7.4565750D-01	-0.0001124	0.0007059	0.3501065		
P	3.1331620D-01	0.0000180	0.0000293	0.0533373		
P	2.8825100D-03	-0.0000001	-0.0000002	0.0000502		
	D	3D	4D			
BASIS/ORB. ENERGY	-15.8424720	-0.7201049				
D	3.1542040D+03	0.0001732	-0.0000589			
D	8.8102700D+02	0.0015081	-0.0005070			
D	3.2449920D+02	0.0090327	-0.0030871			
D	1.3702920D+02	0.0393855	-0.0134145			
D	6.1981320D+01	0.1256291	-0.0438642			

D	2.9315420D+01	0.2777851	-0.0960825
D	1.4046690D+01	0.3972008	-0.1331433
D	6.7551600D+00	0.3057927	-0.0450142
D	3.1051580D+00	0.0826375	0.2474222
D	1.3765190D+00	0.0025076	0.4514913
D	5.6989430D-01	0.0008595	0.3799833
D	2.1089270D-01	-0.0002197	0.1443811

INDIUM K(2)L(8)M(18)4S(2)4P(6)5S(2)4D(10)5P(1), 2P

CHARGE = 49.000000

SYMMETRY SPECIES	S	P	D
NUMBER OF BASIS FUNCTIONS	23	19	12
NUMBER OF CLOSED SHELLS	5	3	2
NUMBER OF OPEN SHELLS	0	1	0
OPEN SHELL OCCUPATION NUMBER	0	1	0

*** FINAL SCF RESULTS ***

E = -5878.480575294

ORBITAL ENERGIES AND EXPANSION COEFFICIENTS

	S	1S	2S	3S	4S	5S
BASIS/ORB. ENERGY		-1031.9995000	-157.8552000	-31.3924800	-5.3060662	-0.3958355
S	1.3098780D+09	0.0000183	-0.0000063	-0.0000027	0.0000012	0.0000003
S	1.3476720D+08	0.0000707	-0.0000242	-0.0000106	0.0000046	0.0000013
S	2.2385440D+07	0.0002147	-0.0000734	-0.0000323	0.0000139	0.0000039
S	4.7896100D+06	0.0005758	-0.0001970	-0.0000866	0.0000372	0.0000103
S	1.2106390D+06	0.0014175	-0.0004858	-0.0002137	0.0000917	0.0000255
S	3.4932170D+05	0.0032739	-0.0011257	-0.0004951	0.0002128	0.0000592
S	1.1212090D+05	0.0073218	-0.0025334	-0.0011163	0.0004791	0.0001332
S	3.9228990D+04	0.0161207	-0.0056337	-0.0024821	0.0010680	0.0002973
S	1.4810670D+04	0.0351575	-0.0125189	-0.0055445	0.0023785	0.0006608
S	5.9657590D+03	0.0756410	-0.0278070	-0.0123247	0.0053210	0.0014831
S	2.5406890D+03	0.1530448	-0.0599316	-0.0269663	0.0115721	0.0032131
S	1.1333360D+03	0.2677600	-0.1180211	-0.0536311	0.0233633	0.0065262
S	5.2220260D+02	0.3412300	-0.1892622	-0.0903757	0.0389905	0.0108243
S	2.4566030D+02	0.2320878	-0.1611065	-0.0789206	0.0358298	0.0101228
S	1.1154350D+02	0.0464546	0.1780743	0.1094724	-0.0534559	-0.0153485

S	5.5455420D+01	-0.0022974	0.5779869	0.5013195	-0.2400931	-0.0677210
S	2.7427970D+01	0.0013938	0.3835880	0.3871838	-0.2192459	-0.0647943
S	1.1668550D+01	-0.0006669	0.0445399	-0.6198895	0.4881060	0.1533091
S	5.7753090D+00	0.0002894	-0.0043127	-0.6949465	0.7480472	0.2433067
S	2.0480420D+00	-0.0001014	0.0010917	-0.0634418	-0.7322165	-0.3241175
S	9.0779270D-01	0.0000435	-0.0005096	0.0078309	-0.6840963	-0.4169262
S	1.6799980D-01	-0.0000099	0.0001033	-0.0016799	-0.0245940	0.6732011
S	6.2279750D-02	0.0000042	-0.0000436	0.0006896	0.0067672	0.5218830
	P	2P	3P	4P	5P	
BASIS/ORB. ENERGY		-141.4913300	-25.8884840	-3.5780216	-0.1942708	
P	1.4835180D+06	0.0000249	-0.0000114	0.0000047	0.0000009	
P	2.1926550D+05	0.0000973	-0.0000447	0.0000183	0.0000037	
P	4.8768660D+04	0.0003573	-0.0001643	0.0000672	0.0000134	
P	1.3830440D+04	0.0012804	-0.0005909	0.0002423	0.0000485	
P	4.7112640D+03	0.0044681	-0.0020699	0.0008468	0.0001680	
P	1.8330070D+03	0.0149527	-0.0070013	0.0028817	0.0005787	
P	7.8205490D+02	0.0461597	-0.0219592	0.0090225	0.0017874	
P	3.5533830D+02	0.1236939	-0.0609665	0.0253544	0.0051077	
P	1.6828210D+02	0.2614037	-0.1350636	0.0563391	0.0111504	
P	8.2127020D+01	0.3745851	-0.2058180	0.0879038	0.0179259	
P	4.0882440D+01	0.2836041	-0.1006205	0.0346692	0.0060317	
P	2.0046560D+01	0.0777540	0.2892613	-0.1641817	-0.0326112	
P	1.0011930D+01	0.0022328	0.5547146	-0.3640127	-0.0810905	
P	5.0461630D+00	0.0012884	0.2720310	-0.0781821	-0.0045278	
P	2.4150960D+00	-0.0006357	0.0287597	0.5213305	0.1225002	
P	1.1175090D+00	0.0002043	0.0011495	0.5324506	0.1767069	
P	4.8950680D-01	-0.0000931	0.0001532	0.1307062	-0.0515427	
P	1.3954350D-01	0.0000225	-0.0000009	0.0031856	-0.5549453	
P	4.4444100D-02	-0.0000072	-0.0000045	0.0000698	-0.5353268	
	D	3D	4D			
BASIS/ORB. ENERGY		-17.3374390	-1.0107228			
D	3.9468670D+03	0.0001328	-0.0000474			
D	1.0118900D+03	0.0013920	-0.0004937			
D	3.4235370D+02	0.0096808	-0.0034763			
D	1.3816580D+02	0.0439697	-0.0158069			

D	6.1665420D+01	0.1369982	-0.0503893
D	2.9300080D+01	0.2876924	-0.1048259
D	1.4248400D+01	0.3915734	-0.1370195
D	6.9975390D+00	0.2875856	-0.0364756
D	3.3209260D+00	0.0775667	0.2574974
D	1.5117360D+00	0.0033633	0.4553451
D	6.4948000D-01	0.0005747	0.3678310
D	2.5233690D-01	-0.0001427	0.1224939

TIN K(2)L(8)M(18)4S(2)4P(6)5S(2)4D(10)5P(2), 3P

CHARGE = 50.000000

SYMMETRY SPECIES	S	P	D
NUMBER OF BASIS FUNCTIONS	23	19	12
NUMBER OF CLOSED SHELLS	5	3	2
NUMBER OF OPEN SHELLS	0	1	0
OPEN SHELL OCCUPATION NUMBER	0	2	0

*** FINAL SCF RESULTS ***

E = -6174.017712224

ORBITAL ENERGIES AND EXPANSION COEFFICIENTS

	S	1S	2S	3S	4S	5S
BASIS/ORB. ENERGY		-1078.5080000	-166.2286900	-33.5463490	-5.8810289	-0.5064140
S	1.3432880D+09	0.0000192	-0.0000066	-0.0000029	0.0000013	-0.0000004
S	1.3851420D+08	0.0000752	-0.0000258	-0.0000114	0.0000050	-0.0000015
S	2.2415860D+07	0.0002320	-0.0000796	-0.0000352	0.0000153	-0.0000046
S	4.7773820D+06	0.0006154	-0.0002113	-0.0000933	0.0000406	-0.0000122
S	1.2109210D+06	0.0015118	-0.0005202	-0.0002299	0.0001000	-0.0000300
S	3.4915710D+05	0.0034864	-0.0012037	-0.0005320	0.0002316	-0.0000695
S	1.1212160D+05	0.0077773	-0.0027029	-0.0011966	0.0005204	-0.0001561
S	3.9180990D+04	0.0171050	-0.0060060	-0.0026591	0.0011592	-0.0003481
S	1.4787450D+04	0.0371194	-0.0132926	-0.0059161	0.0025718	-0.0007710
S	5.9629570D+03	0.0792413	-0.0293251	-0.0130660	0.0057154	-0.0017178
S	2.5404210D+03	0.1595650	-0.0630733	-0.0285358	0.0124123	-0.0037205
S	1.1309210D+03	0.2751863	-0.1229418	-0.0562365	0.0248291	-0.0074772
S	5.2262180D+02	0.3378761	-0.1911308	-0.0919865	0.0402367	-0.0120667
S	2.4750390D+02	0.2204407	-0.1507841	-0.0742000	0.0342369	-0.0104158

S	1.1172140D+02	0.0416402	0.2092877	0.1318954	-0.0650194	0.0200300
S	5.5480780D+01	-0.0027750	0.5864350	0.5240771	-0.2561007	0.0782887
S	2.7527550D+01	0.0015452	0.3518016	0.3472612	-0.2031880	0.0649310
S	1.1957690D+01	-0.0007754	0.0371291	-0.6614271	0.5388876	-0.1833647
S	5.9659470D+00	0.0003544	-0.0031477	-0.6573993	0.7287567	-0.2589264
S	2.2137980D+00	-0.0001301	0.0007645	-0.0600847	-0.7384898	0.3580178
S	9.9637830D-01	0.0000554	-0.0003870	0.0065543	-0.6934195	0.4668187
S	2.0585600D-01	-0.0000132	0.0000793	-0.0014879	-0.0260830	-0.7001009
S	7.7917830D-02	0.0000054	-0.0000318	0.0005927	0.0064306	-0.5241018

	P	2P	3P	4P	5P
BASIS/ORB. ENERGY		-149.0393500	-27.7778410	-4.0477379	-0.2625819
P	1.5547130D+06	0.0000263	-0.0000121	-0.0000051	0.0000012
P	2.2268520D+05	0.0001059	-0.0000489	-0.0000204	0.0000048
P	4.8836280D+04	0.0003887	-0.0001799	-0.0000749	0.0000175
P	1.3824970D+04	0.0013900	-0.0006456	-0.0002695	0.0000631
P	4.7004290D+03	0.0048444	-0.0022590	-0.0009413	0.0002196
P	1.8316950D+03	0.0160467	-0.0075671	-0.0031698	0.0007442
P	7.8288450D+02	0.0492795	-0.0236249	-0.0098910	0.0023063
P	3.5550190D+02	0.1309050	-0.0651079	-0.0275688	0.0064881
P	1.6834000D+02	0.2715830	-0.1417471	-0.0603086	0.0140737
P	8.2183830D+01	0.3768834	-0.2086420	-0.0906840	0.0215239
P	4.0912480D+01	0.2701636	-0.0821924	-0.0259841	0.0053313
P	2.0014470D+01	0.0679450	0.3241976	0.1890658	-0.0453881
P	1.0006760D+01	0.0012844	0.5548911	0.3766917	-0.0970028
P	5.0146660D+00	0.0011381	0.2396439	0.0224211	0.0075566
P	2.4031970D+00	-0.0005929	0.0205749	-0.5716867	0.1688338
P	1.1036420D+00	0.0001835	0.0014445	-0.5027367	0.1935612
P	4.5817940D-01	-0.0000887	-0.0001032	-0.0867961	-0.1058361
P	1.6309450D-01	0.0000302	0.0000568	0.0009059	-0.6001228
P	5.6755960D-02	-0.0000088	-0.0000236	-0.0009404	-0.4513322

	D	3D	4D
BASIS/ORB. ENERGY		-18.8865780	-1.3061377
D	2.9981590D+03	0.0002393	-0.0000891
D	8.4131040D+02	0.0020192	-0.0007499
D	3.1774710D+02	0.0111410	-0.0041797

D	1.3890840D+02	0.0440335	-0.0165687
D	6.5247370D+01	0.1294842	-0.0497447
D	3.2196210D+01	0.2656388	-0.1014855
D	1.6222610D+01	0.3727601	-0.1373691
D	8.1605430D+00	0.3077197	-0.0619979
D	3.9382840D+00	0.0990937	0.2259330
D	1.8140800D+00	0.0059758	0.4626716
D	7.8774250D-01	0.0006466	0.3883591
D	3.0855790D-01	-0.0001667	0.1228287

ANTIMONY K(2)L(8)M(18)4S(2)4P(6)5S(2)4D(10)5P(3), 4S

CHARGE = 51.000000

SYMMETRY SPECIES	S	P	D
NUMBER OF BASIS FUNCTIONS	23	19	12
NUMBER OF CLOSED SHELLS	5	3	2
NUMBER OF OPEN SHELLS	0	1	0
OPEN SHELL OCCUPATION NUMBER	0	3	0

*** FINAL SCF RESULTS ***

E = -6478.255497828

ORBITAL ENERGIES AND EXPANSION COEFFICIENTS

	S	1S	2S	3S	4S	5S
BASIS/ORB. ENERGY		-1126.1726000	-174.8579000	-35.7777490	-6.4753563	-0.6191705
S	1.3192050D+09	0.0000210	-0.0000072	-0.0000032	0.0000014	-0.0000004
S	1.3630630D+08	0.0000807	-0.0000278	-0.0000123	0.0000054	-0.0000017
S	2.2598840D+07	0.0002452	-0.0000844	-0.0000375	0.0000165	-0.0000052
S	4.8169040D+06	0.0006565	-0.0002263	-0.0001004	0.0000443	-0.0000140
S	1.2139340D+06	0.0016135	-0.0005575	-0.0002475	0.0001090	-0.0000346
S	3.4885820D+05	0.0037226	-0.0012906	-0.0005730	0.0002526	-0.0000802
S	1.1163490D+05	0.0082924	-0.0028950	-0.0012873	0.0005670	-0.0001799
S	3.9026160D+04	0.0181224	-0.0063932	-0.0028446	0.0012557	-0.0003988
S	1.4750000D+04	0.0391507	-0.0141027	-0.0063037	0.0027760	-0.0008806
S	5.9536340D+03	0.0830535	-0.0309362	-0.0138633	0.0061401	-0.0019513
S	2.5393930D+03	0.1656024	-0.0661090	-0.0300414	0.0132420	-0.0042014
S	1.1317840D+03	0.2812815	-0.1272252	-0.0586474	0.0262202	-0.0083465
S	5.2356350D+02	0.3360534	-0.1939204	-0.0938111	0.0416174	-0.0132224

S	2.4835160D+02	0.2088082	-0.1391208	-0.0691797	0.0323789	-0.0103917
S	1.1186190D+02	0.0362971	0.2399900	0.1562144	-0.0777298	0.0252221
S	5.5841460D+01	-0.0026510	0.5841091	0.5327998	-0.2654650	0.0862422
S	2.8008870D+01	0.0014244	0.3263988	0.3227759	-0.1941083	0.0655837
S	1.2643170D+01	-0.0007259	0.0337465	-0.6592350	0.5468994	-0.1970254
S	6.3499160D+00	0.0003198	-0.0021018	-0.6612867	0.7465493	-0.2839626
S	2.4099320D+00	-0.0001174	0.0004771	-0.0640302	-0.7174160	0.3743187
S	1.1048950D+00	0.0000506	-0.0002857	0.0068136	-0.7219490	0.5168292
S	2.4158080D-01	-0.0000121	0.0000566	-0.0015255	-0.0293265	-0.7302388
S	9.2734580D-02	0.0000048	-0.0000215	0.0006022	0.0068455	-0.5169847
	P	2P	3P	4P	5P	
BASIS/ORB. ENERGY	-156.8022800	-29.7345300	-4.5326332	-0.3327822		
P	1.5913790D+06	0.0000279	-0.0000130	-0.0000055	0.0000014	
P	2.2925350D+05	0.0001129	-0.0000525	-0.0000222	0.0000058	
P	4.9011810D+04	0.0004276	-0.0001990	-0.0000843	0.0000218	
P	1.3697750D+04	0.0015193	-0.0007100	-0.0003013	0.0000781	
P	4.6902410D+03	0.0052004	-0.0024406	-0.0010354	0.0002682	
P	1.8335570D+03	0.0172177	-0.0081743	-0.0034813	0.0009029	
P	7.8294770D+02	0.0526132	-0.0254176	-0.0108401	0.0028100	
P	3.5569870D+02	0.1380484	-0.0692590	-0.0298260	0.0077495	
P	1.6846870D+02	0.2815587	-0.1484379	-0.0644125	0.0167405	
P	8.2240830D+01	0.3783725	-0.2106287	-0.0929538	0.0242529	
P	4.0923930D+01	0.2563690	-0.0624633	-0.0164573	0.0037752	
P	2.0006210D+01	0.0588914	0.3580168	0.2153141	-0.0587389	
P	1.0007870D+01	0.0007993	0.5507004	0.3837306	-0.1077524	
P	4.9749960D+00	0.0008899	0.2092620	-0.0364090	0.0236842	
P	2.4005970D+00	-0.0004931	0.0139819	-0.6103168	0.2129114	
P	1.1009880D+00	0.0001329	0.0017239	-0.4646312	0.1901076	
P	4.1327880D-01	-0.0000683	-0.0003214	-0.0572798	-0.2075661	
P	1.7102240D-01	0.0000310	0.0001552	0.0050313	-0.6100682	
P	6.4936180D-02	-0.0000088	-0.0000489	-0.0014360	-0.3508829	
	D	3D	4D			
BASIS/ORB. ENERGY	-20.4955670	-1.6138310				
D	2.9704100D+03	0.0002709	-0.0001048			
D	8.3670590D+02	0.0022568	-0.0008712			

D	3.1529580D+02	0.0125683	-0.0048988
D	1.3719390D+02	0.0488804	-0.0191359
D	6.4964030D+01	0.1378431	-0.0551028
D	3.2272890D+01	0.2767781	-0.1097873
D	1.6285140D+01	0.3751941	-0.1424888
D	8.2896380D+00	0.2869106	-0.0489781
D	4.1242600D+00	0.0894583	0.2381158
D	1.9534350D+00	0.0065149	0.4623803
D	8.7427330D-01	0.0003192	0.3759226
D	3.5112610D-01	-0.0000818	0.1102929

TELLURIUM K(2)L(8)M(18)4S(2)4P(6)5S(2)4D(10)5P(4), 3P

CHARGE = 52.000000

SYMMETRY SPECIES	S	P	D
NUMBER OF BASIS FUNCTIONS	23	19	12
NUMBER OF CLOSED SHELLS	5	3	2
NUMBER OF OPEN SHELLS	0	1	0
OPEN SHELL OCCUPATION NUMBER	0	4	0

*** FINAL SCF RESULTS ***

E = -6791.194123300

ORBITAL ENERGIES AND EXPANSION COEFFICIENTS

	S	1S	2S	3S	4S	5S
BASIS/ORB. ENERGY		-1175.0234000	-183.7646400	-38.1059430	-7.1074663	-0.7464163
S	1.3679460D+09	0.0000221	-0.0000076	-0.0000034	0.0000015	-0.0000005
S	1.3840070D+08	0.0000864	-0.0000299	-0.0000133	0.0000059	-0.0000020
S	2.2653740D+07	0.0002631	-0.0000910	-0.0000405	0.0000181	-0.0000060
S	4.8087910D+06	0.0007019	-0.0002429	-0.0001083	0.0000483	-0.0000161
S	1.2145840D+06	0.0017130	-0.0005942	-0.0002649	0.0001181	-0.0000393
S	3.4944390D+05	0.0039609	-0.0013788	-0.0006149	0.0002744	-0.0000913
S	1.1127380D+05	0.0088427	-0.0031010	-0.0013849	0.0006175	-0.0002055
S	3.8892950D+04	0.0191498	-0.0067880	-0.0030341	0.0013555	-0.0004514
S	1.4740350D+04	0.0411607	-0.0149126	-0.0066955	0.0029848	-0.0009935
S	5.9493830D+03	0.0870671	-0.0326475	-0.0147046	0.0065917	-0.0021962
S	2.5369970D+03	0.1718392	-0.0692741	-0.0316362	0.0141201	-0.0047024
S	1.1318960D+03	0.2871226	-0.1315397	-0.0610366	0.0276281	-0.0092176

S	5.2436790D+02	0.3331758	-0.1960039	-0.0954490	0.0428960	-0.0143191
S	2.4943870D+02	0.1973318	-0.1265765	-0.0631912	0.0300384	-0.0100729
S	1.1168480D+02	0.0318275	0.2750007	0.1837339	-0.0924897	0.0313709
S	5.5564540D+01	-0.0027602	0.5874056	0.5520041	-0.2805621	0.0961368
S	2.7901800D+01	0.0014619	0.2933899	0.2756363	-0.1724543	0.0610122
S	1.2897780D+01	-0.0007851	0.0268387	-0.7004936	0.6023932	-0.2283706
S	6.5154310D+00	0.0003585	-0.0011560	-0.6214358	0.7206175	-0.2918531
S	2.5788470D+00	-0.0001368	0.0001955	-0.0586759	-0.7353442	0.4092394
S	1.1970580D+00	0.0000582	-0.0001816	0.0051326	-0.7214649	0.5522288
S	2.8282710D-01	-0.0000142	0.0000343	-0.0011816	-0.0299328	-0.7529509
S	1.0920250D-01	0.0000054	-0.0000115	0.0004588	0.0061888	-0.5210030
	P	2P	3P	4P	5P	
BASIS/ORB. ENERGY	-164.7998700	-31.7772260	-5.0510582	-0.3580673		
P	1.5049580D+06	0.0000316	-0.0000148	-0.0000064	0.0000018	
P	2.2049710D+05	0.0001250	-0.0000584	-0.0000252	0.0000070	
P	4.8494470D+04	0.0004600	-0.0002154	-0.0000927	0.0000258	
P	1.3771370D+04	0.0016209	-0.0007618	-0.0003285	0.0000913	
P	4.7166030D+03	0.0055821	-0.0026369	-0.0011368	0.0003159	
P	1.8323020D+03	0.0186324	-0.0089004	-0.0038515	0.0010715	
P	7.7736320D+02	0.0569426	-0.0277361	-0.0120265	0.0033450	
P	3.5286710D+02	0.1462105	-0.0739755	-0.0323920	0.0090292	
P	1.6852540D+02	0.2863152	-0.1525350	-0.0673417	0.0187832	
P	8.3523740D+01	0.3698129	-0.2065470	-0.0926407	0.0259338	
P	4.2277110D+01	0.2461241	-0.0558518	-0.0132632	0.0031046	
P	2.1125040D+01	0.0582002	0.3467756	0.2125492	-0.0624233	
P	1.0777520D+01	0.0013351	0.5411591	0.3853770	-0.1166398	
P	5.4825470D+00	0.0007749	0.2237680	-0.0076263	0.0161856	
P	2.6663100D+00	-0.0004370	0.0191622	-0.5982678	0.2277873	
P	1.2446870D+00	0.0001065	0.0012555	-0.4862726	0.2170049	
P	4.8850810D-01	-0.0000584	-0.0001222	-0.0652608	-0.2171784	
P	2.0170690D-01	0.0000250	0.0000493	0.0038797	-0.6112459	
P	7.4612940D-02	-0.0000065	-0.0000253	-0.0015715	-0.3551264	
	D	3D	4D			
BASIS/ORB. ENERGY	-22.1829400	-1.9523718				
D	2.9748340D+03	0.0003014	-0.0001207			

D	8.3510790D+02	0.0025059	-0.0009996
D	3.1511590D+02	0.0138234	-0.0055811
D	1.3690400D+02	0.0534725	-0.0216554
D	6.4812320D+01	0.1475963	-0.0612127
D	3.2292150D+01	0.2875359	-0.1175945
D	1.6335140D+01	0.3776473	-0.1476994
D	8.3150830D+00	0.2717871	-0.0288015
D	4.1069480D+00	0.0762828	0.2770301
D	1.9639020D+00	0.0040570	0.4694738
D	8.9960090D-01	0.0004550	0.3386363
D	3.6986900D-01	-0.0001375	0.0848022

IODINE K(2)L(8)M(18)4S(2)4P(6)5S(2)4D(10)5P(5), 2P

CHARGE = 53.000000

SYMMETRY SPECIES	S	P	D
NUMBER OF BASIS FUNCTIONS	23	19	12
NUMBER OF CLOSED SHELLS	5	3	2
NUMBER OF OPEN SHELLS	0	1	0
OPEN SHELL OCCUPATION NUMBER	0	5	0

*** FINAL SCF RESULTS ***

E = -7113.035966885

ORBITAL ENERGIES AND EXPANSION COEFFICIENTS

	S	1S	2S	3S	4S	5S
BASIS/ORB. ENERGY		-1225.0505000	-192.9312000	-40.5111080	-7.7578370	-0.8762305
S	1.3507610D+09	0.0000238	-0.0000083	-0.0000037	0.0000017	0.0000006
S	1.4074100D+08	0.0000904	-0.0000314	-0.0000140	0.0000063	0.0000022
S	2.3304840D+07	0.0002761	-0.0000959	-0.0000429	0.0000193	0.0000067
S	4.8817400D+06	0.0007505	-0.0002608	-0.0001167	0.0000526	0.0000182
S	1.2114910D+06	0.0018437	-0.0006422	-0.0002875	0.0001297	0.0000448
S	3.4688040D+05	0.0042236	-0.0014764	-0.0006612	0.0002984	0.0001032
S	1.1090750D+05	0.0093486	-0.0032933	-0.0014769	0.0006662	0.0002303
S	3.8854140D+04	0.0202376	-0.0072074	-0.0032360	0.0014623	0.0005057
S	1.4707510D+04	0.0433946	-0.0158153	-0.0071306	0.0032163	0.0011123
S	5.9402180D+03	0.0909646	-0.0343355	-0.0155440	0.0070471	0.0024376
S	2.5375450D+03	0.1777585	-0.0723739	-0.0332018	0.0150000	0.0051921

S	1.1326500D+03	0.2931494	-0.1359825	-0.0635318	0.0290855	0.0100705
S	5.2429710D+02	0.3307305	-0.1984686	-0.0972073	0.0442649	0.0153751
S	2.4955940D+02	0.1853026	-0.1121040	-0.0562003	0.0270662	0.0093743
S	1.1131510D+02	0.0272322	0.3116186	0.2142259	-0.1089566	-0.0382830
S	5.5110580D+01	-0.0025378	0.5893614	0.5692008	-0.2955953	-0.1058430
S	2.7496280D+01	0.0013565	0.2596611	0.2259727	-0.1476527	-0.0539043
S	1.3209670D+01	-0.0007806	0.0183690	-0.7338380	0.6511065	0.2569037
S	6.7077410D+00	0.0003589	0.0006525	-0.5875553	0.6999660	0.2993764
S	2.7679910D+00	-0.0001401	-0.0004106	-0.0547284	-0.7453300	-0.4378722
S	1.2992520D+00	0.0000586	0.0000461	0.0036743	-0.7284125	-0.5857618
S	3.2423220D-01	-0.0000144	-0.0000187	-0.0008659	-0.0311663	0.7737527
S	1.2580560D-01	0.0000053	0.0000093	0.0003421	0.0058309	0.5231222
	P	2P	3P	4P	5P	
BASIS/ORB. ENERGY		-173.0122100	-33.8856080	-5.5837300	-0.4017492	
P	1.5601290D+06	0.0000336	-0.0000158	-0.0000069	0.0000020	
P	2.2165690D+05	0.0001365	-0.0000641	-0.0000280	0.0000083	
P	4.8283240D+04	0.0004997	-0.0002353	-0.0001029	0.0000304	
P	1.3753130D+04	0.0017460	-0.0008253	-0.0003611	0.0001064	
P	4.7194560D+03	0.0059945	-0.0028489	-0.0012474	0.0003684	
P	1.8330180D+03	0.0199526	-0.0095915	-0.0042116	0.0012413	
P	7.7729630D+02	0.0606046	-0.0297384	-0.0131031	0.0038760	
P	3.5284850D+02	0.1538163	-0.0784667	-0.0348766	0.0102945	
P	1.6853230D+02	0.2956976	-0.1590743	-0.0714561	0.0212330	
P	8.3534380D+01	0.3694665	-0.2067930	-0.0938997	0.0277130	
P	4.2271890D+01	0.2325087	-0.0351054	-0.0024520	0.0003810	
P	2.1131020D+01	0.0502986	0.3778111	0.2383936	-0.0756681	
P	1.0787440D+01	0.0009601	0.5342766	0.3883489	-0.1231035	
P	5.4456470D+00	0.0005688	0.1961700	-0.0666643	0.0360463	
P	2.6732810D+00	-0.0003605	0.0131779	-0.6252552	0.2659012	
P	1.2646400D+00	0.0000766	0.0015743	-0.4414923	0.1984310	
P	4.8284950D-01	-0.0000419	-0.0003186	-0.0490121	-0.3198024	
P	2.0230920D-01	0.0000198	0.0001173	0.0033712	-0.5919631	
P	7.8017180D-02	-0.0000049	-0.0000514	-0.0016594	-0.2820926	
	D	3D	4D			
BASIS/ORB. ENERGY		-23.9280280	-2.3025924			

D	2.8571150D+03	0.0003585	-0.0001477
D	8.0661310D+02	0.0029530	-0.0012163
D	3.0628700D+02	0.0157909	-0.0065644
D	1.3503150D+02	0.0580245	-0.0242862
D	6.4765720D+01	0.1560122	-0.0666620
D	3.2410230D+01	0.2966837	-0.1252065
D	1.6533210D+01	0.3723363	-0.1478788
D	8.5702670D+00	0.2541217	-0.0190803
D	4.3897500D+00	0.0722022	0.2754392
D	2.1565630D+00	0.0052928	0.4657755
D	1.0106490D+00	0.0001333	0.3365636
D	4.2059200D-01	-0.0000579	0.0825416

XENON K(2)L(8)M(18)4S(2)4P(6)5S(2)4D(10)5P(6), 1S

CHARGE = 54.000000

SYMMETRY SPECIES	S	P	D
NUMBER OF BASIS FUNCTIONS	23	19	12
NUMBER OF CLOSED SHELLS	5	4	2
NUMBER OF OPEN SHELLS	0	0	0
OPEN SHELL OCCUPATION NUMBER	0	0	0

*** FINAL SCF RESULTS ***

E = -7443.894265417

ORBITAL ENERGIES AND EXPANSION COEFFICIENTS

	S	1S	2S	3S	4S	5S
BASIS/ORB. ENERGY		-1276.2660000	-202.3614500	-42.9947080	-8.4276013	-1.0095385
S	1.5571750D+09	0.0000237	-0.0000082	-0.0000037	0.0000017	0.0000006
S	1.4783220D+08	0.0000967	-0.0000337	-0.0000151	0.0000069	0.0000025
S	2.3342500D+07	0.0002993	-0.0001043	-0.0000469	0.0000214	0.0000076
S	4.8370600D+06	0.0008050	-0.0002808	-0.0001262	0.0000575	0.0000205
S	1.2055790D+06	0.0019608	-0.0006857	-0.0003082	0.0001405	0.0000501
S	3.4613750D+05	0.0044824	-0.0015734	-0.0007075	0.0003228	0.0001151
S	1.1075610D+05	0.0099005	-0.0035034	-0.0015774	0.0007193	0.0002566
S	3.8784920D+04	0.0213853	-0.0076531	-0.0034512	0.0015766	0.0005623
S	1.4683320D+04	0.0455974	-0.0167149	-0.0075662	0.0034503	0.0012314
S	5.9370610D+03	0.0949392	-0.0360811	-0.0164164	0.0075249	0.0026836

S	2.5373520D+03	0.1839535	-0.0756258	-0.0348428	0.0159167	0.0056887
S	1.1327690D+03	0.2986621	-0.1403600	-0.0660310	0.0305777	0.0109099
S	5.2460740D+02	0.3269993	-0.1998236	-0.0983745	0.0453041	0.0162728
S	2.5019720D+02	0.1738203	-0.0976705	-0.0491593	0.0240857	0.0085210
S	1.1146130D+02	0.0233917	0.3469047	0.2453093	-0.1263772	-0.0456827
S	5.4341410D+01	-0.0021724	0.6011051	0.5946597	-0.3152251	-0.1172661
S	2.5954400D+01	0.0012283	0.2235009	0.1595887	-0.1143698	-0.0420857
S	1.3300310D+01	-0.0008128	0.0009499	-0.7823587	0.7289810	0.2971231
S	6.7839940D+00	0.0003704	0.0051982	-0.5349859	0.6385637	0.2881194
S	2.8641580D+00	-0.0001470	-0.0020456	-0.0478018	-0.7959025	-0.4971351
S	1.3673320D+00	0.0000619	0.0006822	0.0031565	-0.6889443	-0.5828659
S	3.6615650D-01	-0.0000154	-0.0001710	-0.0007451	-0.0287324	0.8000768
S	1.4223710D-01	0.0000053	0.0000634	0.0003011	0.0045280	0.5207047

	P	2P	3P	4P	5P
BASIS/ORB. ENERGY		-181.4408900	-36.0605740	-6.1317545	-0.4561965
P	1.4141290D+06	0.0000389	-0.0000184	-0.0000081	0.0000025
P	2.1210270D+05	0.0001486	-0.0000702	-0.0000311	0.0000096
P	4.8312330D+04	0.0005299	-0.0002509	-0.0001113	0.0000342
P	1.3855470D+04	0.0018708	-0.0008893	-0.0003947	0.0001212
P	4.7267550D+03	0.0064564	-0.0030854	-0.0013718	0.0004224
P	1.8313610D+03	0.0213639	-0.0103376	-0.0046047	0.0014142
P	7.7710870D+02	0.0643356	-0.0317835	-0.0142281	0.0043891
P	3.5293570D+02	0.1614865	-0.0830907	-0.0374758	0.0115265
P	1.6853030D+02	0.3050497	-0.1655280	-0.0756501	0.0234580
P	8.3480670D+01	0.3684029	-0.2065884	-0.0948383	0.0291194
P	4.2206630D+01	0.2188127	-0.0111884	0.0104274	-0.0036437
P	2.1021800D+01	0.0430355	0.4102894	0.2673546	-0.0891715
P	1.0772700D+01	0.0004213	0.5184610	0.3818732	-0.1257739
P	5.4300830D+00	0.0005172	0.1708677	-0.1228562	0.0594934
P	2.7140930D+00	-0.0003576	0.0090331	-0.6329820	0.2895065
P	1.3194680D+00	0.0000847	0.0018467	-0.4034735	0.1868562
P	5.3091240D-01	-0.0000436	-0.0004492	-0.0431424	-0.3525923
P	2.2440840D-01	0.0000186	0.0001822	0.0026835	-0.5873852
P	8.7721210D-02	-0.0000052	-0.0000549	-0.0008774	-0.2624335

D

3D

4D

BASIS/ORB. ENERGY	-25.7314210	-2.6654986
D 2.7170610D+03	0.0004323	-0.0001829
D 7.8249400D+02	0.0033653	-0.0014244
D 3.0489690D+02	0.0170311	-0.0072773
D 1.3543650D+02	0.0626213	-0.0269589
D 6.4687880D+01	0.1670299	-0.0734186
D 3.2341750D+01	0.3080294	-0.1332976
D 1.6524130D+01	0.3719807	-0.1496127
D 8.5701600D+00	0.2373691	0.0051559
D 4.3730760D+00	0.0610655	0.3113689
D 2.1629240D+00	0.0034070	0.4677171
D 1.0300830D+00	0.0002127	0.2985182
D 4.3499870D-01	-0.0000942	0.0640163

CESIUM [XE]6S(1), 2S

CHARGE = 55.000000

SYMMETRY SPECIES	S	P	D
NUMBER OF BASIS FUNCTIONS	27	23	15
NUMBER OF CLOSED SHELLS	5	4	2
NUMBER OF OPEN SHELLS	1	0	0
OPEN SHELL OCCUPATION NUMBER	1	0	0

*** FINAL SCF RESULTS ***

E = -7783.506391326

ORBITAL ENERGIES AND EXPANSION COEFFICIENTS

	S	1S	2S	3S	4S	5S	6S
BASIS/ORB. ENERGY	-1328.8980000	-212.2724900	-45.7701930	-9.3277745	-1.3086786	-0.1278289	
S 3.3751277D+10	0.0000028	-0.0000010	-0.0000004	0.0000002	0.0000001	0.0000000	
S 3.2916445D+09	0.0000101	-0.0000035	-0.0000016	0.0000007	0.0000003	-0.0000001	
S 7.0216287D+08	0.0000242	-0.0000085	-0.0000038	0.0000018	0.0000007	-0.0000002	
S 1.6079783D+08	0.0000713	-0.0000250	-0.0000113	0.0000052	0.0000019	-0.0000004	
S 3.8050111D+07	0.0001846	-0.0000646	-0.0000291	0.0000134	0.0000050	-0.0000012	
S 1.0087667D+07	0.0004441	-0.0001555	-0.0000701	0.0000323	0.0000121	-0.0000028	
S 2.8878548D+06	0.0010139	-0.0003553	-0.0001603	0.0000739	0.0000278	-0.0000064	
S 9.1888437D+05	0.0021140	-0.0007430	-0.0003353	0.0001545	0.0000581	-0.0000133	
S 3.2018475D+05	0.0043462	-0.0015321	-0.0006917	0.0003189	0.0001199	-0.0000275	

S	1.1673952D+05	0.0091379	-0.0032477	-0.0014680	0.0006763	0.0002543	-0.0000583
S	4.3840534D+04	0.0194663	-0.0069839	-0.0031613	0.0014593	0.0005487	-0.0001256
S	1.7034634D+04	0.0415504	-0.0152556	-0.0069293	0.0031933	0.0012009	-0.0002756
S	6.8954193D+03	0.0876390	-0.0332360	-0.0151708	0.0070231	0.0026412	-0.0006041
S	2.9063094D+03	0.1747027	-0.0713764	-0.0329541	0.0152192	0.0057286	-0.0013157
S	1.2710359D+03	0.2951901	-0.1367813	-0.0644535	0.0301079	0.0113361	-0.0025906
S	5.7642624D+02	0.3379080	-0.2027436	-0.0997624	0.0465101	0.0175682	-0.0040452
S	2.7018571D+02	0.1877560	-0.1096515	-0.0556898	0.0272123	0.0102551	-0.0023134
S	1.1773485D+02	0.0265118	0.3404010	0.2419140	-0.1255723	-0.0481085	0.0109558
S	5.7199090D+01	-0.0030209	0.6029756	0.5958988	-0.3205174	-0.1252678	0.0290691
S	2.7494259D+01	0.0017849	0.2269414	0.1729410	-0.1219246	-0.0488649	0.0107365
S	1.4161049D+01	-0.0011872	0.0035666	-0.7694551	0.7197897	0.3132294	-0.0719723
S	7.2550575D+00	0.0005702	0.0045518	-0.5516013	0.6755830	0.3188732	-0.0770129
S	3.1159224D+00	-0.0002411	-0.0018405	-0.0525203	-0.7711520	-0.5032081	0.1269924
S	1.5077524D+00	0.0001057	0.0006217	0.0034102	-0.7214142	-0.6675402	0.1690583
S	4.4209740D-01	-0.0000308	-0.0001818	-0.0009142	-0.0361986	0.7587885	-0.2371814
S	1.8937484D-01	0.0000121	0.0000761	0.0004078	0.0059730	0.5941562	-0.3405963
S	2.1388343D-02	-0.0000013	-0.0000077	-0.0000375	-0.0005127	0.0076302	1.1101246
	P	2P	3P	4P	5P		
BASIS/ORB. ENERGY	-190.3003000	-38.5141450	-6.9043292	-0.6805787			
P	4.9266422D+07	0.0000027	-0.0000013	-0.0000006	-0.0000002		
P	7.1555927D+06	0.0000089	-0.0000042	-0.0000019	-0.0000006		
P	1.4937391D+06	0.0000266	-0.0000126	-0.0000057	-0.0000019		
P	3.7844540D+05	0.0000750	-0.0000356	-0.0000160	-0.0000054		
P	1.1258271D+05	0.0002053	-0.0000976	-0.0000439	-0.0000147		
P	3.7774967D+04	0.0005739	-0.0002733	-0.0001229	-0.0000411		
P	1.4015011D+04	0.0016218	-0.0007749	-0.0003487	-0.0001169		
P	5.6872591D+03	0.0046606	-0.0022372	-0.0010076	-0.0003373		
P	2.4740438D+03	0.0133789	-0.0064794	-0.0029235	-0.0009808		
P	1.1419148D+03	0.0367132	-0.0180467	-0.0081676	-0.0027359		
P	5.5343456D+02	0.0911602	-0.0460692	-0.0209697	-0.0070484		
P	2.7934109D+02	0.1900103	-0.0999893	-0.0459057	-0.0154109		
P	1.4531004D+02	0.3055816	-0.1698107	-0.0789853	-0.0266849		
P	7.7294283D+01	0.3252396	-0.1778318	-0.0821124	-0.0274870		
P	4.1481309D+01	0.1830044	0.0170261	0.0258280	0.0095927		

P	2.2052273D+01	0.0386089	0.3781671	0.2492254	0.0903343
P	1.1907965D+01	0.0014872	0.4939685	0.3745800	0.1369314
P	6.3685109D+00	0.0002473	0.2051168	-0.0322996	-0.0296798
P	3.2260643D+00	-0.0002117	0.0213910	-0.5965761	-0.2927864
P	1.5888705D+00	0.0000080	0.0007295	-0.4798162	-0.2663148
P	6.7620066D-01	-0.0000181	0.0000499	-0.0674564	0.2937982
P	2.9604244D-01	0.0000070	-0.0000278	0.0029169	0.6463759
P	1.1819731D-01	-0.0000018	0.0000035	-0.0009779	0.2689443
	D	3D	4D		
BASIS/ORB. ENERGY		-27.8053130	-3.2502977		
D	1.0218687D+04	0.0000412	-0.0000178		
D	3.0727965D+03	0.0002703	-0.0001174		
D	1.1180421D+03	0.0016427	-0.0007117		
D	4.6271444D+02	0.0081650	-0.0035674		
D	2.0873415D+02	0.0325891	-0.0143012		
D	9.9633969D+01	0.1001838	-0.0447550		
D	4.9790638D+01	0.2242027	-0.1008657		
D	2.5675450D+01	0.3411442	-0.1494965		
D	1.3656560D+01	0.3255977	-0.1145915		
D	7.3809680D+00	0.1614567	0.0918758		
D	3.9861239D+00	0.0337332	0.3404591		
D	2.1433568D+00	0.0021616	0.4045673		
D	1.1592979D+00	0.0000186	0.2435987		
D	6.2040623D-01	-0.0000274	0.0780012		
D	2.9841162D-01	-0.0000193	0.0100478		

BARIUM [XE]6S(2), 1S

CHARGE = 56.000000

SYMMETRY SPECIES S P D

NUMBER OF BASIS FUNCTIONS 27 23 15

NUMBER OF CLOSED SHELLS 6 4 2

NUMBER OF OPEN SHELLS 0 0 0

OPEN SHELL OCCUPATION NUMBER 0 0 0

*** FINAL SCF RESULTS ***

E = -8132.095988033

ORBITAL ENERGIES AND EXPANSION COEFFICIENTS

	S	1S	2S	3S	4S	5S	6S
BASIS/ORB. ENERGY	-1382.7535000	-222.4636900	-48.6344830	-10.2548760	-1.6031313	-0.1630222	
S 2.3173338D+10	0.0000034	-0.0000012	0.0000005	0.0000002	0.0000001	0.0000000	
S 3.5331827D+09	0.0000097	-0.0000034	0.0000015	0.0000007	0.0000003	0.0000001	
S 6.4677280D+08	0.0000314	-0.0000110	0.0000050	0.0000023	0.0000009	0.0000003	
S 1.3583776D+08	0.0000847	-0.0000298	0.0000135	0.0000063	0.0000025	0.0000007	
S 3.4276864D+07	0.0002007	-0.0000705	0.0000319	0.0000149	0.0000058	0.0000016	
S 9.7841927D+06	0.0004547	-0.0001599	0.0000724	0.0000337	0.0000133	0.0000037	
S 2.9828642D+06	0.0010226	-0.0003596	0.0001629	0.0000758	0.0000298	0.0000083	
S 9.5915884D+05	0.0021808	-0.0007700	0.0003486	0.0001623	0.0000639	0.0000178	
S 3.3316130D+05	0.0044768	-0.0015829	0.0007178	0.0003341	0.0001315	0.0000367	
S 1.2145151D+05	0.0093307	-0.0033351	0.0015116	0.0007042	0.0002774	0.0000773	
S 4.5954089D+04	0.0194851	-0.0070031	0.0031872	0.0014838	0.0005839	0.0001629	
S 1.8125830D+04	0.0405662	-0.0149997	0.0068226	0.0031829	0.0012548	0.0003497	
S 7.4396235D+03	0.0848115	-0.0321074	0.0147561	0.0068787	0.0027066	0.0007556	
S 3.1323450D+03	0.1723597	-0.0708399	0.0326808	0.0153072	0.0060419	0.0016831	
S 1.3442693D+03	0.3017715	-0.1388487	0.0660270	0.0309724	0.0121978	0.0034080	
S 5.9189171D+02	0.3499504	-0.2142639	0.1049318	0.0499303	0.0197963	0.0055107	
S 2.6868156D+02	0.1829874	-0.0880096	0.0462494	0.0217596	0.0084941	0.0023987	
S 1.0792889D+02	0.0194710	0.4652013	-0.3572386	-0.1851599	-0.0743695	-0.0208850	
S 4.9008609D+01	-0.0024908	0.6042422	-0.6261918	-0.3595914	-0.1490097	-0.0416653	
S 1.8756479D+01	0.0011707	0.1142647	0.3737260	0.3159423	0.1439724	0.0403672	
S 9.6247157D+00	-0.0007866	-0.0222088	0.8639195	0.9962927	0.4778659	0.1385159	
S 3.5941872D+00	0.0003813	0.0081384	0.1264023	-0.5008852	-0.3426868	-0.1067294	
S 1.8128841D+00	-0.0001996	-0.0042207	-0.0211247	-0.9061840	-0.8400478	-0.2642567	
S 5.0369287D-01	0.0000718	0.0014398	0.0057502	-0.0673444	0.7057616	0.2818283	
S 2.4029736D-01	-0.0000386	-0.0007604	-0.0029957	0.0184677	0.6421780	0.4604226	
S 4.7101954D-02	0.0000106	0.0002093	0.0007851	-0.0040266	0.0228623	-0.6671509	
S 2.0323929D-02	-0.0000049	-0.0000975	-0.0003647	0.0018178	-0.0071080	-0.5397595	
	P	2P	3P	4P	5P		
BASIS/ORB. ENERGY	-199.3878000	-41.0432210	-7.6987291	-0.8990551			
P 5.2412462D+07	0.0000028	-0.0000014	-0.0000006	-0.0000002			
P 7.1721942D+06	0.0000098	-0.0000047	-0.0000021	-0.0000008			
P 1.4897786D+06	0.0000286	-0.0000136	-0.0000062	-0.0000022			

P	3.8042765D+05	0.0000805	-0.0000384	-0.0000175	-0.0000062
P	1.1266547D+05	0.0002225	-0.0001063	-0.0000484	-0.0000173
P	3.7747242D+04	0.0006164	-0.0002950	-0.0001344	-0.0000480
P	1.4038281D+04	0.0017415	-0.0008363	-0.0003810	-0.0001365
P	5.6846149D+03	0.0050019	-0.0024143	-0.0011015	-0.0003931
P	2.4756452D+03	0.0142555	-0.0069428	-0.0031716	-0.0011380
P	1.1421328D+03	0.0390945	-0.0193416	-0.0088709	-0.0031671
P	5.5305758D+02	0.0962020	-0.0489654	-0.0225735	-0.0081202
P	2.7937904D+02	0.1976218	-0.1048564	-0.0488206	-0.0174578
P	1.4542437D+02	0.3116858	-0.1746480	-0.0823091	-0.0298245
P	7.7342909D+01	0.3210362	-0.1735869	-0.0808590	-0.0285934
P	4.1441118D+01	0.1710800	0.0396825	0.0398501	0.0149843
P	2.2071772D+01	0.0326841	0.4017848	0.2709387	0.1066893
P	1.1968891D+01	0.0013795	0.4811545	0.3725209	0.1433250
P	6.3973447D+00	0.0000242	0.1843275	-0.0854758	-0.0530308
P	3.2435863D+00	-0.0001146	0.0166000	-0.6202269	-0.3419842
P	1.6194795D+00	-0.0000295	0.0008334	-0.4387129	-0.2454973
P	6.7663659D-01	0.0000005	-0.0000920	-0.0546786	0.4003437
P	3.0623076D-01	-0.0000006	0.0000282	0.0041344	0.6315272
P	1.2627262D-01	0.0000002	-0.0000083	-0.0010032	0.1827693
	D	3D	4D		
BASIS/ORB. ENERGY		-29.9461210	-3.8540696		
D	1.7086789D+04	0.0000232	-0.0000102		
D	3.8927145D+03	0.0002272	-0.0001009		
D	1.2348634D+03	0.0016294	-0.0007223		
D	4.8159603D+02	0.0085844	-0.0038390		
D	2.1319864D+02	0.0345050	-0.0155003		
D	1.0086916D+02	0.1065621	-0.0487935		
D	4.9953994D+01	0.2381576	-0.1096139		
D	2.5455172D+01	0.3562758	-0.1591411		
D	1.3408888D+01	0.3171829	-0.1036250		
D	7.2160589D+00	0.1403369	0.1342824		
D	3.8636778D+00	0.0255664	0.3783404		
D	2.0773504D+00	0.0007608	0.3922810		
D	1.1422155D+00	0.0002522	0.1957536		

D	6.5557124D-01	-0.0001499	0.0584945
D	3.3802366D-01	0.0000117	0.0084974

LANTHANUM [XE]6S(2)5D(1), 2D

CHARGE = 57.000000

SYMMETRY SPECIES	S	P	D
NUMBER OF BASIS FUNCTIONS	27	23	15
NUMBER OF CLOSED SHELLS	6	4	2
NUMBER OF OPEN SHELLS	0	0	1
OPEN SHELL OCCUPATION NUMBER	0	0	1

*** FINAL SCF RESULTS ***

E = -8489.786238002

ORBITAL ENERGIES AND EXPANSION COEFFICIENTS

	S	1S	2S	3S	4S	5S	6S
BASIS/ORB. ENERGY	-1437.7696000	-232.8585400	-51.5082910	-11.1296620	-1.8196443	-0.1792231	
S 6.1193083D+10	0.0000021	-0.0000007	0.0000003	0.0000002	0.0000001	0.0000000	
S 5.1845856D+09	0.0000100	-0.0000035	0.0000016	0.0000008	0.0000003	-0.0000001	
S 6.9801037D+08	0.0000353	-0.0000124	0.0000057	0.0000027	0.0000011	-0.0000003	
S 1.3273684D+08	0.0000938	-0.0000331	0.0000150	0.0000071	0.0000029	-0.0000008	
S 3.4486860D+07	0.0002029	-0.0000715	0.0000325	0.0000153	0.0000062	-0.0000018	
S 1.0307668D+07	0.0004616	-0.0001630	0.0000740	0.0000348	0.0000141	-0.0000041	
S 3.1263430D+06	0.0010602	-0.0003744	0.0001702	0.0000799	0.0000324	-0.0000094	
S 9.8886512D+05	0.0023225	-0.0008231	0.0003741	0.0001758	0.0000714	-0.0000207	
S 3.3297659D+05	0.0048351	-0.0017174	0.0007816	0.0003672	0.0001490	-0.0000431	
S 1.2105841D+05	0.0097791	-0.0035098	0.0015967	0.0007507	0.0003050	-0.0000882	
S 4.6349242D+04	0.0201119	-0.0072665	0.0033191	0.0015598	0.0006329	-0.0001832	
S 1.8441072D+04	0.0417379	-0.0154981	0.0070771	0.0033320	0.0013548	-0.0003918	
S 7.5568870D+03	0.0877939	-0.0334714	0.0154388	0.0072662	0.0029475	-0.0008536	
S 3.1652360D+03	0.1775399	-0.0734209	0.0340284	0.0160850	0.0065497	-0.0018942	
S 1.3567040D+03	0.3059016	-0.1425185	0.0680797	0.0322554	0.0130930	-0.0037936	
S 5.9767854D+02	0.3472561	-0.2144271	0.1056418	0.0507436	0.0207736	-0.0060076	
S 2.7138582D+02	0.1737224	-0.0782429	0.0409241	0.0193917	0.0077301	-0.0022547	
S 1.1161606D+02	0.0169997	0.4696041	-0.3630664	-0.1904607	-0.0788231	0.0229377	
S 5.0909647D+01	-0.0016328	0.5973447	-0.6245018	-0.3627053	-0.1556277	0.0452908	
S 1.9859904D+01	0.0006826	0.1134906	0.3636392	0.3098342	0.1472584	-0.0432517	

S	1.0201197D+01	-0.0004645	-0.0206232	0.8707365	1.0170588	0.5034784	-0.1511954
S	3.8668523D+00	0.0002280	0.0077816	0.1345255	-0.4701921	-0.3290930	0.1056270
S	1.9737859D+00	-0.0001211	-0.0041790	-0.0229864	-0.9324622	-0.9132026	0.3046497
S	6.0076870D-01	0.0000443	0.0014497	0.0063946	-0.0739145	0.6304050	-0.2748795
S	2.8877334D-01	-0.0000219	-0.0006986	-0.0030383	0.0162246	0.7440407	-0.4950378
S	5.0747731D-02	0.0000051	0.0001630	0.0006674	-0.0029021	0.0292973	0.7761975
S	2.0810819D-02	-0.0000024	-0.0000756	-0.0003088	0.0012995	-0.0096392	0.4284293
	P	2P	3P	4P	5P		
BASIS/ORB. ENERGY	-208.6243800	-43.5680520	-8.4369321	-1.0526112			
P	5.0400664D+07	0.0000031	-0.0000015	-0.0000007	-0.0000003		
P	7.1932041D+06	0.0000105	-0.0000050	-0.0000023	-0.0000009		
P	1.4918768D+06	0.0000309	-0.0000148	-0.0000068	-0.0000025		
P	3.8208245D+05	0.0000863	-0.0000414	-0.0000190	-0.0000071		
P	1.1329834D+05	0.0002382	-0.0001143	-0.0000527	-0.0000196		
P	3.7981497D+04	0.0006589	-0.0003169	-0.0001460	-0.0000543		
P	1.4101175D+04	0.0018640	-0.0008995	-0.0004148	-0.0001547		
P	5.6983906D+03	0.0053480	-0.0025953	-0.0011978	-0.0004452		
P	2.4771636D+03	0.0152292	-0.0074566	-0.0034492	-0.0012886		
P	1.1415298D+03	0.0415388	-0.0206839	-0.0095973	-0.0035690		
P	5.5284412D+02	0.1013883	-0.0519553	-0.0242683	-0.0090911		
P	2.7902807D+02	0.2061509	-0.1103124	-0.0519790	-0.0193644		
P	1.4518431D+02	0.3172478	-0.1790777	-0.0856182	-0.0323224		
P	7.7477249D+01	0.3128597	-0.1670840	-0.0779961	-0.0286389		
P	4.1810393D+01	0.1599938	0.0588364	0.0511996	0.0200772		
P	2.2271866D+01	0.0294765	0.4216105	0.2927345	0.1206687		
P	1.2080507D+01	0.0007905	0.4699942	0.3652469	0.1460498		
P	6.4545360D+00	0.0001520	0.1657177	-0.1263473	-0.0759492		
P	3.3218938D+00	-0.0001928	0.0134271	-0.6291303	-0.3699560		
P	1.6873198D+00	0.0000122	0.0009662	-0.4086952	-0.2372921		
P	7.4125825D-01	-0.0000151	-0.0001807	-0.0490141	0.4324059		
P	3.4058093D-01	0.0000065	0.0000531	0.0023087	0.6259323		
P	1.4104679D-01	-0.0000016	-0.0000158	-0.0005532	0.1687526		
	D	3D	4D	5D			
BASIS/ORB. ENERGY	-32.0742930	-4.4000025	-0.2352980				
D	8.4346934D+03	0.0000723	-0.0000325	0.0000082			

D	2.7448862D+03	0.0003145	-0.0001439	0.0000365
D	1.2592925D+03	0.0013492	-0.0006075	0.0001536
D	5.3720066D+02	0.0075789	-0.0034701	0.0008806
D	2.3112971D+02	0.0341770	-0.0156616	0.0039719
D	1.0531172D+02	0.1115184	-0.0522608	0.0133042
D	5.0906060D+01	0.2523398	-0.1184962	0.0301454
D	2.5349935D+01	0.3786903	-0.1725822	0.0438182
D	1.2858561D+01	0.3213057	-0.0850468	0.0182396
D	6.4407130D+00	0.1121932	0.2459105	-0.0762947
D	3.1373651D+00	0.0089992	0.5066888	-0.1536201
D	1.4741848D+00	0.0003736	0.3467686	-0.0706457
D	6.2011004D-01	-0.0001924	0.0630023	0.2769122
D	2.3008974D-01	0.0000490	-0.0008009	0.5631635
D	7.6359519D-02	-0.0000172	0.0006202	0.3761203

CERIUM [XE]6S(2)5D(1)4F(1), 1G

CHARGE = 58.000000

SYMMETRY SPECIES	S	P	D	F
NUMBER OF BASIS FUNCTIONS	27	23	15	10
NUMBER OF CLOSED SHELLS	6	4	2	0
NUMBER OF OPEN SHELLS	0	0	1	1
OPEN SHELL OCCUPATION NUMBER	0	0	1	1

*** FINAL SCF RESULTS ***

E = -8856.903630035

ORBITAL ENERGIES AND EXPANSION COEFFICIENTS

	S	1S	2S	3S	4S	5S	6S
BASIS/ORB. ENERGY		-1493.7401000	-243.2123400	-54.0965520	-11.6889860	-1.8795461	-0.1804378
S	3.4002773D+10	0.0000033	-0.0000012	0.0000005	0.0000003	0.0000001	0.0000000
S	3.6821855D+09	0.0000122	-0.0000043	0.0000020	0.0000009	0.0000004	-0.0000001
S	6.3306242D+08	0.0000361	-0.0000128	0.0000058	0.0000028	0.0000011	-0.0000003
S	1.3593059D+08	0.0000967	-0.0000342	0.0000156	0.0000074	0.0000030	-0.0000008
S	3.3661849D+07	0.0002362	-0.0000836	0.0000381	0.0000180	0.0000073	-0.0000021
S	9.4546455D+06	0.0005283	-0.0001873	0.0000854	0.0000403	0.0000163	-0.0000046
S	2.9434908D+06	0.0011267	-0.0003995	0.0001822	0.0000860	0.0000348	-0.0000099
S	9.8444848D+05	0.0023411	-0.0008333	0.0003800	0.0001794	0.0000727	-0.0000206

S	3.4744049D+05	0.0048218	-0.0017196	0.0007853	0.0003706	0.0001501	-0.0000426
S	1.2784612D+05	0.0098573	-0.0035521	0.0016220	0.0007661	0.0003105	-0.0000881
S	4.8945120D+04	0.0203550	-0.0073854	0.0033840	0.0015980	0.0006469	-0.0001837
S	1.9242127D+04	0.0429098	-0.0159982	0.0073355	0.0034692	0.0014073	-0.0003991
S	7.7939669D+03	0.0896352	-0.0343543	0.0158947	0.0075182	0.0030431	-0.0008644
S	3.2639051D+03	0.1784221	-0.0741861	0.0345404	0.0164005	0.0066628	-0.0018889
S	1.4057617D+03	0.3036157	-0.1420661	0.0680605	0.0324150	0.0131290	-0.0037321
S	6.2432795D+02	0.3426366	-0.2116276	0.1047627	0.0505294	0.0206384	-0.0058474
S	2.8605480D+02	0.1760726	-0.0806290	0.0418032	0.0199834	0.0079616	-0.0022880
S	1.1742270D+02	0.0188268	0.4603482	-0.3556700	-0.1877848	-0.0775781	0.0221673
S	5.3713756D+01	-0.0021931	0.6012844	-0.6317752	-0.3680984	-0.1575313	0.0448771
S	2.1268210D+01	0.0010210	0.1186464	0.3310220	0.2822343	0.1339180	-0.0383103
S	1.0898494D+01	-0.0006806	-0.0199803	0.8923129	1.0429765	0.5153219	-0.1520662
S	4.1719807D+00	0.0003342	0.0074861	0.1435604	-0.4269800	-0.3008405	0.0957527
S	2.1176082D+00	-0.0001747	-0.0038950	-0.0227472	-0.9687084	-0.9275494	0.3000578
S	6.1848114D-01	0.0000636	0.0013357	0.0063167	-0.0795404	0.6441450	-0.2686411
S	2.9824948D-01	-0.0000330	-0.0006772	-0.0031592	0.0199016	0.7193490	-0.4854452
S	5.6298194D-02	0.0000084	0.0001737	0.0007661	-0.0039770	0.0296163	0.6502643
S	2.4044171D-02	-0.0000039	-0.0000810	-0.0003566	0.0017959	-0.0094193	0.5521293
	P	2P	3P	4P	5P		
BASIS/ORB. ENERGY	-217.7671500	-45.7950390	-8.8684195	-1.0807256			
P	4.9656588D+07	0.0000034	-0.0000016	-0.0000008	-0.0000003		
P	7.1956823D+06	0.0000112	-0.0000054	-0.0000025	-0.0000009		
P	1.5032424D+06	0.0000333	-0.0000160	-0.0000074	-0.0000027		
P	3.8118893D+05	0.0000937	-0.0000451	-0.0000209	-0.0000077		
P	1.1330273D+05	0.0002546	-0.0001228	-0.0000569	-0.0000211		
P	3.8093303D+04	0.0007086	-0.0003425	-0.0001587	-0.0000587		
P	1.4078256D+04	0.0020034	-0.0009716	-0.0004507	-0.0001673		
P	5.7048089D+03	0.0056947	-0.0027777	-0.0012891	-0.0004770		
P	2.4778324D+03	0.0162747	-0.0080126	-0.0037289	-0.0013867		
P	1.1409415D+03	0.0439920	-0.0220395	-0.0102855	-0.0038072		
P	5.5310796D+02	0.1066400	-0.0550306	-0.0258733	-0.0096490		
P	2.7888026D+02	0.2142994	-0.1155808	-0.0548018	-0.0203227		
P	1.4520820D+02	0.3219996	-0.1831526	-0.0882141	-0.0331672		
P	7.7499776D+01	0.3072044	-0.1607072	-0.0746141	-0.0271497		

P	4.1795282D+01	0.1483836	0.0824664	0.0657147	0.0255986
P	2.2298162D+01	0.0249992	0.4436702	0.3144850	0.1295271
P	1.2099286D+01	0.0006280	0.4535800	0.3502528	0.1380939
P	6.4633354D+00	0.0000706	0.1454265	-0.1787283	-0.1007709
P	3.3301176D+00	-0.0001579	0.0105697	-0.6405199	-0.3809047
P	1.6913757D+00	0.0000045	0.0008423	-0.3697819	-0.1995020
P	7.4891759D-01	-0.0000099	-0.0001573	-0.0392782	0.4661997
P	3.4066318D-01	0.0000044	0.0000422	0.0012802	0.6064693
P	1.4035439D-01	-0.0000010	-0.0000121	-0.0003025	0.1500742
	D	3D	4D	5D	
BASIS/ORB. ENERGY	-33.9024140	-4.6655514	-0.2644536		
D	8.5871753D+03	0.0000870	-0.0000395	0.0000104	
D	2.5294137D+03	0.0003530	-0.0001638	0.0000440	
D	1.3393875D+03	0.0012766	-0.0005787	0.0001517	
D	5.4596423D+02	0.0083824	-0.0038778	0.0010327	
D	2.3085975D+02	0.0370914	-0.0171722	0.0045440	
D	1.0535430D+02	0.1186398	-0.0562564	0.0150204	
D	5.0954813D+01	0.2637820	-0.1249775	0.0331474	
D	2.5360260D+01	0.3843876	-0.1760720	0.0469955	
D	1.2871011D+01	0.3078746	-0.0674093	0.0130637	
D	6.4460893D+00	0.0989099	0.2763074	-0.0881357	
D	3.1430631D+00	0.0068562	0.5102379	-0.1658179	
D	1.4712040D+00	0.0003970	0.3204659	-0.0453232	
D	6.0389343D-01	-0.0001680	0.0506593	0.3265730	
D	2.2905715D-01	0.0000607	-0.0013738	0.5549350	
D	7.9096585D-02	-0.0000142	0.0006438	0.3219397	
	F	4F			
BASIS/ORB. ENERGY	-0.5501431				
F	3.7591040D+02	-0.0002847			
F	1.2980203D+02	-0.0024430			
F	5.6167429D+01	-0.0126930			
F	2.6239296D+01	-0.0441964			
F	1.2591573D+01	-0.1199382			
F	6.1042442D+00	-0.2377827			
F	2.8869783D+00	-0.3367312			

F 1.3071566D+00 -0.3437236
 F 5.5124383D-01 -0.2410269
 F 2.0550452D-01 -0.0936654

 PRASEODYMIUM [XE]6S(2)5D(0)4F(3), 41

CHARGE = 59.000000

SYMMETRY SPECIES	S	P	D	F
NUMBER OF BASIS FUNCTIONS	27	23	15	10
NUMBER OF CLOSED SHELLS	6	4	2	0
NUMBER OF OPEN SHELLS	0	0	0	1
OPEN SHELL OCCUPATION NUMBER	0	0	0	3

*** FINAL SCF RESULTS ***

E = -9233.707382305

ORBITAL ENERGIES AND EXPANSION COEFFICIENTS

	S	1S	2S	3S	4S	5S	6S
BASIS/ORB. ENERGY	-1550.6828000	-253.5328900	-56.4044480	-11.9410560	-1.7936266	-0.1711363	
S 4.9230765D+10	0.0000030	-0.0000011	0.0000005	0.0000002	0.0000001	0.0000000	
S 3.8789882D+09	0.0000138	-0.0000049	0.0000022	0.0000011	0.0000004	0.0000001	
S 5.9318815D+08	0.0000420	-0.0000149	0.0000068	0.0000032	0.0000013	0.0000003	
S 1.2540535D+08	0.0001076	-0.0000383	0.0000175	0.0000083	0.0000032	0.0000009	
S 3.2524318D+07	0.0002468	-0.0000878	0.0000401	0.0000190	0.0000075	0.0000020	
S 9.5292205D+06	0.0005505	-0.0001959	0.0000896	0.0000423	0.0000166	0.0000044	
S 2.9615650D+06	0.0012035	-0.0004286	0.0001961	0.0000926	0.0000364	0.0000097	
S 9.8352823D+05	0.0024805	-0.0008866	0.0004057	0.0001917	0.0000753	0.0000201	
S 3.4922538D+05	0.0050387	-0.0018051	0.0008273	0.0003907	0.0001535	0.0000410	
S 1.2893890D+05	0.0103432	-0.0037432	0.0017148	0.0008107	0.0003188	0.0000851	
S 4.9198751D+04	0.0213671	-0.0077937	0.0035849	0.0016934	0.0006653	0.0001779	
S 1.9315976D+04	0.0448329	-0.0168007	0.0077281	0.0036594	0.0014397	0.0003845	
S 7.8112677D+03	0.0933302	-0.0360319	0.0167455	0.0079216	0.0031122	0.0008326	
S 3.2695886D+03	0.1838427	-0.0770550	0.0359977	0.0171239	0.0067458	0.0018009	
S 1.4087527D+03	0.3088612	-0.1464200	0.0705852	0.0336095	0.0132185	0.0035393	
S 6.2417113D+02	0.3404348	-0.2129412	0.1057919	0.0512212	0.0202737	0.0054076	
S 2.8532902D+02	0.1640267	-0.0652164	0.0338495	0.0157603	0.0060991	0.0016603	
S 1.1950661D+02	0.0155058	0.4759610	-0.3743287	-0.1976394	-0.0794108	-0.0213712	
S 5.4804971D+01	-0.0012996	0.5889398	-0.6211001	-0.3657023	-0.1515739	-0.0406228	

S	2.1557200D+01	0.0005086	0.1103740	0.3838476	0.3386696	0.1544578	0.0415793
S	1.1085975D+01	-0.0003464	-0.0194828	0.8631186	1.0104624	0.4867270	0.1350181
S	4.1973320D+00	0.0001610	0.0069592	0.1271209	-0.5283481	-0.3689966	-0.1093919
S	2.1111952D+00	-0.0000794	-0.0035350	-0.0205147	-0.8959400	-0.8234612	-0.2476624
S	5.9179526D-01	0.0000273	0.0011526	0.0054399	-0.0640019	0.7105489	0.2679733
S	2.7548221D-01	-0.0000141	-0.0005788	-0.0027021	0.0162726	0.6393462	0.4374796
S	5.0025313D-02	0.0000037	0.0001550	0.0006896	-0.0034768	0.0215198	-0.6893151
S	2.1368062D-02	-0.0000018	-0.0000738	-0.0003279	0.0016108	-0.0070762	-0.5028281
	P	2P	3P	4P	5P		
BASIS/ORB. ENERGY	-226.8209500	-47.7285890	-9.0010080	-0.9924792			
P	5.1093673D+07	0.0000036	-0.0000017	-0.0000008	-0.0000003		
P	7.2150462D+06	0.0000122	-0.0000059	-0.0000027	-0.0000010		
P	1.4890556D+06	0.0000359	-0.0000173	-0.0000080	-0.0000029		
P	3.8379255D+05	0.0000995	-0.0000481	-0.0000223	-0.0000079		
P	1.1372872D+05	0.0002753	-0.0001333	-0.0000618	-0.0000219		
P	3.8075062D+04	0.0007580	-0.0003681	-0.0001706	-0.0000605		
P	1.4131287D+04	0.0021379	-0.0010418	-0.0004834	-0.0001719		
P	5.7033863D+03	0.0061087	-0.0029949	-0.0013903	-0.0004926		
P	2.4778855D+03	0.0172711	-0.0085490	-0.0039809	-0.0014174		
P	1.1418199D+03	0.0466171	-0.0234970	-0.0109713	-0.0038891		
P	5.5268940D+02	0.1122438	-0.0583233	-0.0274508	-0.0098020		
P	2.7870202D+02	0.2221278	-0.1207565	-0.0573130	-0.0203539		
P	1.4516744D+02	0.3267548	-0.1871654	-0.0902941	-0.0325096		
P	7.7462378D+01	0.3005769	-0.1530203	-0.0700935	-0.0243060		
P	4.1758039D+01	0.1370016	0.1070397	0.0807979	0.0300966		
P	2.2346049D+01	0.0208933	0.4616901	0.3318074	0.1309558		
P	1.2160891D+01	0.0006509	0.4341239	0.3286116	0.1223937		
P	6.5240612D+00	-0.0000626	0.1289279	-0.2178396	-0.1136277		
P	3.3796572D+00	-0.0000848	0.0090131	-0.6333826	-0.3592042		
P	1.7169726D+00	-0.0000235	0.0007766	-0.3505490	-0.1712866		
P	7.5073577D-01	0.0000022	-0.0001019	-0.0368752	0.4387480		
P	3.3859350D-01	-0.0000010	0.0000305	0.0013744	0.6020001		
P	1.3995024D-01	0.0000002	-0.0000071	-0.0003580	0.1686149		
	D	3D	4D				
BASIS/ORB. ENERGY	-35.4343470	-4.6566207					

D	1.2713148D+04	0.0000469	-0.0000214
D	3.3541165D+03	0.0003491	-0.0001597
D	1.2207718D+03	0.0019377	-0.0008882
D	5.2304242D+02	0.0086559	-0.0039896
D	2.4730016D+02	0.0309628	-0.0143753
D	1.2414225D+02	0.0883755	-0.0416426
D	6.4954192D+01	0.1947284	-0.0928791
D	3.4766164D+01	0.3126875	-0.1459761
D	1.8896568D+01	0.3372854	-0.1376552
D	1.0329810D+01	0.1980598	0.0459341
D	5.5740750D+00	0.0503916	0.3272853
D	2.9513049D+00	0.0036421	0.4376200
D	1.5332733D+00	0.0002524	0.2686230
D	7.5787953D-01	-0.0000343	0.0687516
D	3.1169924D-01	0.0000105	0.0041181

F

4F

BASIS/ORB. ENERGY -0.3960176

F	3.8258496D+02	-0.0002925
F	1.3369373D+02	-0.0026062
F	5.6360841D+01	-0.0141275
F	2.6158584D+01	-0.0476623
F	1.2665608D+01	-0.1242638
F	6.1921268D+00	-0.2388501
F	2.9282665D+00	-0.3347808
F	1.3081764D+00	-0.3436361
F	5.3607490D-01	-0.2439819
F	1.9322252D-01	-0.0977491

NEODIUM [XE]6S(2)5D(0)4F(4), 51

CHARGE = 60.000000

SYMMETRY SPECIES	S	P	D	F
NUMBER OF BASIS FUNCTIONS	27	23	15	10
NUMBER OF CLOSED SHELLS	6	4	2	0
NUMBER OF OPEN SHELLS	0	0	0	1
OPEN SHELL OCCUPATION NUMBER	0	0	0	4

*** FINAL SCF RESULTS ***

E = -9620.368528785

ORBITAL ENERGIES AND EXPANSION COEFFICIENTS

	S	1S	2S	3S	4S	5S	6S
BASIS/ORB. ENERGY	-1609.1241000	-264.3924300	-59.0884480	-12.4964680	-1.8494977	-0.1734712	
S 2.9095464D+10	0.0000041	-0.0000015	0.0000007	0.0000003	0.0000001	0.0000000	
S 3.5474248D+09	0.0000138	-0.0000049	0.0000023	0.0000011	0.0000004	-0.0000001	
S 6.2660415D+08	0.0000418	-0.0000149	0.0000069	0.0000032	0.0000013	-0.0000003	
S 1.3247865D+08	0.0001133	-0.0000405	0.0000186	0.0000088	0.0000034	-0.0000009	
S 3.2558625D+07	0.0002751	-0.0000982	0.0000451	0.0000214	0.0000084	-0.0000022	
S 9.1881109D+06	0.0006022	-0.0002152	0.0000988	0.0000468	0.0000183	-0.0000048	
S 2.9315518D+06	0.0012400	-0.0004434	0.0002036	0.0000965	0.0000378	-0.0000100	
S 1.0008688D+06	0.0025742	-0.0009239	0.0004241	0.0002011	0.0000788	-0.0000208	
S 3.5389774D+05	0.0053098	-0.0019108	0.0008785	0.0004164	0.0001631	-0.0000431	
S 1.3037114D+05	0.0107832	-0.0039190	0.0018013	0.0008547	0.0003351	-0.0000884	
S 4.9842271D+04	0.0222042	-0.0081409	0.0037565	0.0017810	0.0006976	-0.0001843	
S 1.9521555D+04	0.0467296	-0.0175953	0.0081228	0.0038604	0.0015143	-0.0003995	
S 7.8510058D+03	0.0972674	-0.0378255	0.0176383	0.0083750	0.0032808	-0.0008671	
S 3.2730637D+03	0.1899726	-0.0802547	0.0376571	0.0179829	0.0070635	-0.0018630	
S 1.4102050D+03	0.3129487	-0.1503503	0.0728080	0.0348040	0.0136489	-0.0036104	
S 6.2666120D+02	0.3351248	-0.2117965	0.1058200	0.0514756	0.0203204	-0.0053547	
S 2.8753121D+02	0.1544400	-0.0528809	0.0267724	0.0122206	0.0046683	-0.0012623	
S 1.2276019D+02	0.0135809	0.4817222	-0.3822602	-0.2029313	-0.0813321	0.0216226	
S 5.6635177D+01	-0.0008156	0.5801374	-0.6165149	-0.3656437	-0.1512579	0.0400553	
S 2.2562431D+01	0.0002476	0.1082338	0.3898408	0.3471996	0.1580672	-0.0420791	
S 1.1584069D+01	-0.0001790	-0.0182374	0.8616617	1.0143370	0.4875526	-0.1334950	
S 4.4274956D+00	0.0000796	0.0064850	0.1260358	-0.5342920	-0.3720851	0.1085552	
S 2.2154057D+00	-0.0000360	-0.0032512	-0.0192295	-0.8959827	-0.8197312	0.2435086	
S 6.2284904D-01	0.0000122	0.0010489	0.0050627	-0.0633007	0.7013590	-0.2599035	
S 2.8814518D-01	-0.0000063	-0.0005168	-0.0024680	0.0156213	0.6469881	-0.4327512	
S 5.0162524D-02	0.0000016	0.0001354	0.0006143	-0.0032617	0.0219282	0.7103886	
S 2.1350077D-02	-0.0000008	-0.0000653	-0.0002957	0.0015313	-0.0074689	0.4759315	
	P	2P	3P	4P	5P		
BASIS/ORB. ENERGY	-236.3468300	-50.0205640	-9.4215805	-1.0172260			
P 4.8217378D+07	0.0000040	-0.0000019	-0.0000009	-0.0000003			

P	7.2613553D+06	0.0000128	-0.0000062	-0.0000029	-0.0000010
P	1.5073401D+06	0.0000387	-0.0000188	-0.0000087	-0.0000031
P	3.8235630D+05	0.0001078	-0.0000524	-0.0000244	-0.0000086
P	1.1381377D+05	0.0002935	-0.0001428	-0.0000664	-0.0000235
P	3.8195061D+04	0.0008122	-0.0003961	-0.0001844	-0.0000650
P	1.4131438D+04	0.0022905	-0.0011214	-0.0005226	-0.0001848
P	5.7042242D+03	0.0065142	-0.0032086	-0.0014962	-0.0005272
P	2.4781889D+03	0.0183557	-0.0091344	-0.0042729	-0.0015132
P	1.1422855D+03	0.0492687	-0.0249728	-0.0117152	-0.0041297
P	5.5255985D+02	0.1179650	-0.0617203	-0.0291951	-0.0103706
P	2.7845795D+02	0.2299257	-0.1259033	-0.0600694	-0.0212131
P	1.4526851D+02	0.3298649	-0.1902637	-0.0922810	-0.0330694
P	7.7536685D+01	0.2943162	-0.1444460	-0.0653272	-0.0223520
P	4.1634185D+01	0.1265215	0.1323483	0.0972266	0.0359821
P	2.2368480D+01	0.0168207	0.4777592	0.3494995	0.1377611
P	1.2189504D+01	0.0008993	0.4143113	0.3058593	0.1110877
P	6.5377726D+00	-0.0002970	0.1127333	-0.2648314	-0.1341215
P	3.3940219D+00	0.0000355	0.0071423	-0.6315696	-0.3623269
P	1.7295041D+00	-0.0000719	0.0007176	-0.3192268	-0.1372745
P	7.5379370D-01	0.0000229	-0.0000956	-0.0311411	0.4632934
P	3.3887829D-01	-0.0000097	0.0000286	0.0012302	0.5844264
P	1.3960772D-01	0.0000026	-0.0000062	-0.0003116	0.1531668
	D	3D	4D		
BASIS/ORB. ENERGY		-37.3088230	-4.9083092		
D	1.2677919D+04	0.0000517	-0.0000238		
D	3.3468628D+03	0.0003830	-0.0001766		
D	1.2195618D+03	0.0021144	-0.0009765		
D	5.2306807D+02	0.0093875	-0.0043634		
D	2.4731472D+02	0.0333560	-0.0156115		
D	1.2413536D+02	0.0942268	-0.0448243		
D	6.4965013D+01	0.2041826	-0.0981123		
D	3.4760943D+01	0.3207313	-0.1505958		
D	1.8905104D+01	0.3323567	-0.1316222		
D	1.0333931D+01	0.1837705	0.0698769		
D	5.5709417D+00	0.0430452	0.3476103		

D	2.9519905D+00	0.0028033	0.4313625
D	1.5328380D+00	0.0002624	0.2478214
D	7.5575620D-01	-0.0000220	0.0586992
D	3.0598871D-01	0.0000122	0.0032204
	F	4F	
BASIS/ORB.ENERGY			
F	3.7959709D+02	-0.0003538	
F	1.3109244D+02	-0.0031276	
F	5.6143064D+01	-0.0158540	
F	2.6350663D+01	-0.0526287	
F	1.2769647D+01	-0.1356307	
F	6.2466792D+00	-0.2511032	
F	2.9709753D+00	-0.3361944	
F	1.3491672D+00	-0.3288720	
F	5.6686572D-01	-0.2286271	
F	2.0819149D-01	-0.0909939	

PROMETHIUM [XE]6S(2)5D(0)4F(5), 6H

CHARGE = 61.000000

SYMMETRY SPECIES	S	P	D	F
NUMBER OF BASIS FUNCTIONS	27	23	15	10
NUMBER OF CLOSED SHELLS	6	4	2	0
NUMBER OF OPEN SHELLS	0	0	0	1
OPEN SHELL OCCUPATION NUMBER	0	0	0	5

*** FINAL SCF RESULTS ***

E = -10016.963947165

ORBITAL ENERGIES AND EXPANSION COEFFICIENTS

	S	1S	2S	3S	4S	5S	6S
BASIS/ORB.ENERGY	-1668.8318000	-275.5211900	-61.8339000	-13.0597960	-1.9050934	-0.1757013	
S	6.9230958D+10	0.0000029	-0.0000010	0.0000005	0.0000002	0.0000001	0.0000000
S	4.1782939D+09	0.0000163	-0.0000058	0.0000027	0.0000013	0.0000005	-0.0000001
S	5.5670649D+08	0.0000523	-0.0000188	0.0000086	0.0000041	0.0000016	-0.0000004
S	1.1894984D+08	0.0001196	-0.0000429	0.0000197	0.0000094	0.0000037	-0.0000010
S	3.3354640D+07	0.0002712	-0.0000972	0.0000448	0.0000213	0.0000083	-0.0000022
S	9.4636465D+06	0.0006471	-0.0002322	0.0001069	0.0000508	0.0000199	-0.0000052

S	2.9146408D+06	0.0013431	-0.0004824	0.0002222	0.0001056	0.0000413	-0.0000108
S	9.9751535D+05	0.0026858	-0.0009680	0.0004457	0.0002120	0.0000829	-0.0000216
S	3.5878916D+05	0.0054843	-0.0019823	0.0009142	0.0004347	0.0001698	-0.0000444
S	1.3275153D+05	0.0112262	-0.0040974	0.0018892	0.0008992	0.0003515	-0.0000918
S	5.0422403D+04	0.0233054	-0.0085883	0.0039755	0.0018913	0.0007386	-0.0001931
S	1.9620511D+04	0.0488033	-0.0184716	0.0085558	0.0040790	0.0015956	-0.0004166
S	7.8842289D+03	0.1007958	-0.0394733	0.0184719	0.0088024	0.0034376	-0.0008995
S	3.2824340D+03	0.1957521	-0.0833688	0.0392695	0.0188132	0.0073702	-0.0019232
S	1.4129422D+03	0.3172537	-0.1543493	0.0751079	0.0360493	0.0140911	-0.0036916
S	6.2855151D+02	0.3300073	-0.2108327	0.1058250	0.0516553	0.0203529	-0.0053017
S	2.8914278D+02	0.1448257	-0.0385279	0.0185753	0.0081825	0.0030106	-0.0008316
S	1.2515307D+02	0.0117721	0.4926947	-0.3962172	-0.2118650	-0.0846251	0.0223049
S	5.8008532D+01	-0.0005084	0.5677368	-0.6069936	-0.3622566	-0.1498291	0.0391863
S	2.3250915D+01	0.0000979	0.1030000	0.4179608	0.3741224	0.1707740	-0.0447815
S	1.1974734D+01	-0.0000888	-0.0175351	0.8412256	1.0076674	0.4825209	-0.1312732
S	4.7467597D+00	0.0000376	0.0062301	0.1215371	-0.5297025	-0.3607434	0.1050164
S	2.3444303D+00	-0.0000138	-0.0030071	-0.0150815	-0.9102782	-0.8340315	0.2429255
S	6.7464215D-01	0.0000047	0.0009784	0.0040738	-0.0664651	0.6455411	-0.2262346
S	3.1145248D-01	-0.0000025	-0.0004735	-0.0019524	0.0155696	0.6984962	-0.4538783
S	5.3807906D-02	0.0000006	0.0001261	0.0004881	-0.0032904	0.0278898	0.6266646
S	2.3582913D-02	-0.0000003	-0.0000622	-0.0002404	0.0015803	-0.0099138	0.5526011
	P	2P	3P	4P	5P		
BASIS/ORB. ENERGY	-246.0758600	-52.3573420	-9.8456383	-1.0412026			
P	5.1833132D+07	0.0000042	-0.0000020	-0.0000009	-0.0000003		
P	7.3684136D+06	0.0000139	-0.0000068	-0.0000032	-0.0000011		
P	1.5238966D+06	0.0000411	-0.0000200	-0.0000093	-0.0000033		
P	3.8821576D+05	0.0001144	-0.0000558	-0.0000260	-0.0000091		
P	1.1499315D+05	0.0003137	-0.0001532	-0.0000716	-0.0000251		
P	3.8394735D+04	0.0008669	-0.0004246	-0.0001984	-0.0000696		
P	1.4203400D+04	0.0024326	-0.0011960	-0.0005597	-0.0001967		
P	5.7292780D+03	0.0069179	-0.0034238	-0.0016027	-0.0005619		
P	2.4835172D+03	0.0194913	-0.0097460	-0.0045785	-0.0016115		
P	1.1426786D+03	0.0520911	-0.0265591	-0.0125106	-0.0043888		
P	5.5274934D+02	0.1233841	-0.0649561	-0.0308725	-0.0108989		
P	2.7870834D+02	0.2374466	-0.1310216	-0.0627961	-0.0220778		

P	1.4534124D+02	0.3335559	-0.1933107	-0.0942374	-0.0335431
P	7.7645304D+01	0.2853584	-0.1347456	-0.0598265	-0.0202945
P	4.1946785D+01	0.1165241	0.1520901	0.1098441	0.0406769
P	2.2692210D+01	0.0150535	0.4833344	0.3596241	0.1408673
P	1.2434808D+01	0.0006445	0.4004892	0.2867689	0.1027935
P	6.6594496D+00	-0.0001928	0.1048399	-0.2873889	-0.1455739
P	3.4879427D+00	-0.0000196	0.0056382	-0.6252749	-0.3557318
P	1.7846806D+00	-0.0000425	0.0009961	-0.3053558	-0.1304103
P	8.0109477D-01	0.0000116	-0.0002060	-0.0294983	0.4445104
P	3.6268475D-01	-0.0000047	0.0000737	0.0004116	0.5868753
P	1.5088131D-01	0.0000012	-0.0000179	-0.0001419	0.1704736

D

3D

4D

BASIS/ORB. ENERGY -39.2178910 -5.1607807

D	1.2635104D+04	0.0000569	-0.0000263
D	3.3375861D+03	0.0004199	-0.0001950
D	1.2182956D+03	0.0023014	-0.0010701
D	5.2322078D+02	0.0101604	-0.0047589
D	2.4729887D+02	0.0358843	-0.0169196
D	1.2413041D+02	0.1002210	-0.0480944
D	6.4977687D+01	0.2136772	-0.1033471
D	3.4753801D+01	0.3281012	-0.1547723
D	1.8915051D+01	0.3262323	-0.1240654
D	1.0335007D+01	0.1699517	0.0941353
D	5.5679225D+00	0.0365290	0.3653343
D	2.9529940D+00	0.0022518	0.4231652
D	1.5310765D+00	0.0002345	0.2282455
D	7.5311752D-01	0.0000012	0.0499006
D	3.0231499D-01	0.0000102	0.0025993

F

4F

BASIS/ORB. ENERGY -0.4634308

F	3.7849549D+02	-0.0004102
F	1.3079325D+02	-0.0035879
F	5.6126261D+01	-0.0178660
F	2.6353649D+01	-0.0583917
F	1.2791656D+01	-0.1472355

F	6.2571624D+00	-0.2630284
F	2.9759757D+00	-0.3399078
F	1.3499838D+00	-0.3193889
F	5.6853097D-01	-0.2119487
F	2.1117426D-01	-0.0803619

SAMARIUM [XE]6S(2)5D(0)4F(6), 7F

CHARGE = 62.000000

SYMMETRY SPECIES	S	P	D	F
NUMBER OF BASIS FUNCTIONS	27	23	15	10
NUMBER OF CLOSED SHELLS	6	4	2	0
NUMBER OF OPEN SHELLS	0	0	0	1
OPEN SHELL OCCUPATION NUMBER	0	0	0	6

*** FINAL SCF RESULTS ***

E = -10423.677523827

ORBITAL ENERGIES AND EXPANSION COEFFICIENTS

	S	1S	2S	3S	4S	5S	6S
BASIS/ORB. ENERGY	-1729.8170000	-286.9186000	-64.6364830	-13.6269360	-1.9594284	-0.1779880	
S 4.1998563D+10	0.0000037	-0.0000013	0.0000006	0.0000003	0.0000001	0.0000000	
S 4.5941055D+09	0.0000139	-0.0000050	0.0000023	0.0000011	0.0000004	-0.0000001	
S 7.5303931D+08	0.0000430	-0.0000155	0.0000071	0.0000034	0.0000013	-0.0000003	
S 1.5776780D+08	0.0001134	-0.0000409	0.0000189	0.0000090	0.0000035	-0.0000009	
S 3.9364524D+07	0.0002697	-0.0000971	0.0000448	0.0000214	0.0000083	-0.0000022	
S 1.1131390D+07	0.0006039	-0.0002176	0.0001004	0.0000479	0.0000187	-0.0000048	
S 3.4234974D+06	0.0012996	-0.0004685	0.0002164	0.0001032	0.0000402	-0.0000104	
S 1.1274699D+06	0.0027064	-0.0009794	0.0004523	0.0002158	0.0000840	-0.0000217	
S 3.9382672D+05	0.0054775	-0.0019869	0.0009190	0.0004383	0.0001706	-0.0000441	
S 1.4565122D+05	0.0109079	-0.0039985	0.0018488	0.0008826	0.0003438	-0.0000888	
S 5.6081151D+04	0.0220783	-0.0081549	0.0037859	0.0018059	0.0007028	-0.0001817	
S 2.2223641D+04	0.0450987	-0.0171220	0.0079503	0.0038019	0.0014816	-0.0003826	
S 9.0709666D+03	0.0919770	-0.0359146	0.0168453	0.0080468	0.0031317	-0.0008101	
S 3.8006495D+03	0.1803802	-0.0763529	0.0360017	0.0172964	0.0067487	-0.0017421	
S 1.6301057D+03	0.3042471	-0.1446502	0.0703036	0.0338004	0.0131696	-0.0034092	
S 7.1903282D+02	0.3414180	-0.2121365	0.1062048	0.0519291	0.0203537	-0.0052504	
S 3.2762992D+02	0.1722232	-0.0707182	0.0365260	0.0171619	0.0065980	-0.0017314	

S	1.3574405D+02	0.0178199	0.4697952	-0.3739898	-0.1998849	-0.0796422	0.0207166
S	6.2190130D+01	-0.0018237	0.5929745	-0.6293230	-0.3757011	-0.1543250	0.0400044
S	2.4514689D+01	0.0008057	0.1130897	0.3868293	0.3536833	0.1603309	-0.0417914
S	1.2662047D+01	-0.0005372	-0.0202475	0.8631241	1.0190714	0.4871007	-0.1304046
S	4.8593173D+00	0.0002502	0.0071370	0.1260945	-0.5481771	-0.3815482	0.1085460
S	2.4220756D+00	-0.0001230	-0.0035142	-0.0187971	-0.8892722	-0.8038532	0.2330349
S	6.7732450D-01	0.0000413	0.0011165	0.0048923	-0.0615917	0.7024055	-0.2518423
S	3.0935797D-01	-0.0000206	-0.0005440	-0.0023534	0.0150156	0.6418487	-0.4223327
S	5.2779368D-02	0.0000054	0.0001422	0.0005854	-0.0031478	0.0213493	0.7031279
S	2.2246041D-02	-0.0000026	-0.0000687	-0.0002822	0.0014816	-0.0072952	0.4779751
	P	2P	3P	4P	5P		
BASIS/ORB. ENERGY	-256.0043900	-54.7339330	-10.2691730	-1.0639055			
P	5.1833132D+07	0.0000045	-0.0000022	-0.0000010	-0.0000004		
P	7.3871989D+06	0.0000149	-0.0000073	-0.0000034	-0.0000012		
P	1.5277399D+06	0.0000441	-0.0000215	-0.0000101	-0.0000035		
P	3.8907912D+05	0.0001226	-0.0000600	-0.0000281	-0.0000098		
P	1.1515005D+05	0.0003360	-0.0001648	-0.0000772	-0.0000270		
P	3.8447979D+04	0.0009264	-0.0004557	-0.0002137	-0.0000745		
P	1.4216709D+04	0.0025964	-0.0012820	-0.0006019	-0.0002102		
P	5.7322363D+03	0.0073627	-0.0036605	-0.0017201	-0.0005994		
P	2.4843655D+03	0.0206736	-0.0103873	-0.0048964	-0.0017125		
P	1.1426487D+03	0.0549858	-0.0281919	-0.0133349	-0.0046506		
P	5.5273574D+02	0.1290557	-0.0683693	-0.0326154	-0.0114419		
P	2.7863778D+02	0.2453214	-0.1363556	-0.0656741	-0.0229589		
P	1.4524812D+02	0.3364674	-0.1958857	-0.0957865	-0.0338754		
P	7.7646235D+01	0.2766236	-0.1238271	-0.0537856	-0.0179841		
P	4.1975876D+01	0.1069990	0.1765586	0.1266946	0.0467722		
P	2.2717827D+01	0.0124608	0.4980584	0.3756494	0.1464053		
P	1.2413124D+01	0.0006281	0.3786492	0.2591644	0.0900362		
P	6.6771692D+00	-0.0002614	0.0893977	-0.3328575	-0.1659142		
P	3.4902043D+00	0.0000201	0.0052748	-0.6187449	-0.3542127		
P	1.7886776D+00	-0.0000557	0.0005354	-0.2748031	-0.0990130		
P	8.0913759D-01	0.0000183	-0.0000418	-0.0247763	0.4582446		
P	3.6603668D-01	-0.0000072	0.0000070	0.0001870	0.5752259		
P	1.5134571D-01	0.0000019	-0.0000001	-0.0000846	0.1598422		

D	3D	4D
BASIS/ORB. ENERGY	-41.1562030	-5.4103273
D 1.2216870D+04	0.0000646	-0.0000301
D 3.3156361D+03	0.0004560	-0.0002132
D 1.2193760D+03	0.0024977	-0.0011683
D 5.2294735D+02	0.0110077	-0.0051917
D 2.4725139D+02	0.0384793	-0.0182631
D 1.2415130D+02	0.1064272	-0.0514817
D 6.4980980D+01	0.2231274	-0.1085098
D 3.4756012D+01	0.3345912	-0.1583999
D 1.8924652D+01	0.3193997	-0.1150381
D 1.0328493D+01	0.1564874	0.1184096
D 5.5671676D+00	0.0307910	0.3799736
D 2.9537767D+00	0.0019152	0.4145429
D 1.5212792D+00	0.0001875	0.2106593
D 7.4548492D-01	0.0000241	0.0401805
D 3.6712920D-01	0.0000081	0.0028098

F	4F
BASIS/ORB. ENERGY	-0.4947225
F 3.7773288D+02	-0.0004760
F 1.3012154D+02	-0.0041005
F 5.6174664D+01	-0.0199197
F 2.6353745D+01	-0.0646210
F 1.2809689D+01	-0.1582991
F 6.2713685D+00	-0.2742172
F 2.9770012D+00	-0.3425427
F 1.3504876D+00	-0.3091745
F 5.6805858D-01	-0.1977897
F 2.1060250D-01	-0.0695974

EUROPIUM [XE]6S(2)5D(0)4F(7), 8S

CHARGE = 63.000000

SYMMETRY SPECIES	S	P	D	F
NUMBER OF BASIS FUNCTIONS	27	23	15	10
NUMBER OF CLOSED SHELLS	6	4	2	0

NUMBER OF OPEN SHELLS 0 0 0 1
OPEN SHELL OCCUPATION NUMBER 0 0 0 7

*** FINAL SCF RESULTS ***

E = -10840.673984354

ORBITAL ENERGIES AND EXPANSION COEFFICIENTS

	S	1S	2S	3S	4S	5S	6S
BASIS/ORB. ENERGY	-1792.0937000	-298.5877200	-67.4958360	-14.1966490	-2.0115439	-0.1801071	
S 4.1753920D+10	0.0000041	-0.0000015	0.0000007	0.0000003	0.0000001	0.0000000	
S 4.3317072D+09	0.0000156	-0.0000057	0.0000026	0.0000013	0.0000005	0.0000001	
S 7.2947825D+08	0.0000459	-0.0000166	0.0000077	0.0000037	0.0000014	0.0000004	
S 1.5829665D+08	0.0001184	-0.0000428	0.0000198	0.0000095	0.0000037	0.0000009	
S 3.9990152D+07	0.0002853	-0.0001031	0.0000478	0.0000228	0.0000089	0.0000023	
S 1.1163095D+07	0.0006449	-0.0002334	0.0001080	0.0000517	0.0000200	0.0000051	
S 3.4372229D+06	0.0013645	-0.0004941	0.0002288	0.0001094	0.0000424	0.0000109	
S 1.1363016D+06	0.0028508	-0.0010359	0.0004797	0.0002295	0.0000890	0.0000228	
S 3.9560522D+05	0.0057661	-0.0021015	0.0009747	0.0004660	0.0001807	0.0000462	
S 1.4645177D+05	0.0114135	-0.0042013	0.0019483	0.0009325	0.0003617	0.0000925	
S 5.6443635D+04	0.0229817	-0.0085358	0.0039741	0.0019008	0.0007368	0.0001886	
S 2.2455761D+04	0.0465071	-0.0177359	0.0082613	0.0039605	0.0015372	0.0003931	
S 9.1658731D+03	0.0952133	-0.0374517	0.0176190	0.0084404	0.0032721	0.0008381	
S 3.8161544D+03	0.1866076	-0.0795076	0.0376335	0.0181258	0.0070433	0.0018006	
S 1.6309487D+03	0.3094405	-0.1491650	0.0727952	0.0351134	0.0136305	0.0034936	
S 7.1913229D+02	0.3377736	-0.2116012	0.1064762	0.0522105	0.0203793	0.0052061	
S 3.2790922D+02	0.1613453	-0.0582072	0.0293569	0.0136128	0.0051898	0.0013532	
S 1.3955141D+02	0.0151237	0.4740948	-0.3801606	-0.2042072	-0.0811159	-0.0208902	
S 6.4324029D+01	-0.0009825	0.5852215	-0.6252697	-0.3748154	-0.1533344	-0.0393646	
S 2.5733026D+01	0.0003338	0.1119259	0.3830453	0.3507101	0.1580676	0.0408228	
S 1.3290671D+01	-0.0002307	-0.0189232	0.8658530	1.0276739	0.4898945	0.1297093	
S 5.1892966D+00	0.0001009	0.0065797	0.1291282	-0.5214607	-0.3624611	-0.1016817	
S 2.5674576D+00	-0.0000444	-0.0031089	-0.0172246	-0.9156653	-0.8118517	-0.2328808	
S 6.9145127D-01	0.0000144	0.0009556	0.0044194	-0.0649418	0.7183073	0.2566840	
S 3.1445469D-01	-0.0000074	-0.0004743	-0.0021735	0.0171968	0.6184480	0.4094119	
S 5.4105050D-02	0.0000019	0.0001252	0.0005467	-0.0036987	0.0189202	-0.7073835	
S 2.2436888D-02	-0.0000009	-0.0000597	-0.0002603	0.0017238	-0.0062212	-0.4740385	
P	2P	3P	4P	5P			

BASIS/ORB. ENERGY	-266.1317200	-57.1488620	-10.6906480	-1.0844358
P 5.2080119D+07	0.0000048	-0.0000024	-0.0000011	-0.0000004
P 7.4269735D+06	0.0000160	-0.0000078	-0.0000037	-0.0000013
P 1.5337467D+06	0.0000472	-0.0000232	-0.0000109	-0.0000038
P 3.9030835D+05	0.0001313	-0.0000645	-0.0000303	-0.0000105
P 1.1541793D+05	0.0003592	-0.0001769	-0.0000832	-0.0000288
P 3.8522264D+04	0.0009888	-0.0004883	-0.0002297	-0.0000795
P 1.4239528D+04	0.0027654	-0.0013711	-0.0006458	-0.0002240
P 5.7385665D+03	0.0078278	-0.0039086	-0.0018422	-0.0006378
P 2.4851756D+03	0.0219120	-0.0110626	-0.0052324	-0.0018170
P 1.1427122D+03	0.0579601	-0.0298761	-0.0141775	-0.0049131
P 5.5265847D+02	0.1349026	-0.0719165	-0.0344408	-0.0119955
P 2.7857730D+02	0.2527871	-0.1414753	-0.0683915	-0.0237649
P 1.4526948D+02	0.3385941	-0.1979346	-0.0971575	-0.0340944
P 7.7631138D+01	0.2683562	-0.1119130	-0.0466971	-0.0153572
P 4.1915706D+01	0.0975523	0.2012170	0.1432979	0.0527800
P 2.2844802D+01	0.0100997	0.5018404	0.3849173	0.1489894
P 1.2537810D+01	0.0007059	0.3611783	0.2298287	0.0770926
P 6.6693163D+00	-0.0003304	0.0801060	-0.3720436	-0.1849192
P 3.4870357D+00	0.0000590	0.0031071	-0.6106745	-0.3486783
P 1.7790295D+00	-0.0000688	0.0009306	-0.2449196	-0.0708456
P 8.2039295D-01	0.0000252	-0.0002236	-0.0195226	0.4680414
P 3.7091560D-01	-0.0000098	0.0000789	-0.0004597	0.5633384
P 1.5381136D-01	0.0000025	-0.0000187	0.0000701	0.1539485
D	3D	4D		
BASIS/ORB. ENERGY	-43.1218280	-5.6552646		
D 2.3454048D+04	0.0000268	-0.0000125		
D 5.3074341D+03	0.0002432	-0.0001144		
D 1.6819736D+03	0.0016648	-0.0007813		
D 6.4736034D+02	0.0088590	-0.0041981		
D 2.8282798D+02	0.0358349	-0.0170675		
D 1.3385854D+02	0.1092032	-0.0531051		
D 6.6865751D+01	0.2413546	-0.1179386		
D 3.4395987D+01	0.3615515	-0.1714348		
D 1.8106742D+01	0.3188445	-0.0974864		

D	9.5219755D+00	0.1292122	0.1930447
D	4.9157870D+00	0.0171401	0.4467922
D	2.4845815D+00	0.0009379	0.3844440
D	1.1876889D+00	0.0000417	0.1341823
D	4.4422386D-01	0.0000710	0.0123724
D	3.1169105D-01	-0.0000326	-0.0018503
	F	4F	
BASIS/ORB.ENERGY		-0.5314230	
F	3.8360428D+02	-0.0005192	
F	1.3179513D+02	-0.0045610	
F	5.6259741D+01	-0.0223727	
F	2.6332277D+01	-0.0706279	
F	1.2927491D+01	-0.1652979	
F	6.4360919D+00	-0.2727642	
F	3.1366325D+00	-0.3304033	
F	1.4670690D+00	-0.2993032	
F	6.3278294D-01	-0.1979628	
F	2.3742282D-01	-0.0736616	

GADOLINIUM [XE]6S(2)5D(1)4F(7), 9D

CHARGE = 64.000000

SYMMETRY SPECIES	S	P	D	F
NUMBER OF BASIS FUNCTIONS	27	23	15	10
NUMBER OF CLOSED SHELLS	6	4	2	0
NUMBER OF OPEN SHELLS	0	0	1	1
OPEN SHELL OCCUPATION NUMBER	0	0	1	7

*** FINAL SCF RESULTS ***

E = -11267.957204634

ORBITAL ENERGIES AND EXPANSION COEFFICIENTS

	S	1S	2S	3S	4S	5S	6S
BASIS/ORB.ENERGY		-1855.9611000	-310.8421000	-70.7613590	-15.0988510	-2.2301949	-0.1965770
S	3.7001721D+10	0.0000046	-0.0000017	0.0000008	0.0000004	0.0000001	0.0000000
S	4.4233374D+09	0.0000161	-0.0000059	0.0000027	0.0000013	0.0000005	0.0000001
S	7.3662746D+08	0.0000495	-0.0000180	0.0000083	0.0000040	0.0000016	0.0000004
S	1.5746694D+08	0.0001272	-0.0000462	0.0000214	0.0000103	0.0000041	0.0000011

S	3.9988049D+07	0.0003000	-0.0001089	0.0000506	0.0000243	0.0000096	0.0000026
S	1.1295642D+07	0.0006791	-0.0002467	0.0001145	0.0000550	0.0000218	0.0000058
S	3.4429112D+06	0.0014594	-0.0005307	0.0002465	0.0001184	0.0000469	0.0000126
S	1.1344016D+06	0.0030016	-0.0010953	0.0005086	0.0002444	0.0000968	0.0000260
S	3.9695784D+05	0.0060606	-0.0022190	0.0010320	0.0004957	0.0001962	0.0000527
S	1.4656447D+05	0.0120161	-0.0044427	0.0020659	0.0009934	0.0003934	0.0001056
S	5.6594524D+04	0.0239351	-0.0089369	0.0041730	0.0020052	0.0007936	0.0002132
S	2.2562053D+04	0.0483639	-0.0185379	0.0086589	0.0041711	0.0016530	0.0004437
S	9.2067332D+03	0.0984656	-0.0390025	0.0184088	0.0088595	0.0035067	0.0009423
S	3.8301031D+03	0.1921732	-0.0824893	0.0391705	0.0189614	0.0075239	0.0020196
S	1.6305186D+03	0.3155921	-0.1540936	0.0755481	0.0366152	0.0145113	0.0039013
S	7.1619740D+02	0.3347743	-0.2119078	0.1070520	0.0528137	0.0210620	0.0056531
S	3.2513703D+02	0.1496201	-0.0407384	0.0193612	0.0084589	0.0032009	0.0008725
S	1.4113836D+02	0.0116850	0.4898508	-0.3988308	-0.2157145	-0.0875186	-0.0236261
S	6.5402596D+01	-0.0000949	0.5686166	-0.6114755	-0.3708007	-0.1553609	-0.0419667
S	2.6424389D+01	-0.0001757	0.1042905	0.4157609	0.3863907	0.1788164	0.0488376
S	1.3671169D+01	0.0000979	-0.0171813	0.8457283	1.0128530	0.4942229	0.1372001
S	5.3756862D+00	-0.0000557	0.0060202	0.1246899	-0.5501639	-0.3898483	-0.1141988
S	2.6791504D+00	0.0000337	-0.0029289	-0.0173078	-0.8963124	-0.8317035	-0.2551241
S	7.6814741D-01	-0.0000117	0.0009390	0.0046309	-0.0641435	0.7073324	0.2783621
S	3.5394983D-01	0.0000056	-0.0004545	-0.0022252	0.0153750	0.6501453	0.4263774
S	6.2875056D-02	-0.0000015	0.0001154	0.0005362	-0.0031197	0.0222235	-0.7087876
S	2.5554319D-02	0.0000007	-0.0000534	-0.0002478	0.0014043	-0.0069671	-0.4814360
	P	2P	3P	4P	5P		
BASIS/ORB. ENERGY	-276.7643900	-59.9490560	-11.4286420	-1.2378127			
P	5.2152768D+07	0.0000052	-0.0000025	-0.0000012	-0.0000004		
P	7.4402182D+06	0.0000172	-0.0000084	-0.0000040	-0.0000014		
P	1.5354844D+06	0.0000506	-0.0000249	-0.0000118	-0.0000042		
P	3.9055957D+05	0.0001406	-0.0000694	-0.0000328	-0.0000117		
P	1.1546969D+05	0.0003842	-0.0001899	-0.0000898	-0.0000321		
P	3.8541383D+04	0.0010556	-0.0005233	-0.0002476	-0.0000883		
P	1.4246672D+04	0.0029458	-0.0014664	-0.0006948	-0.0002482		
P	5.7402012D+03	0.0083179	-0.0041708	-0.0019781	-0.0007056		
P	2.4852794D+03	0.0231966	-0.0117648	-0.0055980	-0.0020028		
P	1.1427899D+03	0.0610067	-0.0316112	-0.0150996	-0.0053916		

P	5.5263076D+02	0.1408306	-0.0755261	-0.0364002	-0.0130640
P	2.7851980D+02	0.2600872	-0.1465478	-0.0713609	-0.0255540
P	1.4530926D+02	0.3399721	-0.1992790	-0.0983367	-0.0355625
P	7.7642981D+01	0.2596932	-0.0993257	-0.0395192	-0.0131030
P	4.1886077D+01	0.0888164	0.2263958	0.1618147	0.0615723
P	2.2880971D+01	0.0082179	0.5085319	0.3964945	0.1587494
P	1.2554862D+01	0.0006463	0.3397977	0.1975921	0.0644179
P	6.6694959D+00	-0.0003349	0.0689867	-0.4144230	-0.2123694
P	3.4809842D+00	0.0000609	0.0024465	-0.6025136	-0.3649169
P	1.7661486D+00	-0.0000638	0.0007456	-0.2123690	-0.0238145
P	8.1730209D-01	0.0000247	-0.0001932	-0.0133856	0.5316629
P	3.7081054D-01	-0.0000093	0.0000613	-0.0006675	0.5256148
P	1.5135526D-01	0.0000024	-0.0000149	0.0001570	0.1105104

	D	3D	4D	5D
BASIS/ORB. ENERGY		-45.4554350	-6.1909376	-0.2443993
D	1.9762544D+04	0.0000355	-0.0000167	0.0000039
D	4.9529396D+03	0.0002846	-0.0001356	0.0000321
D	1.6932815D+03	0.0016253	-0.0007692	0.0001807
D	6.9838712D+02	0.0079708	-0.0038253	0.0009064
D	3.0548376D+02	0.0344507	-0.0165596	0.0039034
D	1.4053492D+02	0.1127529	-0.0554877	0.0131862
D	6.7860905D+01	0.2603625	-0.1284788	0.0303813
D	3.3708372D+01	0.3885084	-0.1850682	0.0439162
D	1.7123250D+01	0.3112253	-0.0678112	0.0115457
D	8.6140811D+00	0.0990965	0.2888452	-0.0826972
D	4.1984878D+00	0.0074803	0.5113711	-0.1463889
D	1.9508518D+00	0.0005797	0.3116912	-0.0331038
D	7.8058449D-01	-0.0000554	0.0472700	0.2990590
D	2.8167361D-01	0.0000528	-0.0013306	0.5426581
D	9.0559037D-02	-0.0000016	0.0006641	0.3791899

	F	4F
BASIS/ORB. ENERGY		-0.8354171
F	3.8357372D+02	-0.0006113
F	1.3168830D+02	-0.0053383
F	5.6216693D+01	-0.0258038

F	2.6307294D+01	-0.0801640
F	1.2948024D+01	-0.1825816
F	6.4445078D+00	-0.2926782
F	3.1334851D+00	-0.3405758
F	1.4695379D+00	-0.2809911
F	6.5277113D-01	-0.1574307
F	2.6165607D-01	-0.0456485

TERBIUM [XE]6S(2)5D(0)4F(9), 6H

CHARGE = 65.000000

SYMMETRY SPECIES	S	P	D	F
NUMBER OF BASIS FUNCTIONS	27	23	15	10
NUMBER OF CLOSED SHELLS	6	4	2	0
NUMBER OF OPEN SHELLS	0	0	0	1
OPEN SHELL OCCUPATION NUMBER	0	0	0	9

*** FINAL SCF RESULTS ***

E = -11705.457488201

ORBITAL ENERGIES AND EXPANSION COEFFICIENTS

	S	1S	2S	3S	4S	5S	6S
BASIS/ORB. ENERGY		-1920.6679000	-322.8458300	-73.4852100	-15.4232950	-2.1340722	-0.1848542
S 4.9360640D+10	0.0000040	-0.0000015	0.0000007	0.0000003	0.0000001	0.0000000	0.0000000
S 5.9264583D+09	0.0000138	-0.0000050	0.0000023	0.0000011	0.0000004	0.0000001	0.0000001
S 1.0081574D+09	0.0000430	-0.0000157	0.0000073	0.0000035	0.0000014	0.0000003	0.0000003
S 2.0493014D+08	0.0001171	-0.0000427	0.0000199	0.0000096	0.0000037	0.0000009	0.0000009
S 4.9630464D+07	0.0002836	-0.0001034	0.0000481	0.0000231	0.0000089	0.0000022	0.0000022
S 1.3544932D+07	0.0006467	-0.0002360	0.0001098	0.0000528	0.0000204	0.0000051	0.0000051
S 4.0559339D+06	0.0014029	-0.0005122	0.0002385	0.0001146	0.0000443	0.0000111	0.0000111
S 1.2986886D+06	0.0029710	-0.0010886	0.0005068	0.0002437	0.0000941	0.0000236	0.0000236
S 4.3927233D+05	0.0061276	-0.0022520	0.0010501	0.0005047	0.0001949	0.0000489	0.0000489
S 1.5724531D+05	0.0123258	-0.0045766	0.0021341	0.0010267	0.0003967	0.0000995	0.0000995
S 5.9168630D+04	0.0248437	-0.0093129	0.0043595	0.0020959	0.0008092	0.0002032	0.0002032
S 2.3125261D+04	0.0501374	-0.0193266	0.0090543	0.0043643	0.0016872	0.0004230	0.0004230
S 9.4396358D+03	0.0985156	-0.0391785	0.0185454	0.0089282	0.0034475	0.0008660	0.0008660
S 4.0214097D+03	0.1842781	-0.0795162	0.0378508	0.0183403	0.0070997	0.0017793	0.0017793
S 1.7590605D+03	0.3009742	-0.1456963	0.0715315	0.0346552	0.0133976	0.0033684	0.0033684

S	7.8687046D+02	0.3326395	-0.2081368	0.1050819	0.0518581	0.0201656	0.0050492
S	3.6147966D+02	0.1678883	-0.0628193	0.0317846	0.0147259	0.0055946	0.0014318
S	1.5176439D+02	0.0176505	0.4683488	-0.3783461	-0.2042459	-0.0808322	-0.0204198
S	6.9825610D+01	-0.0016540	0.5897696	-0.6305982	-0.3813188	-0.1554691	-0.0391189
S	2.7831612D+01	0.0007076	0.1138665	0.3869765	0.3649075	0.1644008	0.0415959
S	1.4399732D+01	-0.0004654	-0.0196199	0.8663487	1.0246950	0.4864943	0.1263374
S	5.5394069D+00	0.0002117	0.0068086	0.1268219	-0.5652986	-0.3939456	-0.1084172
S	2.7507356D+00	-0.0001017	-0.0032981	-0.0187478	-0.8798589	-0.7825348	-0.2193676
S	7.6206539D-01	0.0000333	0.0010235	0.0048194	-0.0595204	0.7082261	0.2432701
S	3.4217580D-01	-0.0000165	-0.0004933	-0.0022911	0.0144366	0.6307656	0.4073649
S	5.7736431D-02	0.0000043	0.0001302	0.0005776	-0.0030844	0.0204093	-0.6751971
S	2.4079136D-02	-0.0000021	-0.0000628	-0.0002780	0.0014512	-0.0068895	-0.4998414

	P	2P	3P	4P	5P
BASIS/ORB. ENERGY		-287.0728100	-62.1902760	-11.6018710	-1.1364290
P	5.2333798D+07	0.0000055	-0.0000027	-0.0000013	-0.0000004
P	7.4572061D+06	0.0000184	-0.0000091	-0.0000043	-0.0000015
P	1.5378049D+06	0.0000542	-0.0000268	-0.0000127	-0.0000044
P	3.9072744D+05	0.0001506	-0.0000746	-0.0000353	-0.0000121
P	1.1548108D+05	0.0004108	-0.0002038	-0.0000964	-0.0000331
P	3.8572565D+04	0.0011248	-0.0005598	-0.0002649	-0.0000910
P	1.4259328D+04	0.0031366	-0.0015676	-0.0007429	-0.0002555
P	5.7400579D+03	0.0088358	-0.0044491	-0.0021110	-0.0007252
P	2.4856897D+03	0.0245159	-0.0124916	-0.0059461	-0.0020474
P	1.1429397D+03	0.0641863	-0.0334332	-0.0159818	-0.0054962
P	5.5253907D+02	0.1468276	-0.0792204	-0.0382091	-0.0131968
P	2.7847833D+02	0.2673206	-0.1516324	-0.0739376	-0.0255072
P	1.4529343D+02	0.3409243	-0.2002323	-0.0987553	-0.0343398
P	7.7649292D+01	0.2504246	-0.0854354	-0.0312161	-0.0097127
P	4.1847251D+01	0.0806830	0.2516301	0.1797902	0.0660839
P	2.2928841D+01	0.0064708	0.5114642	0.4023571	0.1546915
P	1.2598230D+01	0.0006977	0.3184566	0.1622269	0.0472383
P	6.6886655D+00	-0.0003851	0.0598318	-0.4445489	-0.2189631
P	3.4919036D+00	0.0000943	0.0020122	-0.5839877	-0.3377214
P	1.7678640D+00	-0.0000758	0.0006850	-0.1943769	-0.0063830
P	8.1982907D-01	0.0000300	-0.0001595	-0.0119939	0.5019262

P	3.7009424D-01	-0.0000116	0.0000555	-0.0007748	0.5280509
P	1.5285821D-01	0.0000030	-0.0000123	0.0001584	0.1277469
	D	3D	4D		
BASIS/ORB. ENERGY		-47.2282840	-6.1980316		
D	1.5348021D+04	0.0000587	-0.0000278		
D	3.9866409D+03	0.0004319	-0.0002054		
D	1.4205545D+03	0.0024368	-0.0011582		
D	5.9617142D+02	0.0110383	-0.0052954		
D	2.7748593D+02	0.0394451	-0.0190360		
D	1.3768273D+02	0.1109682	-0.0546564		
D	7.1297139D+01	0.2339778	-0.1156940		
D	3.7819030D+01	0.3453933	-0.1658183		
D	2.0482492D+01	0.3132005	-0.1037259		
D	1.1127340D+01	0.1406559	0.1527661		
D	5.9959803D+00	0.0244629	0.3963308		
D	3.2176917D+00	0.0016877	0.3877541		
D	1.7116602D+00	0.0001795	0.1875391		
D	8.7911028D-01	0.0000762	0.0416875		
D	3.7772273D-01	0.0000081	0.0030354		
	F	4F			
BASIS/ORB. ENERGY		-0.5060820			
F	3.8285976D+02	-0.0006623			
F	1.3139572D+02	-0.0057397			
F	5.6151133D+01	-0.0272461			
F	2.6289163D+01	-0.0833867			
F	1.2954128D+01	-0.1846146			
F	6.4572824D+00	-0.2851809			
F	3.1444537D+00	-0.3274630			
F	1.4609985D+00	-0.2829040			
F	6.2713883D-01	-0.1810361			
F	2.3443126D-01	-0.0678210			

DYSPROSIUM [XE]6S(2)5D(0)4F(10), 51

CHARGE = 66.000000

SYMMETRY SPECIES

S P D F

NUMBER OF BASIS FUNCTIONS	27	23	15	10
NUMBER OF CLOSED SHELLS	6	4	2	0
NUMBER OF OPEN SHELLS	0	0	0	1
OPEN SHELL OCCUPATION NUMBER	0	0	0	10

*** FINAL SCF RESULTS ***

E = -12153.820544143

ORBITAL ENERGIES AND EXPANSION COEFFICIENTS

	S	1S	2S	3S	4S	5S	6S
BASIS/ORB. ENERGY	-1986.9660000	-335.4072500	-76.5759490	-16.0461510	-2.1935972	-0.1871304	
S 6.7214502D+10	0.0000037	-0.0000014	0.0000006	0.0000003	-0.0000001	0.0000000	
S 6.0775684D+09	0.0000160	-0.0000059	0.0000027	0.0000013	-0.0000005	0.0000001	
S 9.4489080D+08	0.0000470	-0.0000172	0.0000080	0.0000039	-0.0000015	0.0000004	
S 2.0829563D+08	0.0001185	-0.0000434	0.0000202	0.0000098	-0.0000038	0.0000009	
S 5.1192202D+07	0.0002976	-0.0001090	0.0000509	0.0000245	-0.0000094	0.0000023	
S 1.3811530D+07	0.0006823	-0.0002500	0.0001167	0.0000562	-0.0000216	0.0000054	
S 4.1137560D+06	0.0014717	-0.0005397	0.0002519	0.0001213	-0.0000467	0.0000116	
S 1.3171498D+06	0.0031126	-0.0011454	0.0005346	0.0002576	-0.0000992	0.0000247	
S 4.4333668D+05	0.0064505	-0.0023816	0.0011133	0.0005362	-0.0002065	0.0000513	
S 1.5787993D+05	0.0129536	-0.0048317	0.0022589	0.0010891	-0.0004197	0.0001043	
S 5.9337899D+04	0.0259214	-0.0097678	0.0045847	0.0022092	-0.0008508	0.0002115	
S 2.3240251D+04	0.0519544	-0.0201344	0.0094587	0.0045692	-0.0017620	0.0004375	
S 9.4869961D+03	0.1019354	-0.0408154	0.0193775	0.0093517	-0.0036021	0.0008961	
S 4.0345400D+03	0.1891457	-0.0822551	0.0392815	0.0190765	-0.0073665	0.0018285	
S 1.7670468D+03	0.3037182	-0.1486020	0.0732513	0.0355854	-0.0137237	0.0034169	
S 7.9234108D+02	0.3284352	-0.2072382	0.1049935	0.0519472	-0.0201532	0.0049980	
S 3.6508060D+02	0.1598558	-0.0513801	0.0251679	0.0113852	-0.0042727	0.0010876	
S 1.5518941D+02	0.0159808	0.4760230	-0.3884458	-0.2107363	0.0832385	-0.0208188	
S 7.1730390D+01	-0.0013077	0.5805977	-0.6231160	-0.3785023	0.1540491	-0.0384017	
S 2.8704884D+01	0.0005249	0.1106779	0.4061107	0.3847647	-0.1730875	0.0434433	
S 1.4882839D+01	-0.0003533	-0.0193743	0.8529325	1.0178471	-0.4826114	0.1240075	
S 5.8379975D+00	0.0001589	0.0067149	0.1234142	-0.5686331	0.3933431	-0.1067267	
S 2.8749545D+00	-0.0000730	-0.0031595	-0.0162689	-0.8843970	0.7838174	-0.2178478	
S 7.9567065D-01	0.0000236	0.0009681	0.0041655	-0.0594427	-0.7039295	0.2396972	
S 3.5452398D-01	-0.0000115	-0.0004591	-0.0019502	0.0141410	-0.6342414	0.4015254	
S 5.7593463D-02	0.0000030	0.0001187	0.0004795	-0.0029636	-0.0197774	-0.7032714	

S	2.3811901D-02	-0.0000014	-0.0000576	-0.0002323	0.0014050	0.0067771	-0.4678142
P		2P	3P	4P	5P		
BASIS/ORB. ENERGY	-297.8516800	-64.7756750	-12.0588220	-1.1602894			
P 5.2440248D+07	0.0000059	-0.0000029	-0.0000014	-0.0000005			
P 7.4695536D+06	0.0000197	-0.0000098	-0.0000046	-0.0000016			
P 1.5413073D+06	0.0000581	-0.0000288	-0.0000137	-0.0000047			
P 3.9039757D+05	0.0001616	-0.0000803	-0.0000381	-0.0000130			
P 1.1542459D+05	0.0004378	-0.0002180	-0.0001034	-0.0000353			
P 3.8636406D+04	0.0011981	-0.0005984	-0.0002840	-0.0000971			
P 1.4258544D+04	0.0033409	-0.0016761	-0.0007964	-0.0002725			
P 5.7411601D+03	0.0093635	-0.0047338	-0.0022526	-0.0007702			
P 2.4860723D+03	0.0259118	-0.0132618	-0.0063298	-0.0021686			
P 1.1429163D+03	0.0674208	-0.0352962	-0.0169269	-0.0057947			
P 5.5253606D+02	0.1529148	-0.0829875	-0.0401474	-0.0137967			
P 2.7840180D+02	0.2743507	-0.1566247	-0.0766725	-0.0263374			
P 1.4532206D+02	0.3410209	-0.2004061	-0.0989523	-0.0342124			
P 7.7666359D+01	0.2412003	-0.0709554	-0.0226336	-0.0066355			
P 4.1830357D+01	0.0729347	0.2765458	0.1986101	0.0729056			
P 2.2958915D+01	0.0052251	0.5132365	0.4075870	0.1558482			
P 1.2605134D+01	0.0005948	0.2969597	0.1253231	0.0312074			
P 6.6942933D+00	-0.0003454	0.0508782	-0.4762067	-0.2339355			
P 3.4934723D+00	0.0000761	0.0018726	-0.5659299	-0.3281773			
P 1.7632603D+00	-0.0000625	0.0004890	-0.1727190	0.0237566			
P 8.1966381D-01	0.0000249	-0.0000917	-0.0094724	0.5136367			
P 3.6998079D-01	-0.0000095	0.0000297	-0.0008174	0.5111671			
P 1.5250069D-01	0.0000024	-0.0000056	0.0001723	0.1173626			
D	3D	4D					
BASIS/ORB. ENERGY	-49.3277210	-6.4659827					
D 1.5533206D+04	0.0000627	-0.0000298					
D 4.0077213D+03	0.0004672	-0.0002231					
D 1.4191338D+03	0.0026462	-0.0012641					
D 5.9580893D+02	0.0118573	-0.0057174					
D 2.7757910D+02	0.0420930	-0.0204276					
D 1.3768029D+02	0.1172672	-0.0581054					
D 7.1305743D+01	0.2430142	-0.1206894					

D	3.7813342D+01	0.3506929	-0.1683102
D	2.0476260D+01	0.3042615	-0.0919112
D	1.1125700D+01	0.1287468	0.1758390
D	5.9868311D+00	0.0208335	0.4062141
D	3.2165010D+00	0.0013987	0.3746692
D	1.7146562D+00	0.0001994	0.1727857
D	8.8136054D-01	0.0000704	0.0367126
D	3.7694426D-01	0.0000108	0.0026439
	F	4F	
BASIS/ORB.ENERGY		-0.5074471	
F	3.8249412D+02	0.0007445	
F	1.3123976D+02	0.0064024	
F	5.6119260D+01	0.0298917	
F	2.6280782D+01	0.0901251	
F	1.2964015D+01	0.1942171	
F	6.4603455D+00	0.2908969	
F	3.1471031D+00	0.3245215	
F	1.4636831D+00	0.2738744	
F	6.2963362D-01	0.1729950	
F	2.3567072D-01	0.0645683	

HOLMIUM [XE]6S(2)5D(0)4F(11), 4I

CHARGE = 67.000000

SYMMETRY SPECIES	S	P	D	F
NUMBER OF BASIS FUNCTIONS	27	23	15	10
NUMBER OF CLOSED SHELLS	6	4	2	0
NUMBER OF OPEN SHELLS	0	0	0	1
OPEN SHELL OCCUPATION NUMBER	0	0	0	11

*** FINAL SCF RESULTS ***

E = -12612.972427060

ORBITAL ENERGIES AND EXPANSION COEFFICIENTS

	S	1S	2S	3S	4S	5S	6S
BASIS/ORB.ENERGY		-2054.6366000	-348.2719500	-79.7413760	-16.6828740	-2.2540362	-0.1893934
S	5.7876523D+10	0.0000042	-0.0000016	0.0000007	0.0000004	-0.0000001	0.0000000
S	6.2850111D+09	0.0000156	-0.0000057	0.0000027	0.0000013	-0.0000005	0.0000001

S	1.0452967D+09	0.0000484	-0.0000178	0.0000083	0.0000040	-0.0000015	0.0000004
S	2.0945137D+08	0.0001307	-0.0000481	0.0000225	0.0000109	-0.0000042	0.0000010
S	5.1656671D+07	0.0003079	-0.0001132	0.0000530	0.0000256	-0.0000098	0.0000024
S	1.4119209D+07	0.0007161	-0.0002636	0.0001233	0.0000595	-0.0000229	0.0000056
S	4.1524601D+06	0.0015629	-0.0005756	0.0002694	0.0001300	-0.0000500	0.0000123
S	1.3247094D+06	0.0032638	-0.0012062	0.0005644	0.0002725	-0.0001047	0.0000258
S	4.4802274D+05	0.0067179	-0.0024916	0.0011676	0.0005636	-0.0002166	0.0000534
S	1.5920876D+05	0.0136274	-0.0051060	0.0023932	0.0011563	-0.0004445	0.0001095
S	5.9306917D+04	0.0272895	-0.0103389	0.0048653	0.0023493	-0.0009027	0.0002225
S	2.3231077D+04	0.0539260	-0.0210136	0.0098982	0.0047921	-0.0018432	0.0004537
S	9.5046756D+03	0.1055152	-0.0425508	0.0202609	0.0097984	-0.0037657	0.0009286
S	4.0333879D+03	0.1947974	-0.0853985	0.0409126	0.0199177	-0.0076710	0.0018875
S	1.7684847D+03	0.3060004	-0.1514631	0.0749747	0.0364994	-0.0140474	0.0034674
S	7.9758700D+02	0.3222616	-0.2048867	0.1041130	0.0516858	-0.0199942	0.0049144
S	3.6973108D+02	0.1525314	-0.0409419	0.0190781	0.0081801	-0.0030373	0.0007756
S	1.5906501D+02	0.0147026	0.4817908	-0.3967413	-0.2159370	0.0851945	-0.0211263
S	7.3772579D+01	-0.0010384	0.5731163	-0.6171510	-0.3770550	0.1530284	-0.0378073
S	2.9699605D+01	0.0003784	0.1073688	0.4207132	0.4024672	-0.1802574	0.0448465
S	1.5394413D+01	-0.0002581	-0.0183134	0.8448999	1.0098767	-0.4789566	0.1220047
S	6.0531880D+00	0.0001141	0.0062747	0.1204644	-0.5871213	0.4078294	-0.1095879
S	2.9751088D+00	-0.0000507	-0.0029294	-0.0157196	-0.8722503	0.7682296	-0.2114658
S	8.1915905D-01	0.0000163	0.0008926	0.0040245	-0.0573757	-0.7158837	0.2414019
S	3.6381960D-01	-0.0000080	-0.0004246	-0.0018923	0.0137638	-0.6204867	0.3940769
S	5.9858954D-02	0.0000021	0.0001111	0.0004714	-0.0029267	-0.0195080	-0.6840715
S	2.4686956D-02	-0.0000010	-0.0000536	-0.0002273	0.0013804	0.0066372	-0.4863544
	P	2P	3P	4P	5P		
BASIS/ORB. ENERGY	-308.8457000	-67.4134770	-12.5234220	-1.1840603			
P	5.1644258D+07	0.0000064	-0.0000032	-0.0000015	-0.0000005		
P	7.5767609D+06	0.0000208	-0.0000104	-0.0000049	-0.0000017		
P	1.5408846D+06	0.0000629	-0.0000313	-0.0000149	-0.0000051		
P	3.8872284D+05	0.0001725	-0.0000860	-0.0000409	-0.0000139		
P	1.1573723D+05	0.0004660	-0.0002328	-0.0001107	-0.0000377		
P	3.8629098D+04	0.0012787	-0.0006409	-0.0003050	-0.0001038		
P	1.4264854D+04	0.0035481	-0.0017866	-0.0008509	-0.0002898		
P	5.7410463D+03	0.0099272	-0.0050386	-0.0024043	-0.0008183		

P	2.4864297D+03	0.0273422	-0.0140547	-0.0067251	-0.0022929
P	1.1429128D+03	0.0707748	-0.0372379	-0.0179139	-0.0061055
P	5.5252518D+02	0.1590095	-0.0867862	-0.0421026	-0.0143987
P	2.7835243D+02	0.2812814	-0.1615961	-0.0794126	-0.0271648
P	1.4529153D+02	0.3407032	-0.2000346	-0.0987898	-0.0339650
P	7.7670045D+01	0.2314608	-0.0555256	-0.0134642	-0.0033743
P	4.1832990D+01	0.0658069	0.3009231	0.2176881	0.0797990
P	2.2974308D+01	0.0041755	0.5137356	0.4106412	0.1561061
P	1.2583574D+01	0.0005246	0.2751725	0.0864368	0.0143652
P	6.7000124D+00	-0.0003259	0.0425051	-0.5035943	-0.2467821
P	3.4996619D+00	0.0000709	0.0019844	-0.5453964	-0.3171310
P	1.7641719D+00	-0.0000561	0.0002445	-0.1541211	0.0523166
P	8.1892405D-01	0.0000226	-0.0000009	-0.0076890	0.5243444
P	3.6975839D-01	-0.0000086	-0.0000046	-0.0007738	0.4931037
P	1.5265564D-01	0.0000022	0.0000033	0.0001664	0.1083447
	D	3D	4D		
BASIS/ORB. ENERGY		-51.4664570	-6.7375325		
D	1.6015423D+04	0.0000664	-0.0000317		
D	4.0094325D+03	0.0005105	-0.0002450		
D	1.4167510D+03	0.0028563	-0.0013707		
D	5.9601133D+02	0.0127213	-0.0061649		
D	2.7754372D+02	0.0448925	-0.0218981		
D	1.3769700D+02	0.1236117	-0.0616097		
D	7.1309138D+01	0.2521384	-0.1256772		
D	3.7808077D+01	0.3548863	-0.1701714		
D	2.0478399D+01	0.2948463	-0.0787252		
D	1.1112848D+01	0.1177077	0.1980555		
D	5.9822558D+00	0.0174400	0.4134097		
D	3.2156846D+00	0.0013427	0.3622880		
D	1.7131879D+00	0.0001349	0.1587317		
D	8.8302399D-01	0.0000951	0.0320142		
D	3.7752870D-01	0.0000062	0.0023764		
	F	4F			
BASIS/ORB. ENERGY		-0.5060055			
F	3.8182905D+02	0.0008353			

F	1.3100528D+02	0.0071226
F	5.6068719D+01	0.0326710
F	2.6275594D+01	0.0969716
F	1.2975211D+01	0.2033995
F	6.4614937D+00	0.2959872
F	3.1490364D+00	0.3205140
F	1.4679062D+00	0.2652930
F	6.3169612D-01	0.1659881
F	2.3710188D-01	0.0617090

ERBIUM [XE]6S(2)5D(0)4F(12), 3H

CHARGE = 68.000000

SYMMETRY SPECIES	S	P	D	F
NUMBER OF BASIS FUNCTIONS	27	23	15	10
NUMBER OF CLOSED SHELLS	6	4	2	0
NUMBER OF OPEN SHELLS	0	0	0	1
OPEN SHELL OCCUPATION NUMBER	0	0	0	12

*** FINAL SCF RESULTS ***

E = -13083.063992565

ORBITAL ENERGIES AND EXPANSION COEFFICIENTS

	S	1S	2S	3S	4S	5S	6S
BASIS/ORB. ENERGY	-2123.6997000	-361.4461700	-82.9836990	-17.3343580	-2.3157311	-0.1916624	
S 6.8154237D+10	0.0000042	-0.0000016	0.0000007	0.0000004	0.0000001	0.0000000	
S 6.4947250D+09	0.0000170	-0.0000063	0.0000029	0.0000014	0.0000005	-0.0000001	
S 1.0534344D+09	0.0000504	-0.0000186	0.0000087	0.0000042	0.0000016	-0.0000004	
S 2.1973865D+08	0.0001344	-0.0000497	0.0000233	0.0000113	0.0000043	-0.0000011	
S 5.2529925D+07	0.0003335	-0.0001232	0.0000578	0.0000279	0.0000107	-0.0000026	
S 1.4149958D+07	0.0007491	-0.0002769	0.0001298	0.0000628	0.0000241	-0.0000059	
S 4.2523312D+06	0.0016122	-0.0005965	0.0002798	0.0001353	0.0000519	-0.0000127	
S 1.3455095D+06	0.0034633	-0.0012855	0.0006030	0.0002917	0.0001118	-0.0000273	
S 4.4930791D+05	0.0070847	-0.0026401	0.0012401	0.0005998	0.0002299	-0.0000562	
S 1.5971536D+05	0.0142495	-0.0053634	0.0025201	0.0012200	0.0004679	-0.0001142	
S 5.9453997D+04	0.0285330	-0.0108697	0.0051274	0.0024809	0.0009511	-0.0002324	
S 2.3261386D+04	0.0561435	-0.0219924	0.0103880	0.0050390	0.0019338	-0.0004719	
S 9.5019423D+03	0.1095486	-0.0445163	0.0212524	0.0103005	0.0039500	-0.0009657	

S	4.0261089D+03	0.2001442	-0.0884286	0.0425128	0.0207392	0.0079700	-0.0019440
S	1.7690924D+03	0.3084454	-0.1546073	0.0768014	0.0374826	0.0143946	-0.0035228
S	7.9938698D+02	0.3179871	-0.2032029	0.1036785	0.0515908	0.0199170	-0.0048517
S	3.7018641D+02	0.1436534	-0.0281198	0.0111734	0.0041050	0.0014391	-0.0003813
S	1.6256866D+02	0.0123298	0.4875147	-0.4045939	-0.2211658	-0.0871009	0.0214185
S	7.5868112D+01	-0.0003620	0.5632612	-0.6105031	-0.3745905	-0.1518050	0.0371684
S	3.0977104D+01	-0.0000012	0.1048627	0.4246129	0.4067450	0.1818342	-0.0448250
S	1.6025216D+01	-0.0000153	-0.0168342	0.8438360	1.0136999	0.4798209	-0.1211626
S	6.3763779D+00	0.0000003	0.0057449	0.1207507	-0.5793040	-0.4004875	0.1065849
S	3.1168067D+00	0.0000048	-0.0026304	-0.0145291	-0.8826374	-0.7728867	0.2105502
S	8.5401130D-01	-0.0000016	0.0007925	0.0037204	-0.0585254	0.7074681	-0.2350443
S	3.7820352D-01	0.0000007	-0.0003746	-0.0017400	0.0140581	0.6261364	-0.3922633
S	6.0993770D-02	-0.0000002	0.0000967	0.0004267	-0.0029536	0.0199598	0.6869902
S	2.4968154D-02	0.0000001	-0.0000467	-0.0002059	0.0013961	-0.0068776	0.4808710
	P	2P	3P	4P	5P		
BASIS/ORB. ENERGY	-320.0568100	-70.1047490	-12.9962550	-1.2080184			
P	5.3962859D+07	0.0000067	-0.0000033	-0.0000016	-0.0000005		
P	7.6891130D+06	0.0000221	-0.0000110	-0.0000053	-0.0000018		
P	1.5832796D+06	0.0000651	-0.0000325	-0.0000155	-0.0000052		
P	4.0139694D+05	0.0001802	-0.0000901	-0.0000429	-0.0000145		
P	1.1818708D+05	0.0004912	-0.0002462	-0.0001173	-0.0000397		
P	3.9214589D+04	0.0013461	-0.0006769	-0.0003229	-0.0001094		
P	1.4420880D+04	0.0037322	-0.0018862	-0.0009004	-0.0003052		
P	5.7870444D+03	0.0104519	-0.0053244	-0.0025472	-0.0008633		
P	2.4958116D+03	0.0288246	-0.0148805	-0.0071370	-0.0024216		
P	1.1438780D+03	0.0743722	-0.0393158	-0.0189696	-0.0064394		
P	5.5176959D+02	0.1657926	-0.0910196	-0.0442751	-0.0150675		
P	2.7774049D+02	0.2883023	-0.1666170	-0.0821868	-0.0280132		
P	1.4504343D+02	0.3393552	-0.1988608	-0.0981555	-0.0335323		
P	7.7627461D+01	0.2210165	-0.0385445	-0.0033078	0.0001467		
P	4.1891579D+01	0.0591420	0.3209595	0.2341795	0.0858422		
P	2.3200157D+01	0.0033863	0.5040627	0.4041579	0.1525431		
P	1.2837524D+01	0.0005091	0.2593131	0.0675833	0.0070336		
P	6.9988955D+00	-0.0003203	0.0403694	-0.4848500	-0.2367397		
P	3.7391982D+00	0.0000682	0.0026655	-0.5388181	-0.3089572		

P	1.9277859D+00	-0.0000544	0.0000942	-0.1717702	0.0156170
P	9.1250304D-01	0.0000206	0.0000784	-0.0107877	0.4843262
P	4.1494170D-01	-0.0000075	-0.0000327	-0.0008427	0.5249274
P	1.7231357D-01	0.0000019	0.0000104	0.0001530	0.1396918
	D	3D	4D		
BASIS/ORB. ENERGY		-53.6450410	-7.0130821		
D	1.6417391D+04	0.0000674	-0.0000323		
D	4.2431585D+03	0.0004913	-0.0002367		
D	1.5042434D+03	0.0027678	-0.0013340		
D	6.2451900D+02	0.0127807	-0.0062176		
D	2.8525007D+02	0.0468925	-0.0229863		
D	1.3883011D+02	0.1320444	-0.0661203		
D	7.0914605D+01	0.2660362	-0.1331397		
D	3.7410418D+01	0.3600377	-0.1715940		
D	2.0252880D+01	0.2818003	-0.0611840		
D	1.0984365D+01	0.1046809	0.2268499		
D	5.8503062D+00	0.0141199	0.4319685		
D	3.0768316D+00	0.0009605	0.3518860		
D	1.5694702D+00	0.0001821	0.1332568		
D	7.2945606D-01	0.0000579	0.0182403		
D	2.1192635D-01	0.0000050	0.0005347		
	F	4F			
BASIS/ORB. ENERGY		-0.5022401			
F	3.8116322D+02	-0.0009338			
F	1.3081426D+02	-0.0078892			
F	5.6032337D+01	-0.0355740			
F	2.6274195D+01	-0.1039754			
F	1.2979990D+01	-0.2123685			
F	6.4604670D+00	-0.2999274			
F	3.1503517D+00	-0.3166355			
F	1.4689142D+00	-0.2570714			
F	6.3280707D-01	-0.1595331			
F	2.3624462D-01	-0.0591904			

 THULIUM [XE]6S(2)5D(0)4F(13), 2F

CHARGE = 69.000000

SYMMETRY SPECIES	S	P	D	F
NUMBER OF BASIS FUNCTIONS	27	23	15	10
NUMBER OF CLOSED SHELLS	6	4	2	0
NUMBER OF OPEN SHELLS	0	0	0	1
OPEN SHELL OCCUPATION NUMBER	0	0	0	13

*** FINAL SCF RESULTS ***

E = -13564.306186169

ORBITAL ENERGIES AND EXPANSION COEFFICIENTS

	S	1S	2S	3S	4S	5S	6S
BASIS/ORB. ENERGY	-2194.1707000	-374.9306300	-86.2987720	-17.9963420	-2.3771509	-0.1938784	
S 6.9527140D+10	0.0000044	-0.0000016	0.0000008	0.0000004	0.0000001	0.0000000	
S 6.9235429D+09	0.0000174	-0.0000065	0.0000030	0.0000015	0.0000006	-0.0000001	
S 1.0786059D+09	0.0000550	-0.0000204	0.0000096	0.0000047	0.0000018	-0.0000004	
S 2.1464164D+08	0.0001458	-0.0000541	0.0000254	0.0000123	0.0000047	-0.0000011	
S 5.2986807D+07	0.0003414	-0.0001267	0.0000595	0.0000288	0.0000110	-0.0000027	
S 1.4544765D+07	0.0007861	-0.0002918	0.0001371	0.0000664	0.0000254	-0.0000062	
S 4.2788435D+06	0.0017223	-0.0006400	0.0003009	0.0001458	0.0000557	-0.0000135	
S 1.3499876D+06	0.0036276	-0.0013525	0.0006358	0.0003081	0.0001179	-0.0000285	
S 4.5157974D+05	0.0074548	-0.0027910	0.0013141	0.0006367	0.0002435	-0.0000590	
S 1.5981914D+05	0.0149517	-0.0056545	0.0026629	0.0012915	0.0004941	-0.0001196	
S 5.9606978D+04	0.0297218	-0.0113825	0.0053832	0.0026093	0.0009980	-0.0002417	
S 2.3271552D+04	0.0586467	-0.0231038	0.0109379	0.0053162	0.0020351	-0.0004923	
S 9.4970149D+03	0.1130394	-0.0462626	0.0221568	0.0107575	0.0041160	-0.0009975	
S 4.0357864D+03	0.2046361	-0.0911491	0.0439269	0.0214788	0.0082329	-0.0019910	
S 1.7716584D+03	0.3122636	-0.1582563	0.0789875	0.0386141	0.0147991	-0.0035901	
S 8.0071134D+02	0.3124155	-0.2011163	0.1027279	0.0513006	0.0197487	-0.0047696	
S 3.7228123D+02	0.1351279	-0.0139362	0.0030029	-0.0002950	-0.0002504	0.0000330	
S 1.6541548D+02	0.0109689	0.4953536	-0.4171692	-0.2287456	-0.0899875	0.0219310	
S 7.7559435D+01	-0.0002063	0.5533025	-0.5975874	-0.3691351	-0.1492117	0.0362296	
S 3.1407479D+01	-0.0000661	0.1005324	0.4623154	0.4506297	0.2010453	-0.0492216	
S 1.6330112D+01	0.0000221	-0.0176471	0.8170635	0.9827809	0.4654818	-0.1164652	
S 6.5157128D+00	-0.0000149	0.0060326	0.1122830	-0.6242215	-0.4323235	0.1137013	
S 3.1840936D+00	0.0000117	-0.0027625	-0.0136307	-0.8494644	-0.7451687	0.2016511	
S 8.8247619D-01	-0.0000038	0.0008342	0.0034936	-0.0538923	0.7210374	-0.2384187	

S	3.8709567D-01	0.0000017	-0.0003892	-0.0016125	0.0124609	0.6149095	-0.3834994
S	6.2378669D-02	-0.0000005	0.0001017	0.0004002	-0.0026536	0.0189570	0.6815732
S	2.5653829D-02	0.0000002	-0.0000493	-0.0001940	0.0012592	-0.0065245	0.4840897
	P	2P	3P	4P	5P		
BASIS/ORB. ENERGY							
		-331.4813700	-72.8442750	-13.4729560	-1.2310624		
P	5.4105389D+07	0.0000071	-0.0000036	-0.0000017	-0.0000006		
P	7.6992702D+06	0.0000237	-0.0000119	-0.0000057	-0.0000019		
P	1.5870519D+06	0.0000694	-0.0000348	-0.0000166	-0.0000056		
P	4.0229735D+05	0.0001923	-0.0000965	-0.0000461	-0.0000155		
P	1.1819372D+05	0.0005240	-0.0002635	-0.0001258	-0.0000424		
P	3.9241105D+04	0.0014293	-0.0007212	-0.0003448	-0.0001162		
P	1.4433194D+04	0.0039618	-0.0020093	-0.0009612	-0.0003242		
P	5.7871832D+03	0.0110576	-0.0056541	-0.0027114	-0.0009147		
P	2.4965258D+03	0.0303630	-0.0157404	-0.0075664	-0.0025549		
P	1.1438901D+03	0.0779249	-0.0413918	-0.0200258	-0.0067670		
P	5.5166947D+02	0.1720978	-0.0950032	-0.0463302	-0.0156913		
P	2.7768866D+02	0.2944954	-0.1711902	-0.0847306	-0.0287552		
P	1.4509849D+02	0.3377793	-0.1971462	-0.0971910	-0.0330098		
P	7.7601940D+01	0.2116657	-0.0216130	0.0070716	0.0037929		
P	4.1855518D+01	0.0526167	0.3448093	0.2537116	0.0928194		
P	2.3206092D+01	0.0028721	0.4985117	0.4008367	0.1502829		
P	1.2842759D+01	0.0002860	0.2394030	0.0292885	-0.0093313		
P	7.0046016D+00	-0.0001949	0.0341954	-0.5069015	-0.2471642		
P	3.7467982D+00	0.0000042	0.0024457	-0.5188077	-0.2978259		
P	1.9334966D+00	-0.0000202	0.0000157	-0.1545467	0.0397426		
P	9.1673759D-01	0.0000065	0.0000995	-0.0091861	0.4912820		
P	4.1782262D-01	-0.0000020	-0.0000399	-0.0007727	0.5116354		
P	1.7376625D-01	0.0000005	0.0000122	0.0001395	0.1328443		
	D	3D	4D				
BASIS/ORB. ENERGY							
		-55.8578300	-7.2885220				
D	1.6617409D+04	0.0000718	-0.0000346				
D	4.2816678D+03	0.0005225	-0.0002526				
D	1.5144344D+03	0.0029541	-0.0014302				
D	6.2637186D+02	0.0136682	-0.0066751				
D	2.8542760D+02	0.0499020	-0.0245860				

D	1.3881170D+02	0.1389473	-0.0698954
D	7.0874392D+01	0.2752269	-0.1382343
D	3.7377733D+01	0.3625099	-0.1716877
D	2.0252334D+01	0.2702334	-0.0462499
D	1.1019065D+01	0.0952039	0.2451512
D	5.8625400D+00	0.0123110	0.4372795
D	3.0653484D+00	0.0008150	0.3408880
D	1.5440675D+00	0.0002079	0.1196435
D	7.2768718D-01	0.0000369	0.0137534
D	3.8004566D-01	0.0000130	0.0012039

F 4F

BASIS/ORB. ENERGY -0.5020701

F	3.7973766D+02	-0.0010478
F	1.3035791D+02	-0.0087344
F	5.5982592D+01	-0.0385724
F	2.6281061D+01	-0.1111073
F	1.2984346D+01	-0.2210285
F	6.4587573D+00	-0.3033077
F	3.1526147D+00	-0.3120770
F	1.4724500D+00	-0.2491082
F	6.3595283D-01	-0.1528909
F	2.3902390D-01	-0.0569822

 YTTERBIUM [XE]6S(2)5D(0)4F(14), 1S

CHARGE = 70.000000

SYMMETRY SPECIES	S	P	D	F
NUMBER OF BASIS FUNCTIONS	27	23	15	10
NUMBER OF CLOSED SHELLS	6	4	2	1
NUMBER OF OPEN SHELLS	0	0	0	0
OPEN SHELL OCCUPATION NUMBER	0	0	0	0

*** FINAL SCF RESULTS ***

E = -14056.882464022

ORBITAL ENERGIES AND EXPANSION COEFFICIENTS

	S	1S	2S	3S	4S	5S	6S
BASIS/ORB. ENERGY		-2266.0687000	-388.7295300	-89.6861660	-18.6674040	-2.4377243	-0.1960545

S	7.1671917D+10	0.0000047	-0.0000017	0.0000008	0.0000004	0.0000002	0.0000000
S	6.8528417D+09	0.0000188	-0.0000070	0.0000033	0.0000016	0.0000006	-0.0000001
S	1.1061794D+09	0.0000558	-0.0000208	0.0000098	0.0000048	0.0000018	-0.0000004
S	2.2963152D+08	0.0001483	-0.0000553	0.0000261	0.0000126	0.0000048	-0.0000012
S	5.5103176D+07	0.0003616	-0.0001348	0.0000635	0.0000308	0.0000118	-0.0000028
S	1.4844859D+07	0.0008285	-0.0003090	0.0001455	0.0000706	0.0000269	-0.0000065
S	4.3300353D+06	0.0018155	-0.0006777	0.0003193	0.0001549	0.0000591	-0.0000142
S	1.3622927D+06	0.0038027	-0.0014240	0.0006710	0.0003257	0.0001243	-0.0000298
S	4.5512954D+05	0.0078208	-0.0029420	0.0013882	0.0006737	0.0002570	-0.0000617
S	1.6028405D+05	0.0157226	-0.0059734	0.0028198	0.0013699	0.0005228	-0.0001255
S	5.9517787D+04	0.0311898	-0.0120130	0.0056938	0.0027647	0.0010547	-0.0002534
S	2.3205185D+04	0.0610612	-0.0241852	0.0114816	0.0055898	0.0021344	-0.0005121
S	9.4862964D+03	0.1167757	-0.0481702	0.0231237	0.0112482	0.0042925	-0.0010317
S	4.0347972D+03	0.2093711	-0.0939541	0.0454424	0.0222594	0.0085110	-0.0020413
S	1.7768299D+03	0.3132768	-0.1607199	0.0804426	0.0394098	0.0150646	-0.0036243
S	8.0629235D+02	0.3070363	-0.1977545	0.1014274	0.0507519	0.0194927	-0.0046686
S	3.7530396D+02	0.1284376	-0.0041984	-0.0035719	-0.0037501	-0.0016002	0.0003571
S	1.7009758D+02	0.0094732	0.4955776	-0.4187375	-0.2303403	-0.0903930	0.0218465
S	8.0217510D+01	0.0002394	0.5470838	-0.5962181	-0.3694265	-0.1490329	0.0358900
S	3.3235814D+01	-0.0003020	0.0998510	0.4430861	0.4307726	0.1915752	-0.0465149
S	1.7206244D+01	0.0001664	-0.0151171	0.8335879	1.0028499	0.4731165	-0.1172484
S	6.8859131D+00	-0.0000810	0.0050670	0.1183673	-0.5948668	-0.4110173	0.1069372
S	3.3580384D+00	0.0000425	-0.0022831	-0.0139550	-0.8733133	-0.7567972	0.2029014
S	9.1181315D-01	-0.0000134	0.0006704	0.0035427	-0.0570593	0.7172613	-0.2352054
S	3.9903684D-01	0.0000062	-0.0003132	-0.0016425	0.0137610	0.6134338	-0.3785756
S	6.3049721D-02	-0.0000016	0.0000807	0.0004025	-0.0029081	0.0184312	0.6959891
S	2.5566065D-02	0.0000008	-0.0000390	-0.0001946	0.0013782	-0.0063261	0.4679346

	P	2P	3P	4P	5P
BASIS/ORB. ENERGY	-343.1188200	-75.6304060	-13.9519420	-1.2527622	
P	5.4522375D+07	0.0000076	-0.0000038	-0.0000018	-0.0000006
P	7.7564022D+06	0.0000252	-0.0000127	-0.0000061	-0.0000020
P	1.5914503D+06	0.0000743	-0.0000373	-0.0000178	-0.0000060
P	4.0199082D+05	0.0002052	-0.0001033	-0.0000494	-0.0000166
P	1.1840033D+05	0.0005565	-0.0002807	-0.0001343	-0.0000450
P	3.9288989D+04	0.0015201	-0.0007695	-0.0003686	-0.0001237

P	1.4434444D+04	0.0042022	-0.0021385	-0.0010251	-0.0003440
P	5.7896417D+03	0.0116766	-0.0059927	-0.0028798	-0.0009667
P	2.4978170D+03	0.0319629	-0.0166372	-0.0080147	-0.0026922
P	1.1436688D+03	0.0816320	-0.0435683	-0.0211296	-0.0071052
P	5.5153591D+02	0.1782898	-0.0989491	-0.0483763	-0.0162990
P	2.7768476D+02	0.3007287	-0.1758045	-0.0872676	-0.0294787
P	1.4498333D+02	0.3361353	-0.1949917	-0.0959788	-0.0323851
P	7.7528112D+01	0.2014290	-0.0032859	0.0185438	0.0077758
P	4.1794548D+01	0.0469497	0.3680963	0.2729436	0.0996442
P	2.3212546D+01	0.0021383	0.4886964	0.3940934	0.1465764
P	1.2922397D+01	0.0003172	0.2203050	-0.0081142	-0.0248075
P	7.0191983D+00	-0.0002249	0.0308632	-0.5257252	-0.2568381
P	3.7516719D+00	0.0000284	0.0015258	-0.4999586	-0.2852881
P	1.9301856D+00	-0.0000299	0.0002848	-0.1378703	0.0623134
P	9.2262189D-01	0.0000112	-0.0000251	-0.0075346	0.4946682
P	4.2161742D-01	-0.0000039	0.0000086	-0.0007899	0.5003459
P	1.7537191D-01	0.0000009	-0.0000002	0.0001435	0.1273297

D		3D	4D		
BASIS/ORB. ENERGY		-58.1026550	-7.5622322		
D	1.8187932D+04	0.0000653	-0.0000315		
D	4.6937060D+03	0.0004965	-0.0002408		
D	1.5745195D+03	0.0030959	-0.0015043		
D	6.3046752D+02	0.0147855	-0.0072487		
D	2.8453395D+02	0.0533919	-0.0264222		
D	1.3857521D+02	0.1456631	-0.0736181		
D	7.0877663D+01	0.2835102	-0.1427357		
D	3.7391735D+01	0.3642756	-0.1714365		
D	2.0235405D+01	0.2599438	-0.0296759		
D	1.0979157D+01	0.0858883	0.2654354		
D	5.8495286D+00	0.0101726	0.4381655		
D	3.0566918D+00	0.0008431	0.3270260		
D	1.5229958D+00	0.0001670	0.1091691		
D	6.5156983D-01	0.0000547	0.0110874		
D	8.5728077D-02	0.0000018	0.0001275		
F		4F			

BASIS/ORB.ENERGY	-0.5061899
F 9.3647925D+02	-0.0001883
F 2.3616785D+02	-0.0030612
F 8.8823830D+01	-0.0200904
F 3.8899260D+01	-0.0740193
F 1.8234384D+01	-0.1834065
F 8.7416685D+00	-0.2984601
F 4.0993797D+00	-0.3410314
F 1.8355451D+00	-0.2866114
F 7.5881066D-01	-0.1793203
F 2.7270801D-01	-0.0689486

LUTECIUM [XE]6S(2)5D(1)4F(14), 2D

CHARGE = 71.000000

SYMMETRY SPECIES	S	P	D	F
NUMBER OF BASIS FUNCTIONS	27	23	15	10
NUMBER OF CLOSED SHELLS	6	4	2	1
NUMBER OF OPEN SHELLS	0	0	1	0
OPEN SHELL OCCUPATION NUMBER	0	0	1	0

*** FINAL SCF RESULTS ***

E = -14560.876057985

ORBITAL ENERGIES AND EXPANSION COEFFICIENTS

	S	1S	2S	3S	4S	5S	6S
BASIS/ORB.ENERGY	-2339.7104000	-403.1665400	-93.4968140	-19.6892710	-2.6990209	-0.2212884	
S 6.7013119D+10	0.0000051	-0.0000019	0.0000009	0.0000004	-0.0000002	0.0000000	
S 7.2167178D+09	0.0000189	-0.0000071	0.0000033	0.0000016	-0.0000006	0.0000002	
S 1.1715292D+09	0.0000583	-0.0000218	0.0000103	0.0000050	-0.0000019	0.0000005	
S 2.3523312D+08	0.0001577	-0.0000591	0.0000279	0.0000136	-0.0000053	0.0000014	
S 5.5877724D+07	0.0003825	-0.0001432	0.0000676	0.0000329	-0.0000128	0.0000033	
S 1.4949778D+07	0.0008772	-0.0003286	0.0001551	0.0000755	-0.0000293	0.0000076	
S 4.3630170D+06	0.0019018	-0.0007131	0.0003367	0.0001639	-0.0000636	0.0000165	
S 1.3753405D+06	0.0039949	-0.0015027	0.0007095	0.0003454	-0.0001342	0.0000348	
S 4.5654052D+05	0.0082471	-0.0031171	0.0014740	0.0007174	-0.0002787	0.0000724	
S 1.6043537D+05	0.0164542	-0.0062815	0.0029717	0.0014478	-0.0005626	0.0001460	
S 5.9637104D+04	0.0324880	-0.0125803	0.0059763	0.0029103	-0.0011304	0.0002936	

S	2.3233144D+04	0.0635719	-0.0253232	0.0120498	0.0058840	-0.0022877	0.0005938
S	9.4740409D+03	0.1209216	-0.0502461	0.0241857	0.0117990	-0.0045846	0.0011910
S	4.0327313D+03	0.2138696	-0.0967788	0.0469376	0.0230679	-0.0089825	0.0023311
S	1.7797539D+03	0.3152734	-0.1635249	0.0821645	0.0403697	-0.0157106	0.0040836
S	8.0787768D+02	0.3023321	-0.1953703	0.1003796	0.0504409	-0.0197404	0.0051224
S	3.7492607D+02	0.1204765	0.0118700	-0.0136806	-0.0092261	0.0038277	-0.0009876
S	1.7216227D+02	0.0075023	0.5044887	-0.4321178	-0.2388498	0.0954559	-0.0249019
S	8.1759054D+01	0.0006427	0.5328907	-0.5811365	-0.3630577	0.1495102	-0.0390680
S	3.4046202D+01	-0.0005157	0.0952358	0.4674130	0.4600643	-0.2093811	0.0553969
S	1.7673598D+01	0.0002981	-0.0146720	0.8170867	0.9848103	-0.4733789	0.1265645
S	7.0840926D+00	-0.0001426	0.0050065	0.1149692	-0.6177934	0.4342762	-0.1215094
S	3.4795073D+00	0.0000735	-0.0023332	-0.0144446	-0.8547540	0.7698560	-0.2278067
S	9.9316525D-01	-0.0000245	0.0007287	0.0038702	-0.0571479	-0.7064890	0.2630686
S	4.4583214D-01	0.0000116	-0.0003435	-0.0018085	0.0131822	-0.6383991	0.4087380
S	7.7213035D-02	-0.0000030	0.0000872	0.0004360	-0.0026920	-0.0224235	-0.6913818
S	3.0533522D-02	0.0000014	-0.0000401	-0.0002001	0.0012044	0.0069976	-0.4912698

	P	2P	3P	4P	5P
BASIS/ORB. ENERGY		-355.2852100	-78.8116270	-14.7653610	-1.4363369
P	5.5602773D+07	0.0000081	-0.0000041	-0.0000019	-0.0000007
P	7.7657459D+06	0.0000271	-0.0000136	-0.0000065	-0.0000023
P	1.5895843D+06	0.0000794	-0.0000400	-0.0000192	-0.0000066
P	4.0181095D+05	0.0002186	-0.0001103	-0.0000530	-0.0000183
P	1.1860334D+05	0.0005911	-0.0002991	-0.0001436	-0.0000495
P	3.9300000D+04	0.0016178	-0.0008216	-0.0003950	-0.0001363
P	1.4430354D+04	0.0044489	-0.0022717	-0.0010929	-0.0003772
P	5.7931246D+03	0.0123286	-0.0063496	-0.0030632	-0.0010576
P	2.4978215D+03	0.0336297	-0.0175752	-0.0084993	-0.0029362
P	1.1437173D+03	0.0853550	-0.0457625	-0.0222876	-0.0077097
P	5.5139771D+02	0.1846254	-0.1030102	-0.0505732	-0.0175250
P	2.7775014D+02	0.3061693	-0.1799120	-0.0897325	-0.0311900
P	1.4503033D+02	0.3339410	-0.1922122	-0.0945203	-0.0327554
P	7.7447456D+01	0.1918674	0.0155381	0.0304712	0.0123265
P	4.1750155D+01	0.0413832	0.3894856	0.2920836	0.1101100
P	2.3226948D+01	0.0018459	0.4786942	0.3857347	0.1471518
P	1.2936387D+01	0.0001456	0.2027366	-0.0452374	-0.0419622

P	7.0260649D+00	-0.0001347	0.0261195	-0.5460101	-0.2776896
P	3.7445047D+00	-0.0000153	0.0014643	-0.4822376	-0.2855291
P	1.8991908D+00	-0.0000062	0.0001518	-0.1179453	0.1086467
P	9.1463474D-01	0.0000018	0.0000044	-0.0042649	0.5364111
P	4.2267369D-01	-0.0000002	-0.0000058	-0.0009455	0.4616558
P	1.7333636D-01	0.0000001	0.0000025	0.0002074	0.0932713
	D	3D	4D	5D	
BASIS/ORB. ENERGY	-60.7226650	-8.1475931	-0.1871820		
D	1.6241493D+04	0.0000852	-0.0000414	0.0000075	
D	4.2789882D+03	0.0006039	-0.0002955	0.0000550	
D	1.5245971D+03	0.0033232	-0.0016240	0.0002953	
D	6.4085771D+02	0.0146793	-0.0072575	0.0013510	
D	2.9556552D+02	0.0525668	-0.0261618	0.0047763	
D	1.4352658D+02	0.1484782	-0.0756438	0.0141333	
D	7.1896175D+01	0.3011086	-0.1523893	0.0278038	
D	3.6657075D+01	0.3884762	-0.1808164	0.0338000	
D	1.8884237D+01	0.2499433	0.0209112	-0.0110891	
D	9.5104568D+00	0.0590224	0.3860507	-0.0813242	
D	4.6208226D+00	0.0031479	0.4872880	-0.1108898	
D	2.1120086D+00	0.0005732	0.2233572	0.0313446	
D	7.5168436D-01	-0.0000027	0.0212526	0.3196606	
D	2.5140270D-01	0.0000219	-0.0013991	0.5155096	
D	7.5471915D-02	-0.0000063	0.0004610	0.3965297	
	F	4F			
BASIS/ORB. ENERGY	-0.8187475				
F	1.5731113D+03	-0.0000910			
F	2.9592915D+02	-0.0021717			
F	1.0834588D+02	-0.0153078			
F	4.7088440D+01	-0.0617284			
F	2.1825954D+01	-0.1658741			
F	1.0480024D+01	-0.2878062			
F	4.9886532D+00	-0.3424209			
F	2.3047615D+00	-0.2963283			
F	9.9952257D-01	-0.1869062			
F	3.8102157D-01	-0.0690409			

HAFNIUM [XE]4F(14)6S(2)5D(2), 3F

CHARGE = 72.000000

SYMMETRY SPECIES	S	P	D	F
NUMBER OF BASIS FUNCTIONS	27	23	15	10
NUMBER OF CLOSED SHELLS	6	4	2	1
NUMBER OF OPEN SHELLS	0	0	1	0
OPEN SHELL OCCUPATION NUMBER	0	0	2	0

*** FINAL SCF RESULTS ***

E = -15076.250511600

ORBITAL ENERGIES AND EXPANSION COEFFICIENTS

	S	1S	2S	3S	4S	5S	6S
BASIS/ORB. ENERGY	-2414.8412000	-417.9527400	-97.4121000	-20.7404970	-2.9433191	-0.2362307	
S 8.7704213D+10	0.0000048	-0.0000018	0.0000009	0.0000004	-0.0000002	0.0000000	
S 7.7970269D+09	0.0000203	-0.0000077	0.0000036	0.0000018	-0.0000007	0.0000002	
S 1.1833914D+09	0.0000627	-0.0000236	0.0000112	0.0000054	-0.0000022	0.0000006	
S 2.3839233D+08	0.0001643	-0.0000618	0.0000292	0.0000143	-0.0000056	0.0000015	
S 5.7504405D+07	0.0003978	-0.0001496	0.0000708	0.0000345	-0.0000136	0.0000037	
S 1.5279318D+07	0.0009221	-0.0003469	0.0001641	0.0000801	-0.0000316	0.0000085	
S 4.4241047D+06	0.0020065	-0.0007558	0.0003576	0.0001746	-0.0000690	0.0000185	
S 1.3815280D+06	0.0042201	-0.0015946	0.0007545	0.0003684	-0.0001456	0.0000391	
S 4.5812199D+05	0.0086272	-0.0032762	0.0015524	0.0007580	-0.0002994	0.0000805	
S 1.6102325D+05	0.0172391	-0.0066127	0.0031351	0.0015321	-0.0006055	0.0001627	
S 5.9644584D+04	0.0339572	-0.0132214	0.0062942	0.0030749	-0.0012148	0.0003265	
S 2.3252256D+04	0.0658814	-0.0263927	0.0125889	0.0061658	-0.0024380	0.0006551	
S 9.4813012D+03	0.1249614	-0.0523058	0.0252372	0.0123540	-0.0048825	0.0013127	
S 4.0309921D+03	0.2188864	-0.0998615	0.0485815	0.0239486	-0.0094832	0.0025482	
S 1.7813455D+03	0.3167312	-0.1661416	0.0837526	0.0413081	-0.0163542	0.0043984	
S 8.1014078D+02	0.2967510	-0.1919352	0.0988549	0.0498161	-0.0198224	0.0053286	
S 3.7525819D+02	0.1132778	0.0271458	-0.0238249	-0.0145859	0.0060359	-0.0016273	
S 1.7453191D+02	0.0058120	0.5116623	-0.4430410	-0.2465653	0.1003595	-0.0270860	
S 8.3439875D+01	0.0010077	0.5191318	-0.5684144	-0.3570357	0.1496522	-0.0405456	
S 3.5198825D+01	-0.0007138	0.0911034	0.4801761	0.4732179	-0.2191922	0.0602307	
S 1.8293630D+01	0.0004215	-0.0134412	0.8074093	0.9835137	-0.4827293	0.1336126	
S 7.4872863D+00	-0.0002015	0.0046148	0.1152849	-0.6010505	0.4305731	-0.1246138	

S	3.6780189D+00	0.0001007	-0.0021229	-0.0131238	-0.8743852	0.8038874	-0.2488925
S	1.0597761D+00	-0.0000342	0.0006744	0.0036225	-0.0612681	-0.7154448	0.2868660
S	4.8417790D-01	0.0000167	-0.0003249	-0.0017373	0.0146644	-0.6387569	0.4143144
S	9.0249496D-02	-0.0000043	0.0000829	0.0004196	-0.0030021	-0.0242258	-0.6533012
S	3.5111885D-02	0.0000019	-0.0000366	-0.0001849	0.0012858	0.0069594	-0.5389458
	P	2P	3P	4P	5P		
BASIS/ORB. ENERGY	-367.6887700	-82.0689410	-15.5978640	-1.6023257			
P	5.4404988D+07	0.0000087	-0.0000044	-0.0000021	-0.0000007		
P	7.7488644D+06	0.0000288	-0.0000146	-0.0000070	-0.0000025		
P	1.5931436D+06	0.0000844	-0.0000426	-0.0000205	-0.0000073		
P	4.0358704D+05	0.0002323	-0.0001176	-0.0000567	-0.0000200		
P	1.1875463D+05	0.0006287	-0.0003190	-0.0001538	-0.0000544		
P	3.9432452D+04	0.0017057	-0.0008689	-0.0004194	-0.0001483		
P	1.4502016D+04	0.0046880	-0.0024013	-0.0011601	-0.0004102		
P	5.8122978D+03	0.0129834	-0.0067103	-0.0032502	-0.0011504		
P	2.5023327D+03	0.0353314	-0.0185345	-0.0090023	-0.0031864		
P	1.1441524D+03	0.0892445	-0.0480685	-0.0235112	-0.0083396		
P	5.5091456D+02	0.1915510	-0.1074154	-0.0529905	-0.0188127		
P	2.7695575D+02	0.3130464	-0.1849498	-0.0926691	-0.0330488		
P	1.4449133D+02	0.3301528	-0.1877427	-0.0922286	-0.0326433		
P	7.7304950D+01	0.1808615	0.0353374	0.0433699	0.0173130		
P	4.1691019D+01	0.0367814	0.4120824	0.3122562	0.1214351		
P	2.3084638D+01	0.0012962	0.4711973	0.3789742	0.1469084		
P	1.2784288D+01	0.0001891	0.1810119	-0.1004651	-0.0673852		
P	6.8898813D+00	-0.0001818	0.0209038	-0.5690756	-0.3037737		
P	3.7023937D+00	0.0000228	0.0009351	-0.4428081	-0.2675505		
P	1.9057350D+00	-0.0000233	0.0002334	-0.1001077	0.1382895		
P	9.6136763D-01	0.0000105	-0.0000595	-0.0032732	0.5303901		
P	4.5938150D-01	-0.0000033	0.0000147	-0.0009896	0.4484480		
P	1.9184705D-01	0.0000008	-0.0000034	0.0002026	0.0945570		
	D	3D	4D	5D			
BASIS/ORB. ENERGY	-63.4023030	-8.7437577	-0.2625143				
D	1.4778667D+04	0.0001053	-0.0000516	0.0000109			
D	4.0909068D+03	0.0006659	-0.0003282	0.0000706			
D	1.5291219D+03	0.0034530	-0.0017002	0.0003579			

D	6.4578378D+02	0.0155869	-0.0077638	0.0016697
D	2.9552552D+02	0.0560539	-0.0281319	0.0059503
D	1.4339328D+02	0.1552037	-0.0797154	0.0172153
D	7.2045069D+01	0.3077354	-0.1567309	0.0331172
D	3.6826605D+01	0.3874187	-0.1791665	0.0385496
D	1.8954163D+01	0.2396024	0.0399306	-0.0175780
D	9.4983091D+00	0.0528442	0.4065213	-0.0999353
D	4.6160122D+00	0.0024808	0.4766927	-0.1250416
D	2.1348639D+00	0.0005506	0.2017948	0.0499559
D	7.9574421D-01	-0.0000258	0.0181827	0.3641307
D	2.8636074D-01	0.0000259	-0.0010305	0.5132639
D	9.3422636D-02	-0.0000083	0.0003568	0.3185836

F 4F

BASIS/ORB. ENERGY -1.1351790

F	9.2286221D+02	-0.0001699
F	3.2238834D+02	-0.0016554
F	1.3097201D+02	-0.0109413
F	5.8432577D+01	-0.0471050
F	2.7266952D+01	-0.1370828
F	1.3239044D+01	-0.2615937
F	6.4122373D+00	-0.3415237
F	2.9886790D+00	-0.3242041
F	1.2933181D+00	-0.2106655
F	4.9178595D-01	-0.0734901

TANTALUM [XE]4F(14)6S(2)5D(3), 4F

CHARGE = 73.000000

SYMMETRY SPECIES	S	P	D	F
NUMBER OF BASIS FUNCTIONS	27	23	15	10
NUMBER OF CLOSED SHELLS	6	4	2	1
NUMBER OF OPEN SHELLS	0	0	1	0
OPEN SHELL OCCUPATION NUMBER	0	0	3	0

*** FINAL SCF RESULTS ***

E = -15603.134461732

ORBITAL ENERGIES AND EXPANSION COEFFICIENTS

	S	1S	2S	3S	4S	5S	6S
BASIS/ORB. ENERGY		-2491.5001000	-433.1102800	-101.4477500	-21.8354560	-3.1907508	-0.2492141
S 7.7668131D+10	0.0000053	-0.0000020	0.0000010	0.0000005	-0.0000002	0.0000001	
S 7.9415652D+09	0.0000207	-0.0000079	0.0000037	0.0000018	-0.0000007	0.0000002	
S 1.2530631D+09	0.0000638	-0.0000241	0.0000114	0.0000056	-0.0000022	0.0000006	
S 2.5117343D+08	0.0001717	-0.0000649	0.0000308	0.0000151	-0.0000060	0.0000017	
S 5.8837842D+07	0.0004229	-0.0001598	0.0000757	0.0000371	-0.0000149	0.0000041	
S 1.5468056D+07	0.0009712	-0.0003671	0.0001739	0.0000852	-0.0000342	0.0000094	
S 4.4590629D+06	0.0021214	-0.0008028	0.0003805	0.0001864	-0.0000748	0.0000206	
S 1.3829207D+06	0.0044573	-0.0016920	0.0008022	0.0003930	-0.0001577	0.0000433	
S 4.5833146D+05	0.0090525	-0.0034543	0.0016401	0.0008033	-0.0003225	0.0000886	
S 1.6125681D+05	0.0179978	-0.0069374	0.0032958	0.0016159	-0.0006488	0.0001782	
S 5.9825101D+04	0.0353356	-0.0138329	0.0065995	0.0032345	-0.0012984	0.0003568	
S 2.3267054D+04	0.0686348	-0.0276549	0.0132204	0.0064965	-0.0026099	0.0007170	
S 9.4657916D+03	0.1290693	-0.0544277	0.0263282	0.0129303	-0.0051931	0.0014273	
S 4.0301852D+03	0.2232672	-0.1027066	0.0501008	0.0247858	-0.0099724	0.0027399	
S 1.7830107D+03	0.3186430	-0.1689817	0.0854931	0.0423065	-0.0170230	0.0046802	
S 8.1063696D+02	0.2913738	-0.1883712	0.0971225	0.0491553	-0.0198730	0.0054636	
S 3.7387525D+02	0.1057063	0.0452698	-0.0358085	-0.0211765	0.0088302	-0.0024384	
S 1.7609612D+02	0.0040261	0.5190956	-0.4560702	-0.2552472	0.1056962	-0.0291635	
S 8.4883788D+01	0.0013656	0.5034578	-0.5503190	-0.3486371	0.1486995	-0.0412336	
S 3.5969722D+01	-0.0008974	0.0866686	0.5063724	0.5054616	-0.2386110	0.0671795	
S 1.8730490D+01	0.0005341	-0.0131850	0.7892312	0.9639736	-0.4823626	0.1366460	
S 7.6785878D+00	-0.0002565	0.0046200	0.1104601	-0.6324624	0.4629644	-0.1374107	
S 3.7924093D+00	0.0001301	-0.0021897	-0.0132281	-0.8510834	0.8105412	-0.2595355	
S 1.1451710D+00	-0.0000455	0.0007204	0.0037275	-0.0580481	-0.7255767	0.3061177	
S 5.2478918D-01	0.0000218	-0.0003393	-0.0017473	0.0124953	-0.6478819	0.4182999	
S 1.0080020D-01	-0.0000054	0.0000845	0.0004104	-0.0024536	-0.0252668	-0.6475579	
S 3.8120496D-02	0.0000023	-0.0000360	-0.0001746	0.0010080	0.0068504	-0.5508834	
	P	2P	3P	4P	5P		
BASIS/ORB. ENERGY		-380.3463600	-85.4167150	-16.4636120	-1.7692728		
P 5.4530298D+07	0.0000093	-0.0000047	-0.0000023	0.0000008			
P 7.7507418D+06	0.0000308	-0.0000156	-0.0000075	0.0000027			
P 1.5941988D+06	0.0000899	-0.0000456	-0.0000220	0.0000080			
P 4.0360495D+05	0.0002474	-0.0001256	-0.0000608	0.0000220			

P	1.1880151D+05	0.0006678	-0.0003399	-0.0001646	0.0000595
P	3.9458963D+04	0.0018082	-0.0009239	-0.0004478	0.0001620
P	1.4512986D+04	0.0049559	-0.0025467	-0.0012355	0.0004468
P	5.8158421D+03	0.0136900	-0.0070996	-0.0034537	0.0012502
P	2.5028355D+03	0.0371068	-0.0195413	-0.0095333	0.0034511
P	1.1441201D+03	0.0931736	-0.0504070	-0.0247697	0.0089867
P	5.5071494D+02	0.1980050	-0.1116020	-0.0553198	0.0200877
P	2.7689574D+02	0.3181270	-0.1888328	-0.0950884	0.0346935
P	1.4445926D+02	0.3266492	-0.1832864	-0.0898217	0.0324516
P	7.7223449D+01	0.1713124	0.0552486	0.0565077	-0.0227613
P	4.1662410D+01	0.0322182	0.4312372	0.3307786	-0.1320364
P	2.3067833D+01	0.0011508	0.4585693	0.3658948	-0.1442717
P	1.2772359D+01	0.0000485	0.1643924	-0.1406098	0.0881220
P	6.8745760D+00	-0.0001062	0.0175366	-0.5846789	0.3242076
P	3.6964445D+00	-0.0000142	0.0007976	-0.4160898	0.2578798
P	1.9108749D+00	-0.0000018	0.0001805	-0.0848081	-0.1865494
P	9.6537180D-01	0.0000010	-0.0000570	-0.0026446	-0.5530466
P	4.6481369D-01	0.0000004	0.0000108	-0.0007321	-0.4089697
P	1.9463813D-01	0.0000000	-0.0000034	0.0001500	-0.0764832
	D	3D	4D	5D	
BASIS/ORB. ENERGY		-66.1555100	-9.3654521	-0.3201903	
D	1.7225445D+04	0.0000924	-0.0000456	0.0000106	
D	4.3938967D+03	0.0006741	-0.0003344	0.0000785	
D	1.5543978D+03	0.0037037	-0.0018398	0.0004253	
D	6.4874369D+02	0.0164813	-0.0082676	0.0019432	
D	2.9749476D+02	0.0584757	-0.0296144	0.0068710	
D	1.4448283D+02	0.1607707	-0.0831915	0.0196469	
D	7.2614064D+01	0.3134693	-0.1608882	0.0372932	
D	3.7248619D+01	0.3839092	-0.1762843	0.0412835	
D	1.9285001D+01	0.2304325	0.0501076	-0.0220050	
D	9.7781089D+00	0.0502578	0.4060449	-0.1102582	
D	4.8149253D+00	0.0026344	0.4705685	-0.1351641	
D	2.2610103D+00	0.0004743	0.1998642	0.0541738	
D	8.7403946D-01	-0.0000105	0.0183492	0.3848197	
D	3.2592289D-01	0.0000168	-0.0008764	0.5102259	

D	1.0959136D-01	-0.0000060	0.0003147	0.2855141
	F	4F		
BASIS/ORB.ENERGY		-1.4725493		
F	1.1878438D+03	-0.0001239		
F	3.5301992D+02	-0.0016590		
F	1.3444056D+02	-0.0120721		
F	5.8627888D+01	-0.0520353		
F	2.7303576D+01	-0.1477767		
F	1.3248721D+01	-0.2758059		
F	6.4051161D+00	-0.3483516		
F	3.0133576D+00	-0.3119179		
F	1.3376813D+00	-0.1869815		
F	5.2922518D-01	-0.0574666		

TUNGSTEN [XE]4F(14)6S(2)5D(4), 5D

CHARGE = 74.000000

SYMMETRY SPECIES	S	P	D	F
NUMBER OF BASIS FUNCTIONS	27	23	15	10
NUMBER OF CLOSED SHELLS	6	4	2	1
NUMBER OF OPEN SHELLS	0	0	1	0
OPEN SHELL OCCUPATION NUMBER	0	0	4	0

*** FINAL SCF RESULTS ***

E = -16141.675753694

ORBITAL ENERGIES AND EXPANSION COEFFICIENTS

	S	1S	2S	3S	4S	5S	6S
BASIS/ORB.ENERGY	-2569.7095000	-448.6437300	-105.6022300	-22.9711920	-3.4419686	-0.2607662	
S	7.7444361D+10	0.0000058	-0.0000022	0.0000011	0.0000005	-0.0000002	0.0000001
S	7.8061015D+09	0.0000223	-0.0000085	0.0000040	0.0000020	-0.0000008	0.0000002
S	1.2763080D+09	0.0000657	-0.0000250	0.0000119	0.0000058	-0.0000024	0.0000007
S	2.6213421D+08	0.0001780	-0.0000676	0.0000321	0.0000158	-0.0000064	0.0000018
S	6.0304759D+07	0.0004477	-0.0001700	0.0000807	0.0000396	-0.0000162	0.0000045
S	1.5700853D+07	0.0010200	-0.0003873	0.0001839	0.0000903	-0.0000368	0.0000103
S	4.5438689D+06	0.0021960	-0.0008348	0.0003965	0.0001948	-0.0000794	0.0000221
S	1.4199071D+06	0.0046005	-0.0017543	0.0008333	0.0004096	-0.0001669	0.0000465
S	4.6849215D+05	0.0094433	-0.0036204	0.0017222	0.0008463	-0.0003448	0.0000961

S	1.6310518D+05	0.0188736	-0.0073097	0.0034800	0.0017117	-0.0006976	0.0001945
S	5.9928441D+04	0.0371137	-0.0146097	0.0069832	0.0034341	-0.0013993	0.0003902
S	2.3169383D+04	0.0716305	-0.0290335	0.0139145	0.0068601	-0.0027974	0.0007798
S	9.4304454D+03	0.1330693	-0.0565509	0.0274120	0.0135099	-0.0055078	0.0015359
S	4.0231447D+03	0.2279161	-0.1057157	0.0517445	0.0256871	-0.0104906	0.0029250
S	1.7829351D+03	0.3193072	-0.1712447	0.0868516	0.0431395	-0.0176221	0.0049153
S	8.1463179D+02	0.2834389	-0.1827307	0.0944927	0.0479995	-0.0196977	0.0054974
S	3.7858995D+02	0.0999885	0.0558905	-0.0435919	-0.0254542	0.0107418	-0.0030151
S	1.8051598D+02	0.0037704	0.5180616	-0.4569254	-0.2570399	0.1081350	-0.0302704
S	8.7513697D+01	0.0012920	0.4970300	-0.5477517	-0.3486533	0.1510637	-0.0425506
S	3.7759665D+01	-0.0008322	0.0855982	0.4960401	0.4947028	-0.2371248	0.0678712
S	1.9595190D+01	0.0004824	-0.0114415	0.7986307	0.9820998	-0.5002605	0.1439186
S	8.1267225D+00	-0.0002325	0.0039960	0.1142979	-0.6040435	0.4508423	-0.1359572
S	4.0232341D+00	0.0001174	-0.0018814	-0.0126284	-0.8775898	0.8486050	-0.2774277
S	1.2203991D+00	-0.0000412	0.0006165	0.0035530	-0.0628283	-0.7338542	0.3233699
S	5.6409649D-01	0.0000199	-0.0002919	-0.0016812	0.0139220	-0.6489774	0.4152328
S	1.1177350D-01	-0.0000050	0.0000727	0.0003926	-0.0027441	-0.0260050	-0.6252128
S	4.1966778D-02	0.0000021	-0.0000304	-0.0001637	0.0011048	0.0067512	-0.5756317
	P	2P	3P	4P	5P		
BASIS/ORB. ENERGY	-393.2569300	-88.8519840	-17.3594650	-1.9378580			
P	5.4530298D+07	0.0000099	-0.0000050	-0.0000024	-0.0000009		
P	7.7507418D+06	0.0000329	-0.0000167	-0.0000081	-0.0000030		
P	1.5935863D+06	0.0000959	-0.0000487	-0.0000237	-0.0000087		
P	4.0360495D+05	0.0002632	-0.0001340	-0.0000651	-0.0000240		
P	1.1883930D+05	0.0007091	-0.0003619	-0.0001760	-0.0000649		
P	3.9486337D+04	0.0019151	-0.0009813	-0.0004777	-0.0001764		
P	1.4526332D+04	0.0052342	-0.0026981	-0.0013147	-0.0004852		
P	5.8215213D+03	0.0144139	-0.0074999	-0.0036647	-0.0013542		
P	2.5037406D+03	0.0389658	-0.0205987	-0.0100944	-0.0037294		
P	1.1437299D+03	0.0972201	-0.0528260	-0.0260834	-0.0096612		
P	5.5054038D+02	0.2043726	-0.1157702	-0.0576640	-0.0213705		
P	2.7681422D+02	0.3231198	-0.1926352	-0.0975028	-0.0363302		
P	1.4434462D+02	0.3227552	-0.1780937	-0.0869114	-0.0319491		
P	7.7087392D+01	0.1616778	0.0760313	0.0703949	0.0286517		
P	4.1627755D+01	0.0280167	0.4486689	0.3487289	0.1427246		

P	2.3041088D+01	0.0010696	0.4452109	0.3497640	0.1393729
P	1.2725048D+01	-0.0000850	0.1485516	-0.1809830	-0.1094530
P	6.8570117D+00	-0.0000341	0.0141460	-0.5969950	-0.3447579
P	3.6864894D+00	-0.0000495	0.0008889	-0.3889664	-0.2420310
P	1.9073753D+00	0.0000190	0.0000326	-0.0702908	0.2374130
P	9.7047703D-01	-0.0000083	-0.0000090	-0.0021310	0.5645651
P	4.6991339D-01	0.0000039	-0.0000097	-0.0005261	0.3717759
P	1.9619857D-01	-0.0000007	0.0000006	0.0001030	0.0615326

	D	3D	4D	5D
BASIS/ORB. ENERGY		-68.9788450	-10.0099020	-0.3725972
D	1.6747285D+04	0.0001021	-0.0000508	0.0000126
D	4.3995633D+03	0.0007102	-0.0003548	0.0000889
D	1.5663560D+03	0.0039241	-0.0019657	0.0004874
D	6.4936900D+02	0.0176440	-0.0089178	0.0022379
D	2.9699548D+02	0.0618838	-0.0316271	0.0078704
D	1.4463746D+02	0.1668987	-0.0870479	0.0219574
D	7.2846508D+01	0.3204460	-0.1656568	0.0412049
D	3.7346907D+01	0.3834513	-0.1737858	0.0430761
D	1.9271827D+01	0.2191820	0.0711861	-0.0294598
D	9.7599996D+00	0.0441545	0.4232258	-0.1245394
D	4.8219740D+00	0.0022968	0.4583712	-0.1387209
D	2.2886607D+00	0.0003664	0.1802736	0.0720097
D	9.2259124D-01	0.0000040	0.0155213	0.4061236
D	3.5484542D-01	0.0000063	-0.0004533	0.4984984
D	1.2275926D-01	-0.0000033	0.0001780	0.2556776

	F	4F
BASIS/ORB. ENERGY		-1.8292106
F	6.3213520D+02	-0.0005114
F	2.5495032D+02	-0.0026976
F	1.3040476D+02	-0.0106734
F	6.5640906D+01	-0.0422659
F	3.2042239D+01	-0.1262065
F	1.5730900D+01	-0.2583397
F	7.6233340D+00	-0.3510374
F	3.5844936D+00	-0.3307609

F 1.5857610D+00 -0.2008781
F 6.2238864D-01 -0.0585080

RHENIUM [XE]4F(14)6S(2)5D(5), 6S

CHARGE = 75.000000

SYMMETRY SPECIES	S	P	D	F
NUMBER OF BASIS FUNCTIONS	27	23	15	10
NUMBER OF CLOSED SHELLS	6	4	2	1
NUMBER OF OPEN SHELLS	0	0	1	0
OPEN SHELL OCCUPATION NUMBER	0	0	5	0

*** FINAL SCF RESULTS ***

E =-16692.058502205

ORBITAL ENERGIES AND EXPANSION COEFFICIENTS

	S	1S	2S	3S	4S	5S	6S
BASIS/ORB. ENERGY		-2649.4904000	-464.5559200	-109.8724200	-24.1431580	-3.6946336	-0.2704227
S 1.0105214D+11	0.0000051	-0.0000020	0.0000009	0.0000005	-0.0000002	-0.0000001	
S 9.9178402D+09	0.0000212	-0.0000081	0.0000039	0.0000019	-0.0000008	-0.0000002	
S 1.4004048D+09	0.0000721	-0.0000275	0.0000131	0.0000065	-0.0000027	-0.0000007	
S 2.5711410D+08	0.0001969	-0.0000751	0.0000357	0.0000176	-0.0000073	-0.0000020	
S 5.9901854D+07	0.0004681	-0.0001785	0.0000849	0.0000419	-0.0000173	-0.0000049	
S 1.5843201D+07	0.0010691	-0.0004078	0.0001940	0.0000956	-0.0000395	-0.0000111	
S 4.5989738D+06	0.0022960	-0.0008769	0.0004173	0.0002057	-0.0000850	-0.0000238	
S 1.4359158D+06	0.0048297	-0.0018502	0.0008806	0.0004342	-0.0001794	-0.0000503	
S 4.7003033D+05	0.0099637	-0.0038385	0.0018295	0.0009021	-0.0003726	-0.0001046	
S 1.6269448D+05	0.0198451	-0.0077246	0.0036846	0.0018184	-0.0007512	-0.0002108	
S 5.9724337D+04	0.0386961	-0.0153187	0.0073376	0.0036207	-0.0014959	-0.0004198	
S 2.3161222D+04	0.0740595	-0.0301960	0.0145010	0.0071731	-0.0029648	-0.0008320	
S 9.4327451D+03	0.1373187	-0.0587888	0.0285700	0.0141313	-0.0058425	-0.0016394	
S 4.0166927D+03	0.2330449	-0.1090085	0.0534863	0.0266417	-0.0110261	-0.0030957	
S 1.7814294D+03	0.3201982	-0.1736208	0.0884030	0.0440845	-0.0182729	-0.0051261	
S 8.1488614D+02	0.2770230	-0.1777161	0.0917910	0.0467725	-0.0194226	-0.0054665	
S 3.7788345D+02	0.0930052	0.0740332	-0.0557820	-0.0321388	0.0136205	0.0038739	
S 1.8225026D+02	0.0026057	0.5226779	-0.4682288	-0.2653041	0.1135187	0.0319281	
S 8.9086366D+01	0.0014161	0.4826284	-0.5283576	-0.3382066	0.1482914	0.0421963	
S 3.8481558D+01	-0.0008789	0.0818788	0.5191299	0.5226337	-0.2536510	-0.0735012	

S	2.0117040D+01	0.0005142	-0.0117454	0.7776672	0.9644660	-0.5021459	-0.1449976
S	8.4970481D+00	-0.0002457	0.0041294	0.1125849	-0.6001622	0.4604098	0.1389083
S	4.2217471D+00	0.0001206	-0.0018997	-0.0116320	-0.8870203	0.8669141	0.2888680
S	1.2715109D+00	-0.0000410	0.0006051	0.0032302	-0.0641204	-0.7810784	-0.3626824
S	5.8489144D-01	0.0000196	-0.0002843	-0.0015311	0.0146253	-0.6143917	-0.3819826
S	1.1453393D-01	-0.0000048	0.0000699	0.0003530	-0.0028883	-0.0215866	0.6728652
S	4.2256862D-02	0.0000020	-0.0000290	-0.0001462	0.0011588	0.0054647	0.5271216
	P	2P	3P	4P	5P		
BASIS/ORB. ENERGY	-406.4174700	-92.3701280	-18.2805020	-2.1061242			
P	5.4553082D+07	0.0000106	-0.0000054	-0.0000026	-0.0000010		
P	7.7507418D+06	0.0000351	-0.0000178	-0.0000087	-0.0000033		
P	1.5934334D+06	0.0001021	-0.0000520	-0.0000254	-0.0000095		
P	4.0366373D+05	0.0002799	-0.0001429	-0.0000697	-0.0000262		
P	1.1883930D+05	0.0007531	-0.0003855	-0.0001882	-0.0000707		
P	3.9486337D+04	0.0020280	-0.0010422	-0.0005096	-0.0001916		
P	1.4537295D+04	0.0055232	-0.0028558	-0.0013977	-0.0005254		
P	5.8257865D+03	0.0151758	-0.0079225	-0.0038886	-0.0014637		
P	2.5040419D+03	0.0408789	-0.0216910	-0.0106789	-0.0040185		
P	1.1434914D+03	0.1013226	-0.0552947	-0.0274333	-0.0103516		
P	5.5039936D+02	0.2107366	-0.1199574	-0.0600489	-0.0226689		
P	2.7680865D+02	0.3275371	-0.1960768	-0.0997371	-0.0378679		
P	1.4430410D+02	0.3184934	-0.1721770	-0.0835707	-0.0311899		
P	7.6944728D+01	0.1524447	0.0971093	0.0849042	0.0350158		
P	4.1603149D+01	0.0241107	0.4642942	0.3654179	0.1529284		
P	2.3022137D+01	0.0011082	0.4304563	0.3314347	0.1329507		
P	1.2696295D+01	-0.0002554	0.1339752	-0.2202765	-0.1312236		
P	6.8469580D+00	0.0000630	0.0115243	-0.6055401	-0.3637652		
P	3.6841190D+00	-0.0000997	0.0008836	-0.3617722	-0.2216892		
P	1.9041662D+00	0.0000476	-0.0000536	-0.0582597	0.2907233		
P	9.7102201D-01	-0.0000215	0.0000138	-0.0016166	0.5693369		
P	4.7204599D-01	0.0000089	-0.0000204	-0.0004194	0.3330452		
P	1.9661870D-01	-0.0000018	0.0000026	0.0000801	0.0488789		
	D	3D	4D	5D			
BASIS/ORB. ENERGY	-71.8671780	-10.6723970	-0.4336206				
D	1.7746359D+04	0.0001031	-0.0000517	0.0000136			

D	4.4469144D+03	0.0007686	-0.0003868	0.0001022
D	1.5616227D+03	0.0042103	-0.0021270	0.0005586
D	6.5062171D+02	0.0186208	-0.0094842	0.0025107
D	2.9756038D+02	0.0652745	-0.0336626	0.0088723
D	1.4472488D+02	0.1740530	-0.0915041	0.0243517
D	7.2910863D+01	0.3276136	-0.1705318	0.0449479
D	3.7417531D+01	0.3807349	-0.1698084	0.0439396
D	1.9294708D+01	0.2080412	0.0919390	-0.0372887
D	9.7517951D+00	0.0391280	0.4403652	-0.1387812
D	4.8121284D+00	0.0019161	0.4482922	-0.1396885
D	2.2834578D+00	0.0003050	0.1590723	0.0958943
D	9.5800244D-01	0.0000008	0.0116439	0.4246883
D	3.8057095D-01	0.0000045	0.0000277	0.4817551
D	1.3585956D-01	-0.0000024	-0.0000398	0.2282425
	F	4F		
BASIS/ORB. ENERGY				
F	8.5206756D+02	0.0002812		
F	3.1904614D+02	0.0021697		
F	1.3897068D+02	0.0122335		
F	6.6108754D+01	0.0456331		
F	3.3268171D+01	0.1201515		
F	1.7262090D+01	0.2350406		
F	8.7627437D+00	0.3343301		
F	4.2440777D+00	0.3374378		
F	1.9191791D+00	0.2169076		
F	7.6395347D-01	0.0668083		

OSMIUM [XE]4F(14)6S(2)5D(6), 5D

CHARGE = 76.000000

SYMMETRY SPECIES	S	P	D	F
NUMBER OF BASIS FUNCTIONS	27	23	15	10
NUMBER OF CLOSED SHELLS	6	4	2	1
NUMBER OF OPEN SHELLS	0	0	1	0
OPEN SHELL OCCUPATION NUMBER	0	0	6	0

*** FINAL SCF RESULTS ***

E =-17254.270006956

ORBITAL ENERGIES AND EXPANSION COEFFICIENTS

	S	1S	2S	3S	4S	5S	6S
BASIS/ORB. ENERGY		-2730.8926000	-480.8772700	-114.2823100	-25.3733790	-3.9694385	-0.2841982
S 1.6533730D+11		0.0000039	-0.0000015	0.0000007	0.0000004	0.0000001	0.0000000
S 1.6450041D+10		0.0000155	-0.0000060	0.0000028	0.0000014	0.0000006	-0.0000002
S 2.5734617D+09		0.0000477	-0.0000183	0.0000087	0.0000043	0.0000018	-0.0000005
S 5.1602382D+08		0.0001263	-0.0000484	0.0000231	0.0000114	0.0000048	-0.0000014
S 1.2386770D+08		0.0002986	-0.0001144	0.0000545	0.0000270	0.0000113	-0.0000032
S 3.3755743D+07		0.0006665	-0.0002554	0.0001217	0.0000602	0.0000252	-0.0000072
S 9.9145483D+06		0.0014468	-0.0005544	0.0002643	0.0001307	0.0000547	-0.0000156
S 3.0969574D+06		0.0029961	-0.0011512	0.0005487	0.0002715	0.0001137	-0.0000324
S 1.0285530D+06		0.0060377	-0.0023252	0.0011093	0.0005488	0.0002297	-0.0000655
S 3.5742837D+05		0.0119890	-0.0046572	0.0022234	0.0011005	0.0004608	-0.0001313
S 1.2985763D+05		0.0234305	-0.0091766	0.0043918	0.0021739	0.0009101	-0.0002594
S 4.9115804D+04		0.0454741	-0.0182447	0.0087512	0.0043376	0.0018172	-0.0005179
S 1.9341982D+04		0.0868185	-0.0357308	0.0172569	0.0085570	0.0035834	-0.0010214
S 7.9016192D+03		0.1614467	-0.0710887	0.0345957	0.0172173	0.0072209	-0.0020582
S 3.3021777D+03		0.2751639	-0.1323044	0.0657792	0.0328219	0.0137634	-0.0039233
S 1.4106157D+03		0.3460485	-0.2047111	0.1048144	0.0528957	0.0222614	-0.0063502
S 6.1864959D+02		0.2239547	-0.1100431	0.0560173	0.0278382	0.0116436	-0.0033134
S 2.4567379D+02		0.0348079	0.4056341	-0.3305270	-0.1850506	-0.0797045	0.0227991
S 1.1122219D+02		-0.0048091	0.6290830	-0.6725662	-0.4149007	-0.1834048	0.0527705
S 4.4716532D+01		0.0026809	0.1458269	0.2734616	0.2815261	0.1396583	-0.0410700
S 2.3297712D+01		-0.0017846	-0.0243983	0.9277245	1.1161238	0.5807463	-0.1709392
S 9.3212246D+00		0.0008704	0.0091041	0.1623286	-0.4229260	-0.3384407	0.1046648
S 4.6722302D+00		-0.0004364	-0.0043567	-0.0209333	-0.9992733	-0.9674380	0.3243869
S 1.3565983D+00		0.0001545	0.0014527	0.0057201	-0.0812404	0.7489507	-0.3567509
S 6.4138041D-01		-0.0000796	-0.0007345	-0.0028296	0.0208071	0.6391389	-0.3994624
S 1.3063625D-01		0.0000194	0.0001794	0.0006560	-0.0040290	0.0258525	0.6274420
S 4.7541380D-02		-0.0000078	-0.0000723	-0.0002638	0.0015670	-0.0062836	0.5777940
	P	2P	3P	4P	5P		
BASIS/ORB. ENERGY		-419.8528600	-95.9939600	-19.2485480	-2.2919057		
P 5.4369194D+07		0.0000113	-0.0000058	-0.0000028	-0.0000011		
P 7.7421807D+06		0.0000374	-0.0000191	-0.0000093	-0.0000036		

P	1.5947917D+06	0.0001086	-0.0000555	-0.0000272	-0.0000104
P	4.0372204D+05	0.0002979	-0.0001524	-0.0000747	-0.0000286
P	1.1875146D+05	0.0007996	-0.0004104	-0.0002013	-0.0000770
P	3.9489176D+04	0.0021451	-0.0011055	-0.0005429	-0.0002078
P	1.4546855D+04	0.0058278	-0.0030224	-0.0014859	-0.0005687
P	5.8287506D+03	0.0159668	-0.0083627	-0.0041232	-0.0015801
P	2.5043916D+03	0.0428495	-0.0228209	-0.0112878	-0.0043248
P	1.1432245D+03	0.1055140	-0.0578289	-0.0288285	-0.0110764
P	5.5029017D+02	0.2170395	-0.1241385	-0.0624568	-0.0240089
P	2.7683061D+02	0.3316072	-0.1992617	-0.1018475	-0.0393795
P	1.4426916D+02	0.3138182	-0.1655250	-0.0797499	-0.0301963
P	7.6795405D+01	0.1434289	0.1186246	0.1000550	0.0419142
P	4.1587288D+01	0.0205865	0.4777673	0.3807010	0.1627665
P	2.3013150D+01	0.0011781	0.4149541	0.3108076	0.1251065
P	1.2665653D+01	-0.0004141	0.1206667	-0.2586121	-0.1537612
P	6.8412648D+00	0.0001553	0.0092051	-0.6103190	-0.3814796
P	3.6864177D+00	-0.0001469	0.0009314	-0.3346683	-0.1969853
P	1.9004196D+00	0.0000742	-0.0001538	-0.0481982	0.3463868
P	9.6768755D-01	-0.0000339	0.0000470	-0.0011646	0.5675261
P	4.7339406D-01	0.0000137	-0.0000344	-0.0003547	0.2920526
P	1.9717399D-01	-0.0000028	0.0000053	0.0000652	0.0389948
	D	3D	4D	5D	
BASIS/ORB. ENERGY	-74.8427430	-11.3745610	-0.4508356		
D	1.7143743D+04	0.0001148	-0.0000581	0.0000159	
D	4.4281331D+03	0.0008150	-0.0004132	0.0001136	
D	1.5691091D+03	0.0044590	-0.0022704	0.0006229	
D	6.5226703D+02	0.0197270	-0.0101266	0.0027894	
D	2.9799642D+02	0.0687494	-0.0357589	0.0098463	
D	1.4479761D+02	0.1813027	-0.0960870	0.0266082	
D	7.3018190D+01	0.3335134	-0.1746415	0.0481202	
D	3.7600135D+01	0.3761461	-0.1651559	0.0439119	
D	1.9413692D+01	0.1986465	0.1109226	-0.0446628	
D	9.7558259D+00	0.0352702	0.4590530	-0.1530800	
D	4.7821248D+00	0.0014614	0.4386983	-0.1365831	
D	2.2458991D+00	0.0002988	0.1368709	0.1288507	

D	9.7226157D-01	-0.0000271	0.0076075	0.4393179
D	3.9195833D-01	0.0000090	0.0006707	0.4593388
D	1.4108079D-01	-0.0000053	-0.0001187	0.2101190
	F	4F		
BASIS/ORB.ENERGY		-2.6098175		
F	1.0327856D+03	0.0002349		
F	3.2820297D+02	0.0024976		
F	1.3686844D+02	0.0140344		
F	6.5596999D+01	0.0492317		
F	3.3371014D+01	0.1277231		
F	1.7297401D+01	0.2472903		
F	8.7805324D+00	0.3391710		
F	4.3009337D+00	0.3269171		
F	1.9824156D+00	0.1988272		
F	8.0765539D-01	0.0563222		

IRIDIUM [XE]4F(14)6S(2)5D(7), 4F

CHARGE = 77.000000

SYMMETRY SPECIES	S	P	D	F
NUMBER OF BASIS FUNCTIONS	27	23	15	10
NUMBER OF CLOSED SHELLS	6	4	2	1
NUMBER OF OPEN SHELLS	0	0	1	0
OPEN SHELL OCCUPATION NUMBER	0	0	7	0

*** FINAL SCF RESULTS ***

E = -17828.640193122

ORBITAL ENERGIES AND EXPANSION COEFFICIENTS

	S	1S	2S	3S	4S	5S	6S
BASIS/ORB.ENERGY	-2813.9189000	-497.5919100	-118.8095700	-26.6380250	-4.2454588	-0.2960343	
S	1.5407728D+11	0.0000043	-0.0000017	0.0000008	0.0000004	0.0000002	0.0000000
S	1.6236210D+10	0.0000166	-0.0000064	0.0000031	0.0000015	0.0000006	-0.0000002
S	2.5647660D+09	0.0000503	-0.0000194	0.0000093	0.0000046	0.0000019	-0.0000006
S	5.3657014D+08	0.0001279	-0.0000493	0.0000235	0.0000117	0.0000050	-0.0000014
S	1.3078862D+08	0.0003075	-0.0001184	0.0000565	0.0000280	0.0000119	-0.0000034
S	3.5093707D+07	0.0006981	-0.0002688	0.0001283	0.0000637	0.0000270	-0.0000078
S	1.0210191D+07	0.0015023	-0.0005785	0.0002762	0.0001371	0.0000581	-0.0000167

S	3.1853167D+06	0.0031144	-0.0012022	0.0005741	0.0002849	0.0001208	-0.0000347
S	1.0479788D+06	0.0063286	-0.0024490	0.0011705	0.0005810	0.0002462	-0.0000708
S	3.6160683D+05	0.0125109	-0.0048829	0.0023354	0.0011598	0.0004917	-0.0001413
S	1.3090626D+05	0.0244411	-0.0096234	0.0046142	0.0022917	0.0009713	-0.0002791
S	4.9287476D+04	0.0473313	-0.0190896	0.0091743	0.0045626	0.0019353	-0.0005561
S	1.9392295D+04	0.0895550	-0.0371001	0.0179558	0.0089342	0.0037878	-0.0010884
S	7.9359883D+03	0.1648843	-0.0730836	0.0356468	0.0178021	0.0075602	-0.0021729
S	3.3249459D+03	0.2777295	-0.1346705	0.0671294	0.0336150	0.0142697	-0.0041005
S	1.4237126D+03	0.3436063	-0.2043779	0.1048885	0.0531256	0.0226469	-0.0065157
S	6.2697354D+02	0.2169216	-0.1022195	0.0514572	0.0255270	0.0107738	-0.0030842
S	2.5228449D+02	0.0330464	0.4095227	-0.3352638	-0.1885615	-0.0822169	0.0236994
S	1.1459108D+02	-0.0042426	0.6239474	-0.6686733	-0.4144038	-0.1857814	0.0539608
S	4.6252410D+01	0.0023449	0.1452435	0.2776146	0.2875622	0.1452654	-0.0432640
S	2.4128959D+01	-0.0015704	-0.0245352	0.9238403	1.1170603	0.5889044	-0.1747011
S	9.7366503D+00	0.0007776	0.0093759	0.1634695	-0.4135266	-0.3343579	0.1038556
S	4.9080511D+00	-0.0003951	-0.0045574	-0.0207904	-1.0069522	-0.9986552	0.3404797
S	1.4827094D+00	0.0001413	0.0015378	0.0057108	-0.0849340	0.7142159	-0.3505833
S	7.0513974D-01	-0.0000701	-0.0007482	-0.0027133	0.0199701	0.6855759	-0.4114292
S	1.3623170D-01	0.0000161	0.0001724	0.0005887	-0.0036177	0.0295057	0.6420305
S	4.9774537D-02	-0.0000067	-0.0000710	-0.0002419	0.0014377	-0.0077533	0.5581394
	P	2P	3P	4P	5P		
BASIS/ORB. ENERGY	-433.5392900	-99.6985750	-20.2387810	-2.4769364			
P	5.3288951D+07	0.0000123	-0.0000063	-0.0000031	-0.0000012		
P	7.5748706D+06	0.0000405	-0.0000207	-0.0000102	-0.0000040		
P	1.5641272D+06	0.0001169	-0.0000599	-0.0000295	-0.0000115		
P	3.9941160D+05	0.0003168	-0.0001625	-0.0000800	-0.0000311		
P	1.1874375D+05	0.0008407	-0.0004326	-0.0002131	-0.0000829		
P	3.9762614D+04	0.0022479	-0.0011617	-0.0005730	-0.0002229		
P	1.4630867D+04	0.0061347	-0.0031908	-0.0015757	-0.0006129		
P	5.8393648D+03	0.0168175	-0.0088366	-0.0043764	-0.0017042		
P	2.5037540D+03	0.0449314	-0.0240171	-0.0119353	-0.0046482		
P	1.1428892D+03	0.1096854	-0.0603713	-0.0302398	-0.0118069		
P	5.5021367D+02	0.2236017	-0.1284914	-0.0649772	-0.0253946		
P	2.7630742D+02	0.3369363	-0.2031630	-0.1043239	-0.0409840		
P	1.4362535D+02	0.3085241	-0.1574101	-0.0749610	-0.0287477		

P	7.6371145D+01	0.1331080	0.1428418	0.1173676	0.0500036
P	4.1444913D+01	0.0174605	0.4902838	0.3956508	0.1722519
P	2.2920241D+01	0.0010380	0.3974485	0.2858908	0.1149798
P	1.2596815D+01	-0.0004148	0.1067264	-0.2994641	-0.1793984
P	6.8110112D+00	0.0001481	0.0074571	-0.6130534	-0.3967097
P	3.6709846D+00	-0.0001363	0.0007687	-0.3034803	-0.1690830
P	1.9291885D+00	0.0000690	-0.0001367	-0.0387509	0.3903404
P	9.7137476D-01	-0.0000283	0.0000194	-0.0019078	0.5750121
P	4.6320896D-01	0.0000111	-0.0000242	-0.0000214	0.2567050
P	1.8076245D-01	-0.0000022	0.0000028	-0.0000025	0.0252900

	D	3D	4D	5D
BASIS/ORB. ENERGY		-77.8800950	-12.0918510	-0.4835845
D	1.7150290D+04	0.0001231	-0.0000628	0.0000179
D	4.4301401D+03	0.0008716	-0.0004450	0.0001269
D	1.5700663D+03	0.0047507	-0.0024390	0.0006961
D	6.5255850D+02	0.0209275	-0.0108220	0.0030928
D	2.9798838D+02	0.0724119	-0.0380036	0.0108873
D	1.4481227D+02	0.1885477	-0.1006651	0.0289224
D	7.3049089D+01	0.3402262	-0.1793339	0.0514328
D	3.7643600D+01	0.3723580	-0.1593481	0.0433016
D	1.9406176D+01	0.1876554	0.1325419	-0.0535235
D	9.7536543D+00	0.0307870	0.4725317	-0.1654776
D	4.7830041D+00	0.0013753	0.4254695	-0.1316652
D	2.2284709D+00	0.0001754	0.1196660	0.1642531
D	9.7365018D-01	0.0000026	0.0047445	0.4597784
D	3.9305112D-01	-0.0000073	0.0010056	0.4369166
D	1.4264963D-01	-0.0000014	-0.0001607	0.1803440

	F	4F
BASIS/ORB. ENERGY		-3.0312712
F	8.3274020D+02	0.0003687
F	3.1533614D+02	0.0026692
F	1.3946640D+02	0.0145464
F	6.6563591D+01	0.0530908
F	3.3441924D+01	0.1382197
F	1.7262282D+01	0.2581772

F	8.8247886D+00	0.3389145
F	4.4024321D+00	0.3142808
F	2.0738695D+00	0.1849582
F	8.5810590D-01	0.0493539

PLATINUM [XE]4F(14)6S(1)5D(9), 3D

CHARGE = 78.000000

SYMMETRY SPECIES	S	P	D	F
NUMBER OF BASIS FUNCTIONS	27	23	15	10
NUMBER OF CLOSED SHELLS	5	4	2	1
NUMBER OF OPEN SHELLS	1	0	1	0
OPEN SHELL OCCUPATION NUMBER	1	0	9	0

*** FINAL SCF RESULTS ***

E = -18415.319144481

ORBITAL ENERGIES AND EXPANSION COEFFICIENTS

	S	1S	2S	3S	4S	5S	6S
BASIS/ORB. ENERGY	-2898.4822000	-514.5865200	-123.3345200	-27.8153430	-4.4052654	-0.2910502	
S 1.8472855D+11	0.0000043	-0.0000017	0.0000008	0.0000004	0.0000002	0.0000000	
S 1.7665223D+10	0.0000171	-0.0000066	0.0000032	0.0000016	0.0000007	-0.0000002	
S 2.7896841D+09	0.0000510	-0.0000198	0.0000095	0.0000047	0.0000020	-0.0000006	
S 5.6774131D+08	0.0001347	-0.0000522	0.0000250	0.0000124	0.0000053	-0.0000015	
S 1.3407865D+08	0.0003264	-0.0001263	0.0000604	0.0000301	0.0000128	-0.0000036	
S 3.5741727D+07	0.0007293	-0.0002822	0.0001349	0.0000672	0.0000287	-0.0000080	
S 1.0452539D+07	0.0015601	-0.0006036	0.0002887	0.0001437	0.0000614	-0.0000171	
S 3.2592628D+06	0.0032413	-0.0012571	0.0006013	0.0002994	0.0001279	-0.0000356	
S 1.0675873D+06	0.0066118	-0.0025711	0.0012309	0.0006130	0.0002618	-0.0000730	
S 3.6473522D+05	0.0131734	-0.0051663	0.0024754	0.0012333	0.0005268	-0.0001468	
S 1.3101415D+05	0.0255612	-0.0101188	0.0048602	0.0024218	0.0010343	-0.0002883	
S 4.9393816D+04	0.0490067	-0.0198725	0.0095695	0.0047748	0.0020406	-0.0005685	
S 1.9432965D+04	0.0926709	-0.0386436	0.0187382	0.0093550	0.0039967	-0.0011144	
S 7.9434799D+03	0.1688908	-0.0753868	0.0368607	0.0184703	0.0079030	-0.0022015	
S 3.3428936D+03	0.2789300	-0.1363833	0.0681382	0.0342407	0.0146487	-0.0040873	
S 1.4418872D+03	0.3391396	-0.2026910	0.1042881	0.0530012	0.0227616	-0.0063387	
S 6.3936911D+02	0.2115453	-0.0958565	0.0475461	0.0235485	0.0100115	-0.0028105	
S 2.5957531D+02	0.0322670	0.4116989	-0.3380245	-0.1909905	-0.0839984	0.0235820	

S	1.1829514D+02	-0.0040677	0.6186101	-0.6658055	-0.4142932	-0.1871651	0.0524894
S	4.8496136D+01	0.0022472	0.1446500	0.2666165	0.2771794	0.1409150	-0.0399327
S	2.5205052D+01	-0.0014861	-0.0221035	0.9297510	1.1278511	0.6009425	-0.1746560
S	1.0220688D+01	0.0007382	0.0085077	0.1699230	-0.3880796	-0.3223568	0.1011596
S	5.1647690D+00	-0.0003740	-0.0041229	-0.0214928	-1.0269968	-1.0224557	0.3316692
S	1.5505902D+00	0.0001354	0.0014023	0.0060077	-0.0884588	0.7382854	-0.3385830
S	7.3329681D-01	-0.0000708	-0.0007175	-0.0030093	0.0222134	0.6635327	-0.4063044
S	1.6979756D-01	0.0000181	0.0001834	0.0007283	-0.0045261	0.0322224	0.4387033
S	5.9344671D-02	-0.0000066	-0.0000672	-0.0002667	0.0016112	-0.0065692	0.7577751
	P	2P	3P	4P	5P		
BASIS/ORB. ENERGY	-447.3582500	-103.3638800	-21.1308240	-2.5597108			
P	5.2551826D+07	0.0000132	-0.0000068	-0.0000033	-0.0000013		
P	7.5446465D+06	0.0000431	-0.0000221	-0.0000109	-0.0000043		
P	1.5602497D+06	0.0001249	-0.0000641	-0.0000317	-0.0000124		
P	3.9786606D+05	0.0003365	-0.0001731	-0.0000856	-0.0000336		
P	1.1893982D+05	0.0008877	-0.0004580	-0.0002267	-0.0000890		
P	3.9790141D+04	0.0023799	-0.0012333	-0.0006110	-0.0002399		
P	1.4639627D+04	0.0064593	-0.0033695	-0.0016715	-0.0006563		
P	5.8425603D+03	0.0176911	-0.0093252	-0.0046389	-0.0018234		
P	2.5026396D+03	0.0470340	-0.0252320	-0.0125991	-0.0049533		
P	1.1430125D+03	0.1139107	-0.0629581	-0.0316839	-0.0124876		
P	5.5014265D+02	0.2300554	-0.1328105	-0.0675138	-0.0266410		
P	2.7624427D+02	0.3403162	-0.2057971	-0.1061309	-0.0420855		
P	1.4358046D+02	0.3027062	-0.1490493	-0.0700728	-0.0269940		
P	7.6283759D+01	0.1245895	0.1645497	0.1335424	0.0574494		
P	4.1438911D+01	0.0149073	0.5006546	0.4083695	0.1798786		
P	2.2887043D+01	0.0009969	0.3805690	0.2614192	0.1035906		
P	1.2581973D+01	-0.0004589	0.0947678	-0.3362618	-0.2018508		
P	6.8032374D+00	0.0001700	0.0063895	-0.6133544	-0.4094862		
P	3.6625440D+00	-0.0001430	0.0005176	-0.2755639	-0.1320966		
P	1.9322378D+00	0.0000738	-0.0000700	-0.0307683	0.4312057		
P	9.7138065D-01	-0.0000293	-0.0000228	-0.0019365	0.5579140		
P	4.5992982D-01	0.0000114	-0.0000129	0.0000051	0.2319543		
P	1.7625277D-01	-0.0000021	-0.0000013	-0.0000454	0.0207505		
	D	3D	4D	5D			

BASIS/ORB. ENERGY	-80.8589250	-12.7048720	-0.4118064
D 1.7132605D+04	0.0001319	-0.0000678	0.0000194
D 4.4330328D+03	0.0009316	-0.0004789	0.0001365
D 1.5707842D+03	0.0050544	-0.0026162	0.0007490
D 6.5307126D+02	0.0221690	-0.0115478	0.0032999
D 2.9793171D+02	0.0762462	-0.0403720	0.0116023
D 1.4482256D+02	0.1957045	-0.1052417	0.0302289
D 7.3095243D+01	0.3466809	-0.1838885	0.0529440
D 3.7674886D+01	0.3681553	-0.1526639	0.0406576
D 1.9391481D+01	0.1766864	0.1544888	-0.0605833
D 9.7570972D+00	0.0267894	0.4836356	-0.1716608
D 4.7940839D+00	0.0013063	0.4108474	-0.1191876
D 2.2117054D+00	0.0000758	0.1044088	0.1923352
D 9.7497560D-01	0.0000224	0.0028210	0.4530582
D 3.8981252D-01	-0.0000224	0.0014625	0.4219673
D 1.3667229D-01	-0.0000005	-0.0000865	0.1897757

F 4F

BASIS/ORB. ENERGY	-3.3455868
F 1.4380312D+03	0.0001284
F 4.5867494D+02	0.0014422
F 1.8197510D+02	0.0100108
F 8.1000401D+01	0.0448538
F 3.8248610D+01	0.1345728
F 1.8816155D+01	0.2694461
F 9.2984602D+00	0.3572838
F 4.5320724D+00	0.3189917
F 2.1117028D+00	0.1709260
F 8.7343243D-01	0.0408919

GOLD [XE]4F(14)6S(1)5D(10), 2S

CHARGE = 79.000000

SYMMETRY SPECIES	S	P	D	F
NUMBER OF BASIS FUNCTIONS	27	23	15	10
NUMBER OF CLOSED SHELLS	5	4	3	1
NUMBER OF OPEN SHELLS	1	0	0	0

OPEN SHELL OCCUPATION NUMBER 1 0 0 0

*** FINAL SCF RESULTS ***

E = -19014.506992841

ORBITAL ENERGIES AND EXPANSION COEFFICIENTS

	S	1S	2S	3S	4S	5S	6S
BASIS/ORB. ENERGY	-2984.8419000	-532.1085300	-128.0977800	-29.1456300	-4.6831212	-0.2898901	
S 1.8292916D+11	0.0000046	-0.0000018	0.0000009	0.0000004	0.0000002	-0.0000001	
S 1.7915395D+10	0.0000182	-0.0000071	0.0000034	0.0000017	0.0000007	-0.0000002	
S 2.7914950D+09	0.0000549	-0.0000214	0.0000102	0.0000051	0.0000022	-0.0000006	
S 5.7042440D+08	0.0001419	-0.0000552	0.0000265	0.0000132	0.0000057	-0.0000016	
S 1.3760160D+08	0.0003354	-0.0001304	0.0000625	0.0000312	0.0000135	-0.0000037	
S 3.7040264D+07	0.0007612	-0.0002959	0.0001417	0.0000708	0.0000305	-0.0000084	
S 1.0608426D+07	0.0016621	-0.0006462	0.0003096	0.0001546	0.0000667	-0.0000183	
S 3.2762261D+06	0.0034016	-0.0013256	0.0006352	0.0003173	0.0001369	-0.0000375	
S 1.0788147D+06	0.0068629	-0.0026819	0.0012861	0.0006426	0.0002772	-0.0000759	
S 3.7001856D+05	0.0136332	-0.0053724	0.0025786	0.0012890	0.0005562	-0.0001522	
S 1.3300838D+05	0.0264282	-0.0105171	0.0050604	0.0025298	0.0010915	-0.0002987	
S 4.9955339D+04	0.0508309	-0.0207176	0.0099950	0.0050039	0.0021600	-0.0005910	
S 1.9510300D+04	0.0962939	-0.0404222	0.0196389	0.0098372	0.0042459	-0.0011624	
S 7.9342639D+03	0.1736455	-0.0780576	0.0382547	0.0192373	0.0083135	-0.0022744	
S 3.3483330D+03	0.2808028	-0.1385571	0.0694037	0.0349928	0.0151275	-0.0041435	
S 1.4528423D+03	0.3352020	-0.2013294	0.1038161	0.0529702	0.0229706	-0.0062853	
S 6.4758292D+02	0.2047319	-0.0878313	0.0427271	0.0210083	0.0090256	-0.0024794	
S 2.6628397D+02	0.0305218	0.4157540	-0.3428243	-0.1944413	-0.0865115	0.0238209	
S 1.2175325D+02	-0.0035003	0.6128134	-0.6618115	-0.4141143	-0.1889554	0.0521324	
S 5.0355493D+01	0.0018808	0.1431181	0.2681648	0.2812560	0.1440265	-0.0403853	
S 2.6104885D+01	-0.0012244	-0.0207381	0.9301988	1.1307309	0.6114106	-0.1741004	
S 1.0566874D+01	0.0006048	0.0080245	0.1705558	-0.3910475	-0.3347088	0.1021631	
S 5.3726006D+00	-0.0003048	-0.0038940	-0.0221410	-1.0274633	-1.0340742	0.3326120	
S 1.6183897D+00	0.0001045	0.0012558	0.0058349	-0.0853460	0.7834060	-0.3660667	
S 7.5175030D-01	-0.0000512	-0.0006011	-0.0027480	0.0199194	0.6362243	-0.3587159	
S 1.5000327D-01	0.0000121	0.0001426	0.0006166	-0.0037928	0.0254508	0.5528581	
S 5.2826349D-02	-0.0000048	-0.0000567	-0.0002439	0.0014618	-0.0054577	0.6337879	
	P	2P	3P	4P	5P		
BASIS/ORB. ENERGY	-461.5483100	-107.2270300	-22.1616220	-2.7427377			

P	5.2550552D+07	0.0000142	-0.0000073	-0.0000036	-0.0000014
P	7.3441452D+06	0.0000469	-0.0000241	-0.0000120	-0.0000048
P	1.5427204D+06	0.0001321	-0.0000680	-0.0000338	-0.0000134
P	3.9776968D+05	0.0003565	-0.0001839	-0.0000913	-0.0000363
P	1.1892102D+05	0.0009392	-0.0004859	-0.0002415	-0.0000960
P	3.9903694D+04	0.0025035	-0.0013009	-0.0006473	-0.0002576
P	1.4671297D+04	0.0068095	-0.0035622	-0.0017749	-0.0007063
P	5.8432763D+03	0.0186032	-0.0098375	-0.0049157	-0.0019580
P	2.5019242D+03	0.0491931	-0.0264828	-0.0132844	-0.0052941
P	1.1429128D+03	0.1182335	-0.0656241	-0.0331833	-0.0132543
P	5.5015701D+02	0.2363550	-0.1370425	-0.0700092	-0.0280090
P	2.7617684D+02	0.3435252	-0.2083234	-0.1079144	-0.0433576
P	1.4347346D+02	0.2967303	-0.1396647	-0.0643466	-0.0249786
P	7.6033991D+01	0.1163448	0.1871178	0.1505124	0.0657565
P	4.1438478D+01	0.0121925	0.5068619	0.4183377	0.1870340
P	2.2907685D+01	0.0012133	0.3641875	0.2342097	0.0912229
P	1.2526282D+01	-0.0006479	0.0849703	-0.3722602	-0.2269354
P	6.7923370D+00	0.0002882	0.0046080	-0.6082638	-0.4193234
P	3.6542217D+00	-0.0002069	0.0007149	-0.2484760	-0.0939975
P	1.9405845D+00	0.0001075	-0.0002164	-0.0243354	0.4715999
P	9.6818459D-01	-0.0000418	0.0000283	-0.0019714	0.5474702
P	4.5156405D-01	0.0000153	-0.0000306	0.0000706	0.1994192
P	1.6468148D-01	-0.0000029	0.0000026	-0.0000521	0.0140070
	D	3D	4D	5D	
BASIS/ORB. ENERGY	-84.0149930	-13.4485390	-0.4523359		
D	1.6934048D+04	0.0001424	-0.0000737	0.0000217	
D	4.4539466D+03	0.0009786	-0.0005069	0.0001487	
D	1.5803312D+03	0.0053527	-0.0027921	0.0008242	
D	6.5318404D+02	0.0235748	-0.0123786	0.0036417	
D	2.9776176D+02	0.0800280	-0.0427365	0.0126669	
D	1.4494472D+02	0.2027544	-0.1098954	0.0324952	
D	7.3143912D+01	0.3530829	-0.1882611	0.0559134	
D	3.7729467D+01	0.3623977	-0.1453565	0.0389939	
D	1.9439955D+01	0.1664797	0.1755918	-0.0697469	
D	9.7693369D+00	0.0237466	0.4946741	-0.1828869	

D	4.8084185D+00	0.0010826	0.3941129	-0.1090222
D	2.2101367D+00	0.0000684	0.0909117	0.2270153
D	9.7822853D-01	0.0000242	0.0011783	0.4629546
D	3.9580645D-01	-0.0000113	0.0010697	0.3983602
D	1.4203377D-01	0.0000032	-0.0002709	0.1653877
F		4F		
BASIS/ORB.ENERGY		-3.7885708		
F	1.2733749D+03	0.0001814		
F	4.3181235D+02	0.0017153		
F	1.8223462D+02	0.0101823		
F	8.5326812D+01	0.0417933		
F	4.1900789D+01	0.1208065		
F	2.1305811D+01	0.2457928		
F	1.0796232D+01	0.3467892		
F	5.3227245D+00	0.3354098		
F	2.4860055D+00	0.1917093		
F	1.0232078D+00	0.0476742		

MERCURY [XE]4F(14)6S(2)5D(10), 1S

CHARGE = 80.000000

SYMMETRY SPECIES	S	P	D	F
NUMBER OF BASIS FUNCTIONS	27	23	15	10
NUMBER OF CLOSED SHELLS	6	4	3	1
NUMBER OF OPEN SHELLS	0	0	0	0
OPEN SHELL OCCUPATION NUMBER	0	0	0	0

*** FINAL SCF RESULTS ***

E = -19626.258988046

ORBITAL ENERGIES AND EXPANSION COEFFICIENTS

	S	1S	2S	3S	4S	5S	6S
BASIS/ORB.ENERGY		-3073.0571000	-550.1964500	-133.1302900	-30.6573580	-5.1029328	-0.3265558
S	1.9277921D+11	0.0000048	-0.0000019	0.0000009	0.0000005	0.0000002	-0.0000001
S	1.9187256D+10	0.0000185	-0.0000073	0.0000035	0.0000017	0.0000008	-0.0000002
S	3.0313463D+09	0.0000559	-0.0000219	0.0000105	0.0000053	0.0000023	-0.0000007
S	6.0468256D+08	0.0001482	-0.0000580	0.0000278	0.0000139	0.0000061	-0.0000018
S	1.4229863D+08	0.0003555	-0.0001389	0.0000667	0.0000334	0.0000146	-0.0000042

S	3.7651363D+07	0.0008003	-0.0003127	0.0001500	0.0000752	0.0000329	-0.0000096
S	1.0819765D+07	0.0017344	-0.0006776	0.0003252	0.0001630	0.0000713	-0.0000207
S	3.3141332D+06	0.0035956	-0.0014079	0.0006758	0.0003388	0.0001482	-0.0000430
S	1.0841614D+06	0.0071865	-0.0028224	0.0013558	0.0006797	0.0002974	-0.0000864
S	3.7243776D+05	0.0142177	-0.0056305	0.0027071	0.0013577	0.0005942	-0.0001726
S	1.3349760D+05	0.0275895	-0.0110390	0.0053207	0.0026690	0.0011679	-0.0003392
S	5.0068919D+04	0.0526989	-0.0215973	0.0104388	0.0052434	0.0022957	-0.0006667
S	1.9574362D+04	0.0990874	-0.0418688	0.0203814	0.0102448	0.0044844	-0.0013028
S	7.9576083D+03	0.1781986	-0.0806482	0.0396122	0.0199867	0.0087616	-0.0025449
S	3.3486115D+03	0.2849383	-0.1419169	0.0712703	0.0360695	0.0158121	-0.0045947
S	1.4564912D+03	0.3309280	-0.1998867	0.1033077	0.0528870	0.0232746	-0.0067655
S	6.5379251D+02	0.1966102	-0.0780779	0.0368433	0.0179699	0.0077737	-0.0022524
S	2.7233151D+02	0.0287666	0.4210573	-0.3490562	-0.1990478	-0.0898007	0.0262112
S	1.2503871D+02	-0.0030884	0.6056553	-0.6563680	-0.4124551	-0.1912730	0.0561488
S	5.2166627D+01	0.0016468	0.1411578	0.2714720	0.2847221	0.1488208	-0.0446886
S	2.7064125D+01	-0.0010766	-0.0198110	0.9260369	1.1337082	0.6220237	-0.1877524
S	1.1086042D+01	0.0005394	0.0078225	0.1736701	-0.3746736	-0.3241773	0.1040229
S	5.6518041D+00	-0.0002751	-0.0038452	-0.0219928	-1.0396882	-1.0745926	0.3725489
S	1.7715031D+00	0.0000983	0.0012905	0.0060698	-0.0913748	0.7371335	-0.3780950
S	8.4168566D-01	-0.0000478	-0.0006122	-0.0028308	0.0201248	0.6938915	-0.4064625
S	1.7000436D-01	0.0000108	0.0001388	0.0006031	-0.0035967	0.0293632	0.6083517
S	5.9566537D-02	-0.0000042	-0.0000543	-0.0002353	0.0013506	-0.0069353	0.5961531
	P	2P	3P	4P	5P		
BASIS/ORB. ENERGY	-476.1401400	-111.3167400	-23.3585200	-3.0452764			
P	6.0414736D+07	0.0000137	-0.0000071	-0.0000035	0.0000014		
P	8.2308540D+06	0.0000468	-0.0000241	-0.0000120	0.0000049		
P	1.6574806D+06	0.0001357	-0.0000700	-0.0000349	0.0000141		
P	4.1752952D+05	0.0003682	-0.0001903	-0.0000949	0.0000384		
P	1.2258379D+05	0.0009813	-0.0005088	-0.0002539	0.0001029		
P	4.0494991D+04	0.0026389	-0.0013750	-0.0006871	0.0002782		
P	1.4758870D+04	0.0071463	-0.0037482	-0.0018755	0.0007603		
P	5.8874150D+03	0.0192702	-0.0102234	-0.0051311	0.0020791		
P	2.5253016D+03	0.0508632	-0.0274635	-0.0138362	0.0056190		
P	1.1502125D+03	0.1224527	-0.0682481	-0.0346731	0.0140833		
P	5.5102488D+02	0.2441106	-0.1420711	-0.0729174	0.0297548		

P	2.7459985D+02	0.3518474	-0.2140566	-0.1113721	0.0454176
P	1.4058609D+02	0.2945605	-0.1259529	-0.0551175	0.0217686
P	7.2343928D+01	0.1020912	0.2513864	0.1995835	-0.0897832
P	3.8501327D+01	0.0059286	0.5443365	0.4574091	-0.2067098
P	2.0598712D+01	0.0015859	0.3052960	0.1108545	-0.0306609
P	1.0845765D+01	-0.0010106	0.0455138	-0.5436245	0.3484713
P	5.6872593D+00	0.0005144	0.0019414	-0.5549956	0.3931511
P	2.7468201D+00	-0.0003698	-0.0000921	-0.1239789	-0.1988091
P	1.4989635D+00	0.0002880	0.0000986	0.0080284	-0.5395299
P	8.2735001D-01	-0.0001654	-0.0001250	-0.0063407	-0.3543090
P	4.5652704D-01	0.0000640	0.0000358	0.0018629	-0.1363996
P	1.9008268D-01	-0.0000108	-0.0000084	-0.0002962	-0.0153630

	D	3D	4D	5D
BASIS/ORB. ENERGY		-87.3763020	-14.3495760	-0.6031993
D	1.7129664D+04	0.0001520	-0.0000792	0.0000247
D	4.4531659D+03	0.0010379	-0.0005412	0.0001680
D	1.6017309D+03	0.0054825	-0.0028820	0.0009003
D	6.6526822D+02	0.0242085	-0.0127967	0.0039841
D	3.0116853D+02	0.0835857	-0.0450008	0.0141163
D	1.4532736D+02	0.2115948	-0.1154582	0.0361355
D	7.3035413D+01	0.3601804	-0.1930151	0.0606433
D	3.7706699D+01	0.3550477	-0.1358705	0.0376130
D	1.9502164D+01	0.1557255	0.1933777	-0.0807351
D	9.8922531D+00	0.0213432	0.4941549	-0.1945217
D	4.9397414D+00	0.0010510	0.3793341	-0.1073075
D	2.3245438D+00	0.0000357	0.0873260	0.2413619
D	1.0531057D+00	0.0000335	0.0017496	0.4720389
D	4.4136883D-01	-0.0000154	0.0008798	0.3843347
D	1.6624377D-01	0.0000044	-0.0002191	0.1403632

	F	4F
BASIS/ORB. ENERGY		-4.3870032
F	1.3232654D+03	0.0001859
F	4.4237913D+02	0.0017978
F	1.8499816D+02	0.0108977
F	8.6046064D+01	0.0446719

F	4.2132399D+01	0.1285281
F	2.1345359D+01	0.2571650
F	1.0820075D+01	0.3504523
F	5.3886113D+00	0.3240899
F	2.5606799D+00	0.1767002
F	1.0806275D+00	0.0414019

TALLIUM [XE]4F(14)6S(2)5D(10)6P(1), 2P

CHARGE = 81.000000

SYMMETRY SPECIES	S	P	D	F
NUMBER OF BASIS FUNCTIONS	27	23	15	10
NUMBER OF CLOSED SHELLS	6	4	3	1
NUMBER OF OPEN SHELLS	0	1	0	0
OPEN SHELL OCCUPATION NUMBER	0	1	0	0

*** FINAL SCF RESULTS ***

E = -20250.536178182

ORBITAL ENERGIES AND EXPANSION COEFFICIENTS

	S	1S	2S	3S	4S	5S	6S
BASIS/ORB. ENERGY	-3163.1227000	-568.8153900	-138.3895800	-32.3052130	-5.6204574	-0.4477927	
S 2.0232234D+11	0.0000049	-0.0000020	0.0000009	0.0000005	0.0000002	-0.0000001	
S 2.0259966D+10	0.0000194	-0.0000076	0.0000037	0.0000018	0.0000008	-0.0000003	
S 3.1155926D+09	0.0000589	-0.0000232	0.0000112	0.0000056	0.0000025	-0.0000008	
S 6.2557525D+08	0.0001544	-0.0000607	0.0000292	0.0000147	0.0000065	-0.0000021	
S 1.4547281D+08	0.0003784	-0.0001486	0.0000714	0.0000359	0.0000159	-0.0000050	
S 3.7733841D+07	0.0008566	-0.0003363	0.0001616	0.0000813	0.0000360	-0.0000114	
S 1.0816442D+07	0.0018224	-0.0007155	0.0003439	0.0001729	0.0000766	-0.0000243	
S 3.3427946D+06	0.0037523	-0.0014765	0.0007098	0.0003570	0.0001582	-0.0000501	
S 1.0912002D+06	0.0075605	-0.0029842	0.0014360	0.0007222	0.0003200	-0.0001013	
S 3.7312667D+05	0.0148869	-0.0059256	0.0028535	0.0014357	0.0006363	-0.0002014	
S 1.3376345D+05	0.0287256	-0.0115558	0.0055804	0.0028085	0.0012446	-0.0003941	
S 5.0138728D+04	0.0547081	-0.0225488	0.0109156	0.0055008	0.0024390	-0.0007721	
S 1.9591169D+04	0.1022663	-0.0434934	0.0212223	0.0107032	0.0047453	-0.0015027	
S 7.9642342D+03	0.1824064	-0.0831624	0.0409096	0.0207111	0.0091943	-0.0029113	
S 3.3517937D+03	0.2885887	-0.1449644	0.0730607	0.0371049	0.0164771	-0.0052192	
S 1.4563509D+03	0.3288787	-0.1999118	0.1033376	0.0530908	0.0236593	-0.0074977	

S	6.5426556D+02	0.1875835	-0.0649282	0.0292836	0.0139491	0.0060705	-0.0019127
S	2.7473519D+02	0.0258506	0.4370450	-0.3673927	-0.2107336	-0.0964115	0.0306857
S	1.2626532D+02	-0.0025473	0.5953146	-0.6444320	-0.4077197	-0.1917213	0.0614042
S	5.1889216D+01	0.0013419	0.1321277	0.3299261	0.3461136	0.1834259	-0.0601508
S	2.7235744D+01	-0.0009176	-0.0220325	0.8882331	1.1028152	0.6165371	-0.2033835
S	1.1391258D+01	0.0004701	0.0087239	0.1595825	-0.4203519	-0.3643050	0.1279454
S	5.8286016D+00	-0.0002418	-0.0043187	-0.0188419	-1.0143592	-1.0808052	0.4134512
S	1.9124685D+00	0.0000899	0.0015119	0.0053556	-0.0906026	0.7225900	-0.4115964
S	9.2040810D-01	-0.0000436	-0.0007146	-0.0024829	0.0185761	0.7254344	-0.4721318
S	1.9733417D-01	0.0000101	0.0001666	0.0005384	-0.0033675	0.0320290	0.6926824
S	7.2144355D-02	-0.0000040	-0.0000650	-0.0002092	0.0012580	-0.0074970	0.5425239
	P	2P	3P	4P	5P	6P	
BASIS/ORB. ENERGY	-491.0924400	-115.5901600	-24.6783600	-3.4422544	-0.1853159		
P	5.8291947D+07	0.0000148	-0.0000077	-0.0000038	-0.0000016	-0.0000003	
P	8.2641230D+06	0.0000488	-0.0000252	-0.0000126	-0.0000052	-0.0000011	
P	1.6903653D+06	0.0001416	-0.0000732	-0.0000366	-0.0000151	-0.0000033	
P	4.2472689D+05	0.0003866	-0.0002003	-0.0001003	-0.0000413	-0.0000089	
P	1.2380619D+05	0.0010361	-0.0005386	-0.0002699	-0.0001113	-0.0000240	
P	4.0665653D+04	0.0027803	-0.0014524	-0.0007288	-0.0003005	-0.0000647	
P	1.4806764D+04	0.0075085	-0.0039498	-0.0019849	-0.0008194	-0.0001771	
P	5.8925590D+03	0.0202442	-0.0107712	-0.0054295	-0.0022399	-0.0004818	
P	2.5261879D+03	0.0530325	-0.0287421	-0.0145457	-0.0060166	-0.0013027	
P	1.1515387D+03	0.1267631	-0.0709091	-0.0361911	-0.0149662	-0.0032146	
P	5.5121142D+02	0.2507398	-0.1466319	-0.0756259	-0.0314418	-0.0068320	
P	2.7432566D+02	0.3546127	-0.2158155	-0.1127136	-0.0467684	-0.0099787	
P	1.4047882D+02	0.2862328	-0.1146938	-0.0480971	-0.0191806	-0.0044061	
P	7.2605915D+01	0.0943754	0.2713228	0.2155055	0.0990238	0.0223619	
P	3.8658712D+01	0.0054973	0.5454847	0.4627823	0.2128632	0.0451224	
P	2.0617630D+01	0.0010810	0.2901805	0.0731162	0.0110362	0.0045233	
P	1.0661808D+01	-0.0006607	0.0391242	-0.5940807	-0.3949060	-0.0962051	
P	5.5055026D+00	0.0002638	0.0009796	-0.5221408	-0.3732876	-0.0781728	
P	2.5985549D+00	-0.0001356	0.0000710	-0.0867649	0.3571719	0.0902151	
P	1.2618990D+00	0.0000689	-0.0000768	0.0020807	0.6530451	0.2296542	
P	5.6273636D-01	-0.0000204	-0.0000085	-0.0012734	0.2478368	0.0039346	
P	1.4545317D-01	0.0000049	-0.0000008	0.0002434	0.0105861	-0.5371463	

P	4.4688491D-02	-0.0000016	0.0000003	-0.0000713	-0.0011766	-0.5780662
	D	3D	4D	5D		
BASIS/ORB. ENERGY		-90.8997560	-15.3657180	-0.8407541		
D	1.6081381D+04	0.0001777	-0.0000932	0.0000306		
D	4.2201581D+03	0.0012224	-0.0006424	0.0002109		
D	1.5131209D+03	0.0064335	-0.0034052	0.0011195		
D	6.4035780D+02	0.0263684	-0.0140561	0.0046265		
D	3.0042141D+02	0.0835721	-0.0453266	0.0149709		
D	1.5037046D+02	0.2005541	-0.1102612	0.0364950		
D	7.7992852D+01	0.3389594	-0.1832761	0.0605379		
D	4.1314732D+01	0.3528276	-0.1478655	0.0451564		
D	2.1882602D+01	0.1764007	0.1411941	-0.0666511		
D	1.1372795D+01	0.0310244	0.4572373	-0.1886690		
D	5.8559360D+00	0.0015208	0.4137543	-0.1528662		
D	2.9260748D+00	0.0001800	0.1301775	0.1658117		
D	1.3535144D+00	0.0000002	0.0090632	0.4730925		
D	5.7731191D-01	-0.0000017	0.0003209	0.4314314		
D	2.2032967D-01	0.0000005	-0.0000551	0.1550957		
	F	4F				
BASIS/ORB. ENERGY		-5.0980388				
F	1.6622083D+03	0.0001367				
F	4.8485710D+02	0.0017460				
F	1.9046172D+02	0.0116968				
F	8.6394508D+01	0.0487388				
F	4.1945751D+01	0.1382036				
F	2.1263502D+01	0.2666840				
F	1.0852911D+01	0.3506886				
F	5.4735966D+00	0.3124238				
F	2.6447503D+00	0.1636205				
F	1.1422553D+00	0.0363133				

LEAD [XE]4F(14)6S(2)5D(10)6P(2), 3P

CHARGE = 82.000000

SYMMETRY SPECIES	S	P	D	F
NUMBER OF BASIS FUNCTIONS	27	23	15	10

NUMBER OF CLOSED SHELLS	6	4	3	1
NUMBER OF OPEN SHELLS	0	1	0	0
OPEN SHELL OCCUPATION NUMBER	0	2	0	0

*** FINAL SCF RESULTS ***

E = -20887.626301558

ORBITAL ENERGIES AND EXPANSION COEFFICIENTS

S	1S	2S	3S	4S	5S	6S
BASIS/ORB. ENERGY	-3254.9803000	-587.8846900	-143.7868200	-33.9981530	-6.1437570	-0.5622533
S 2.3499268D+11	0.0000049	-0.0000019	0.0000009	0.0000005	0.0000002	-0.0000001
S 2.2281446D+10	0.0000197	-0.0000078	0.0000038	0.0000019	0.0000009	-0.0000003
S 3.3921974D+09	0.0000604	-0.0000239	0.0000115	0.0000058	0.0000026	-0.0000009
S 6.6184910D+08	0.0001608	-0.0000636	0.0000306	0.0000154	0.0000069	-0.0000023
S 1.5342763D+08	0.0003863	-0.0001525	0.0000734	0.0000370	0.0000166	-0.0000056
S 4.0151044D+07	0.0008693	-0.0003430	0.0001651	0.0000833	0.0000374	-0.0000125
S 1.1448208D+07	0.0018766	-0.0007405	0.0003565	0.0001798	0.0000807	-0.0000271
S 3.4834135D+06	0.0038967	-0.0015408	0.0007419	0.0003743	0.0001679	-0.0000564
S 1.1232785D+06	0.0078676	-0.0031211	0.0015042	0.0007589	0.0003405	-0.0001143
S 3.8012709D+05	0.0155183	-0.0062069	0.0029940	0.0015113	0.0006782	-0.0002277
S 1.3532618D+05	0.0298622	-0.0120795	0.0058424	0.0029498	0.0013236	-0.0004445
S 5.0509879D+04	0.0566872	-0.0234868	0.0113914	0.0057593	0.0025857	-0.0008681
S 1.9673845D+04	0.1055539	-0.0452025	0.0220924	0.0111786	0.0050184	-0.0016854
S 7.9748712D+03	0.1871273	-0.0858685	0.0423469	0.0215109	0.0096698	-0.0032472
S 3.3526520D+03	0.2917519	-0.1480110	0.0747406	0.0380880	0.0171268	-0.0057539
S 1.4595502D+03	0.3250958	-0.1980120	0.1026415	0.0529184	0.0238828	-0.0080261
S 6.5829504D+02	0.1794506	-0.0553198	0.0230343	0.0105913	0.0046054	-0.0015374
S 2.8203427D+02	0.0237908	0.4374686	-0.3681381	-0.2120037	-0.0982495	0.0331845
S 1.3054573D+02	-0.0018474	0.5880933	-0.6407931	-0.4072018	-0.1940712	0.0659323
S 5.4944971D+01	0.0008994	0.1332676	0.3034166	0.3199211	0.1719559	-0.0598086
S 2.8651790D+01	-0.0005932	-0.0189234	0.9049897	1.1225263	0.6358522	-0.2230797
S 1.1942760D+01	0.0002990	0.0076708	0.1708791	-0.3805805	-0.3407166	0.1281006
S 6.1563706D+00	-0.0001534	-0.0038709	-0.0214538	-1.0392912	-1.1190254	0.4559374
S 2.0214087D+00	0.0000587	0.0013960	0.0063288	-0.0986602	0.7133371	-0.4389304
S 9.9548772D-01	-0.0000299	-0.0006904	-0.0030730	0.0217778	0.7385776	-0.5225588
S 2.3245102D-01	0.0000073	0.0001680	0.0007012	-0.0040802	0.0337980	0.7171527
S 8.7367227D-02	-0.0000028	-0.0000639	-0.0002647	0.0014844	-0.0072886	0.5475533

	P	2P	3P	4P	5P	6P
BASIS/ORB. ENERGY		-506.3154900	-119.9557300	-26.0286320	-3.8379694	-0.2505977
P 5.8513559D+07	0.0000158	-0.0000082	-0.0000041	-0.0000017	-0.0000004	
P 8.2879185D+06	0.0000518	-0.0000268	-0.0000135	-0.0000057	-0.0000014	
P 1.6942523D+06	0.0001501	-0.0000778	-0.0000391	-0.0000164	-0.0000041	
P 4.2539473D+05	0.0004094	-0.0002127	-0.0001069	-0.0000449	-0.0000113	
P 1.2391025D+05	0.0010957	-0.0005710	-0.0002874	-0.0001207	-0.0000303	
P 4.0684536D+04	0.0029339	-0.0015366	-0.0007742	-0.0003249	-0.0000815	
P 1.4808510D+04	0.0079023	-0.0041685	-0.0021038	-0.0008843	-0.0002225	
P 5.8928396D+03	0.0212231	-0.0113270	-0.0057338	-0.0024074	-0.0006034	
P 2.5263830D+03	0.0553368	-0.0300950	-0.0152995	-0.0064456	-0.0016241	
P 1.1515518D+03	0.1313306	-0.0737591	-0.0378137	-0.0159120	-0.0039841	
P 5.5116897D+02	0.2569271	-0.1508887	-0.0782091	-0.0331349	-0.0083743	
P 2.7427899D+02	0.3564697	-0.2171160	-0.1137658	-0.0479767	-0.0119480	
P 1.4044470D+02	0.2786380	-0.1025459	-0.0404566	-0.0162966	-0.0043387	
P 7.2545970D+01	0.0872419	0.2938386	0.2344134	0.1102505	0.0288014	
P 3.8664235D+01	0.0044116	0.5441196	0.4643074	0.2166272	0.0538616	
P 2.0608668D+01	0.0010151	0.2719660	0.0361915	-0.0076796	-0.0002618	
P 1.0667929D+01	-0.0006324	0.0336477	-0.6165743	-0.4263821	-0.1203162	
P 5.5198214D+00	0.0002497	0.0009608	-0.4966124	-0.3497238	-0.0864136	
P 2.5679298D+00	-0.0001254	-0.0000477	-0.0741429	0.4305505	0.1360621	
P 1.2440634D+00	0.0000680	-0.0000345	0.0029829	0.6358482	0.2654861	
P 5.6570886D-01	-0.0000227	-0.0000190	-0.0014156	0.1978740	-0.0218788	
P 1.7276808D-01	0.0000063	0.0000031	0.0003351	0.0076321	-0.5943590	
P 5.7668369D-02	-0.0000020	-0.0000008	-0.0000937	-0.0003210	-0.5114442	
	D	3D	4D	5D		
BASIS/ORB. ENERGY		-94.4930180	-16.4039470	-1.0729339		
D 1.6085869D+04	0.0001907	0.0001008	0.0000346			
D 4.1933524D+03	0.0013207	0.0006987	0.0002397			
D 1.5044436D+03	0.0068803	0.0036679	0.0012629			
D 6.3847001D+02	0.0279048	0.0149807	0.0051533			
D 3.0013277D+02	0.0874068	0.0477819	0.0165341			
D 1.5055759D+02	0.2068213	0.1144634	0.0395828			
D 7.8122687D+01	0.3446156	0.1872135	0.0648174			
D 4.1359848D+01	0.3484568	0.1407789	0.0437880			

D	2.1886127D+01	0.1665518	-0.1615378	-0.0778407
D	1.1382111D+01	0.0274153	-0.4677500	-0.2045900
D	5.8721267D+00	0.0013358	-0.4002848	-0.1455253
D	2.9223768D+00	0.0001197	-0.1158987	0.1989093
D	1.3859686D+00	0.0000110	-0.0064080	0.4830012
D	6.1337030D-01	-0.0000069	-0.0006049	0.4065559
D	2.4333943D-01	0.0000022	0.0001535	0.1280734
	F	4F		
BASIS/ORB.ENERGY		-5.8288055		
F	1.2930021D+03	0.0002319		
F	4.4341623D+02	0.0021015		
F	1.8994925D+02	0.0117304		
F	9.1874226D+01	0.0432809		
F	4.7213791D+01	0.1156225		
F	2.5138176D+01	0.2277850		
F	1.3351898D+01	0.3280388		
F	6.8580381D+00	0.3387534		
F	3.3099138D+00	0.2060610		
F	1.4143033D+00	0.0510319		

BISMUTH [XE]4F(14)6S(2)5D(10)6P(3), 4S

CHARGE = 83.000000

SYMMETRY SPECIES	S	P	D	F
NUMBER OF BASIS FUNCTIONS	27	23	15	10
NUMBER OF CLOSED SHELLS	6	4	3	1
NUMBER OF OPEN SHELLS	0	1	0	0
OPEN SHELL OCCUPATION NUMBER	0	3	0	0

*** FINAL SCF RESULTS ***

E = -21537.718824263

ORBITAL ENERGIES AND EXPANSION COEFFICIENTS

	S	1S	2S	3S	4S	5S	6S
BASIS/ORB.ENERGY		-3348.6733000	-607.4221600	-149.3317600	-35.7438400	-6.6802339	-0.6777410
S	2.4062858D+11	0.0000052	-0.0000021	0.0000010	0.0000005	0.0000002	-0.0000001
S	2.2809639D+10	0.0000209	-0.0000084	0.0000040	0.0000020	0.0000009	-0.0000003
S	3.4462821D+09	0.0000641	-0.0000255	0.0000123	0.0000062	0.0000028	-0.0000010

S	6.7450223D+08	0.0001697	-0.0000674	0.0000325	0.0000165	0.0000075	-0.0000026
S	1.5569479D+08	0.0004082	-0.0001619	0.0000781	0.0000395	0.0000179	-0.0000063
S	4.0651160D+07	0.0009166	-0.0003635	0.0001752	0.0000887	0.0000403	-0.0000141
S	1.1560254D+07	0.0019732	-0.0007825	0.0003773	0.0001909	0.0000867	-0.0000304
S	3.5127552D+06	0.0040948	-0.0016273	0.0007848	0.0003972	0.0001804	-0.0000633
S	1.1280140D+06	0.0082640	-0.0032951	0.0015906	0.0008051	0.0003656	-0.0001283
S	3.8096930D+05	0.0162385	-0.0065289	0.0031541	0.0015972	0.0007254	-0.0002547
S	1.3537905D+05	0.0311545	-0.0126716	0.0061398	0.0031097	0.0014125	-0.0004959
S	5.0527834D+04	0.0587303	-0.0244766	0.0118896	0.0060306	0.0027403	-0.0009620
S	1.9697323D+04	0.1087496	-0.0468732	0.0229602	0.0116545	0.0052964	-0.0018598
S	7.9790262D+03	0.1917033	-0.0886288	0.0437756	0.0223130	0.0101515	-0.0035644
S	3.3497459D+03	0.2954804	-0.1511730	0.0765993	0.0391588	0.0178282	-0.0062628
S	1.4574575D+03	0.3218529	-0.1970457	0.1021102	0.0528505	0.0241355	-0.0084806
S	6.5841402D+02	0.1706225	-0.0410043	0.0145294	0.0059105	0.0025158	-0.0008719
S	2.8409184D+02	0.0212850	0.4522740	-0.3861499	-0.2235245	-0.1050215	0.0371087
S	1.3178503D+02	-0.0014845	0.5767410	-0.6265485	-0.4011761	-0.1936933	0.0688394
S	5.4629074D+01	0.0006907	0.1247582	0.3625899	0.3854326	0.2098903	-0.0764040
S	2.8745817D+01	-0.0004743	-0.0210439	0.8679192	1.0871696	0.6276842	-0.2310092
S	1.2110242D+01	0.0002447	0.0086391	0.1550723	-0.4423393	-0.3989302	0.1579308
S	6.3011136D+00	-0.0001276	-0.0044625	-0.0195680	-1.0007806	-1.1098849	0.4780398
S	2.1494104D+00	0.0000502	0.0016683	0.0058286	-0.0951042	0.7266775	-0.4736337
S	1.0677106D+00	-0.0000257	-0.0008274	-0.0028274	0.0199660	0.7456398	-0.5635569
S	2.6714109D-01	0.0000064	0.0002068	0.0006594	-0.0038145	0.0341511	0.7428017
S	1.0206999D-01	-0.0000024	-0.0000763	-0.0002405	0.0013457	-0.0067402	0.5496555
	P	2P	3P	4P	5P	6P	
BASIS/ORB. ENERGY	-521.8184100	-124.4208700	-27.4160290	-4.2402153	-0.3165808		
P	5.8730496D+07	0.0000167	-0.0000087	-0.0000044	-0.0000019	0.0000005	
P	8.3144760D+06	0.0000550	-0.0000285	-0.0000144	-0.0000061	0.0000017	
P	1.6976188D+06	0.0001591	-0.0000827	-0.0000417	-0.0000178	0.0000049	
P	4.2605330D+05	0.0004333	-0.0002256	-0.0001139	-0.0000486	0.0000135	
P	1.2403012D+05	0.0011585	-0.0006052	-0.0003058	-0.0001307	0.0000362	
P	4.0689092D+04	0.0030952	-0.0016254	-0.0008223	-0.0003511	0.0000971	
P	1.4811776D+04	0.0083078	-0.0043944	-0.0022272	-0.0009527	0.0002641	
P	5.8931265D+03	0.0222471	-0.0119101	-0.0060541	-0.0025860	0.0007149	
P	2.5262925D+03	0.0576904	-0.0314825	-0.0160772	-0.0068937	0.0019134	

P	1.1517227D+03	0.1359504	-0.0766581	-0.0394719	-0.0168975	0.0046680
P	5.5107472D+02	0.2631128	-0.1551600	-0.0808224	-0.0348643	0.0097017
P	2.7424988D+02	0.3577030	-0.2179129	-0.1145143	-0.0490821	0.0135025
P	1.4046722D+02	0.2708886	-0.0898191	-0.0323702	-0.0130153	0.0037963
P	7.2494510D+01	0.0805910	0.3161062	0.2537027	0.1218684	-0.0349063
P	3.8653022D+01	0.0034574	0.5414060	0.4636939	0.2195562	-0.0605793
P	2.0583442D+01	0.0009676	0.2538328	-0.0014026	-0.0283727	0.0069816
P	1.0692111D+01	-0.0006159	0.0286534	-0.6338195	-0.4543278	0.1408678
P	5.5586880D+00	0.0002436	0.0010496	-0.4704317	-0.3259136	0.0897324
P	2.5810616D+00	-0.0001179	-0.0001772	-0.0649156	0.4907571	-0.1803802
P	1.2386791D+00	0.0000650	0.0000176	0.0029674	0.6267627	-0.2908346
P	5.5495678D-01	-0.0000237	-0.0000359	-0.0013690	0.1528430	0.0598137
P	1.9599244D-01	0.0000078	0.0000101	0.0004003	0.0034033	0.6307895
P	6.9345825D-02	-0.0000023	-0.0000028	-0.0001101	0.0003251	0.4585952

	D	3D	4D	5D
BASIS/ORB. ENERGY		-98.1628420	-17.4708320	-1.3085010
D	1.6038922D+04	0.0002052	0.0001091	0.0000390
D	4.1627671D+03	0.0014278	0.0007604	0.0002711
D	1.4932680D+03	0.0073787	0.0039615	0.0014191
D	6.3617893D+02	0.0294442	0.0159166	0.0056911
D	3.0019669D+02	0.0911349	0.0502071	0.0180813
D	1.5071473D+02	0.2137840	0.1190729	0.0427922
D	7.8150152D+01	0.3500132	0.1909388	0.0687929
D	4.1403834D+01	0.3426366	0.1324741	0.0415923
D	2.1913244D+01	0.1573210	-0.1811124	-0.0894072
D	1.1392226D+01	0.0242163	-0.4789062	-0.2199987
D	5.8708730D+00	0.0011899	-0.3857984	-0.1352772
D	2.9079721D+00	0.0000524	-0.1015090	0.2397726
D	1.3928501D+00	0.0000290	-0.0042943	0.4964586
D	6.3220087D-01	-0.0000148	-0.0006428	0.3725961
D	2.5747463D-01	0.0000048	0.0001865	0.1007645

	F	4F
BASIS/ORB. ENERGY		-6.5858355
F	1.2931490D+03	0.0002558
F	4.4245050D+02	0.0023003

F	1.8992104D+02	0.0127464
F	9.1584137D+01	0.0469483
F	4.7062874D+01	0.1226971
F	2.5131198D+01	0.2368570
F	1.3357806D+01	0.3323572
F	6.9337984D+00	0.3267702
F	3.4247290D+00	0.1915664
F	1.5159795D+00	0.0472214

POLONIUM [XE]4F(14)6S(2)5D(10)6P(4), 3P

CHARGE = 84.000000

SYMMETRY SPECIES	S	P	D	F
NUMBER OF BASIS FUNCTIONS	27	23	15	10
NUMBER OF CLOSED SHELLS	6	4	3	1
NUMBER OF OPEN SHELLS	0	1	0	0
OPEN SHELL OCCUPATION NUMBER	0	4	0	0

*** FINAL SCF RESULTS ***

E = -22200.901491442

ORBITAL ENERGIES AND EXPANSION COEFFICIENTS

	S	1S	2S	3S	4S	5S	6S
BASIS/ORB. ENERGY		-3444.2577000	-627.4569000	-155.0447400	-37.5602610	-7.2474170	-0.8069083
S	3.0382570D+11	0.0000048	-0.0000019	0.0000009	0.0000005	0.0000002	-0.0000001
S	2.7956576D+10	0.0000197	-0.0000079	0.0000038	0.0000019	0.0000009	-0.0000003
S	4.2117674D+09	0.0000604	-0.0000242	0.0000117	0.0000059	0.0000027	-0.0000010
S	8.0736545D+08	0.0001634	-0.0000653	0.0000315	0.0000160	0.0000074	-0.0000027
S	1.8111687D+08	0.0004029	-0.0001607	0.0000776	0.0000394	0.0000181	-0.0000066
S	4.5526749D+07	0.0009292	-0.0003704	0.0001788	0.0000908	0.0000417	-0.0000152
S	1.2517696D+07	0.0020275	-0.0008081	0.0003903	0.0001981	0.0000910	-0.0000332
S	3.7074113D+06	0.0042465	-0.0016959	0.0008191	0.0004158	0.0001911	-0.0000697
S	1.1679185D+06	0.0085950	-0.0034445	0.0016652	0.0008454	0.0003885	-0.0001417
S	3.8953830D+05	0.0169227	-0.0068379	0.0033087	0.0016806	0.0007723	-0.0002818
S	1.3667635D+05	0.0326655	-0.0133600	0.0064833	0.0032940	0.0015138	-0.0005524
S	5.0455141D+04	0.0614453	-0.0257552	0.0125337	0.0063770	0.0029320	-0.0010699
S	1.9602527D+04	0.1123946	-0.0487922	0.0239424	0.0121927	0.0056061	-0.0020461
S	7.9710239D+03	0.1947132	-0.0906684	0.0448853	0.0229515	0.0105667	-0.0038569

S	3.3738125D+03	0.2944813	-0.1518290	0.0770778	0.0395374	0.0182102	-0.0066484
S	1.4802229D+03	0.3167270	-0.1938059	0.1005746	0.0522030	0.0241321	-0.0088168
S	6.7243376D+02	0.1669655	-0.0361167	0.0111321	0.0040859	0.0016603	-0.0005851
S	2.9333007D+02	0.0208236	0.4495644	-0.3840997	-0.2232654	-0.1061167	0.0389676
S	1.3654197D+02	-0.0012323	0.5742945	-0.6258622	-0.4017946	-0.1965594	0.0726942
S	5.7353962D+01	0.0005384	0.1265780	0.3420448	0.3647165	0.2017815	-0.0765931
S	3.0110985D+01	-0.0003634	-0.0195999	0.8795857	1.1044973	0.6449129	-0.2468811
S	1.2713100D+01	0.0001847	0.0081864	0.1638702	-0.4093619	-0.3759616	0.1548009
S	6.6407521D+00	-0.0000958	-0.0042969	-0.0211110	-1.0221881	-1.1530134	0.5204407
S	2.3100669D+00	0.0000387	0.0016530	0.0065167	-0.1021076	0.6928898	-0.4791788
S	1.1662976D+00	-0.0000200	-0.0008254	-0.0031809	0.0209272	0.7867820	-0.6215269
S	2.9978687D-01	0.0000049	0.0002046	0.0007371	-0.0038783	0.0373421	0.7773932
S	1.1596341D-01	-0.0000018	-0.0000747	-0.0002651	0.0013525	-0.0071767	0.5382406
	P	2P	3P	4P	5P	6P	
BASIS/ORB. ENERGY	-537.6207900	-129.0034700	-28.8578870	-4.6665868	-0.3386646		
P	5.8771546D+07	0.0000178	-0.0000092	-0.0000047	-0.0000020	0.0000006	
P	8.3373778D+06	0.0000582	-0.0000303	-0.0000153	-0.0000067	0.0000020	
P	1.7039690D+06	0.0001685	-0.0000877	-0.0000444	-0.0000193	0.0000057	
P	4.2638362D+05	0.0004596	-0.0002399	-0.0001216	-0.0000528	0.0000156	
P	1.2401720D+05	0.0012229	-0.0006404	-0.0003249	-0.0001411	0.0000417	
P	4.0735342D+04	0.0032605	-0.0017166	-0.0008720	-0.0003784	0.0001118	
P	1.4808201D+04	0.0087464	-0.0046389	-0.0023609	-0.0010264	0.0003038	
P	5.8914147D+03	0.0232857	-0.0125051	-0.0063829	-0.0027709	0.0008187	
P	2.5271432D+03	0.0600881	-0.0328996	-0.0168747	-0.0073545	0.0021794	
P	1.1516893D+03	0.1407540	-0.0796884	-0.0412119	-0.0179319	0.0052963	
P	5.5083106D+02	0.2691724	-0.1593512	-0.0834037	-0.0365769	0.0108619	
P	2.7424247D+02	0.3583331	-0.2182672	-0.1150180	-0.0500751	0.0147459	
P	1.4053069D+02	0.2630790	-0.0763417	-0.0236269	-0.0092096	0.0028432	
P	7.2403607D+01	0.0743873	0.3381699	0.2732263	0.1336992	-0.0407371	
P	3.8646565D+01	0.0025398	0.5359303	0.4602396	0.2211674	-0.0656016	
P	2.0596185D+01	0.0009741	0.2366758	-0.0386473	-0.0505653	0.0151426	
P	1.0716990D+01	-0.0006256	0.0246953	-0.6498431	-0.4809440	0.1589953	
P	5.5922886D+00	0.0002540	0.0009712	-0.4425905	-0.3008355	0.0891548	
P	2.6258951D+00	-0.0001185	-0.0002208	-0.0564409	0.5387895	-0.2208009	
P	1.2496708D+00	0.0000628	0.0000263	0.0019712	0.6197029	-0.3084173	

P	5.3335520D-01	-0.0000236	-0.0000366	-0.0009625	0.1185091	0.1299016
P	2.0732843D-01	0.0000088	0.0000132	0.0003471	-0.0008086	0.6418193
P	7.3837681D-02	-0.0000025	-0.0000031	-0.0000792	0.0014109	0.4093100
	D	3D	4D	5D		
BASIS/ORB. ENERGY	-101.9264300	-18.5836080	-1.5651969			
D	1.5052151D+04	0.0002421	0.0001296	0.0000479		
D	3.9204730D+03	0.0016823	0.0009023	0.0003335		
D	1.4123766D+03	0.0086331	0.0046665	0.0017291		
D	6.0132139D+02	0.0343397	0.0187162	0.0069386		
D	2.8289619D+02	0.1042423	0.0579222	0.0215847		
D	1.4261242D+02	0.2307574	0.1294098	0.0482252		
D	7.5105906D+01	0.3486174	0.1895820	0.0704465		
D	4.0961628D+01	0.3152420	0.1138226	0.0357265		
D	2.2612538D+01	0.1463322	-0.1725186	-0.0890736		
D	1.2214974D+01	0.0272006	-0.4477609	-0.2132599		
D	6.5198907D+00	0.0010737	-0.3947626	-0.1589140		
D	3.3539380D+00	0.0003291	-0.1257686	0.1923578		
D	1.6411025D+00	-0.0000874	-0.0087691	0.4949382		
D	7.5627550D-01	0.0000319	-0.0004547	0.4045763		
D	3.0888188D-01	-0.0000076	0.0001444	0.1129348		
	F	4F				
BASIS/ORB. ENERGY	-7.3862853					
F	1.2594186D+03	0.0002851				
F	4.4454231D+02	0.0024693				
F	1.8997698D+02	0.0138938				
F	9.1459634D+01	0.0503162				
F	4.7073097D+01	0.1298056				
F	2.5139700D+01	0.2460219				
F	1.3361140D+01	0.3377908				
F	6.9399797D+00	0.3203836				
F	3.4346690D+00	0.1758852				
F	1.5357901D+00	0.0385673				

ASTATINE [XE]4F(14)6S(2)5D(10)6P(5), 2P
 CHARGE = 85.000000

SYMMETRY SPECIES	S	P	D	F
NUMBER OF BASIS FUNCTIONS	27	23	15	10
NUMBER OF CLOSED SHELLS	6	4	3	1
NUMBER OF OPEN SHELLS	0	1	0	0
OPEN SHELL OCCUPATION NUMBER	0	5	0	0

*** FINAL SCF RESULTS ***

E = -22877.462946821

ORBITAL ENERGIES AND EXPANSION COEFFICIENTS

	S	1S	2S	3S	4S	5S	6S
BASIS/ORB. ENERGY	-3541.7540000	-647.9819500	-160.9099400	-39.4293890	-7.8273325	-0.9378230	
S 3.7414834D+11	0.0000045	-0.0000018	0.0000009	0.0000005	0.0000002	-0.0000001	
S 3.3690316D+10	0.0000190	-0.0000077	0.0000037	0.0000019	0.0000009	-0.0000003	
S 4.8412550D+09	0.0000606	-0.0000244	0.0000118	0.0000060	0.0000028	-0.0000011	
S 8.9721873D+08	0.0001646	-0.0000661	0.0000320	0.0000163	0.0000076	-0.0000028	
S 1.9864780D+08	0.0004095	-0.0001642	0.0000794	0.0000404	0.0000188	-0.0000071	
S 4.8611909D+07	0.0009637	-0.0003861	0.0001867	0.0000951	0.0000442	-0.0000166	
S 1.3058480D+07	0.0021206	-0.0008496	0.0004109	0.0002092	0.0000972	-0.0000366	
S 3.8005140D+06	0.0044484	-0.0017855	0.0008637	0.0004398	0.0002044	-0.0000769	
S 1.1864105D+06	0.0089973	-0.0036245	0.0017549	0.0008937	0.0004153	-0.0001563	
S 3.9248480D+05	0.0177172	-0.0071962	0.0034876	0.0017768	0.0008257	-0.0003108	
S 1.3718448D+05	0.0340104	-0.0139887	0.0067988	0.0034651	0.0016104	-0.0006062	
S 5.0505962D+04	0.0638670	-0.0269249	0.0131260	0.0066986	0.0031144	-0.0011723	
S 1.9565763D+04	0.1161486	-0.0507755	0.0249587	0.0127516	0.0059301	-0.0022326	
S 7.9541328D+03	0.1990973	-0.0933883	0.0463360	0.0237651	0.0110631	-0.0041657	
S 3.3706250D+03	0.2967481	-0.1543718	0.0785342	0.0404285	0.0188386	-0.0070947	
S 1.4821482D+03	0.3123966	-0.1912899	0.0994142	0.0517299	0.0241669	-0.0091095	
S 6.7492787D+02	0.1593757	-0.0244239	0.0034218	-0.0000801	-0.0002556	0.0001244	
S 2.9858232D+02	0.0187611	0.4544961	-0.3903937	-0.2282370	-0.1099071	0.0416413	
S 1.3989204D+02	-0.0007169	0.5646204	-0.6178333	-0.3979641	-0.1968062	0.0751432	
S 5.9474906D+01	0.0002182	0.1247198	0.3427436	0.3642442	0.2032600	-0.0797477	
S 3.1239587D+01	-0.0001425	-0.0185626	0.8754682	1.1105290	0.6593097	-0.2607932	
S 1.3498944D+01	0.0000610	0.0078262	0.1671667	-0.3774281	-0.3564354	0.1515910	
S 7.0056646D+00	-0.0000253	-0.0039972	-0.0180999	-1.0500285	-1.1917131	0.5580548	
S 2.4258219D+00	0.0000100	0.0015817	0.0058257	-0.1106201	0.6771838	-0.4964864	
S 1.2592656D+00	-0.0000055	-0.0008137	-0.0029407	0.0244162	0.8033702	-0.6551792	

S	3.2875923D-01	0.0000013	0.0001947	0.0006547	-0.0043174	0.0404592	0.8251939
S	1.2676301D-01	-0.0000005	-0.0000698	-0.0002298	0.0014826	-0.0078505	0.5103085
	P	2P	3P	4P	5P	6P	
BASIS/ORB. ENERGY	-553.7058200	-133.6851700	-30.3353650	-5.0991025	-0.3781844		
P	5.9841748D+07	0.0000188	-0.0000098	-0.0000050	-0.0000022	0.0000007	
P	8.3625162D+06	0.0000622	-0.0000324	-0.0000165	-0.0000073	0.0000023	
P	1.6980399D+06	0.0001791	-0.0000934	-0.0000475	-0.0000209	0.0000066	
P	4.2687615D+05	0.0004841	-0.0002532	-0.0001289	-0.0000568	0.0000178	
P	1.2433022D+05	0.0012918	-0.0006782	-0.0003455	-0.0001523	0.0000477	
P	4.0717501D+04	0.0034413	-0.0018164	-0.0009263	-0.0004081	0.0001277	
P	1.4805256D+04	0.0091874	-0.0048863	-0.0024972	-0.0011024	0.0003453	
P	5.8903715D+03	0.0243768	-0.0131295	-0.0067284	-0.0029660	0.0009280	
P	2.5270066D+03	0.0625826	-0.0343854	-0.0177153	-0.0078417	0.0024581	
P	1.1518135D+03	0.1454005	-0.0826265	-0.0429089	-0.0189585	0.0059321	
P	5.5101256D+02	0.2751000	-0.1635369	-0.0860171	-0.0383238	0.0120333	
P	2.7402856D+02	0.3597847	-0.2187218	-0.1154676	-0.0509981	0.0159312	
P	1.4024469D+02	0.2545979	-0.0618547	-0.0141865	-0.0049700	0.0015771	
P	7.2321707D+01	0.0678117	0.3599589	0.2930719	0.1460568	-0.0469172	
P	3.8604492D+01	0.0021048	0.5297901	0.4547741	0.2212291	-0.0699259	
P	2.0568223D+01	0.0007849	0.2192792	-0.0769549	-0.0739793	0.0247308	
P	1.0749893D+01	-0.0005258	0.0209625	-0.6616824	-0.5062567	0.1767011	
P	5.6311137D+00	0.0002060	0.0009666	-0.4160274	-0.2709967	0.0856047	
P	2.6656138D+00	-0.0000928	-0.0002719	-0.0491362	0.5823333	-0.2628843	
P	1.2704067D+00	0.0000492	0.0000396	0.0013961	0.6004919	-0.3141660	
P	5.2236762D-01	-0.0000184	-0.0000387	-0.0006831	0.0953848	0.2057816	
P	2.1515015D-01	0.0000076	0.0000167	0.0002988	-0.0028335	0.6410537	
P	7.8906102D-02	-0.0000021	-0.0000035	-0.0000551	0.0020169	0.3549004	
	D	3D	4D	5D			
BASIS/ORB. ENERGY	-105.7646500	-19.7231540	-1.8252321				
D	1.4832407D+04	0.0002621	0.0001411	0.0000538			
D	3.9078700D+03	0.0017875	0.0009650	0.0003679			
D	1.4112105D+03	0.0091563	0.0049815	0.0019033			
D	6.0080044D+02	0.0361421	0.0198353	0.0075863			
D	2.8292304D+02	0.1087586	0.0608606	0.0233905			
D	1.4257268D+02	0.2380447	0.1343290	0.0516469			

D	7.5076715D+01	0.3525917	0.1920355	0.0734731
D	4.0964885D+01	0.3085505	0.1043202	0.0323314
D	2.2655401D+01	0.1376292	-0.1904419	-0.1006885
D	1.2231504D+01	0.0245076	-0.4583376	-0.2262519
D	6.5287509D+00	0.0007494	-0.3800637	-0.1504856
D	3.3725397D+00	0.0003436	-0.1122823	0.2301965
D	1.6422812D+00	-0.0001061	-0.0071963	0.5188759
D	7.5855452D-01	0.0000398	-0.0001948	0.3693258
D	3.1262997D-01	-0.0000094	0.0001064	0.0850109
	F	4F		
BASIS/ORB.ENERGY		-8.2110314		
F	1.3204374D+03	0.0002972		
F	4.4350317D+02	0.0027449		
F	1.8928527D+02	0.0150711		
F	9.1264573D+01	0.0540350		
F	4.6896839D+01	0.1383617		
F	2.5042136D+01	0.2545829		
F	1.3390283D+01	0.3376090		
F	7.0365352D+00	0.3095451		
F	3.5328137D+00	0.1646575		
F	1.6070145D+00	0.0343919		

RADON [XE]4F(14)6S(2)5D(10)6P(6), 1S

CHARGE = 86.000000

SYMMETRY SPECIES	S	P	D	F
NUMBER OF BASIS FUNCTIONS	27	23	15	10
NUMBER OF CLOSED SHELLS	6	5	3	1
NUMBER OF OPEN SHELLS	0	0	0	0
OPEN SHELL OCCUPATION NUMBER	0	0	0	0

*** FINAL SCF RESULTS ***

E = -23567.609484250

ORBITAL ENERGIES AND EXPANSION COEFFICIENTS

	S	1S	2S	3S	4S	5S	6S
BASIS/ORB.ENERGY		-3641.2041000	-669.0100600	-166.9307000	-41.3522570	-8.4207442	-1.0711905
S	3.8309454D+11	0.0000047	-0.0000019	0.0000009	0.0000005	0.0000002	-0.0000001

S	3.7743015D+10	0.0000183	-0.0000074	0.0000036	0.0000018	0.0000009	-0.0000003
S	5.7282393D+09	0.0000580	-0.0000235	0.0000114	0.0000058	0.0000027	-0.0000011
S	1.0223956D+09	0.0001684	-0.0000680	0.0000329	0.0000168	0.0000079	-0.0000031
S	2.1097773D+08	0.0004361	-0.0001758	0.0000852	0.0000435	0.0000204	-0.0000079
S	4.9758039D+07	0.0010209	-0.0004112	0.0001991	0.0001017	0.0000478	-0.0000184
S	1.3264302D+07	0.0022226	-0.0008951	0.0004336	0.0002214	0.0001040	-0.0000402
S	3.8529432D+06	0.0046602	-0.0018802	0.0009109	0.0004652	0.0002185	-0.0000844
S	1.1959811D+06	0.0094485	-0.0038263	0.0018554	0.0009476	0.0004451	-0.0001719
S	3.9361516D+05	0.0185490	-0.0075741	0.0036763	0.0018786	0.0008825	-0.0003407
S	1.3729434D+05	0.0354443	-0.0146616	0.0071373	0.0036483	0.0017139	-0.0006618
S	5.0442862D+04	0.0664139	-0.0281656	0.0137529	0.0070406	0.0033088	-0.0012777
S	1.9488573D+04	0.1201856	-0.0529114	0.0260593	0.0133522	0.0062768	-0.0024239
S	7.9189237D+03	0.2036474	-0.0962580	0.0478497	0.0246276	0.0115893	-0.0044772
S	3.3603232D+03	0.2992668	-0.1570658	0.0801248	0.0413540	0.0194794	-0.0075237
S	1.4780885D+03	0.3084285	-0.1889635	0.0981865	0.0513198	0.0242377	-0.0093773
S	6.7356917D+02	0.1507233	-0.0093943	-0.0062241	-0.0056373	-0.0029348	0.0011800
S	3.0098021D+02	0.0165005	0.4659998	-0.4047535	-0.2374487	-0.1156762	0.0449488
S	1.4163104D+02	-0.0003973	0.5515566	-0.6042136	-0.3928453	-0.1967285	0.0771687
S	6.0475585D+01	0.0000379	0.1170151	0.3757732	0.4044340	0.2287467	-0.0923228
S	3.1713839D+01	-0.0000245	-0.0170147	0.8609676	1.0911629	0.6572579	-0.2670538
S	1.3451924D+01	-0.0000012	0.0072515	0.1580014	-0.4437491	-0.4248309	0.1862661
S	7.1127543D+00	0.0000083	-0.0039218	-0.0215735	-1.0023039	-1.1712649	0.5703862
S	2.5331097D+00	-0.0000042	0.0015722	0.0068315	-0.1014290	0.7437199	-0.5657971
S	1.3035851D+00	0.0000020	-0.0008124	-0.0034552	0.0212399	0.7677939	-0.6560948
S	3.7059550D-01	-0.0000006	0.0002111	0.0008450	-0.0040509	0.0343690	0.8246451
S	1.4702438D-01	0.0000002	-0.0000734	-0.0002870	0.0013506	-0.0054074	0.5377367
	P	2P	3P	4P	5P	6P	
BASIS/ORB. ENERGY	-570.0758300	-138.4666400	-31.8486000	-5.5384636	-0.4271703		
P	5.8284769D+07	0.0000202	-0.0000105	-0.0000054	-0.0000024	0.0000008	
P	8.3590590D+06	0.0000654	-0.0000341	-0.0000174	-0.0000078	0.0000025	
P	1.7116933D+06	0.0001885	-0.0000986	-0.0000503	-0.0000225	0.0000073	
P	4.2890530D+05	0.0005124	-0.0002687	-0.0001373	-0.0000614	0.0000200	
P	1.2436687D+05	0.0013661	-0.0007189	-0.0003676	-0.0001646	0.0000536	
P	4.0703208D+04	0.0036266	-0.0019192	-0.0009826	-0.0004396	0.0001431	
P	1.4798949D+04	0.0096491	-0.0051452	-0.0026400	-0.0011834	0.0003854	

P	5.8895427D+03	0.0255050	-0.0137802	-0.0070905	-0.0031740	0.0010333
P	2.5267687D+03	0.0651189	-0.0358936	-0.0185708	-0.0083471	0.0027196
P	1.1520800D+03	0.1501647	-0.0856790	-0.0446845	-0.0200511	0.0065305
P	5.5086762D+02	0.2811862	-0.1677457	-0.0886360	-0.0401046	0.0130822
P	2.7378326D+02	0.3602838	-0.2186699	-0.1156727	-0.0518527	0.0168850
P	1.3999795D+02	0.2463535	-0.0460065	-0.0035452	0.0000729	-0.0001265
P	7.2021978D+01	0.0616905	0.3829069	0.3143081	0.1593807	-0.0530638
P	3.8497829D+01	0.0014685	0.5196110	0.4450281	0.2191686	-0.0725656
P	2.0568014D+01	0.0007324	0.2022967	-0.1139189	-0.0979100	0.0351274
P	1.0836951D+01	-0.0004962	0.0180052	-0.6639089	-0.5243888	0.1899543
P	5.7335531D+00	0.0001919	0.0009942	-0.3952109	-0.2465968	0.0822038
P	2.7293647D+00	-0.0000820	-0.0003144	-0.0460831	0.6154591	-0.3008016
P	1.3042112D+00	0.0000426	0.0000517	0.0016574	0.5846871	-0.3125674
P	5.1568313D-01	-0.0000156	-0.0000408	-0.0007396	0.0784200	0.2898364
P	2.1858823D-01	0.0000070	0.0000180	0.0003357	-0.0053841	0.6282458
P	8.3562340D-02	-0.0000020	-0.0000049	-0.0000859	0.0016566	0.2965211

	D	3D	4D	5D
BASIS/ORB. ENERGY		-109.6773600	-20.8893950	-2.0892755
D	1.1985537D+04	0.0003847	0.0002086	0.0000818
D	3.3272140D+03	0.0023920	0.0013002	0.0005093
D	1.2849125D+03	0.0106311	0.0058274	0.0022914
D	5.7811528D+02	0.0385634	0.0213144	0.0083754
D	2.7989145D+02	0.1119638	0.0631354	0.0249778
D	1.4334261D+02	0.2393312	0.1357775	0.0536020
D	7.5989159D+01	0.3542057	0.1937962	0.0763474
D	4.1263308D+01	0.3093355	0.0975982	0.0291290
D	2.2443035D+01	0.1308845	-0.2182436	-0.1169099
D	1.2023139D+01	0.0195419	-0.4722406	-0.2423288
D	6.4285778D+00	0.0009770	-0.3545654	-0.1268595
D	3.3483726D+00	0.0000488	-0.0956042	0.2626725
D	1.6868048D+00	0.0000171	-0.0054017	0.5074467
D	8.1084410D-01	-0.0000088	-0.0002946	0.3461155
D	3.4433112D-01	0.0000042	0.0001464	0.0805606

	F	4F
BASIS/ORB. ENERGY		-9.0599406

F	1.2471719D+03	0.0003626
F	4.3085474D+02	0.0030971
F	1.8802375D+02	0.0161352
F	9.1574864D+01	0.0570172
F	4.7041485D+01	0.1461928
F	2.5009938D+01	0.2651702
F	1.3363832D+01	0.3396620
F	7.0932945D+00	0.2962044
F	3.6330615D+00	0.1522115
F	1.6982621D+00	0.0313477

FRANCIUM [RN]7S(1), 2S

CHARGE = 87.000000

SYMMETRY SPECIES	S	P	D	F
NUMBER OF BASIS FUNCTIONS	35	26	18	13
NUMBER OF CLOSED SHELLS	6	5	3	1
NUMBER OF OPEN SHELLS	1	0	0	0
OPEN SHELL OCCUPATION NUMBER	1	0	0	0

*** FINAL SCF RESULTS ***

E = -24271.221986984

ORBITAL ENERGIES AND EXPANSION COEFFICIENTS

	S	1S	2S	3S	4S	5S	6S	7S
BASIS/ORB. ENERGY		-3742.8407000	-690.7409500	-173.2959800	-43.5147870	-9.2115927	-1.3522130	-0.1316408
S	3.2244469D+12	0.0000011	-0.0000005	0.0000002	0.0000001	-0.0000001	0.0000000	0.0000000
S	3.1047682D+11	0.0000047	-0.0000019	0.0000009	0.0000005	-0.0000002	0.0000001	0.0000000
S	4.8590502D+10	0.0000140	-0.0000057	0.0000028	0.0000014	-0.0000007	0.0000003	-0.0000001
S	1.0054799D+10	0.0000352	-0.0000143	0.0000070	0.0000036	-0.0000017	0.0000007	-0.0000002
S	2.5073787D+09	0.0000793	-0.0000322	0.0000156	0.0000080	-0.0000038	0.0000015	-0.0000004
S	7.2698514D+08	0.0001596	-0.0000647	0.0000314	0.0000161	-0.0000076	0.0000031	-0.0000008
S	2.4170350D+08	0.0002952	-0.0001196	0.0000580	0.0000297	-0.0000141	0.0000057	-0.0000014
S	8.6668624D+07	0.0005592	-0.0002265	0.0001098	0.0000563	-0.0000267	0.0000108	-0.0000027
S	3.0891912D+07	0.0011200	-0.0004534	0.0002199	0.0001126	-0.0000535	0.0000216	-0.0000054
S	1.0730469D+07	0.0022481	-0.0009104	0.0004416	0.0002262	-0.0001073	0.0000433	-0.0000108
S	3.7197889D+06	0.0044004	-0.0017848	0.0008660	0.0004436	-0.0002105	0.0000850	-0.0000211
S	1.3137931D+06	0.0084049	-0.0034208	0.0016608	0.0008508	-0.0004038	0.0001631	-0.0000405

S	4.7990107D+05	0.0154842	-0.0063440	0.0030836	0.0015801	-0.0007500	0.0003030	-0.0000751
S	1.8466920D+05	0.0273268	-0.0113186	0.0055117	0.0028254	-0.0013411	0.0005416	-0.0001344
S	7.5418635D+04	0.0464385	-0.0195771	0.0095627	0.0049068	-0.0023300	0.0009415	-0.0002335
S	3.2773337D+04	0.0756760	-0.0327558	0.0160722	0.0082533	-0.0039187	0.0015822	-0.0003928
S	1.5098341D+04	0.1186786	-0.0535182	0.0264537	0.0136176	-0.0064734	0.0026177	-0.0006485
S	7.2580686D+03	0.1789881	-0.0857279	0.0428356	0.0220893	-0.0104959	0.0042351	-0.0010532
S	3.5800878D+03	0.2445702	-0.1287858	0.0655305	0.0340007	-0.0162053	0.0065647	-0.0016217
S	1.8042970D+03	0.2662136	-0.1569597	0.0816871	0.0425138	-0.0202258	0.0081434	-0.0020376
S	9.2329949D+02	0.1882641	-0.0981617	0.0490686	0.0254631	-0.0122054	0.0050074	-0.0012013
S	4.7077519D+02	0.0573796	0.1690344	-0.1339391	-0.0777165	0.0382835	-0.0157383	0.0038114
S	2.4261042D+02	0.0020664	0.5022704	-0.4697355	-0.2842855	0.1404688	-0.0568966	0.0143647
S	1.2781797D+02	0.0010867	0.3950230	-0.4662436	-0.3092066	0.1588702	-0.0661401	0.0158705
S	7.0357003D+01	-0.0008724	0.0859588	0.2549873	0.2497049	-0.1429614	0.0620341	-0.0141905
S	3.9281200D+01	0.0005878	0.0074644	0.7777247	0.9663361	-0.5762417	0.2409393	-0.0626655
S	2.1527158D+01	-0.0004240	-0.0019463	0.3489125	0.4054825	-0.2507135	0.1164442	-0.0245013
S	1.2221831D+01	0.0002768	0.0011112	0.0231862	-0.8076648	0.7348903	-0.3577505	0.0830865
S	6.7169442D+00	-0.0001327	-0.0006682	0.0060165	-0.7365611	1.0196620	-0.5181681	0.1428750
S	3.2175919D+00	0.0000573	0.0002905	-0.0018719	-0.0900522	-0.5425882	0.3764988	-0.1146793
S	1.6296599D+00	-0.0000257	-0.0001180	0.0006363	0.0052913	-0.9908852	0.9433261	-0.2469653
S	5.9827170D-01	0.0000103	0.0000502	-0.0002946	-0.0020893	-0.1125485	-0.2429637	0.0463928
S	2.9596175D-01	-0.0000056	-0.0000277	0.0001642	0.0010733	0.0227115	-0.9379672	0.4658933
S	1.1688786D-01	0.0000015	0.0000071	-0.0000414	-0.0002473	-0.0047728	-0.1941989	0.1056489
S	2.2660486D-02	-0.0000002	-0.0000010	0.0000058	0.0000345	0.0005993	0.0025235	-1.1210819
	P	2P	3P	4P	5P	6P		
BASIS/ORB. ENERGY	-586.9187600	-143.5332600	-33.5818270	-6.1671510	-0.6216319			
P	4.6144126D+08	0.0000048	-0.0000025	-0.0000013	-0.0000006	0.0000002		
P	6.7302690D+07	0.0000147	-0.0000077	-0.0000039	-0.0000018	0.0000006		
P	1.4438281D+07	0.0000390	-0.0000204	-0.0000105	-0.0000047	0.0000017		
P	3.6463787D+06	0.0000994	-0.0000520	-0.0000267	-0.0000121	0.0000043		
P	1.0406179D+06	0.0002421	-0.0001270	-0.0000651	-0.0000295	0.0000104		
P	3.2868663D+05	0.0005721	-0.0003008	-0.0001543	-0.0000700	0.0000247		
P	1.1492957D+05	0.0013303	-0.0007020	-0.0003604	-0.0001634	0.0000577		
P	4.3433880D+04	0.0031650	-0.0016780	-0.0008625	-0.0003917	0.0001383		
P	1.7540764D+04	0.0076132	-0.0040650	-0.0020927	-0.0009492	0.0003352		
P	7.5555018D+03	0.0183385	-0.0098907	-0.0051053	-0.0023226	0.0008202		

P	3.4449559D+03	0.0436429	-0.0239292	-0.0123992	-0.0056288	0.0019887
P	1.6506219D+03	0.0976788	-0.0549291	-0.0286533	-0.0130809	0.0046214
P	8.2642974D+02	0.1918198	-0.1119454	-0.0589277	-0.0268212	0.0094844
P	4.2796450D+02	0.3007090	-0.1830398	-0.0975961	-0.0449096	0.0158788
P	2.2769364D+02	0.3188099	-0.1825756	-0.0946189	-0.0424821	0.0150206
P	1.2323539D+02	0.1833390	0.0373605	0.0511903	0.0262126	-0.0095803
P	6.6817859D+01	0.0395950	0.4208896	0.3502354	0.1812695	-0.0653734
P	3.6889916D+01	0.0013239	0.4741574	0.3993965	0.1965304	-0.0708843
P	2.0160121D+01	0.0001550	0.1721541	-0.1731564	-0.1358740	0.0533762
P	1.0765118D+01	-0.0001844	0.0146011	-0.6649812	-0.5427314	0.2137767
P	5.7455211D+00	0.0000402	0.0008334	-0.3622280	-0.2086806	0.0745523
P	2.8207962D+00	-0.0000125	-0.0003111	-0.0400271	0.6271089	-0.3422704
P	1.3773655D+00	0.0000115	0.0000484	0.0006263	0.5717067	-0.3330197
P	5.5579289D-01	-0.0000032	-0.0000391	-0.0003717	0.0782113	0.3316307
P	2.4793669D-01	0.0000016	0.0000182	0.0001902	-0.0063902	0.6465271
P	1.0071325D-01	-0.0000004	-0.0000050	-0.0000477	0.0017526	0.2430464

	D	3D	4D	5D
BASIS/ORB. ENERGY		-113.8494300	-22.2666720	-2.5391306
D	3.9623203D+04	0.0000658	-0.0000358	0.0000144
D	9.9788161D+03	0.0004154	-0.0002267	0.0000913
D	3.4890328D+03	0.0020680	-0.0011306	0.0004546
D	1.4378227D+03	0.0088788	-0.0048927	0.0019741
D	6.5927843D+02	0.0315361	-0.0175059	0.0070611
D	3.2622799D+02	0.0903503	-0.0510755	0.0207226
D	1.6982040D+02	0.2025835	-0.1157246	0.0469387
D	9.0903907D+01	0.3282172	-0.1840152	0.0746429
D	4.9770581D+01	0.3344305	-0.1445078	0.0530146
D	2.7491861D+01	0.1772227	0.1161393	-0.0719525
D	1.5141529D+01	0.0394092	0.4032720	-0.2127024
D	8.4717864D+00	0.0025939	0.4058693	-0.2005373
D	4.8163897D+00	0.0004270	0.1781038	0.0525219
D	2.8572907D+00	-0.0001016	0.0352202	0.2881653
D	1.7389284D+00	0.0000538	0.0042473	0.3753602
D	1.0130047D+00	-0.0000204	-0.0000305	0.3114267
D	5.4070390D-01	0.0000077	-0.0000312	0.1303118

D	2.5194248D-01	-0.0000006	-0.0000395	0.0174883
F		4F		
BASIS/ORB.ENERGY		-10.1172090		
F	1.8508172D+03	-0.0001590		
F	6.2432203D+02	-0.0014740		
F	2.6461067D+02	-0.0086514		
F	1.2637520D+02	-0.0350140		
F	6.4371980D+01	-0.1003514		
F	3.4314689D+01	-0.2084858		
F	1.8730220D+01	-0.3035158		
F	1.0317612D+01	-0.3189302		
F	5.5081267D+00	-0.2764104		
F	4.4668327D+00	0.0975915		
F	3.3759831D+00	-0.1261195		
F	1.7493609D+00	-0.0213332		
F	8.1676479D-01	-0.0011920		

RADIUM [RN]7S(2), 1S

CHARGE = 88.000000

SYMMETRY SPECIES	S	P	D	F
NUMBER OF BASIS FUNCTIONS	35	26	18	13
NUMBER OF CLOSED SHELLS	7	5	3	1
NUMBER OF OPEN SHELLS	0	0	0	0
OPEN SHELL OCCUPATION NUMBER	0	0	0	0

*** FINAL SCF RESULTS ***

E = -24988.616996780

ORBITAL ENERGIES AND EXPANSION COEFFICIENTS

	S	1S	2S	3S	4S	5S	6S	7S
BASIS/ORB.ENERGY		-3846.5239000	-713.0058800	-179.8271800	-45.7358250	-10.0184960	-1.6261645	-0.1651272
S	3.2244469D+12	0.0000013	-0.0000005	0.0000003	0.0000001	-0.0000001	0.0000000	0.0000000
S	3.1047682D+11	0.0000051	-0.0000021	0.0000010	0.0000005	-0.0000003	0.0000001	0.0000000
S	4.8590502D+10	0.0000151	-0.0000062	0.0000030	0.0000015	-0.0000007	0.0000003	-0.0000001
S	1.0054799D+10	0.0000379	-0.0000155	0.0000075	0.0000039	-0.0000019	0.0000008	-0.0000002
S	2.5073787D+09	0.0000851	-0.0000348	0.0000169	0.0000087	-0.0000042	0.0000018	-0.0000005
S	7.2698514D+08	0.0001706	-0.0000696	0.0000338	0.0000174	-0.0000083	0.0000035	-0.0000010

S	2.4170350D+08	0.0003147	-0.0001283	0.0000623	0.0000320	-0.0000153	0.0000065	-0.0000019
S	8.6668624D+07	0.0005946	-0.0002421	0.0001176	0.0000604	-0.0000289	0.0000122	-0.0000036
S	3.0891912D+07	0.0011873	-0.0004832	0.0002347	0.0001206	-0.0000578	0.0000243	-0.0000072
S	1.0730469D+07	0.0023756	-0.0009672	0.0004698	0.0002413	-0.0001157	0.0000487	-0.0000144
S	3.7197889D+06	0.0046352	-0.0018901	0.0009184	0.0004718	-0.0002262	0.0000951	-0.0000281
S	1.3137610D+06	0.0088229	-0.0036104	0.0017553	0.0009018	-0.0004323	0.0001818	-0.0000537
S	4.7990400D+05	0.0161955	-0.0066718	0.0032477	0.0016691	-0.0008002	0.0003367	-0.0000993
S	1.8466920D+05	0.0284733	-0.0118604	0.0057841	0.0029736	-0.0014256	0.0005996	-0.0001770
S	7.5418635D+04	0.0481811	-0.0204327	0.0099962	0.0051444	-0.0024676	0.0010385	-0.0003062
S	3.2773337D+04	0.0781375	-0.0340368	0.0167282	0.0086150	-0.0041313	0.0017371	-0.0005132
S	1.5098341D+04	0.1218287	-0.0553192	0.0273935	0.0141450	-0.0067933	0.0028617	-0.0008424
S	7.2580908D+03	0.1823732	-0.0880088	0.0440600	0.0227853	-0.0109325	0.0045929	-0.0013603
S	3.5801424D+03	0.2465637	-0.1308276	0.0667138	0.0347332	-0.0167317	0.0070642	-0.0020715
S	1.8042970D+03	0.2641108	-0.1561749	0.0813627	0.0424363	-0.0203688	0.0085298	-0.0025475
S	9.2330442D+02	0.1818917	-0.0895046	0.0437874	0.0227170	-0.0110439	0.0047529	-0.0013337
S	4.7079316D+02	0.0529798	0.1874558	-0.1489745	-0.0869313	0.0433802	-0.0186219	0.0053452
S	2.4261351D+02	0.0016790	0.5095831	-0.4834117	-0.2942265	0.1467731	-0.0618215	0.0186310
S	1.2776994D+02	0.0009685	0.3789340	-0.4459867	-0.2988348	0.1562725	-0.0682235	0.0193118
S	7.0384491D+01	-0.0007695	0.0760098	0.3039773	0.3010869	-0.1760061	0.0800141	-0.0218518
S	3.9219871D+01	0.0005037	0.0066245	0.7777530	0.9831932	-0.5922282	0.2572005	-0.0801586
S	2.1292988D+01	-0.0003668	-0.0019821	0.3181377	0.3351576	-0.2141073	0.1087645	-0.0254948
S	1.2221818D+01	0.0002457	0.0011327	0.0139661	-0.8611326	0.8247612	-0.4277260	0.1181745
S	6.7171019D+00	-0.0001168	-0.0006604	0.0067120	-0.6865563	0.9686294	-0.5115802	0.1721656
S	3.2145788D+00	0.0000511	0.0002940	-0.0022530	-0.0735379	-0.6591886	0.4779205	-0.1759278
S	1.6484713D+00	-0.0000237	-0.0001233	0.0008163	0.0041226	-0.9210553	0.9798968	-0.3082022
S	6.4486758D-01	0.0000087	0.0000475	-0.0003265	-0.0014166	-0.0873879	-0.4131856	0.1218312
S	2.9782185D-01	-0.0000038	-0.0000215	0.0001502	0.0006076	0.0108329	-0.9561951	0.6633638
S	9.4009563D-02	0.0000010	0.0000057	-0.0000390	-0.0001346	-0.0022441	-0.0869698	-0.1484182
S	2.9444441D-02	-0.0000003	-0.0000015	0.0000105	0.0000354	0.0005395	0.0084725	-1.0398832
	P	2P	3P	4P	5P	6P		
	BASIS/ORB. ENERGY	-604.0551200	-148.7040800	-35.3536100	-6.8040548	-0.8069118		
P	5.1267276D+08	0.0000048	-0.0000025	-0.0000013	-0.0000006	0.0000002		
P	7.1882190D+07	0.0000155	-0.0000081	-0.0000042	-0.0000019	0.0000007		
P	1.4487878D+07	0.0000421	-0.0000221	-0.0000114	-0.0000052	0.0000020		
P	3.6574645D+06	0.0001047	-0.0000549	-0.0000283	-0.0000130	0.0000049		

P	1.0436183D+06	0.0002555	-0.0001343	-0.0000691	-0.0000318	0.0000119
P	3.3112639D+05	0.0005988	-0.0003156	-0.0001625	-0.0000747	0.0000280
P	1.1545176D+05	0.0014085	-0.0007450	-0.0003839	-0.0001764	0.0000662
P	4.3364399D+04	0.0033425	-0.0017765	-0.0009166	-0.0004216	0.0001583
P	1.7541541D+04	0.0079676	-0.0042654	-0.0022042	-0.0010132	0.0003805
P	7.5611426D+03	0.0191887	-0.0103790	-0.0053783	-0.0024781	0.0009309
P	3.4456953D+03	0.0454465	-0.0249962	-0.0130031	-0.0059837	0.0022477
P	1.6513379D+03	0.1011535	-0.0570874	-0.0299035	-0.0138242	0.0051959
P	8.2630518D+02	0.1971264	-0.1154742	-0.0610383	-0.0281738	0.0105911
P	4.2784464D+02	0.3046641	-0.1860002	-0.0995909	-0.0463832	0.0174547
P	2.2758046D+02	0.3158545	-0.1782031	-0.0920012	-0.0418640	0.0157058
P	1.2323320D+02	0.1749152	0.0535237	0.0627346	0.0326041	-0.0125804
P	6.7079527D+01	0.0358508	0.4320359	0.3627500	0.1901084	-0.0731636
P	3.7147237D+01	0.0012326	0.4631765	0.3868497	0.1928740	-0.0737146
P	2.0381263D+01	0.0000671	0.1622383	-0.1951206	-0.1544114	0.0640851
P	1.0964855D+01	-0.0001398	0.0133183	-0.6635903	-0.5518558	0.2337604
P	5.8958036D+00	0.0000211	0.0008221	-0.3488888	-0.2016047	0.0740342
P	2.9839220D+00	-0.0000034	-0.0003348	-0.0390118	0.6200222	-0.3618802
P	1.4909924D+00	0.0000078	0.0000579	-0.0000542	0.5734833	-0.3736536
P	6.5055803D-01	-0.0000017	-0.0000441	-0.0001643	0.0875093	0.3110614
P	2.9672566D-01	0.0000008	0.0000190	0.0000977	-0.0036389	0.6891829
P	1.2027334D-01	-0.0000002	-0.0000050	-0.0000246	0.0009711	0.2371468

	D	3D	4D	5D
BASIS/ORB. ENERGY	-118.0989600	-23.6731030	-2.9937224	
D	3.8358002D+04	0.0000721	0.0000394	0.0000162
D	9.9661515D+03	0.0004361	0.0002394	0.0000988
D	3.4994748D+03	0.0021889	0.0012038	0.0004958
D	1.4368697D+03	0.0094077	0.0052166	0.0021567
D	6.5889404D+02	0.0331120	0.0184967	0.0076434
D	3.2629428D+02	0.0941691	0.0536011	0.0222893
D	1.6984739D+02	0.2089968	0.1200660	0.0498873
D	9.0895189D+01	0.3331748	0.1874257	0.0778754
D	4.9761984D+01	0.3302873	0.1375319	0.0504919
D	2.7460074D+01	0.1684438	-0.1347967	-0.0833805
D	1.5122507D+01	0.0351816	-0.4159037	-0.2261769

D	8.4711397D+00	0.0022594	-0.3966930	-0.1963418
D	4.8087400D+00	0.0002772	-0.1642292	0.0817987
D	2.8585222D+00	-0.0000210	-0.0289510	0.3102448
D	1.7499034D+00	-0.0000007	-0.0036243	0.3818743
D	1.0131640D+00	0.0000048	0.0002107	0.2922620
D	5.4102524D-01	-0.0000002	0.0000026	0.1030403
D	2.5348547D-01	0.0000009	0.0000380	0.0100519

F 4F

BASIS/ORB.ENERGY -11.2009760

F	1.8529220D+03	0.0001728
F	6.2477669D+02	0.0015964
F	2.6468871D+02	0.0093345
F	1.2638692D+02	0.0374326
F	6.4359043D+01	0.1062376
F	3.4315364D+01	0.2170160
F	1.8722787D+01	0.3100045
F	1.0314666D+01	0.3170161
F	5.5034564D+00	0.2622780
F	4.4707126D+00	-0.0899476
F	3.3690040D+00	0.1120381
F	1.7461726D+00	0.0167009
F	8.0733808D-01	0.0007418

 ACTINIUM [RN]7S(2)6D(1), 2D

CHARGE = 89.000000

SYMMETRY SPECIES S P D F

NUMBER OF BASIS FUNCTIONS 35 26 18 13

NUMBER OF CLOSED SHELLS 7 5 3 1

NUMBER OF OPEN SHELLS 0 0 1 0

OPEN SHELL OCCUPATION NUMBER 0 0 1 0

*** FINAL SCF RESULTS ***

E = -25719.991753641

ORBITAL ENERGIES AND EXPANSION COEFFICIENTS

S	1S	2S	3S	4S	5S	6S	7S
BASIS/ORB.ENERGY	-3952.2653000	-735.7792100	-186.4873300	-47.9756450	-10.8008910	-1.8523824	-0.1892183

S	3.2665313D+12	0.0000014	-0.0000006	0.0000003	0.0000001	-0.0000001	0.0000000	0.0000000
S	3.1047682D+11	0.0000055	-0.0000023	0.0000011	0.0000006	-0.0000003	0.0000001	0.0000000
S	4.8590502D+10	0.0000164	-0.0000068	0.0000033	0.0000017	-0.0000008	0.0000004	-0.0000001
S	1.0009456D+10	0.0000410	-0.0000169	0.0000082	0.0000042	-0.0000021	0.0000009	-0.0000003
S	2.5031167D+09	0.0000911	-0.0000374	0.0000182	0.0000094	-0.0000045	0.0000020	-0.0000006
S	7.2698514D+08	0.0001827	-0.0000749	0.0000365	0.0000188	-0.0000091	0.0000039	-0.0000012
S	2.4149867D+08	0.0003357	-0.0001375	0.0000669	0.0000345	-0.0000167	0.0000072	-0.0000023
S	8.6685553D+07	0.0006319	-0.0002587	0.0001258	0.0000648	-0.0000314	0.0000136	-0.0000043
S	3.0891912D+07	0.0012584	-0.0005149	0.0002505	0.0001290	-0.0000624	0.0000271	-0.0000085
S	1.0737389D+07	0.0025083	-0.0010267	0.0004994	0.0002572	-0.0001245	0.0000539	-0.0000170
S	3.7214073D+06	0.0048835	-0.0020021	0.0009742	0.0005018	-0.0002428	0.0001052	-0.0000332
S	1.3137610D+06	0.0092614	-0.0038105	0.0018553	0.0009558	-0.0004625	0.0002004	-0.0000632
S	4.7991151D+05	0.0169362	-0.0070154	0.0034197	0.0017624	-0.0008529	0.0003697	-0.0001166
S	1.8467397D+05	0.0296561	-0.0124245	0.0060684	0.0031286	-0.0015141	0.0006560	-0.0002070
S	7.5418850D+04	0.0499867	-0.0213235	0.0104472	0.0053916	-0.0026103	0.0011318	-0.0003569
S	3.2766976D+04	0.0806384	-0.0353581	0.0174084	0.0089914	-0.0043531	0.0018852	-0.0005951
S	1.5100789D+04	0.1249617	-0.0571165	0.0283259	0.0146677	-0.0071092	0.0030862	-0.0009723
S	7.2573820D+03	0.1857919	-0.0903829	0.0453549	0.0235277	-0.0114000	0.0049303	-0.0015585
S	3.5801131D+03	0.2482841	-0.1325912	0.0677008	0.0353453	-0.0171777	0.0074804	-0.0023525
S	1.8042895D+03	0.2618302	-0.1554262	0.0811625	0.0424629	-0.0205969	0.0088620	-0.0028128
S	9.2328621D+02	0.1754478	-0.0795608	0.0373751	0.0192279	-0.0093794	0.0042272	-0.0012976
S	4.7079868D+02	0.0488640	0.2038718	-0.1623411	-0.0950839	0.0477896	-0.0212440	0.0066331
S	2.4304564D+02	0.0013197	0.5184306	-0.4992652	-0.3060002	0.1545888	-0.0668502	0.0212957
S	1.2653269D+02	0.0009081	0.3669525	-0.4284116	-0.2893183	0.1527018	-0.0695706	0.0216078
S	7.0381385D+01	-0.0007350	0.0577824	0.3624785	0.3593437	-0.2109103	0.1001104	-0.0309325
S	3.9224859D+01	0.0004738	0.0111144	0.7636947	0.9870763	-0.6054938	0.2684442	-0.0870959
S	2.1170375D+01	-0.0003482	-0.0055664	0.2959969	0.2659516	-0.1658658	0.0969942	-0.0279255
S	1.2273438D+01	0.0002395	0.0035417	0.0038637	-0.8901962	0.8793015	-0.4866304	0.1530741
S	6.8079979D+00	-0.0001131	-0.0018203	0.0088917	-0.6457881	0.9305900	-0.4943529	0.1700713
S	3.2109168D+00	0.0000494	0.0008110	-0.0032883	-0.0672295	-0.7877790	0.5806764	-0.2127178
S	1.6364770D+00	-0.0000255	-0.0004029	0.0014564	0.0062614	-0.8320291	1.0396511	-0.3796275
S	7.5968413D-01	0.0000097	0.0001566	-0.0005793	-0.0021529	-0.0579962	-0.5492854	0.2338624
S	3.1751340D-01	-0.0000029	-0.0000473	0.0001793	0.0006396	-0.0029118	-0.9771434	0.6875310
S	7.4446062D-02	0.0000008	0.0000127	-0.0000468	-0.0001460	0.0008275	-0.0557040	-0.4130248
S	3.0673697D-02	-0.0000003	-0.0000052	0.0000192	0.0000598	-0.0003599	0.0124589	-0.8168808

	P	2P	3P	4P	5P	6P
BASIS/ORB. ENERGY		-621.4468000	-153.9391300	-37.1236160	-7.4096774	-0.9534382
P 4.6486755D+08	0.0000053	-0.0000028	-0.0000014	-0.0000007	0.0000003	
P 7.1405815D+07	0.0000160	-0.0000084	-0.0000043	-0.0000020	0.0000008	
P 1.4639391D+07	0.0000448	-0.0000235	-0.0000121	-0.0000056	0.0000022	
P 3.6356151D+06	0.0001120	-0.0000589	-0.0000304	-0.0000142	0.0000055	
P 1.0437547D+06	0.0002678	-0.0001411	-0.0000729	-0.0000339	0.0000133	
P 3.3241273D+05	0.0006338	-0.0003348	-0.0001730	-0.0000805	0.0000315	
P 1.1520230D+05	0.0014898	-0.0007898	-0.0004085	-0.0001901	0.0000744	
P 4.3375379D+04	0.0035084	-0.0018692	-0.0009679	-0.0004508	0.0001765	
P 1.7538207D+04	0.0083697	-0.0044924	-0.0023303	-0.0010846	0.0004249	
P 7.5630690D+03	0.0200360	-0.0108674	-0.0056528	-0.0026371	0.0010325	
P 3.4460589D+03	0.0473874	-0.0261472	-0.0136558	-0.0063633	0.0024941	
P 1.6501671D+03	0.1047881	-0.0593448	-0.0312105	-0.0146100	0.0057220	
P 8.2612660D+02	0.2021295	-0.1188625	-0.0630956	-0.0294932	0.0115741	
P 4.2779024D+02	0.3085276	-0.1888128	-0.1014805	-0.0478614	0.0187517	
P 2.2745755D+02	0.3125104	-0.1734100	-0.0891236	-0.0409376	0.0160806	
P 1.2321108D+02	0.1667739	0.0705233	0.0751820	0.0393407	-0.0159902	
P 6.7169512D+01	0.0323403	0.4450892	0.3771126	0.2006284	-0.0802737	
P 3.7201660D+01	0.0010610	0.4525192	0.3724988	0.1864566	-0.0749388	
P 2.0374766D+01	0.0000099	0.1498906	-0.2309253	-0.1810342	0.0797719	
P 1.0986474D+01	-0.0001096	0.0108478	-0.6680157	-0.5728567	0.2527668	
P 5.9045407D+00	0.0000104	0.0009138	-0.3231655	-0.1554150	0.0569328	
P 2.9978014D+00	0.0000033	-0.0004232	-0.0325316	0.6607873	-0.4181718	
P 1.5054802D+00	0.0000046	0.0000980	-0.0001520	0.5385922	-0.3565942	
P 6.4793753D-01	-0.0000005	-0.0000571	-0.0000468	0.0698988	0.4194263	
P 3.0104212D-01	0.0000003	0.0000258	0.0000546	-0.0041462	0.6586134	
P 1.2294138D-01	-0.0000001	-0.0000067	-0.0000145	0.0008517	0.1754923	
D	3D	4D	5D	6D		
BASIS/ORB. ENERGY		-122.3852600	-25.0684910	-3.4137507	-0.1751691	
D 4.3754266D+04	0.0000650	0.0000358	0.0000151	-0.0000037		
D 1.0733782D+04	0.0004275	0.0002359	0.0000996	-0.0000244		
D 3.5991889D+03	0.0023014	0.0012737	0.0005366	-0.0001316		
D 1.4321884D+03	0.0102284	0.0057032	0.0024126	-0.0005908		
D 6.4912279D+02	0.0359193	0.0202077	0.0085421	-0.0020966		

D	3.2083103D+02	0.1002981	0.0574621	0.0244626	-0.0059942
D	1.6835195D+02	0.2125889	0.1229013	0.0522114	-0.0128315
D	9.1624706D+01	0.3272545	0.1845573	0.0785043	-0.0192043
D	5.0769999D+01	0.3258854	0.1348187	0.0499457	-0.0121072
D	2.7945017D+01	0.1683910	-0.1468595	-0.0919235	0.0238031
D	1.5001727D+01	0.0329443	-0.4557626	-0.2560377	0.0647772
D	8.0084638D+00	0.0013330	-0.4074852	-0.1862905	0.0458833
D	4.1601846D+00	0.0002758	-0.1259103	0.2393005	-0.0766403
D	2.1101549D+00	-0.0000844	-0.0076068	0.5405593	-0.1674237
D	1.0277232D+00	0.0000351	-0.0005050	0.3496881	-0.0802428
D	4.5352361D-01	-0.0000101	0.0002784	0.0626752	0.2588903
D	1.6806913D-01	0.0000039	-0.0000620	-0.0002239	0.5580699
D	5.5246265D-02	-0.0000010	0.0000202	0.0004469	0.4068753

F

4F

BASIS/ORB. ENERGY -12.2708190

F	1.8553256D+03	0.0001875
F	6.2529707D+02	0.0017260
F	2.6477914D+02	0.0100559
F	1.2639122D+02	0.0399584
F	6.4345001D+01	0.1122806
F	3.4315438D+01	0.2254486
F	1.8715140D+01	0.3161255
F	1.0310185D+01	0.3141924
F	5.5055135D+00	0.2451708
F	4.4681569D+00	-0.0790556
F	3.3573012D+00	0.0980103
F	1.7413061D+00	0.0128728
F	8.0470069D-01	0.0004371

 THORIUM [RN]7S(2)6D(2), 3F

CHARGE = 90.000000

SYMMETRY SPECIES	S	P	D	F
NUMBER OF BASIS FUNCTIONS	35	26	18	13
NUMBER OF CLOSED SHELLS	7	5	3	1
NUMBER OF OPEN SHELLS	0	0	1	0

OPEN SHELL OCCUPATION NUMBER 0 0 2 0

*** FINAL SCF RESULTS ***

E =-26465.679259379

ORBITAL ENERGIES AND EXPANSION COEFFICIENTS

	S	1S	2S	3S	4S	5S	6S	7S
BASIS/ORB. ENERGY	-4060.1392000	-759.1011200	-193.3053200	-50.2604340	-11.5851280	-2.0638996	-0.2065769	
S 3.2665313D+12	0.0000015	-0.0000006	0.0000003	0.0000002	-0.0000001	0.0000000	0.0000000	
S 3.1047682D+11	0.0000060	-0.0000025	0.0000012	0.0000006	-0.0000003	0.0000001	0.0000000	
S 4.8590502D+10	0.0000177	-0.0000074	0.0000036	0.0000019	-0.0000009	0.0000004	-0.0000001	
S 1.0009456D+10	0.0000442	-0.0000183	0.0000089	0.0000046	-0.0000023	0.0000010	-0.0000003	
S 2.5031167D+09	0.0000979	-0.0000404	0.0000197	0.0000102	-0.0000050	0.0000022	-0.0000007	
S 7.2698514D+08	0.0001955	-0.0000806	0.0000393	0.0000203	-0.0000099	0.0000044	-0.0000014	
S 2.4149867D+08	0.0003581	-0.0001475	0.0000719	0.0000371	-0.0000181	0.0000080	-0.0000026	
S 8.6685553D+07	0.0006720	-0.0002766	0.0001347	0.0000696	-0.0000340	0.0000151	-0.0000049	
S 3.0891912D+07	0.0013342	-0.0005489	0.0002674	0.0001381	-0.0000674	0.0000299	-0.0000098	
S 1.0737389D+07	0.0026507	-0.0010909	0.0005314	0.0002745	-0.0001340	0.0000595	-0.0000194	
S 3.7214073D+06	0.0051434	-0.0021201	0.0010330	0.0005336	-0.0002605	0.0001156	-0.0000377	
S 1.3137610D+06	0.0097190	-0.0040209	0.0019605	0.0010127	-0.0004944	0.0002195	-0.0000716	
S 4.7991737D+05	0.0177094	-0.0073767	0.0036008	0.0018608	-0.0009086	0.0004034	-0.0001317	
S 1.8460185D+05	0.0309124	-0.0130263	0.0063716	0.0032940	-0.0016083	0.0007139	-0.0002331	
S 7.5356435D+04	0.0518524	-0.0222520	0.0109183	0.0056503	-0.0027602	0.0012258	-0.0004000	
S 3.2757509D+04	0.0831271	-0.0366901	0.0180937	0.0093714	-0.0045771	0.0020314	-0.0006634	
S 1.5103318D+04	0.1281101	-0.0589472	0.0292818	0.0152062	-0.0074377	0.0033058	-0.0010783	
S 7.2584012D+03	0.1891003	-0.0927174	0.0466192	0.0242519	-0.0118522	0.0052567	-0.0017178	
S 3.5788124D+03	0.2502103	-0.1344780	0.0687821	0.0360187	-0.0176734	0.0078713	-0.0025653	
S 1.8033247D+03	0.2588679	-0.1540846	0.0805503	0.0422383	-0.0206428	0.0091288	-0.0029890	
S 9.2423847D+02	0.1689829	-0.0690949	0.0307186	0.0156311	-0.0077365	0.0035304	-0.0011346	
S 4.6958869D+02	0.0453904	0.2222367	-0.1780784	-0.1048628	0.0533418	-0.0241060	0.0078445	
S 2.4308611D+02	0.0005778	0.5221063	-0.5098574	-0.3143872	0.1601498	-0.0713737	0.0234152	
S 1.2633571D+02	0.0011544	0.3513401	-0.4046111	-0.2754314	0.1479741	-0.0683474	0.0222249	
S 7.0381385D+01	-0.0009438	0.0480823	0.4108354	0.4130526	-0.2473450	0.1177780	-0.0384151	
S 3.9224859D+01	0.0006304	0.0113669	0.7498546	0.9863825	-0.6097923	0.2814449	-0.0934139	
S 2.1170957D+01	-0.0004619	-0.0061482	0.2700149	0.1909418	-0.1227728	0.0718363	-0.0227565	
S 1.2267199D+01	0.0003176	0.0039196	0.0010616	-0.9235407	0.9650089	-0.5396873	0.1804748	
S 6.8095844D+00	-0.0001522	-0.0019994	0.0082236	-0.5958419	0.8532579	-0.4806778	0.1678054	

S	3.2116152D+00	0.0000669	0.0008969	-0.0031424	-0.0541981	-0.8943142	0.7278179	-0.2700134
S	1.6377747D+00	-0.0000348	-0.0004517	0.0014035	0.0046600	-0.7593125	0.9869062	-0.3927877
S	7.5934918D-01	0.0000138	0.0001806	-0.0005711	-0.0015873	-0.0374140	-0.6821301	0.3433313
S	3.3378405D-01	-0.0000042	-0.0000567	0.0001844	0.0005082	-0.0035923	-0.9001276	0.6537108
S	7.6225497D-02	0.0000010	0.0000136	-0.0000432	-0.0000997	0.0009037	-0.0446987	-0.5908494
S	3.0635439D-02	-0.0000004	-0.0000055	0.0000174	0.0000403	-0.0003792	0.0102534	-0.6643881
	P	2P	3P	4P	5P	6P		
BASIS/ORB. ENERGY	-639.1206100	-159.2636500	-38.9166820	-8.0093845	-1.0875660			
P	5.1369916D+08	0.0000054	-0.0000029	-0.0000015	-0.0000007	0.0000003		
P	7.2421457D+07	0.0000173	-0.0000091	-0.0000047	-0.0000022	0.0000009		
P	1.4656467D+07	0.0000475	-0.0000250	-0.0000129	-0.0000061	0.0000025		
P	3.6267708D+06	0.0001195	-0.0000630	-0.0000326	-0.0000154	0.0000062		
P	1.0337391D+06	0.0002869	-0.0001515	-0.0000785	-0.0000370	0.0000149		
P	3.2873308D+05	0.0006732	-0.0003564	-0.0001848	-0.0000870	0.0000352		
P	1.1450216D+05	0.0015741	-0.0008364	-0.0004342	-0.0002044	0.0000826		
P	4.3192758D+04	0.0036952	-0.0019737	-0.0010258	-0.0004834	0.0001954		
P	1.7522322D+04	0.0087563	-0.0047117	-0.0024530	-0.0011554	0.0004672		
P	7.5718170D+03	0.0208639	-0.0113492	-0.0059257	-0.0027966	0.0011305		
P	3.4573256D+03	0.0490259	-0.0271296	-0.0142225	-0.0067080	0.0027136		
P	1.6545617D+03	0.1085199	-0.0616769	-0.0325664	-0.0154211	0.0062367		
P	8.2521610D+02	0.2084458	-0.1230033	-0.0655571	-0.0310266	0.0125651		
P	4.2698117D+02	0.3113518	-0.1910890	-0.1031050	-0.0491762	0.0199024		
P	2.2771204D+02	0.3073071	-0.1670039	-0.0852454	-0.0395468	0.0160004		
P	1.2367773D+02	0.1594263	0.0832804	0.0846055	0.0448447	-0.0187383		
P	6.8086756D+01	0.0293950	0.4459502	0.3806054	0.2050246	-0.0849211		
P	3.7999418D+01	0.0014896	0.4441543	0.3640178	0.1843770	-0.0762679		
P	2.0919841D+01	-0.0002908	0.1480308	-0.2327198	-0.1863875	0.0846547		
P	1.1374482D+01	0.0000727	0.0104459	-0.6642590	-0.5781291	0.2656634		
P	6.1564151D+00	-0.0000944	0.0011553	-0.3242961	-0.1650236	0.0616558		
P	3.1859865D+00	0.0000592	-0.0005638	-0.0340518	0.6502959	-0.4269543		
P	1.6291231D+00	-0.0000222	0.0001651	-0.0004773	0.5493999	-0.3921178		
P	7.3712707D-01	0.0000112	-0.0000876	0.0000412	0.0779027	0.3979721		
P	3.4729667D-01	-0.0000047	0.0000379	0.0000268	-0.0028222	0.6809797		
P	1.4257602D-01	0.0000011	-0.0000092	-0.0000053	0.0006066	0.1914477		
	D	3D	4D	5D	6D			

BASIS/ORB. ENERGY	-126.7326200	-26.4772130	-3.8248915	-0.2342636
D 4.9771507D+04	0.0000607	0.0000336	0.0000144	-0.0000040
D 1.1053506D+04	0.0004569	0.0002535	0.0001092	-0.0000303
D 3.5781983D+03	0.0024772	0.0013791	0.0005934	-0.0001642
D 1.4293707D+03	0.0107460	0.0060270	0.0026036	-0.0007228
D 6.4933676D+02	0.0376910	0.0213377	0.0092135	-0.0025496
D 3.2059636D+02	0.1045629	0.0602884	0.0262157	-0.0072885
D 1.6835503D+02	0.2183942	0.1269587	0.0550888	-0.0152405
D 9.1705636D+01	0.3310233	0.1870899	0.0812036	-0.0226243
D 5.0842652D+01	0.3211006	0.1274930	0.0468903	-0.0124312
D 2.7986806D+01	0.1603336	-0.1648269	-0.1038469	0.0297943
D 1.5002607D+01	0.0296275	-0.4677945	-0.2698039	0.0786899
D 8.0047847D+00	0.0010728	-0.3931323	-0.1732561	0.0452383
D 4.1673997D+00	0.0002334	-0.1123565	0.2791396	-0.0977374
D 2.1092299D+00	-0.0000720	-0.0059997	0.5545984	-0.2065340
D 1.0226585D+00	0.0000296	-0.0002901	0.3155663	-0.0422949
D 4.3363914D-01	-0.0000083	0.0002127	0.0429887	0.3494889
D 1.7416264D-01	0.0000039	-0.0000546	-0.0014634	0.5443642
D 6.2967716D-02	-0.0000010	0.0000187	0.0006277	0.3011664

F 4F

BASIS/ORB. ENERGY	-13.3511070
F 1.8577194D+03	0.0002031
F 6.2583883D+02	0.0018629
F 2.6491641D+02	0.0108132
F 1.2638165D+02	0.0426124
F 6.4328107D+01	0.1184265
F 3.4317857D+01	0.2338259
F 1.8703377D+01	0.3218898
F 1.0310295D+01	0.3096766
F 5.5390871D+00	0.2209818
F 4.3932230D+00	-0.0629642
F 3.3531489D+00	0.0871674
F 1.7251519D+00	0.0096799
F 8.3161755D-01	0.0002221

PROTOACTINIUM [RN]7S(2)6D(1)5F(2), 4J

CHARGE = 91.000000

SYMMETRY SPECIES	S	P	D	F
NUMBER OF BASIS FUNCTIONS	35	26	18	13
NUMBER OF CLOSED SHELLS	7	5	3	1
NUMBER OF OPEN SHELLS	0	0	1	1
OPEN SHELL OCCUPATION NUMBER	0	0	1	2

*** FINAL SCF RESULTS ***

E = -27225.991304740

ORBITAL ENERGIES AND EXPANSION COEFFICIENTS

	S	1S	2S	3S	4S	5S	6S	7S
BASIS/ORB. ENERGY	-4169.8848000	-782.6521200	-199.9220400	-52.2293630	-12.0162800	-2.0448556	-0.1937969	
S 3.2665313D+12	0.0000016	-0.0000007	0.0000003	0.0000002	-0.0000001	0.0000000	0.0000000	
S 3.1047682D+11	0.0000066	-0.0000028	0.0000013	0.0000007	-0.0000003	0.0000002	0.0000000	
S 4.8590502D+10	0.0000192	-0.0000080	0.0000039	0.0000020	-0.0000010	0.0000004	-0.0000001	
S 1.0009456D+10	0.0000478	-0.0000199	0.0000097	0.0000050	-0.0000025	0.0000011	-0.0000003	
S 2.4966177D+09	0.0001055	-0.0000439	0.0000214	0.0000111	-0.0000054	0.0000024	-0.0000007	
S 7.2471686D+08	0.0002093	-0.0000868	0.0000424	0.0000219	-0.0000108	0.0000047	-0.0000014	
S 2.4149867D+08	0.0003813	-0.0001580	0.0000771	0.0000399	-0.0000196	0.0000086	-0.0000026	
S 8.6685553D+07	0.0007152	-0.0002961	0.0001444	0.0000748	-0.0000367	0.0000162	-0.0000049	
S 3.0891912D+07	0.0014144	-0.0005852	0.0002854	0.0001478	-0.0000726	0.0000320	-0.0000097	
S 1.0737389D+07	0.0028014	-0.0011594	0.0005655	0.0002928	-0.0001439	0.0000634	-0.0000192	
S 3.7214073D+06	0.0054166	-0.0022451	0.0010954	0.0005672	-0.0002788	0.0001228	-0.0000372	
S 1.3137450D+06	0.0101987	-0.0042429	0.0020715	0.0010728	-0.0005272	0.0002322	-0.0000703	
S 4.7991737D+05	0.0185122	-0.0077548	0.0037906	0.0019638	-0.0009653	0.0004252	-0.0001288	
S 1.8460185D+05	0.0321830	-0.0136410	0.0066816	0.0034629	-0.0017020	0.0007496	-0.0002271	
S 7.5356435D+04	0.0537429	-0.0232043	0.0114023	0.0059159	-0.0029095	0.0012818	-0.0003881	
S 3.2757509D+04	0.0857192	-0.0380800	0.0188081	0.0097662	-0.0048010	0.0021143	-0.0006409	
S 1.5103318D+04	0.1313120	-0.0608419	0.0302748	0.0157634	-0.0077642	0.0034228	-0.0010354	
S 7.2582067D+03	0.1923062	-0.0949899	0.0478466	0.0249540	-0.0122711	0.0054021	-0.0016396	
S 3.5789871D+03	0.2516258	-0.1361650	0.0697784	0.0366442	-0.0181172	0.0080001	-0.0024152	
S 1.8033247D+03	0.2560746	-0.1523655	0.0796515	0.0418404	-0.0205434	0.0090250	-0.0027519	
S 9.2423847D+02	0.1625943	-0.0588686	0.0242014	0.0120843	-0.0060987	0.0027513	-0.0007945	
S 4.6958869D+02	0.0416969	0.2406796	-0.1941744	-0.1149164	0.0590596	-0.0264024	0.0079247	
S 2.4308611D+02	0.0003817	0.5249075	-0.5195982	-0.3222817	0.1650611	-0.0731703	0.0223878	

S	1.2633580D+02	0.0010348	0.3342017	-0.3768564	-0.2581710	0.1412447	-0.0644931	0.0191608
S	7.0381385D+01	-0.0008434	0.0411376	0.4550166	0.4651480	-0.2839268	0.1331441	-0.0396945
S	3.9225458D+01	0.0005565	0.0104551	0.7345409	0.9808746	-0.6081754	0.2804001	-0.0875446
S	2.1170961D+01	-0.0004052	-0.0058190	0.2443485	0.1140327	-0.0786177	0.0474628	-0.0112267
S	1.2267199D+01	0.0002789	0.0036760	-0.0004472	-0.9488753	1.0503496	-0.5828457	0.1770898
S	6.8095844D+00	-0.0001334	-0.0018645	0.0072220	-0.5476567	0.7563876	-0.4258701	0.1428795
S	3.2116152D+00	0.0000585	0.0008367	-0.0027964	-0.0425278	-0.9823424	0.8263841	-0.2915767
S	1.6377547D+00	-0.0000304	-0.0004209	0.0012349	0.0029798	-0.6797565	0.8660999	-0.3033378
S	7.5934918D-01	0.0000120	0.0001681	-0.0005000	-0.0009826	-0.0294765	-0.7100851	0.3021296
S	3.3378608D-01	-0.0000037	-0.0000528	0.0001615	0.0003233	-0.0031246	-0.8569087	0.6014330
S	7.6231056D-02	0.0000009	0.0000127	-0.0000378	-0.0000583	0.0007074	-0.0436015	-0.4766402
S	3.0633838D-02	-0.0000004	-0.0000051	0.0000152	0.0000236	-0.0002963	0.0103735	-0.7509631
	P	2P	3P	4P	5P	6P		
BASIS/ORB. ENERGY	-656.7446500	-164.3158900	-40.3725970	-8.2625293	-1.0401835			
P	5.1155543D+08	0.0000058	-0.0000031	-0.0000016	-0.0000008	0.0000003		
P	7.2013448D+07	0.0000183	-0.0000097	-0.0000050	-0.0000024	0.0000009		
P	1.4731866D+07	0.0000502	-0.0000265	-0.0000138	-0.0000065	0.0000026		
P	3.6188316D+06	0.0001274	-0.0000673	-0.0000350	-0.0000166	0.0000066		
P	1.0316510D+06	0.0003032	-0.0001605	-0.0000834	-0.0000396	0.0000157		
P	3.2847411D+05	0.0007114	-0.0003775	-0.0001964	-0.0000932	0.0000370		
P	1.1439335D+05	0.0016585	-0.0008834	-0.0004601	-0.0002182	0.0000866		
P	4.3203876D+04	0.0038804	-0.0020775	-0.0010833	-0.0005142	0.0002042		
P	1.7519478D+04	0.0091902	-0.0049579	-0.0025904	-0.0012293	0.0004882		
P	7.5703645D+03	0.0217747	-0.0118778	-0.0062225	-0.0029582	0.0011746		
P	3.4589058D+03	0.0509905	-0.0283039	-0.0148945	-0.0070786	0.0028130		
P	1.6540049D+03	0.1123138	-0.0640557	-0.0339404	-0.0161897	0.0064314		
P	8.2522297D+02	0.2133094	-0.1263289	-0.0676109	-0.0322492	0.0128308		
P	4.2701621D+02	0.3149912	-0.1936914	-0.1047991	-0.0503388	0.0200097		
P	2.2743693D+02	0.3034825	-0.1611618	-0.0817023	-0.0380700	0.0151281		
P	1.2370313D+02	0.1510578	0.1004042	0.0977468	0.0521428	-0.0213897		
P	6.8182918D+01	0.0268138	0.4580349	0.3935582	0.2138358	-0.0870234		
P	3.7992905D+01	0.0010561	0.4326492	0.3490388	0.1766511	-0.0717370		
P	2.0963068D+01	-0.0001408	0.1351559	-0.2695275	-0.2145698	0.0956550		
P	1.1382522D+01	-0.0000274	0.0095502	-0.6666986	-0.5944244	0.2693033		
P	6.1580668D+00	-0.0000283	0.0005961	-0.2985310	-0.1115673	0.0315667		

P	3.1837911D+00	0.0000243	-0.0003107	-0.0282191	0.6883278	-0.4473503
P	1.6238247D+00	-0.0000056	0.0000455	-0.0003701	0.5053151	-0.3436844
P	7.4761205D-01	0.0000038	-0.0000336	0.0000140	0.0648255	0.4106699
P	3.4721579D-01	-0.0000015	0.0000142	0.0000316	-0.0005661	0.6622767
P	1.4339047D-01	0.0000004	-0.0000036	-0.0000088	0.0002029	0.1942369
	D	3D	4D	5D	6D	
BASIS/ORB. ENERGY	-130.7812800	-27.5396430	-3.9244007	-0.2237298		
D	3.8409563D+04	0.0000885	0.0000492	0.0000214	-0.0000059	
D	9.6913974D+03	0.0005519	0.0003080	0.0001339	-0.0000367	
D	3.4200290D+03	0.0026528	0.0014851	0.0006455	-0.0001770	
D	1.4306456D+03	0.0109394	0.0061705	0.0026895	-0.0007368	
D	6.5802200D+02	0.0386320	0.0219920	0.0095946	-0.0026322	
D	3.2226426D+02	0.1102281	0.0639338	0.0280453	-0.0076904	
D	1.6657757D+02	0.2325512	0.1358776	0.0596015	-0.0163690	
D	8.9902299D+01	0.3378412	0.1905208	0.0831500	-0.0227596	
D	5.0468770D+01	0.2999046	0.1118133	0.0399837	-0.0106563	
D	2.8934401D+01	0.1487848	-0.1520498	-0.0976347	0.0282930	
D	1.6201400D+01	0.0338297	-0.4287431	-0.2501581	0.0713081	
D	8.9418322D+00	0.0012275	-0.4080603	-0.2025746	0.0558282	
D	4.7686737D+00	0.0005439	-0.1422641	0.2114477	-0.0780282	
D	2.4451016D+00	-0.0002210	-0.0111406	0.5470107	-0.1949123	
D	1.1951296D+00	0.0000891	-0.0003948	0.3671496	-0.0901500	
D	5.2559086D-01	-0.0000337	0.0002108	0.0669237	0.2906214	
D	2.0145363D-01	0.0000112	-0.0000404	-0.0005463	0.5653686	
D	6.8888718D-02	-0.0000036	0.0000209	0.0001481	0.3622849	
	F	4F	5F			
BASIS/ORB. ENERGY	-14.0856430	-0.3177597				
F	3.2508191D+03	-0.0000861	-0.0000244			
F	7.9895277D+02	-0.0013384	-0.0003812			
F	3.0443716D+02	-0.0093181	-0.0026521			
F	1.3804992D+02	-0.0407282	-0.0116549			
F	6.7860968D+01	-0.1213332	-0.0347537			
F	3.5045052D+01	-0.2507246	-0.0709401			
F	1.8387982D+01	-0.3522780	-0.0912241			
F	9.6048780D+00	-0.3262686	-0.0567478			

F	4.8414391D+00	-0.1628622	0.1062203
F	2.2255853D+00	-0.0270092	0.3284036
F	9.7233758D-01	0.0004027	0.4185121
F	3.9388383D-01	-0.0003955	0.3311042
F	1.3942158D-01	0.0000902	0.1518744

URANIUM [RN]7S(2)6D(1)5F(3), 5L

CHARGE = 92.000000

SYMMETRY SPECIES	S	P	D	F
NUMBER OF BASIS FUNCTIONS	35	26	18	13
NUMBER OF CLOSED SHELLS	7	5	3	1
NUMBER OF OPEN SHELLS	0	0	1	1
OPEN SHELL OCCUPATION NUMBER	0	0	1	3

*** FINAL SCF RESULTS ***

E = -28001.366514892

ORBITAL ENERGIES AND EXPANSION COEFFICIENTS

	S	1S	2S	3S	4S	5S	6S	7S
BASIS/ORB. ENERGY		-4282.0074000	-806.9275400	-206.8560500	-54.3977110	-12.6063950	-2.1258069	-0.1962971
S	3.2665313D+12	0.0000018	-0.0000008	0.0000004	0.0000002	-0.0000001	0.0000000	0.0000000
S	3.1047682D+11	0.0000072	-0.0000030	0.0000015	0.0000008	-0.0000004	0.0000002	0.0000000
S	4.8590502D+10	0.0000208	-0.0000088	0.0000043	0.0000022	-0.0000011	0.0000005	-0.0000001
S	1.0009456D+10	0.0000515	-0.0000216	0.0000106	0.0000055	-0.0000027	0.0000012	-0.0000004
S	2.4966177D+09	0.0001134	-0.0000474	0.0000232	0.0000120	-0.0000060	0.0000026	-0.0000008
S	7.2471686D+08	0.0002240	-0.0000935	0.0000457	0.0000237	-0.0000117	0.0000052	-0.0000015
S	2.4149867D+08	0.0004071	-0.0001696	0.0000829	0.0000430	-0.0000213	0.0000094	-0.0000028
S	8.6685553D+07	0.0007606	-0.0003167	0.0001546	0.0000803	-0.0000397	0.0000176	-0.0000052
S	3.0894257D+07	0.0015003	-0.0006242	0.0003048	0.0001582	-0.0000783	0.0000346	-0.0000103
S	1.0739020D+07	0.0029580	-0.0012310	0.0006012	0.0003121	-0.0001544	0.0000683	-0.0000203
S	3.7243158D+06	0.0057029	-0.0023771	0.0011613	0.0006028	-0.0002983	0.0001319	-0.0000392
S	1.3137450D+06	0.0107067	-0.0044794	0.0021898	0.0011369	-0.0005625	0.0002487	-0.0000740
S	4.7991648D+05	0.0193437	-0.0081496	0.0039889	0.0020717	-0.0010253	0.0004534	-0.0001348
S	1.8460081D+05	0.0335027	-0.0142842	0.0070063	0.0036403	-0.0018013	0.0007964	-0.0002369
S	7.5352579D+04	0.0556811	-0.0241891	0.0119034	0.0061914	-0.0030659	0.0013559	-0.0004032
S	3.2757509D+04	0.0883541	-0.0395071	0.0195427	0.0101734	-0.0050348	0.0022259	-0.0006625
S	1.5104669D+04	0.1344782	-0.0627422	0.0312722	0.0163251	-0.0080976	0.0035833	-0.0010647

S	7.2596244D+03	0.1954481	-0.0972521	0.0490718	0.0256591	-0.0126993	0.0056129	-0.0016726
S	3.5789871D+03	0.2529294	-0.1377594	0.0707204	0.0372398	-0.0185517	0.0082220	-0.0024389
S	1.8033247D+03	0.2529768	-0.1502609	0.0785218	0.0413203	-0.0203884	0.0089938	-0.0026910
S	9.2424987D+02	0.1562919	-0.0481663	0.0172662	0.0082571	-0.0042841	0.0019486	-0.0005466
S	4.6958869D+02	0.0381882	0.2589777	-0.2104804	-0.1251664	0.0649462	-0.0291223	0.0086054
S	2.4308611D+02	0.0002665	0.5263139	-0.5280390	-0.3295310	0.1697988	-0.0756454	0.0226973
S	1.2633426D+02	0.0008839	0.3169866	-0.3466808	-0.2384548	0.1328696	-0.0609164	0.0178230
S	7.0371076D+01	-0.0007147	0.0348943	0.4971690	0.5168687	-0.3208746	0.1508232	-0.0444492
S	3.9225458D+01	0.0004611	0.0096288	0.7163366	0.9703148	-0.6038375	0.2804370	-0.0857140
S	2.1170961D+01	-0.0003325	-0.0054898	0.2203091	0.0351407	-0.0294773	0.0230241	-0.0042265
S	1.2266637D+01	0.0002291	0.0034354	-0.0016257	-0.9672650	1.1314130	-0.6352840	0.1913438
S	6.8087533D+00	-0.0001092	-0.0017327	0.0063539	-0.4996422	0.6492871	-0.3641376	0.1197813
S	3.2127131D+00	0.0000476	0.0007782	-0.0025009	-0.0330445	-1.0579409	0.9220727	-0.3179099
S	1.6377547D+00	-0.0000248	-0.0003907	0.0010920	0.0016863	-0.6029514	0.7730269	-0.2677402
S	7.5935845D-01	0.0000098	0.0001557	-0.0004392	-0.0005173	-0.0224121	-0.7891941	0.3386539
S	3.3392057D-01	-0.0000030	-0.0000489	0.0001423	0.0001862	-0.0024488	-0.7885307	0.5562863
S	7.6245555D-02	0.0000007	0.0000117	-0.0000332	-0.0000281	0.0005055	-0.0335897	-0.5102918
S	3.0635202D-02	-0.0000003	-0.0000047	0.0000134	0.0000115	-0.0002107	0.0076592	-0.7177173
	P	2P	3P	4P	5P	6P		
BASIS/ORB. ENERGY	-674.7970600	-169.6093000	-42.0032830	-8.6625765	-1.0717352			
P	5.0421512D+08	0.0000062	-0.0000033	-0.0000017	-0.0000008	0.0000003		
P	7.1035224D+07	0.0000198	-0.0000105	-0.0000054	-0.0000026	0.0000010		
P	1.4357392D+07	0.0000543	-0.0000287	-0.0000150	-0.0000072	0.0000028		
P	3.5466837D+06	0.0001364	-0.0000722	-0.0000377	-0.0000180	0.0000072		
P	1.0127981D+06	0.0003249	-0.0001723	-0.0000899	-0.0000430	0.0000171		
P	3.2373593D+05	0.0007562	-0.0004021	-0.0002099	-0.0001004	0.0000399		
P	1.1335358D+05	0.0017530	-0.0009359	-0.0004890	-0.0002338	0.0000929		
P	4.3002224D+04	0.0040769	-0.0021879	-0.0011448	-0.0005477	0.0002177		
P	1.7519177D+04	0.0095811	-0.0051823	-0.0027166	-0.0012999	0.0005168		
P	7.5854976D+03	0.0227049	-0.0124177	-0.0065287	-0.0031283	0.0012433		
P	3.4604410D+03	0.0530628	-0.0295491	-0.0156029	-0.0074782	0.0029750		
P	1.6541025D+03	0.1160904	-0.0664223	-0.0353315	-0.0169851	0.0067536		
P	8.2444285D+02	0.2190025	-0.1302073	-0.0699328	-0.0336511	0.0134046		
P	4.2636572D+02	0.3178631	-0.1956712	-0.1062610	-0.0514114	0.0204505		
P	2.2738444D+02	0.2982479	-0.1545038	-0.0773804	-0.0362722	0.0144323		

P	1.2391382D+02	0.1437067	0.1168659	0.1099572	0.0592842	-0.0243632
P	6.8446532D+01	0.0242388	0.4653095	0.4040096	0.2212821	-0.0901384
P	3.8286828D+01	0.0009842	0.4200258	0.3302333	0.1674083	-0.0681040
P	2.1203490D+01	-0.0001951	0.1277906	-0.2812184	-0.2272334	0.1018831
P	1.1721141D+01	0.0000117	0.0082771	-0.6529749	-0.5883384	0.2671117
P	6.4360107D+00	-0.0000509	0.0009871	-0.2986283	-0.1256614	0.0395615
P	3.4248631D+00	0.0000361	-0.0004915	-0.0306628	0.6593955	-0.4307069
P	1.7701463D+00	-0.0000101	0.0001127	-0.0009646	0.5379492	-0.3645568
P	7.9569853D-01	0.0000055	-0.0000611	0.0001417	0.0772606	0.3890528
P	3.6927144D-01	-0.0000022	0.0000254	-0.0000210	-0.0030060	0.6698362
P	1.5190133D-01	0.0000006	-0.0000064	0.0000046	0.0008077	0.2031953
	D	3D	4D	5D	6D	
BASIS/ORB. ENERGY	-135.0397500	-28.7661560	-4.1551027	-0.2280231		
D	3.7660811D+04	0.0000959	0.0000536	0.0000235	-0.0000065	
D	9.6167344D+03	0.0005901	0.0003311	0.0001457	-0.0000401	
D	3.4107884D+03	0.0027963	0.0015742	0.0006924	-0.0001905	
D	1.4335911D+03	0.0114715	0.0065052	0.0028701	-0.0007904	
D	6.5807391D+02	0.0405684	0.0232316	0.0102585	-0.0028233	
D	3.2217142D+02	0.1144908	0.0667934	0.0296650	-0.0081779	
D	1.6658431D+02	0.2390946	0.1404095	0.0623245	-0.0171622	
D	8.9830585D+01	0.3414873	0.1925661	0.0849756	-0.0234197	
D	5.0479385D+01	0.2933790	0.1027938	0.0352973	-0.0091924	
D	2.9004616D+01	0.1414856	-0.1672722	-0.1071153	0.0308523	
D	1.6237556D+01	0.0307401	-0.4395770	-0.2614014	0.0754842	
D	8.9528533D+00	0.0010020	-0.3971910	-0.1898546	0.0509468	
D	4.7670824D+00	0.0004596	-0.1285758	0.2463421	-0.0890640	
D	2.4501116D+00	-0.0001953	-0.0087024	0.5521909	-0.2015574	
D	1.1962558D+00	0.0000728	-0.0004502	0.3415233	-0.0646535	
D	5.1833885D-01	-0.0000288	0.0002151	0.0557135	0.3153555	
D	2.0134803D-01	0.0000093	-0.0000510	-0.0009503	0.5547389	
D	6.9324681D-02	-0.0000032	0.0000219	0.0002118	0.3424429	
	F	4F	5F			
BASIS/ORB. ENERGY	-14.9800840	-0.3903638				
F	2.1626449D+03	-0.0001696	-0.0000514			
F	7.2334376D+02	-0.0015536	-0.0004710			

F	3.0701713D+02	-0.0090004	-0.0027389
F	1.4699654D+02	-0.0363561	-0.0110791
F	7.4894952D+01	-0.1056960	-0.0323628
F	3.9606560D+01	-0.2259914	-0.0684108
F	2.1057592D+01	-0.3405166	-0.0961430
F	1.1053894D+01	-0.3425288	-0.0716440
F	5.6286962D+00	-0.1883891	0.0794036
F	2.6805945D+00	-0.0384005	0.3088084
F	1.1979814D+00	-0.0004534	0.4295815
F	4.9108127D-01	-0.0003703	0.3448273
F	1.7513845D-01	0.0000775	0.1494555

NEPTUNIUM [RN]7S(2)6D(1)5F(4), 6L

CHARGE = 93.000000

SYMMETRY SPECIES	S	P	D	F
NUMBER OF BASIS FUNCTIONS	35	26	18	13
NUMBER OF CLOSED SHELLS	7	5	3	1
NUMBER OF OPEN SHELLS	0	0	1	1
OPEN SHELL OCCUPATION NUMBER	0	0	1	4

*** FINAL SCF RESULTS ***

E = -28792.003370771

ORBITAL ENERGIES AND EXPANSION COEFFICIENTS

	S	1S	2S	3S	4S	5S	6S	7S
BASIS/ORB. ENERGY		-4396.4329000	-831.8036600	-213.9592900	-56.6138590	-13.2031800	-2.2060235	-0.1990001
S	3.2870111D+12	0.0000020	-0.0000008	0.0000004	0.0000002	-0.0000001	0.0000000	0.0000000
S	3.0927164D+11	0.0000078	-0.0000033	0.0000016	0.0000008	-0.0000004	0.0000002	-0.0000001
S	4.8590502D+10	0.0000226	-0.0000096	0.0000047	0.0000024	-0.0000012	0.0000005	-0.0000002
S	9.9519574D+09	0.0000561	-0.0000237	0.0000116	0.0000060	-0.0000030	0.0000013	-0.0000004
S	2.4755508D+09	0.0001224	-0.0000515	0.0000252	0.0000131	-0.0000065	0.0000029	-0.0000008
S	7.2245565D+08	0.0002393	-0.0001004	0.0000491	0.0000256	-0.0000127	0.0000056	-0.0000017
S	2.4149867D+08	0.0004344	-0.0001821	0.0000890	0.0000463	-0.0000231	0.0000102	-0.0000030
S	8.6617857D+07	0.0008104	-0.0003393	0.0001659	0.0000863	-0.0000430	0.0000191	-0.0000056
S	3.0900291D+07	0.0015872	-0.0006642	0.0003248	0.0001690	-0.0000841	0.0000373	-0.0000109
S	1.0755812D+07	0.0031254	-0.0013081	0.0006397	0.0003328	-0.0001657	0.0000735	-0.0000215
S	3.7243158D+06	0.0060117	-0.0025200	0.0012327	0.0006414	-0.0003194	0.0001417	-0.0000415

S	1.3136748D+06	0.0112292	-0.0047249	0.0023128	0.0012036	-0.0005993	0.0002658	-0.0000778
S	4.7990476D+05	0.0202181	-0.0085673	0.0041988	0.0021860	-0.0010887	0.0004829	-0.0001413
S	1.8455574D+05	0.0348775	-0.0149592	0.0073473	0.0038268	-0.0019056	0.0008451	-0.0002474
S	7.5318558D+04	0.0576866	-0.0252155	0.0124259	0.0064789	-0.0032288	0.0014322	-0.0004191
S	3.2758743D+04	0.0909417	-0.0409330	0.0202784	0.0105826	-0.0052704	0.0023375	-0.0006846
S	1.5113137D+04	0.1376388	-0.0646563	0.0322776	0.0168919	-0.0084329	0.0037425	-0.0010945
S	7.2610425D+03	0.1986416	-0.0995735	0.0503305	0.0263844	-0.0131398	0.0058272	-0.0017085
S	3.5782733D+03	0.2540567	-0.1391915	0.0715683	0.0377822	-0.0189483	0.0084196	-0.0024591
S	1.8033247D+03	0.2494326	-0.1477699	0.0771676	0.0406772	-0.0201769	0.0089365	-0.0026292
S	9.2520936D+02	0.1500167	-0.0368375	0.0098162	0.0040957	-0.0022295	0.0010176	-0.0002706
S	4.6933040D+02	0.0351888	0.2771866	-0.2271564	-0.1357224	0.0709544	-0.0318630	0.0092856
S	2.4299117D+02	-0.0000251	0.5264697	-0.5351829	-0.3360871	0.1743833	-0.0780844	0.0230254
S	1.2621942D+02	0.0009097	0.2996741	-0.3142392	-0.2163567	0.1223929	-0.0561229	0.0162061
S	7.0359158D+01	-0.0007401	0.0288776	0.5377724	0.5684403	-0.3572716	0.1679248	-0.0489618
S	3.9226176D+01	0.0004833	0.0091088	0.6945505	0.9538516	-0.5973410	0.2799648	-0.0839379
S	2.1236276D+01	-0.0003457	-0.0052836	0.1978338	-0.0433475	0.0265599	-0.0069323	0.0041539
S	1.2266147D+01	0.0002358	0.0032430	-0.0015102	-0.9817953	1.2034930	-0.6811329	0.2035987
S	6.7865439D+00	-0.0001131	-0.0016293	0.0052798	-0.4514897	0.5402195	-0.3007254	0.0969300
S	3.2230029D+00	0.0000493	0.0007309	-0.0021260	-0.0240518	-1.1299079	1.0186505	-0.3439703
S	1.6185017D+00	-0.0000254	-0.0003640	0.0009059	0.0001250	-0.5292108	0.6725799	-0.2314305
S	7.5946583D-01	0.0000104	0.0001493	-0.0003736	0.0000271	-0.0118088	-0.8603634	0.3716749
S	3.3411628D-01	-0.0000032	-0.0000465	0.0001205	0.0000248	-0.0030625	-0.7225964	0.5138741
S	7.6194384D-02	0.0000008	0.0000111	-0.0000278	0.0000081	0.0005944	-0.0262630	-0.5454915
S	3.0511841D-02	-0.0000003	-0.0000044	0.0000112	-0.0000031	-0.0002412	0.0057496	-0.6824717
	P	2P	3P	4P	5P	6P		
BASIS/ORB. ENERGY	-693.1389600	-174.9921100	-43.6564620	-9.0619946	-1.1018954			
P	5.0434089D+08	0.0000066	-0.0000035	-0.0000018	-0.0000009	0.0000004		
P	7.1015026D+07	0.0000210	-0.0000111	-0.0000058	-0.0000028	0.0000011		
P	1.4335463D+07	0.0000577	-0.0000306	-0.0000160	-0.0000077	0.0000031		
P	3.5397464D+06	0.0001446	-0.0000767	-0.0000401	-0.0000193	0.0000077		
P	1.0108196D+06	0.0003438	-0.0001827	-0.0000956	-0.0000461	0.0000183		
P	3.2328415D+05	0.0007983	-0.0004254	-0.0002228	-0.0001073	0.0000426		
P	1.1325789D+05	0.0018458	-0.0009876	-0.0005178	-0.0002494	0.0000991		
P	4.2991890D+04	0.0042807	-0.0023028	-0.0012088	-0.0005827	0.0002315		
P	1.7520483D+04	0.0100314	-0.0054394	-0.0028609	-0.0013792	0.0005484		

P	7.5866545D+03	0.0236945	-0.0129949	-0.0068553	-0.0033090	0.0013150
P	3.4606188D+03	0.0551419	-0.0307998	-0.0163201	-0.0078818	0.0031362
P	1.6540220D+03	0.1198997	-0.0688371	-0.0367480	-0.0177967	0.0070750
P	8.2430639D+02	0.2241027	-0.1336950	-0.0720717	-0.0349528	0.0139288
P	4.2636146D+02	0.3203953	-0.1974974	-0.1075756	-0.0524139	0.0208369
P	2.2735434D+02	0.2939602	-0.1476088	-0.0728956	-0.0342673	0.0136538
P	1.2376895D+02	0.1364260	0.1346104	0.1237918	0.0672786	-0.0277059
P	6.8504786D+01	0.0213683	0.4743796	0.4153177	0.2293869	-0.0933563
P	3.8304414D+01	0.0010247	0.4080013	0.3104775	0.1564264	-0.0637917
P	2.1154801D+01	-0.0003185	0.1169097	-0.3165045	-0.2570412	0.1159173
P	1.1731538D+01	0.0000906	0.0064390	-0.6495693	-0.5975847	0.2714771
P	6.4430042D+00	-0.0000918	0.0010309	-0.2749765	-0.0747403	0.0129786
P	3.4446968D+00	0.0000585	-0.0005377	-0.0253910	0.6842119	-0.4538074
P	1.7852488D+00	-0.0000204	0.0001329	-0.0010611	0.5051788	-0.3299372
P	8.0135881D-01	0.0000094	-0.0000660	0.0002049	0.0668142	0.4255575
P	3.7018595D-01	-0.0000038	0.0000272	-0.0000478	-0.0025792	0.6518597
P	1.5187785D-01	0.0000010	-0.0000068	0.0000105	0.0006703	0.1846669
	D	3D	4D	5D	6D	
BASIS/ORB. ENERGY	-139.3564700	-30.0044880	-4.3837949	-0.2328350		
D	3.4958747D+04	0.0001105	0.0000621	0.0000276	-0.0000076	
D	9.4269414D+03	0.0006203	0.0003497	0.0001556	-0.0000429	
D	3.4270495D+03	0.0029178	0.0016516	0.0007345	-0.0002021	
D	1.4350993D+03	0.0121153	0.0069050	0.0030798	-0.0008490	
D	6.5785675D+02	0.0424386	0.0244474	0.0109155	-0.0030055	
D	3.2221595D+02	0.1189617	0.0697801	0.0313361	-0.0086481	
D	1.6644430D+02	0.2459990	0.1452030	0.0651604	-0.0179483	
D	8.9721051D+01	0.3443669	0.1938936	0.0863456	-0.0238318	
D	5.0481275D+01	0.2865600	0.0935240	0.0303777	-0.0077241	
D	2.9096644D+01	0.1341718	-0.1822965	-0.1166858	0.0335384	
D	1.6287437D+01	0.0281614	-0.4487153	-0.2713934	0.0787028	
D	8.9794227D+00	0.0007117	-0.3856842	-0.1756272	0.0459669	
D	4.7723715D+00	0.0004436	-0.1165472	0.2804692	-0.1006281	
D	2.4523065D+00	-0.0002021	-0.0066924	0.5544816	-0.2044372	
D	1.1963155D+00	0.0000723	-0.0005185	0.3150391	-0.0414230	
D	5.1692597D-01	-0.0000300	0.0002264	0.0468190	0.3334252	

D	2.0259593D-01	0.0000095	-0.0000633	-0.0007990	0.5438517
D	7.0403108D-02	-0.0000034	0.0000230	0.0001895	0.3287867
	F	4F	5F		
BASIS/ORB.ENERGY		-15.8833600	-0.4433905		
F	2.1577817D+03	-0.0001833	-0.0000579		
F	7.2422846D+02	-0.0016715	-0.0005316		
F	3.0690467D+02	-0.0096687	-0.0030732		
F	1.4696749D+02	-0.0386384	-0.0123433		
F	7.4902419D+01	-0.1111931	-0.0355779		
F	3.9634205D+01	-0.2337849	-0.0740488		
F	2.1085597D+01	-0.3452376	-0.1008976		
F	1.1083325D+01	-0.3375252	-0.0700163		
F	5.6394629D+00	-0.1763352	0.1014411		
F	2.6705922D+00	-0.0323655	0.3348601		
F	1.2081720D+00	-0.0001230	0.4236228		
F	5.0721115D-01	-0.0003719	0.3170303		
F	1.8654913D-01	0.0000756	0.1268060		

PLUTONIUM [RN]7S(2)5F(6), 7F

CHARGE = 94.000000

SYMMETRY SPECIES	S	P	D	F
NUMBER OF BASIS FUNCTIONS	35	26	18	13
NUMBER OF CLOSED SHELLS	7	5	3	1
NUMBER OF OPEN SHELLS	0	0	0	1
OPEN SHELL OCCUPATION NUMBER	0	0	0	6

*** FINAL SCF RESULTS ***

E = -29598.167050842

ORBITAL ENERGIES AND EXPANSION COEFFICIENTS

	S	1S	2S	3S	4S	5S	6S	7S
BASIS/ORB.ENERGY		-4513.0574000	-857.1226300	-221.0466800	-58.6888570	-13.6183110	-2.1603404	-0.1860283
S	3.2883756D+12	0.0000022	-0.0000009	0.0000005	0.0000002	-0.0000001	0.0000001	0.0000000
S	3.0912095D+11	0.0000086	-0.0000037	0.0000018	0.0000009	-0.0000005	0.0000002	-0.0000001
S	4.8248284D+10	0.0000247	-0.0000105	0.0000051	0.0000027	-0.0000013	0.0000006	-0.0000002
S	9.9363406D+09	0.0000605	-0.0000257	0.0000126	0.0000066	-0.0000033	0.0000014	-0.0000004
S	2.4755508D+09	0.0001319	-0.0000558	0.0000273	0.0000143	-0.0000071	0.0000031	-0.0000008

S	7.2108264D+08	0.0002570	-0.0001085	0.0000531	0.0000277	-0.0000139	0.0000061	-0.0000016
S	2.4111840D+08	0.0004636	-0.0001955	0.0000957	0.0000499	-0.0000250	0.0000110	-0.0000030
S	8.6617857D+07	0.0008616	-0.0003628	0.0001777	0.0000926	-0.0000464	0.0000203	-0.0000055
S	3.0900291D+07	0.0016848	-0.0007091	0.0003472	0.0001810	-0.0000906	0.0000397	-0.0000107
S	1.0755812D+07	0.0033002	-0.0013892	0.0006802	0.0003547	-0.0001775	0.0000779	-0.0000210
S	3.7274086D+06	0.0063289	-0.0026682	0.0013068	0.0006816	-0.0003411	0.0001496	-0.0000404
S	1.3136926D+06	0.0117863	-0.0049878	0.0024446	0.0012751	-0.0006382	0.0002800	-0.0000756
S	4.7994138D+05	0.0211174	-0.0090012	0.0044173	0.0023049	-0.0011539	0.0005061	-0.0001366
S	1.8455258D+05	0.0362972	-0.0156607	0.0077017	0.0040206	-0.0020129	0.0008830	-0.0002384
S	7.5297126D+04	0.0597546	-0.0262866	0.0129726	0.0067791	-0.0033953	0.0014895	-0.0004018
S	3.2745839D+04	0.0936744	-0.0424318	0.0210487	0.0110115	-0.0055154	0.0024197	-0.0006536
S	1.5113137D+04	0.1407593	-0.0666124	0.0333147	0.0174721	-0.0087615	0.0038446	-0.0010361
S	7.2610425D+03	0.2017883	-0.1017999	0.0515200	0.0270826	-0.0135778	0.0059583	-0.0016120
S	3.5767764D+03	0.2548725	-0.1406656	0.0724909	0.0383362	-0.0192816	0.0084668	-0.0022760
S	1.8029530D+03	0.2460910	-0.1444350	0.0751609	0.0397268	-0.0199092	0.0087367	-0.0023793
S	9.2385183D+02	0.1436562	-0.0268314	0.0033850	0.0003311	-0.0000696	0.0000174	0.0000420
S	4.7246213D+02	0.0316011	0.2935209	-0.2425472	-0.1451589	0.0757213	-0.0335480	0.0089687
S	2.4244783D+02	0.0006117	0.5350585	-0.5497754	-0.3482928	0.1833593	-0.0814481	0.0222429
S	1.2382681D+02	0.0002795	0.2813196	-0.2792362	-0.1899367	0.1055822	-0.0475156	0.0123069
S	7.0399362D+01	-0.0002209	0.0158223	0.5831584	0.6191353	-0.3851715	0.1781663	-0.0472550
S	3.9238956D+01	0.0000936	0.0117840	0.6682254	0.9407893	-0.6082867	0.2846196	-0.0798292
S	2.1290133D+01	-0.0000562	-0.0067137	0.1789635	-0.1489376	0.1409120	-0.0679717	0.0228342
S	1.2030940D+01	0.0000404	0.0040791	-0.0027453	-0.9930845	1.2363475	-0.6960712	0.1880964
S	6.7209943D+00	-0.0000183	-0.0021317	0.0051340	-0.3760135	0.4419451	-0.2384863	0.0764598
S	3.3155266D+00	0.0000069	0.0009163	-0.0021100	-0.0229098	-1.1930571	1.0712579	-0.3373629
S	1.5591702D+00	-0.0000035	-0.0004239	0.0008394	0.0013903	-0.4985666	0.6197576	-0.1823581
S	7.6020952D-01	0.0000016	0.0001880	-0.0003757	-0.0006993	0.0192681	-0.9310253	0.3396773
S	3.2170560D-01	-0.0000004	-0.0000557	0.0001155	0.0002517	-0.0096052	-0.6661615	0.4775594
S	7.7939585D-02	0.0000001	0.0000142	-0.0000286	-0.0000550	0.0022339	-0.0194463	-0.4342115
S	3.0139489D-02	0.0000000	-0.0000054	0.0000109	0.0000212	-0.0008498	0.0032939	-0.7785946
P		2P	3P	4P	5P	6P		
BASIS/ORB. ENERGY	-711.5962400	-180.2752700	-45.1425710	-9.2786209	-1.0327799			
P	5.0414937D+08	0.0000070	-0.0000037	-0.0000020	-0.0000009	0.0000004		
P	7.0978257D+07	0.0000224	-0.0000119	-0.0000062	-0.0000030	0.0000012		
P	1.4299984D+07	0.0000613	-0.0000325	-0.0000171	-0.0000083	0.0000032		

P	3.5336432D+06	0.0001532	-0.0000814	-0.0000427	-0.0000207	0.0000080
P	1.0090143D+06	0.0003638	-0.0001937	-0.0001017	-0.0000492	0.0000191
P	3.2284024D+05	0.0008425	-0.0004499	-0.0002364	-0.0001145	0.0000444
P	1.1315935D+05	0.0019429	-0.0010419	-0.0005479	-0.0002654	0.0001030
P	4.2985918D+04	0.0044920	-0.0024221	-0.0012754	-0.0006180	0.0002398
P	1.7521746D+04	0.0105018	-0.0057088	-0.0030122	-0.0014602	0.0005669
P	7.5874739D+03	0.0247099	-0.0135886	-0.0071917	-0.0034898	0.0013539
P	3.4610310D+03	0.0572833	-0.0320937	-0.0170629	-0.0082871	0.0032196
P	1.6537683D+03	0.1237638	-0.0712920	-0.0381892	-0.0185925	0.0072158
P	8.2424618D+02	0.2291215	-0.1371602	-0.0742039	-0.0361991	0.0140857
P	4.2632439D+02	0.3227876	-0.1991208	-0.1087467	-0.0532371	0.0206571
P	2.2732951D+02	0.2891782	-0.1401856	-0.0680304	-0.0319913	0.0124452
P	1.2369534D+02	0.1293798	0.1524711	0.1379544	0.0755010	-0.0303534
P	6.8549377D+01	0.0188254	0.4825425	0.4257575	0.2364857	-0.0939419
P	3.8321450D+01	0.0010390	0.3950264	0.2888653	0.1440075	-0.0572828
P	2.1126263D+01	-0.0004144	0.1068080	-0.3501588	-0.2867183	0.1264076
P	1.1741960D+01	0.0001550	0.0049701	-0.6454310	-0.6027824	0.2675570
P	6.4272290D+00	-0.0001255	0.0010381	-0.2519044	-0.0202750	-0.0168216
P	3.4583914D+00	0.0000773	-0.0005677	-0.0197723	0.7025259	-0.4560258
P	1.7929288D+00	-0.0000291	0.0001479	-0.0014736	0.4709519	-0.2863747
P	8.0870908D-01	0.0000127	-0.0000705	0.0003511	0.0594025	0.4204136
P	3.6949302D-01	-0.0000051	0.0000281	-0.0001117	-0.0016279	0.6372498
P	1.5216548D-01	0.0000013	-0.0000073	0.0000254	0.0005394	0.1951864
	D	3D	4D	5D		
BASIS/ORB. ENERGY	-143.5427500	-31.0651550	-4.4449628			
D	4.1478171D+04	0.0000947	-0.0000535	-0.0000239		
D	1.0322581D+04	0.0006022	-0.0003411	-0.0001526		
D	3.5425677D+03	0.0030371	-0.0017271	-0.0007726		
D	1.4418116D+03	0.0129012	-0.0073925	-0.0033155		
D	6.5442805D+02	0.0450110	-0.0260650	-0.0117100		
D	3.2047169D+02	0.1239325	-0.0731385	-0.0330333		
D	1.6615699D+02	0.2511888	-0.1488041	-0.0671832		
D	8.9665823D+01	0.3488705	-0.1964972	-0.0877694		
D	4.9944825D+01	0.2866932	-0.0808960	-0.0229936		
D	2.8278501D+01	0.1221363	0.2158314	0.1370927		

D	1.5969977D+01	0.0218705	0.4436052	0.2695543
D	9.1449981D+00	0.0008042	0.3452237	0.1558300
D	5.2647089D+00	0.0004046	0.1164957	-0.2122244
D	3.0122354D+00	-0.0003908	0.0151148	-0.4229578
D	2.0937038D+00	0.0003449	-0.0001005	-0.1431092
D	1.4960356D+00	-0.0001700	0.0005832	-0.2928238
D	8.0532791D-01	0.0000235	-0.0000692	-0.1147755
D	3.6206364D-01	-0.0000052	0.0000023	-0.0121159
	F	4F	5F	
BASIS/ORB. ENERGY		-16.6073680	-0.3373019	
F	2.1278859D+03	-0.0002028	-0.0000642	
F	7.2185999D+02	-0.0017964	-0.0005730	
F	3.0720342D+02	-0.0103258	-0.0032896	
F	1.4707671D+02	-0.0409836	-0.0131319	
F	7.4941263D+01	-0.1168445	-0.0374808	
F	3.9658517D+01	-0.2414836	-0.0765484	
F	2.1136975D+01	-0.3480268	-0.1011175	
F	1.1164745D+01	-0.3306187	-0.0647980	
F	5.6985600D+00	-0.1662148	0.1152156	
F	2.6798856D+00	-0.0281479	0.3479786	
F	1.1937583D+00	0.0000533	0.4206180	
F	4.8925043D-01	-0.0003400	0.3081926	
F	1.7438974D-01	0.0000678	0.1269109	

AMERICIUM [RN]7S(2)5F(7), 8S

CHARGE = 95.000000

SYMMETRY SPECIES	S	P	D	F
NUMBER OF BASIS FUNCTIONS	35	26	18	13
NUMBER OF CLOSED SHELLS	7	5	3	1
NUMBER OF OPEN SHELLS	0	0	0	1
OPEN SHELL OCCUPATION NUMBER	0	0	0	7

*** FINAL SCF RESULTS ***

E = -30420.289361919

ORBITAL ENERGIES AND EXPANSION COEFFICIENTS

S	1S	2S	3S	4S	5S	6S	7S
---	----	----	----	----	----	----	----

BASIS/ORB. ENERGY	-4632.2697000	-883.2479900	-228.4915700	-60.9930370	-14.2187160	-2.2313962	-0.1883271
S 3.2883756D+12	0.0000024	-0.0000010	0.0000005	0.0000003	-0.0000001	0.0000001	0.0000000
S 3.0912095D+11	0.0000094	-0.0000040	0.0000020	0.0000010	-0.0000005	0.0000002	-0.0000001
S 4.8248284D+10	0.0000268	-0.0000115	0.0000056	0.0000029	-0.0000015	0.0000007	-0.0000002
S 9.9363406D+09	0.0000654	-0.0000279	0.0000137	0.0000072	-0.0000036	0.0000016	-0.0000004
S 2.4755508D+09	0.0001420	-0.0000604	0.0000297	0.0000155	-0.0000078	0.0000034	-0.0000009
S 7.2042800D+08	0.0002757	-0.0001171	0.0000574	0.0000300	-0.0000151	0.0000066	-0.0000018
S 2.4111840D+08	0.0004949	-0.0002099	0.0001029	0.0000538	-0.0000271	0.0000119	-0.0000032
S 8.6600941D+07	0.0009179	-0.0003888	0.0001906	0.0000996	-0.0000501	0.0000220	-0.0000059
S 3.0894257D+07	0.0017868	-0.0007564	0.0003708	0.0001938	-0.0000975	0.0000428	-0.0000114
S 1.0761587D+07	0.0034848	-0.0014755	0.0007233	0.0003780	-0.0001903	0.0000836	-0.0000222
S 3.7301088D+06	0.0066652	-0.0028264	0.0013860	0.0007245	-0.0003646	0.0001602	-0.0000426
S 1.3136926D+06	0.0123690	-0.0052650	0.0025836	0.0013507	-0.0006798	0.0002987	-0.0000794
S 4.7994138D+05	0.0220549	-0.0094565	0.0046465	0.0024300	-0.0012232	0.0005374	-0.0001429
S 1.8456962D+05	0.0377528	-0.0163876	0.0080695	0.0042223	-0.0021255	0.0009339	-0.0002484
S 7.5297126D+04	0.0618537	-0.0273815	0.0135313	0.0070873	-0.0035694	0.0015684	-0.0004168
S 3.2749037D+04	0.0964079	-0.0439588	0.0218368	0.0114505	-0.0057668	0.0025341	-0.0006743
S 1.5115773D+04	0.1439804	-0.0686106	0.0343683	0.0180664	-0.0091109	0.0040044	-0.0010634
S 7.2609538D+03	0.2047244	-0.1040100	0.0527186	0.0277798	-0.0140020	0.0061547	-0.0016399
S 3.5767873D+03	0.2554804	-0.1417647	0.0731682	0.0387819	-0.0196223	0.0086301	-0.0022866
S 1.8029530D+03	0.2424094	-0.1412077	0.0732843	0.0387871	-0.0195193	0.0085797	-0.0023000
S 9.2384902D+02	0.1374969	-0.0147768	-0.0047011	-0.0042812	0.0022642	-0.0010163	0.0003113
S 4.7246213D+02	0.0287833	0.3109281	-0.2593244	-0.1559095	0.0819329	-0.0363640	0.0095974
S 2.4244783D+02	0.0005109	0.5323674	-0.5533879	-0.3528047	0.1868388	-0.0831830	0.0223498
S 1.2382718D+02	0.0002086	0.2638160	-0.2415198	-0.1619529	0.0912149	-0.0410976	0.0104826
S 7.0392487D+01	-0.0001614	0.0125107	0.6153037	0.6653961	-0.4196661	0.1946664	-0.0511412
S 3.9240752D+01	0.0000533	0.0105405	0.6449862	0.9168161	-0.5956604	0.2799455	-0.0771183
S 2.1290263D+01	-0.0000268	-0.0059920	0.1588346	-0.2311324	0.2067781	-0.1019204	0.0311759
S 1.2030573D+01	0.0000206	0.0035884	-0.0027800	-0.9886368	1.2928539	-0.7368160	0.1977647
S 6.7209943D+00	-0.0000083	-0.0018629	0.0043103	-0.3336820	0.3065691	-0.1474624	0.0481946
S 3.3155266D+00	0.0000026	0.0007998	-0.0017968	-0.0186722	-1.2156524	1.1174484	-0.3453306
S 1.5588467D+00	-0.0000015	-0.0003689	0.0007017	0.0012904	-0.4358261	0.5185530	-0.1496083
S 7.6020720D-01	0.0000006	0.0001634	-0.0003121	-0.0006627	0.0176369	-0.9604814	0.3528273
S 3.2166633D-01	-0.0000002	-0.0000484	0.0000963	0.0002417	-0.0079825	-0.6159191	0.4489799
S 7.7939546D-02	0.0000000	0.0000123	-0.0000238	-0.0000541	0.0018168	-0.0138486	-0.4623066

S	3.0142432D-02	0.0000000	-0.0000047	0.0000090	0.0000208	-0.0006886	0.0018612	-0.7514596
P		2P	3P	4P	5P	6P		
BASIS/ORB. ENERGY	-730.5131300	-185.8267600	-46.8290910	-9.6661134	-1.0542736			
P	5.0297614D+08	0.0000075	-0.0000040	-0.0000021	-0.0000010	0.0000004		
P	7.0692481D+07	0.0000238	-0.0000127	-0.0000067	-0.0000032	0.0000013		
P	1.4267308D+07	0.0000650	-0.0000346	-0.0000182	-0.0000089	0.0000034		
P	3.5272644D+06	0.0001623	-0.0000864	-0.0000455	-0.0000222	0.0000086		
P	1.0073845D+06	0.0003849	-0.0002054	-0.0001082	-0.0000527	0.0000204		
P	3.2218207D+05	0.0008890	-0.0004758	-0.0002507	-0.0001222	0.0000473		
P	1.1308893D+05	0.0020433	-0.0010982	-0.0005793	-0.0002824	0.0001093		
P	4.2967250D+04	0.0047157	-0.0025486	-0.0013462	-0.0006564	0.0002540		
P	1.7523619D+04	0.0109797	-0.0059835	-0.0031673	-0.0015454	0.0005986		
P	7.5896730D+03	0.0257670	-0.0142083	-0.0075431	-0.0036826	0.0014252		
P	3.4609963D+03	0.0594751	-0.0334224	-0.0178308	-0.0087184	0.0033797		
P	1.6536195D+03	0.1276772	-0.0737886	-0.0396548	-0.0194213	0.0075182		
P	8.2409354D+02	0.2341253	-0.1406262	-0.0763663	-0.0375200	0.0145707		
P	4.2629266D+02	0.3248653	-0.2004576	-0.1096951	-0.0539688	0.0208775		
P	2.2727355D+02	0.2841984	-0.1323100	-0.0629328	-0.0296760	0.0115372		
P	1.2367164D+02	0.1223357	0.1703276	0.1526376	0.0844053	-0.0339089		
P	6.8566837D+01	0.0167442	0.4906173	0.4353555	0.2429347	-0.0961713		
P	3.8277212D+01	0.0008975	0.3810476	0.2669426	0.1321553	-0.0526020		
P	2.1156597D+01	-0.0003915	0.0963506	-0.3838113	-0.3190093	0.1410364		
P	1.1736302D+01	0.0001374	0.0046489	-0.6425493	-0.6054830	0.2677920		
P	6.3628319D+00	-0.0001109	0.0005773	-0.2276899	0.0381878	-0.0480793		
P	3.4723740D+00	0.0000715	-0.0003646	-0.0135926	0.7126789	-0.4663657		
P	1.8077194D+00	-0.0000264	0.0000600	-0.0021384	0.4398874	-0.2527488		
P	8.1629968D-01	0.0000112	-0.0000334	0.0005789	0.0520011	0.4436312		
P	3.7081238D-01	-0.0000044	0.0000129	-0.0001972	-0.0012858	0.6257989		
P	1.5131823D-01	0.0000011	-0.0000034	0.0000462	0.0004233	0.1798889		
D		3D	4D	5D				
BASIS/ORB. ENERGY	-147.9628700	-32.3145230	-4.6590230					
D	4.1531818D+04	0.0001003	-0.0000569	-0.0000257				
D	1.0332260D+04	0.0006365	-0.0003623	-0.0001635				
D	3.5441664D+03	0.0032034	-0.0018309	-0.0008266				
D	1.4419980D+03	0.0135612	-0.0078090	-0.0035340				

D	6.5425482D+02	0.0470711	-0.0274091	-0.0124291
D	3.2041638D+02	0.1285140	-0.0762405	-0.0347507
D	1.6612860D+02	0.2574313	-0.1531772	-0.0697963
D	8.9652315D+01	0.3510520	-0.1972391	-0.0886679
D	4.9936783D+01	0.2802913	-0.0699799	-0.0168865
D	2.8272173D+01	0.1151849	0.2325699	0.1482245
D	1.5963992D+01	0.0193990	0.4510892	0.2776948
D	9.1249252D+00	0.0007163	0.3325230	0.1379590
D	5.2533326D+00	0.0002734	0.1039936	-0.2420143
D	3.0150259D+00	-0.0002724	0.0128354	-0.4258516
D	2.1076638D+00	0.0002200	-0.0003669	-0.1394813
D	1.4993581D+00	-0.0001105	0.0006364	-0.2774620
D	8.0722820D-01	0.0000128	-0.0000751	-0.1023781
D	3.6247888D-01	-0.0000037	0.0000081	-0.0103082

	F	4F	5F	
BASIS/ORB. ENERGY		-17.5153540	-0.3859740	
F	2.1243338D+03	-0.0002214	-0.0000728	
F	7.1533852D+02	-0.0019784	-0.0006501	
F	3.0486178D+02	-0.0111549	-0.0036853	
F	1.4686024D+02	-0.0431994	-0.0142756	
F	7.5161491D+01	-0.1216078	-0.0404511	
F	3.9830148D+01	-0.2485589	-0.0810108	
F	2.1202929D+01	-0.3529559	-0.1057655	
F	1.1216841D+01	-0.3225348	-0.0588744	
F	5.7919738D+00	-0.1538056	0.1241931	
F	2.8282187D+00	-0.0261413	0.3402423	
F	1.3060663D+00	-0.0004228	0.4109305	
F	5.4874312D-01	-0.0001585	0.3071814	
F	1.9793159D-01	0.0000390	0.1263013	

CURIUM [RN]7S(2)6D(1)5F(7), 9D

CHARGE = 96.000000

SYMMETRY SPECIES	S	P	D	F
NUMBER OF BASIS FUNCTIONS	35	26	18	13
NUMBER OF CLOSED SHELLS	7	5	3	1

NUMBER OF OPEN SHELLS 0 0 1 1
OPEN SHELL OCCUPATION NUMBER 0 0 1 7

*** FINAL SCF RESULTS ***

E = -31258.493278873

ORBITAL ENERGIES AND EXPANSION COEFFICIENTS

	S	1S	2S	3S	4S	5S	6S	7S
BASIS/ORB. ENERGY	-4754.1787000	-910.2415600	-236.3407600	-63.5689280	-15.0438640	-2.4473462	-0.2100400	
S 3.2883756D+12	0.0000026	-0.0000012	0.0000006	0.0000003	-0.0000002	0.0000001	0.0000000	
S 3.0900022D+11	0.0000103	-0.0000045	0.0000022	0.0000011	-0.0000006	0.0000003	-0.0000001	
S 4.8248284D+10	0.0000292	-0.0000126	0.0000062	0.0000032	-0.0000016	0.0000007	-0.0000002	
S 9.9363406D+09	0.0000708	-0.0000304	0.0000149	0.0000078	-0.0000040	0.0000018	-0.0000005	
S 2.4755508D+09	0.0001530	-0.0000655	0.0000322	0.0000169	-0.0000085	0.0000038	-0.0000011	
S 7.2042800D+08	0.0002957	-0.0001264	0.0000620	0.0000325	-0.0000165	0.0000073	-0.0000021	
S 2.4112093D+08	0.0005286	-0.0002255	0.0001107	0.0000580	-0.0000294	0.0000131	-0.0000037	
S 8.6600941D+07	0.0009781	-0.0004168	0.0002046	0.0001072	-0.0000542	0.0000242	-0.0000069	
S 3.0893502D+07	0.0018937	-0.0008064	0.0003958	0.0002073	-0.0001050	0.0000468	-0.0000133	
S 1.0774206D+07	0.0036811	-0.0015677	0.0007694	0.0004031	-0.0002040	0.0000910	-0.0000258	
S 3.7314394D+06	0.0070238	-0.0029959	0.0014709	0.0007706	-0.0003901	0.0001740	-0.0000493	
S 1.3136937D+06	0.0129737	-0.0055550	0.0027292	0.0014300	-0.0007240	0.0003229	-0.0000915	
S 4.7987108D+05	0.0230460	-0.0099404	0.0048903	0.0025633	-0.0012979	0.0005789	-0.0001640	
S 1.8448744D+05	0.0392740	-0.0171527	0.0084568	0.0044350	-0.0022458	0.0010018	-0.0002839	
S 7.5267719D+04	0.0640027	-0.0285120	0.0141088	0.0074065	-0.0037522	0.0016738	-0.0004742	
S 3.2749037D+04	0.0991471	-0.0455108	0.0226387	0.0118987	-0.0060281	0.0026895	-0.0007622	
S 1.5119203D+04	0.1472143	-0.0706296	0.0354336	0.0186693	-0.0094703	0.0042255	-0.0011971	
S 7.2609538D+03	0.2074844	-0.1061644	0.0538905	0.0284664	-0.0144342	0.0064426	-0.0018262	
S 3.5785959D+03	0.2557536	-0.1425543	0.0736708	0.0391327	-0.0199151	0.0088900	-0.0025185	
S 1.8029090D+03	0.2389502	-0.1379343	0.0713382	0.0378038	-0.0191322	0.0085432	-0.0024220	
S 9.2297027D+02	0.1312582	-0.0018060	-0.0135027	-0.0093477	0.0049178	-0.0022375	0.0006359	
S 4.7283284D+02	0.0260644	0.3262826	-0.2748804	-0.1660218	0.0877974	-0.0395438	0.0112261	
S 2.4240619D+02	0.0004935	0.5334528	-0.5594061	-0.3588422	0.1915438	-0.0867039	0.0246090	
S 1.2138358D+02	0.0001151	0.2507534	-0.2051456	-0.1338474	0.0758698	-0.0345010	0.0098672	
S 7.0366173D+01	-0.0000925	-0.0017959	0.6535493	0.7161110	-0.4560713	0.2147148	-0.0615231	
S 3.9279946D+01	0.0000077	0.0150569	0.6144715	0.8826472	-0.5790191	0.2779302	-0.0793777	
S 2.1294595D+01	0.0000054	-0.0087983	0.1449264	-0.3066641	0.2774019	-0.1425242	0.0407254	
S 1.2029613D+01	-0.0000007	0.0053382	-0.0055007	-0.9846223	1.3378420	-0.7804764	0.2318525	

S	6.6717852D+00	0.0000025	-0.0027504	0.0050709	-0.2906701	0.1750471	-0.0601542	0.0149595
S	3.3198066D+00	-0.0000020	0.0011889	-0.0022026	-0.0141257	-1.2389623	1.1885673	-0.3814485
S	1.5365784D+00	0.0000007	-0.0005511	0.0009076	0.0009579	-0.3764919	0.4248556	-0.1533388
S	7.6044484D-01	-0.0000003	0.0002518	-0.0004154	-0.0005502	0.0223210	-1.0477458	0.4726278
S	3.2154622D-01	0.0000001	-0.0000736	0.0001256	0.0002141	-0.0077342	-0.5282399	0.3986293
S	7.8529814D-02	0.0000000	0.0000189	-0.0000317	-0.0000495	0.0017642	-0.0043143	-0.6433024
S	3.0609801D-02	0.0000000	-0.0000072	0.0000121	0.0000192	-0.0006660	-0.0007055	-0.5928672
	P	2P	3P	4P	5P	6P		
BASIS/ORB. ENERGY	-749.9322700	-191.6884100	-48.7568410	-10.2620190	-1.1875505			
P	4.9802135D+08	0.0000080	-0.0000043	-0.0000023	-0.0000011	0.0000004		
P	7.0064692D+07	0.0000254	-0.0000135	-0.0000071	-0.0000035	0.0000014		
P	1.4129150D+07	0.0000694	-0.0000370	-0.0000195	-0.0000096	0.0000038		
P	3.4889676D+06	0.0001731	-0.0000924	-0.0000488	-0.0000239	0.0000095		
P	9.9844251D+05	0.0004080	-0.0002182	-0.0001152	-0.0000566	0.0000224		
P	3.2058332D+05	0.0009385	-0.0005033	-0.0002660	-0.0001306	0.0000517		
P	1.1274450D+05	0.0021508	-0.0011585	-0.0006130	-0.0003010	0.0001191		
P	4.2932942D+04	0.0049398	-0.0026759	-0.0014179	-0.0006964	0.0002755		
P	1.7533621D+04	0.0114692	-0.0062655	-0.0033269	-0.0016352	0.0006476		
P	7.5946430D+03	0.0268501	-0.0148455	-0.0079072	-0.0038888	0.0015387		
P	3.4611770D+03	0.0617542	-0.0348063	-0.0186288	-0.0091758	0.0036371		
P	1.6528937D+03	0.1317244	-0.0763795	-0.0411916	-0.0203249	0.0080441		
P	8.2366161D+02	0.2390692	-0.1440581	-0.0784891	-0.0388501	0.0154289		
P	4.2625930D+02	0.3264324	-0.2014204	-0.1105106	-0.0547630	0.0216525		
P	2.2727865D+02	0.2791240	-0.1238770	-0.0571681	-0.0268341	0.0106685		
P	1.2355157D+02	0.1156282	0.1882355	0.1671042	0.0930554	-0.0382595		
P	6.8687559D+01	0.0146006	0.4942420	0.4423254	0.2490884	-0.1008206		
P	3.8408307D+01	0.0009530	0.3686561	0.2427901	0.1170272	-0.0475806		
P	2.1107741D+01	-0.0004763	0.0888351	-0.4142609	-0.3480735	0.1582363		
P	1.1795068D+01	0.0001968	0.0028560	-0.6259515	-0.6016411	0.2724102		
P	6.4509138D+00	-0.0001397	0.0009458	-0.2116257	0.0872049	-0.0764931		
P	3.4904046D+00	0.0000861	-0.0005563	-0.0128691	0.7278057	-0.4965659		
P	1.8192609D+00	-0.0000336	0.0001499	-0.0014918	0.4072934	-0.2223439		
P	8.2582136D-01	0.0000141	-0.0000667	0.0004101	0.0433326	0.4977905		
P	3.7867281D-01	-0.0000056	0.0000265	-0.0001318	-0.0010851	0.6027932		
P	1.5482424D-01	0.0000014	-0.0000067	0.0000300	0.0002707	0.1493226		

	D	3D	4D	5D	6D
BASIS/ORB. ENERGY		-152.6575200	-33.7928960	-5.0611264	-0.2102059
D 4.3051866D+04		0.0001002	0.0000571	0.0000261	-0.0000067
D 1.0766689D+04		0.0006305	0.0003603	0.0001646	-0.0000422
D 3.6597111D+03		0.0032386	0.0018607	0.0008503	-0.0002170
D 1.4667325D+03		0.0140866	0.0081462	0.0037327	-0.0009566
D 6.5424146D+02		0.0503077	0.0294677	0.0135277	-0.0034543
D 3.1554499D+02		0.1382674	0.0824282	0.0380536	-0.0097693
D 1.6282989D+02		0.2668417	0.1595274	0.0735397	-0.0187521
D 8.8976912D+01		0.3405634	0.1898801	0.0862594	-0.0222449
D 5.1136259D+01		0.2598824	0.0651276	0.0150534	-0.0026961
D 3.0202949D+01		0.1179406	-0.2025890	-0.1313928	0.0344105
D 1.7197860D+01		0.0246232	-0.4545230	-0.2872505	0.0786957
D 9.5400764D+00		0.0005566	-0.3701917	-0.1530527	0.0336829
D 5.0620636D+00		0.0003317	-0.1010394	0.3347140	-0.1091003
D 2.6039791D+00		-0.0001777	-0.0045294	0.5533593	-0.1933143
D 1.2582453D+00		0.0000475	-0.0005799	0.2763368	0.0053918
D 5.1240583D-01		-0.0000223	0.0001896	0.0326456	0.3526759
D 1.9639093D-01		0.0000066	-0.0000640	-0.0012990	0.5206033
D 6.6365289D-02		-0.0000026	0.0000206	0.0003367	0.3284120
	F	4F	5F		
BASIS/ORB. ENERGY		-18.6474550	-0.5924535		
F 2.1178227D+03		-0.0002403	-0.0000838		
F 7.1344183D+02		-0.0021348	-0.0007439		
F 3.0439801D+02		-0.0119327	-0.0041803		
F 1.4683060D+02		-0.0456753	-0.0160084		
F 7.5193249D+01		-0.1273712	-0.0449348		
F 3.9851864D+01		-0.2561857	-0.0882982		
F 2.1221476D+01		-0.3565548	-0.1121911		
F 1.1236685D+01		-0.3156741	-0.0542874		
F 5.7979295D+00		-0.1427252	0.1495793		
F 2.8250932D+00		-0.0218802	0.3699619		
F 1.3144705D+00		-0.0002763	0.4061308		
F 5.7117533D-01		-0.0001280	0.2676461		
F 2.1883797D-01		0.0000307	0.0904281		

BERKELIUM [RN]7S(2)6D(1)5F(8), 8H

CHARGE = 97.000000

SYMMETRY SPECIES	S	P	D	F
NUMBER OF BASIS FUNCTIONS	35	26	18	13
NUMBER OF CLOSED SHELLS	7	5	3	1
NUMBER OF OPEN SHELLS	0	0	1	1
OPEN SHELL OCCUPATION NUMBER	0	0	1	8

*** FINAL SCF RESULTS ***

E = -32113.028436026

ORBITAL ENERGIES AND EXPANSION COEFFICIENTS

	S	1S	2S	3S	4S	5S	6S	7S
BASIS/ORB. ENERGY	-4878.5086000	-937.7551300	-244.2031000	-66.0198830	-15.6986110	-2.5405963	-0.2160732	
S 3.2892027D+12	0.0000029	-0.0000013	0.0000006	0.0000003	-0.0000002	0.0000001	0.0000000	
S 3.0899964D+11	0.0000113	-0.0000049	0.0000024	0.0000013	-0.0000006	0.0000003	0.0000001	
S 4.8207415D+10	0.0000318	-0.0000138	0.0000068	0.0000036	-0.0000018	0.0000008	0.0000002	
S 9.9363406D+09	0.0000768	-0.0000332	0.0000163	0.0000086	-0.0000044	0.0000020	0.0000006	
S 2.4639137D+09	0.0001657	-0.0000714	0.0000351	0.0000184	-0.0000094	0.0000042	0.0000012	
S 7.1816264D+08	0.0003169	-0.0001362	0.0000670	0.0000352	-0.0000179	0.0000080	0.0000023	
S 2.4112093D+08	0.0005640	-0.0002421	0.0001190	0.0000625	-0.0000318	0.0000142	0.0000040	
S 8.6786178D+07	0.0010379	-0.0004450	0.0002186	0.0001148	-0.0000584	0.0000261	0.0000074	
S 3.0999086D+07	0.0020070	-0.0008598	0.0004224	0.0002218	-0.0001128	0.0000504	0.0000142	
S 1.0788793D+07	0.0038972	-0.0016697	0.0008204	0.0004307	-0.0002191	0.0000980	0.0000277	
S 3.7314394D+06	0.0074005	-0.0031754	0.0015608	0.0008194	-0.0004169	0.0001864	0.0000526	
S 1.3131806D+06	0.0136178	-0.0058658	0.0028852	0.0015150	-0.0007709	0.0003447	0.0000973	
S 4.7949633D+05	0.0240777	-0.0104481	0.0051462	0.0027032	-0.0013756	0.0006151	0.0001737	
S 1.8441539D+05	0.0408253	-0.0179414	0.0088566	0.0046546	-0.0023690	0.0010594	0.0002992	
S 7.5241162D+04	0.0662203	-0.0296864	0.0147085	0.0077381	-0.0039393	0.0017615	0.0004974	
S 3.2745814D+04	0.1019515	-0.0471174	0.0234707	0.0123626	-0.0062964	0.0028165	0.0007955	
S 1.5119203D+04	0.1504316	-0.0726532	0.0364993	0.0192742	-0.0098217	0.0043920	0.0012402	
S 7.2606193D+03	0.2102215	-0.1083489	0.0550870	0.0291607	-0.0148737	0.0066580	0.0018808	
S 3.5778952D+03	0.2560019	-0.1431936	0.0740620	0.0394307	-0.0201365	0.0090043	0.0025428	
S 1.8028865D+03	0.2347539	-0.1341486	0.0691313	0.0366385	-0.0186991	0.0083847	0.0023680	
S 9.2283438D+02	0.1254006	0.0120039	-0.0231423	-0.0148719	0.0079950	-0.0036611	-0.0010337	
S 4.7224438D+02	0.0235488	0.3416051	-0.2906449	-0.1765256	0.0935294	-0.0421745	-0.0119393	

S	2.4303673D+02	0.0004466	0.5264251	-0.5571950	-0.3591352	0.1937693	-0.0881213	-0.0249171
S	1.2136865D+02	0.0000258	0.2372446	-0.1672515	-0.1043800	0.0569414	-0.0254347	-0.0072971
S	7.0362717D+01	-0.0000097	-0.0060862	0.6814134	0.7621364	-0.4849865	0.2284106	0.0653147
S	3.9241971D+01	-0.0000495	0.0153474	0.5873367	0.8445499	-0.5677466	0.2755586	0.0783299
S	2.1307633D+01	0.0000457	-0.0089988	0.1273559	-0.3805414	0.3672337	-0.1937503	-0.0552203
S	1.2029259D+01	-0.0000263	0.0052374	-0.0047244	-0.9828002	1.3501293	-0.7934147	-0.2356223
S	6.4534654D+00	0.0000152	-0.0026248	0.0041036	-0.2493206	0.0618378	0.0245858	0.0118098
S	3.3025315D+00	-0.0000074	0.0011345	-0.0018448	-0.0034875	-1.2941689	1.2575595	0.4028203
S	1.3208083D+00	0.0000036	-0.0005715	0.0008192	-0.0018537	-0.3298828	0.3401409	0.1295683
S	7.6137158D-01	-0.0000022	0.0003447	-0.0004937	0.0009331	0.0770814	-1.1301538	-0.5171533
S	3.2053513D-01	0.0000006	-0.0000857	0.0001268	-0.0001664	-0.0160984	-0.4668698	-0.3665253
S	8.0533533D-02	-0.0000001	0.0000210	-0.0000305	0.0000442	0.0035521	-0.0036090	0.6772218
S	3.0587145D-02	0.0000000	-0.0000076	0.0000111	-0.0000158	-0.0012767	-0.0005292	0.5636497

	P	2P	3P	4P	5P	6P
BASIS/ORB. ENERGY		-769.4860800	-197.4644900	-50.5289400	-10.6840620	-1.2231982
P	4.9766933D+08	0.0000086	-0.0000046	-0.0000024	-0.0000012	0.0000005
P	6.9915323D+07	0.0000271	-0.0000144	-0.0000076	-0.0000038	0.0000015
P	1.4087366D+07	0.0000737	-0.0000394	-0.0000208	-0.0000103	0.0000041
P	3.4776980D+06	0.0001835	-0.0000981	-0.0000519	-0.0000256	0.0000101
P	9.9569896D+05	0.0004313	-0.0002311	-0.0001224	-0.0000604	0.0000239
P	3.1998383D+05	0.0009895	-0.0005318	-0.0002819	-0.0001391	0.0000550
P	1.1263540D+05	0.0022612	-0.0012206	-0.0006477	-0.0003199	0.0001266
P	4.2923413D+04	0.0051780	-0.0028114	-0.0014941	-0.0007379	0.0002919
P	1.7537005D+04	0.0119871	-0.0065645	-0.0034961	-0.0017282	0.0006844
P	7.5960252D+03	0.0279730	-0.0155079	-0.0082853	-0.0040975	0.0016209
P	3.4611860D+03	0.0640545	-0.0362099	-0.0194421	-0.0096325	0.0038179
P	1.6526864D+03	0.1357322	-0.0789583	-0.0427201	-0.0211964	0.0083871
P	8.2353396D+02	0.2439438	-0.1474576	-0.0806136	-0.0401447	0.0159437
P	4.2624286D+02	0.3279031	-0.2022027	-0.1111450	-0.0553435	0.0218690
P	2.2726215D+02	0.2737389	-0.1149467	-0.0511274	-0.0238446	0.0094830
P	1.2346845D+02	0.1091069	0.2063039	0.1822432	0.1022688	-0.0420704
P	6.8720218D+01	0.0127413	0.4986265	0.4489906	0.2541934	-0.1028204
P	3.8429821D+01	0.0009344	0.3547059	0.2175196	0.1015779	-0.0412543
P	2.1104062D+01	-0.0005109	0.0805371	-0.4449054	-0.3791593	0.1730752
P	1.1817515D+01	0.0002213	0.0021663	-0.6133209	-0.5948726	0.2688763

P	6.4532889D+00	-0.0001491	0.0008344	-0.1927798	0.1444573	-0.1090899
P	3.4948093D+00	0.0000913	-0.0005126	-0.0099508	0.7335656	-0.5058348
P	1.8226846D+00	-0.0000362	0.0001353	-0.0015209	0.3744906	-0.1825442
P	8.2754257D-01	0.0000149	-0.0000594	0.0004348	0.0367747	0.5236273
P	3.7852822D-01	-0.0000059	0.0000235	-0.0001436	-0.0008326	0.5827555
P	1.5436163D-01	0.0000015	-0.0000059	0.0000325	0.0001965	0.1348082
	D	3D	4D	5D	6D	
BASIS/ORB. ENERGY	-157.2325500	-35.1038540	-5.3023512	-0.1898966		
D	4.5059762D+04	0.0000991	0.0000568	0.0000261	-0.0000063	
D	1.1182070D+04	0.0006364	0.0003652	0.0001682	-0.0000405	
D	3.7258842D+03	0.0033664	0.0019437	0.0008955	-0.0002147	
D	1.4735942D+03	0.0148288	0.0086136	0.0039780	-0.0009579	
D	6.5358776D+02	0.0527345	0.0310599	0.0143779	-0.0034488	
D	3.1501255D+02	0.1435632	0.0859837	0.0400129	-0.0096544	
D	1.6240470D+02	0.2736713	0.1643284	0.0763744	-0.0182853	
D	8.8906637D+01	0.3390276	0.1878461	0.0856874	-0.0207941	
D	5.1477445D+01	0.2512490	0.0568999	0.0105711	-0.0013008	
D	3.0567672D+01	0.1143601	-0.2122923	-0.1384995	0.0339443	
D	1.7372994D+01	0.0230028	-0.4605953	-0.2944436	0.0761017	
D	9.6488175D+00	0.0005125	-0.3597094	-0.1389945	0.0270332	
D	5.1238938D+00	0.0002533	-0.0942733	0.3569149	-0.1088623	
D	2.6323700D+00	-0.0001469	-0.0037157	0.5501894	-0.1798671	
D	1.2662372D+00	0.0000304	-0.0006086	0.2604115	0.0198463	
D	4.9650708D-01	-0.0000159	0.0001811	0.0276124	0.3589610	
D	1.8244067D-01	0.0000044	-0.0000617	-0.0015234	0.5178372	
D	6.0430199D-02	-0.0000018	0.0000215	0.0003896	0.3295432	
	F	4F	5F			
BASIS/ORB. ENERGY	-19.6100330	-0.6023390				
F	2.1120694D+03	-0.0002590	-0.0000924			
F	7.1321228D+02	-0.0022930	-0.0008161			
F	3.0406689D+02	-0.0127523	-0.0045688			
F	1.4684618D+02	-0.0482029	-0.0172620			
F	7.5210755D+01	-0.1334542	-0.0481534			
F	3.9847433D+01	-0.2636681	-0.0925288			
F	2.1238294D+01	-0.3595294	-0.1146442			

F	1.1247084D+01	-0.3088417	-0.0462770
F	5.7897264D+00	-0.1314995	0.1702873
F	2.8242064D+00	-0.0181164	0.3814600
F	1.3138584D+00	-0.0004089	0.3967809
F	5.7146932D-01	-0.0001060	0.2510685
F	2.2045794D-01	-0.0000092	0.0822315

CALIFORNIUM [RN]7S(2)5F(10), 5I

CHARGE = 98.000000

SYMMETRY SPECIES	S	P	D	F
NUMBER OF BASIS FUNCTIONS	35	26	18	13
NUMBER OF CLOSED SHELLS	7	5	3	1
NUMBER OF OPEN SHELLS	0	0	0	1
OPEN SHELL OCCUPATION NUMBER	0	0	0	10

*** FINAL SCF RESULTS ***

E = -32984.476957478

ORBITAL ENERGIES AND EXPANSION COEFFICIENTS

	S	1S	2S	3S	4S	5S	6S	7S
BASIS/ORB. ENERGY	-5005.2964000	-965.7702200	-252.0414500	-68.3044400	-16.1416180	-2.4751816	-0.1967740	
S 3.2892027D+12	0.0000032	-0.0000014	0.0000007	0.0000004	-0.0000002	0.0000001	0.0000000	
S 3.0896946D+11	0.0000124	-0.0000054	0.0000027	0.0000014	-0.0000007	0.0000003	0.0000001	
S 4.8169758D+10	0.0000346	-0.0000151	0.0000074	0.0000039	-0.0000020	0.0000009	0.0000002	
S 9.9361591D+09	0.0000832	-0.0000362	0.0000178	0.0000094	-0.0000048	0.0000021	0.0000005	
S 2.4639137D+09	0.0001786	-0.0000774	0.0000381	0.0000201	-0.0000102	0.0000045	0.0000012	
S 7.1816264D+08	0.0003401	-0.0001471	0.0000724	0.0000381	-0.0000195	0.0000086	0.0000022	
S 2.4112093D+08	0.0006032	-0.0002605	0.0001282	0.0000674	-0.0000344	0.0000152	0.0000039	
S 8.6786178D+07	0.0011058	-0.0004769	0.0002346	0.0001234	-0.0000631	0.0000279	0.0000072	
S 3.0999086D+07	0.0021309	-0.0009184	0.0004517	0.0002376	-0.0001214	0.0000537	0.0000138	
S 1.0789847D+07	0.0041191	-0.0017754	0.0008734	0.0004594	-0.0002347	0.0001038	0.0000267	
S 3.7328973D+06	0.0077934	-0.0033641	0.0016555	0.0008709	-0.0004449	0.0001968	0.0000505	
S 1.3131807D+06	0.0142861	-0.0061909	0.0030486	0.0016040	-0.0008195	0.0003625	0.0000931	
S 4.7949633D+05	0.0251397	-0.0109756	0.0054124	0.0028487	-0.0014556	0.0006439	0.0001653	
S 1.8441539D+05	0.0424355	-0.0187654	0.0092744	0.0048841	-0.0024961	0.0011043	0.0002836	
S 7.5241162D+04	0.0684772	-0.0308961	0.0153275	0.0080801	-0.0041305	0.0018274	0.0004692	
S 3.2745814D+04	0.1048310	-0.0487723	0.0243259	0.0128398	-0.0065664	0.0029057	0.0007465	

S	1.5119156D+04	0.1536261	-0.0747088	0.0375884	0.0198902	-0.0101782	0.0045037	0.0011558
S	7.2606415D+03	0.2128221	-0.1104173	0.0562076	0.0298177	-0.0152714	0.0067611	0.0017384
S	3.5778939D+03	0.2560044	-0.1437434	0.0744345	0.0397038	-0.0203620	0.0090132	0.0023103
S	1.8028852D+03	0.2304792	-0.1296803	0.0663972	0.0351935	-0.0180206	0.0079817	0.0020597
S	9.2283438D+02	0.1195321	0.0253788	-0.0324446	-0.0203058	0.0108735	-0.0048778	-0.0012750
S	4.7224439D+02	0.0212940	0.3576126	-0.3075504	-0.1876430	0.0999519	-0.0446673	-0.0114476
S	2.4303673D+02	0.0004073	0.5196600	-0.5547478	-0.3596498	0.1951152	-0.0876935	-0.0226560
S	1.2136865D+02	-0.0000357	0.2203098	-0.1232124	-0.0683010	0.0362303	-0.0160413	-0.0039000
S	7.0362717D+01	0.0000424	-0.0070667	0.7015043	0.7996264	-0.5140360	0.2407036	0.0618799
S	3.9241973D+01	-0.0000828	0.0138110	0.5616800	0.8072102	-0.5461790	0.2615281	0.0687708
S	2.1307633D+01	0.0000688	-0.0080607	0.1107560	-0.4606666	0.4482175	-0.2326940	-0.0626669
S	1.2029259D+01	-0.0000410	0.0046505	-0.0038173	-0.9561186	1.3636191	-0.8042155	-0.2133099
S	6.4534654D+00	0.0000224	-0.0023188	0.0032059	-0.2164520	-0.0834527	0.1418447	0.0383170
S	3.3025290D+00	-0.0000105	0.0010012	-0.0014701	-0.0027062	-1.2602296	1.2151474	0.3580580
S	1.3208083D+00	0.0000052	-0.0005035	0.0006377	-0.0014090	-0.2839438	0.2342578	0.0640583
S	7.6137100D-01	-0.0000031	0.0003035	-0.0003833	0.0006678	0.0648167	-1.0621413	-0.4022071
S	3.2053513D-01	0.0000008	-0.0000755	0.0000988	-0.0001064	-0.0133769	-0.4644972	-0.3660916
S	8.0533502D-02	-0.0000002	0.0000184	-0.0000236	0.0000287	0.0029041	-0.0035827	0.5336768
S	3.0587168D-02	0.0000001	-0.0000067	0.0000086	-0.0000102	-0.0010420	-0.0004978	0.6841799
	P	2P	3P	4P	5P	6P		
BASIS/ORB. ENERGY	-789.1340200	-203.1122700	-52.1023600	-10.8911660	-1.1323831			
P	4.9575168D+08	0.0000091	-0.0000049	-0.0000026	-0.0000013	0.0000005		
P	6.9639169D+07	0.0000288	-0.0000154	-0.0000082	-0.0000040	0.0000016		
P	1.4029526D+07	0.0000784	-0.0000419	-0.0000223	-0.0000110	0.0000043		
P	3.4628311D+06	0.0001946	-0.0001043	-0.0000554	-0.0000274	0.0000106		
P	9.9201277D+05	0.0004562	-0.0002449	-0.0001301	-0.0000645	0.0000249		
P	3.1918927D+05	0.0010431	-0.0005618	-0.0002986	-0.0001480	0.0000571		
P	1.1249616D+05	0.0023765	-0.0012856	-0.0006842	-0.0003392	0.0001310		
P	4.2912494D+04	0.0054249	-0.0029522	-0.0015733	-0.0007802	0.0003010		
P	1.7541815D+04	0.0125222	-0.0068742	-0.0036718	-0.0018225	0.0007039		
P	7.5977688D+03	0.0291316	-0.0161933	-0.0086768	-0.0043083	0.0016624		
P	3.4611860D+03	0.0664120	-0.0376535	-0.0202798	-0.0100903	0.0039006		
P	1.6524162D+03	0.1397960	-0.0815817	-0.0442757	-0.0220560	0.0085130		
P	8.2338063D+02	0.2487421	-0.1508201	-0.0827221	-0.0413790	0.0160284		
P	4.2622371D+02	0.3291062	-0.2026945	-0.1115751	-0.0557339	0.0214804		

P	2.2723604D+02	0.2681393	-0.1055457	-0.0447138	-0.0205830	0.0079650
P	1.2341102D+02	0.1027413	0.2243193	0.1976134	0.1115693	-0.0447258
P	6.8744082D+01	0.0111378	0.5020244	0.4543982	0.2581530	-0.1018797
P	3.8440343D+01	0.0008735	0.3404863	0.1911443	0.0849516	-0.0333525
P	2.1108310D+01	-0.0005085	0.0726830	-0.4740794	-0.4094250	0.1823722
P	1.1844142D+01	0.0002220	0.0017102	-0.5984267	-0.5831717	0.2568004
P	6.4681244D+00	-0.0001444	0.0006786	-0.1752693	0.2003581	-0.1387221
P	3.4992903D+00	0.0000881	-0.0004400	-0.0079341	0.7329227	-0.4915061
P	1.8220443D+00	-0.0000351	0.0001078	-0.0014528	0.3442243	-0.1445345
P	8.3093956D-01	0.0000144	-0.0000483	0.0004059	0.0324260	0.5083755
P	3.7613038D-01	-0.0000056	0.0000186	-0.0001370	-0.0002964	0.5747001
P	1.5435246D-01	0.0000014	-0.0000049	0.0000306	0.0001415	0.1453408
	D	3D	4D	5D		
BASIS/ORB. ENERGY	-161.6441100	-36.2041790	-5.3424027			
D	4.0561832D+04	0.0001237	0.0000712	-0.0000329		
D	1.0077658D+04	0.0007828	0.0004517	-0.0002087		
D	3.4590695D+03	0.0039072	0.0022656	-0.0010489		
D	1.4105926D+03	0.0162238	0.0094790	-0.0043940		
D	6.4314555D+02	0.0545432	0.0322713	-0.0150145		
D	3.1726435D+02	0.1430413	0.0861636	-0.0402352		
D	1.6553876D+02	0.2738377	0.1648094	-0.0770262		
D	8.9744904D+01	0.3538876	0.1965206	-0.0894410		
D	4.9960418D+01	0.2614107	0.0342929	0.0034965		
D	2.8286530D+01	0.0949923	-0.2758896	0.1795270		
D	1.6306974D+01	0.0136799	-0.4391137	0.2771761		
D	9.7375819D+00	0.0007176	-0.2824484	0.1098047		
D	6.1826885D+00	0.0001073	-0.0970377	-0.1867680		
D	3.8255203D+00	-0.0001032	-0.0227034	-0.3818200		
D	2.3507306D+00	0.0000137	-0.0002175	-0.3611402		
D	1.3906715D+00	-0.0000276	-0.0006488	-0.2057122		
D	7.5756491D-01	0.0000009	0.0001294	-0.0582715		
D	3.2775210D-01	-0.0000022	-0.0000293	-0.0048844		
	F	4F	5F			
BASIS/ORB. ENERGY	-20.3596540	-0.4299579				
F	2.0699633D+03	-0.0002917	-0.0001031			

F	7.0521611D+02	-0.0024778	-0.0008736
F	3.0424182D+02	-0.0134875	-0.0047888
F	1.4685433D+02	-0.0511190	-0.0181374
F	7.5147156D+01	-0.1393732	-0.0498372
F	3.9898308D+01	-0.2701977	-0.0936205
F	2.1278249D+01	-0.3622878	-0.1134136
F	1.1287894D+01	-0.3001448	-0.0370624
F	5.8317741D+00	-0.1218026	0.1808047
F	2.8460380D+00	-0.0158685	0.3795185
F	1.3075735D+00	-0.0004386	0.3898400
F	5.5123261D-01	-0.0001563	0.2564310
F	2.0257310D-01	-0.0000344	0.0949711

EINSTEINIUM [RN]7S(2)5F(11), 4I

CHARGE = 99.000000

SYMMETRY SPECIES	S	P	D	F
NUMBER OF BASIS FUNCTIONS	35	26	18	13
NUMBER OF CLOSED SHELLS	7	5	3	1
NUMBER OF OPEN SHELLS	0	0	0	1
OPEN SHELL OCCUPATION NUMBER	0	0	0	11

*** FINAL SCF RESULTS ***

E = -33873.112140296

ORBITAL ENERGIES AND EXPANSION COEFFICIENTS

	S	1S	2S	3S	4S	5S	6S	7S
BASIS/ORB. ENERGY		-5135.0141000	-994.7225700	-260.2966500	-70.8600800	-16.8056610	-2.5557751	-0.1994470
S	3.2892005D+12	0.0000036	-0.0000016	0.0000008	0.0000004	-0.0000002	0.0000001	0.0000000
S	3.0896946D+11	0.0000136	-0.0000060	0.0000030	0.0000016	-0.0000008	0.0000004	0.0000001
S	4.8150946D+10	0.0000379	-0.0000166	0.0000082	0.0000043	-0.0000022	0.0000010	0.0000002
S	9.8781131D+09	0.0000909	-0.0000398	0.0000196	0.0000103	-0.0000053	0.0000024	0.0000006
S	2.4485623D+09	0.0001928	-0.0000841	0.0000415	0.0000219	-0.0000112	0.0000050	0.0000013
S	7.1816264D+08	0.0003641	-0.0001585	0.0000781	0.0000412	-0.0000211	0.0000094	0.0000024
S	2.4116803D+08	0.0006459	-0.0002807	0.0001382	0.0000729	-0.0000374	0.0000166	0.0000042
S	8.6850899D+07	0.0011765	-0.0005106	0.0002514	0.0001325	-0.0000680	0.0000301	0.0000077
S	3.1059691D+07	0.0022573	-0.0009788	0.0004820	0.0002541	-0.0001304	0.0000578	0.0000147
S	1.0819383D+07	0.0043503	-0.0018865	0.0009291	0.0004897	-0.0002513	0.0001113	0.0000283

S	3.7372744D+06	0.0082208	-0.0035703	0.0017589	0.0009271	-0.0004758	0.0002108	0.0000535
S	1.3126678D+06	0.0149907	-0.0065360	0.0032221	0.0016987	-0.0008718	0.0003863	0.0000981
S	4.7949633D+05	0.0262372	-0.0115256	0.0056901	0.0030009	-0.0015402	0.0006824	0.0001733
S	1.8441539D+05	0.0441025	-0.0196253	0.0097106	0.0051241	-0.0026305	0.0011656	0.0002961
S	7.5248511D+04	0.0707769	-0.0321408	0.0159648	0.0084331	-0.0043303	0.0019188	0.0004873
S	3.2746781D+04	0.1077628	-0.0504722	0.0252048	0.0133311	-0.0068484	0.0030350	0.0007711
S	1.5119492D+04	0.1567943	-0.0767729	0.0386833	0.0205115	-0.0105432	0.0046732	0.0011865
S	7.2605529D+03	0.2153348	-0.1124429	0.0573041	0.0304632	-0.0156727	0.0069478	0.0017663
S	3.5778939D+03	0.2557627	-0.1440614	0.0746729	0.0399044	-0.0205553	0.0091176	0.0023131
S	1.8028852D+03	0.2260588	-0.1248028	0.0633766	0.0335764	-0.0172591	0.0076443	0.0019480
S	9.2283438D+02	0.1137552	0.0391810	-0.0421769	-0.0260278	0.0139532	-0.0062364	-0.0015988
S	4.7224439D+02	0.0192291	0.3729722	-0.3242958	-0.1987843	0.1064514	-0.0477169	-0.0121166
S	2.4303673D+02	0.0003638	0.5117266	-0.5503453	-0.3588044	0.1958789	-0.0881024	-0.0224757
S	1.2136865D+02	-0.0000750	0.2038293	-0.0777351	-0.0300035	0.0135790	-0.0059686	-0.0013940
S	7.0362717D+01	0.0000733	-0.0076540	0.7180193	0.8343544	-0.5414326	0.2550713	0.0651382
S	3.9241977D+01	-0.0001005	0.0123174	0.5353685	0.7651751	-0.5219446	0.2498333	0.0646080
S	2.1307633D+01	0.0000808	-0.0071417	0.0954925	-0.5385829	0.5339700	-0.2780727	-0.0730974
S	1.2029259D+01	-0.0000486	0.0040782	-0.0027897	-0.9238707	1.3627909	-0.8161948	-0.2156590
S	6.4534654D+00	0.0000260	-0.0020215	0.0023376	-0.1866502	-0.2237046	0.2574885	0.0715864
S	3.3025290D+00	-0.0000120	0.0008721	-0.0011076	-0.0022516	-1.2217292	1.1900318	0.3454721
S	1.3208083D+00	0.0000060	-0.0004377	0.0004621	-0.0009940	-0.2409711	0.1313329	0.0350382
S	7.6137109D-01	-0.0000036	0.0002636	-0.0002758	0.0004368	0.0538972	-1.0386183	-0.4023201
S	3.2053525D-01	0.0000009	-0.0000655	0.0000717	-0.0000538	-0.0108506	-0.4294025	-0.3412419
S	8.0533471D-02	-0.0000002	0.0000160	-0.0000170	0.0000153	0.0023190	-0.0001254	0.5593513
S	3.0586724D-02	0.0000001	-0.0000058	0.0000062	-0.0000053	-0.0008296	-0.0014317	0.6572207
	P	2P	3P	4P	5P	6P		
BASIS/ORB. ENERGY	-809.2872300	-209.0658200	-53.9112050	-11.3018920	-1.1550667			
P	4.9403095D+08	0.0000097	-0.0000052	-0.0000028	-0.0000014	0.0000005		
P	6.9362480D+07	0.0000306	-0.0000164	-0.0000087	-0.0000043	0.0000017		
P	1.3970464D+07	0.0000833	-0.0000446	-0.0000238	-0.0000118	0.0000046		
P	3.4472613D+06	0.0002064	-0.0001108	-0.0000590	-0.0000294	0.0000113		
P	9.8827004D+05	0.0004823	-0.0002595	-0.0001382	-0.0000688	0.0000265		
P	3.1838115D+05	0.0010994	-0.0005934	-0.0003163	-0.0001575	0.0000606		
P	1.1235789D+05	0.0024965	-0.0013534	-0.0007223	-0.0003599	0.0001386		
P	4.2905634D+04	0.0056811	-0.0030987	-0.0016560	-0.0008252	0.0003177		

P	1.7547522D+04	0.0130757	-0.0071952	-0.0038543	-0.0019228	0.0007410
P	7.5992703D+03	0.0303315	-0.0169054	-0.0090847	-0.0045330	0.0017454
P	3.4610281D+03	0.0688111	-0.0391266	-0.0211380	-0.0105712	0.0040778
P	1.6522594D+03	0.1439038	-0.0842471	-0.0458618	-0.0229588	0.0088423
P	8.2315542D+02	0.2535014	-0.1541506	-0.0848229	-0.0426555	0.0164886
P	4.2625021D+02	0.3298274	-0.2028011	-0.1117616	-0.0560543	0.0215509
P	2.2728433D+02	0.2624686	-0.0957028	-0.0379405	-0.0170997	0.0065907
P	1.2333594D+02	0.0966880	0.2422940	0.2133009	0.1212590	-0.0485161
P	6.8749668D+01	0.0096504	0.5043931	0.4584653	0.2615806	-0.1029891
P	3.8431622D+01	0.0008358	0.3260782	0.1637984	0.0673789	-0.0261303
P	2.1118025D+01	-0.0005135	0.0651526	-0.5023863	-0.4402842	0.1963648
P	1.1866500D+01	0.0002268	0.0014999	-0.5815782	-0.5684221	0.2489867
P	6.4849922D+00	-0.0001421	0.0004517	-0.1586729	0.2564436	-0.1705390
P	3.5001169D+00	0.0000862	-0.0003304	-0.0064702	0.7305560	-0.4923614
P	1.8213640D+00	-0.0000347	0.0000647	-0.0012784	0.3138887	-0.1069669
P	8.3230610D-01	0.0000141	-0.0000305	0.0003568	0.0274764	0.5253730
P	3.7624914D-01	-0.0000055	0.0000116	-0.0001200	-0.0001307	0.5572125
P	1.5437331D-01	0.0000014	-0.0000031	0.0000263	0.0000895	0.1346558

	D	3D	4D	5D
BASIS/ORB. ENERGY	-166.3226000	-37.5266280	-5.5669058	
D	3.9167537D+04	0.0001376	0.0000795	-0.0000370
D	9.7833122D+03	0.0008628	0.0005000	-0.0002327
D	3.3877039D+03	0.0042169	0.0024570	-0.0011454
D	1.3955986D+03	0.0171567	0.0100693	-0.0047010
D	6.3924636D+02	0.0572796	0.0340698	-0.0159644
D	3.1536976D+02	0.1491726	0.0902691	-0.0424581
D	1.6460002D+02	0.2800868	0.1691644	-0.0795911
D	8.9547050D+01	0.3520844	0.1940179	-0.0885399
D	4.9993186D+01	0.2544086	0.0218650	0.0110635
D	2.8175649D+01	0.0899532	-0.2985063	0.1948075
D	1.5973479D+01	0.0112168	-0.4628630	0.2946960
D	9.1234653D+00	0.0007557	-0.2766852	0.0526826
D	5.3650054D+00	-0.0002960	-0.0629384	-0.3032866
D	3.5461826D+00	0.0002282	-0.0098808	-0.2527183
D	2.4689132D+00	-0.0001650	-0.0005035	-0.3540716

D	1.3946180D+00	0.0000220	-0.0004670	-0.2169935
D	7.0545945D-01	-0.0000125	0.0000612	-0.0457336
D	2.7965858D-01	0.0000005	-0.0000189	-0.0025969
	F	4F	5F	
BASIS/ORB.ENERGY		-21.3263140	-0.4495345	
F	2.1037721D+03	-0.0003039	0.0001096	
F	7.0669294D+02	-0.0026875	0.0009658	
F	3.0108295D+02	-0.0147751	0.0053548	
F	1.4567372D+02	-0.0540361	0.0195467	
F	7.5271662D+01	-0.1432578	0.0522966	
F	4.0177192D+01	-0.2752430	0.0969047	
F	2.1406081D+01	-0.3664776	0.1161140	
F	1.1314285D+01	-0.2937477	0.0277462	
F	5.8332098D+00	-0.1115506	-0.1984526	
F	2.8670561D+00	-0.0133796	-0.3829269	
F	1.3297839D+00	-0.0005492	-0.3786842	
F	5.6699566D-01	-0.0001464	-0.2451651	
F	2.1033925D-01	-0.0000576	-0.0904500	

FERMIUM [RN]7S(2)5F(12), 3H

CHARGE =100.000000

SYMMETRY SPECIES	S	P	D	F
NUMBER OF BASIS FUNCTIONS	35	26	18	13
NUMBER OF CLOSED SHELLS	7	5	3	1
NUMBER OF OPEN SHELLS	0	0	0	1
OPEN SHELL OCCUPATION NUMBER	0	0	0	12

*** FINAL SCF RESULTS ***

E =-34779.285928196

ORBITAL ENERGIES AND EXPANSION COEFFICIENTS

	S	1S	2S	3S	4S	5S	6S	7S
BASIS/ORB.ENERGY		-5267.5682000	-1024.4469000	-268.7702300	-73.4822840	-17.4857220	-2.6380610	-0.2022204
S	3.3123875D+12	0.0000040	-0.0000018	0.0000009	0.0000005	-0.0000002	0.0000001	0.0000000
S	3.0841530D+11	0.0000150	-0.0000067	0.0000033	0.0000017	-0.0000009	0.0000004	0.0000001
S	4.7787046D+10	0.0000418	-0.0000185	0.0000091	0.0000048	-0.0000025	0.0000011	0.0000003
S	9.7468927D+09	0.0000993	-0.0000437	0.0000216	0.0000114	-0.0000059	0.0000026	0.0000007

S	2.4324383D+09	0.0002082	-0.0000914	0.0000451	0.0000238	-0.0000123	0.0000054	0.0000014
S	7.1369678D+08	0.0003931	-0.0001722	0.0000849	0.0000449	-0.0000231	0.0000103	0.0000026
S	2.4060031D+08	0.0006869	-0.0003004	0.0001481	0.0000782	-0.0000403	0.0000179	0.0000045
S	8.7250784D+07	0.0012466	-0.0005444	0.0002684	0.0001417	-0.0000730	0.0000324	0.0000082
S	3.1218713D+07	0.0023923	-0.0010439	0.0005146	0.0002717	-0.0001400	0.0000621	0.0000156
S	1.0859057D+07	0.0046016	-0.0020078	0.0009899	0.0005227	-0.0002694	0.0001195	0.0000301
S	3.7387345D+06	0.0086863	-0.0037957	0.0018719	0.0009886	-0.0005095	0.0002261	0.0000569
S	1.3109001D+06	0.0157246	-0.0068984	0.0034045	0.0017983	-0.0009268	0.0004113	0.0001035
S	4.7949633D+05	0.0273735	-0.0120998	0.0059802	0.0031600	-0.0016288	0.0007228	0.0001818
S	1.8430736D+05	0.0458777	-0.0205452	0.0101773	0.0053808	-0.0027741	0.0012312	0.0003097
S	7.5208889D+04	0.0731167	-0.0334203	0.0166204	0.0087967	-0.0045361	0.0020130	0.0005062
S	3.2742543D+04	0.1107025	-0.0521986	0.0260985	0.0138309	-0.0071359	0.0031680	0.0007972
S	1.5116574D+04	0.1600443	-0.0788960	0.0398081	0.0211507	-0.0109172	0.0048448	0.0012177
S	7.2583223D+03	0.2175653	-0.1143332	0.0583323	0.0310699	-0.0160564	0.0071339	0.0017969
S	3.5799909D+03	0.2551775	-0.1440464	0.0747131	0.0400006	-0.0206842	0.0091770	0.0023032
S	1.8018833D+03	0.2220942	-0.1198610	0.0602565	0.0318706	-0.0164551	0.0073260	0.0018543
S	9.2139357D+02	0.1076777	0.0541794	-0.0529108	-0.0323389	0.0174098	-0.0078569	-0.0020029
S	4.7227322D+02	0.0173474	0.3857729	-0.3392026	-0.2089890	0.1124127	-0.0503401	-0.0126356
S	2.4366645D+02	0.0002491	0.5025958	-0.5431779	-0.3557067	0.1955196	-0.0884381	-0.0223958
S	1.2125069D+02	-0.0000095	0.1906536	-0.0350266	0.0070505	-0.0093764	0.0055358	0.0016738
S	7.0362717D+01	-0.0000007	-0.0101504	0.7358215	0.8713287	-0.5692456	0.2670554	0.0672525
S	3.9112596D+01	-0.0000393	0.0123168	0.5071205	0.7169294	-0.4951076	0.2416653	0.0624886
S	2.1307633D+01	0.0000370	-0.0072879	0.0797972	-0.6148902	0.6270165	-0.3370425	-0.0887273
S	1.2042620D+01	-0.0000202	0.0041757	-0.0011381	-0.8860158	1.3393362	-0.8001530	-0.2079706
S	6.4451802D+00	0.0000113	-0.0020785	0.0013289	-0.1618011	-0.3444536	0.3437942	0.0924627
S	3.3204770D+00	-0.0000057	0.0009100	-0.0007064	-0.0010475	-1.1795022	1.1779104	0.3421084
S	1.3208778D+00	0.0000028	-0.0004702	0.0002773	-0.0011096	-0.2124214	-0.0047081	-0.0177182
S	7.6614456D-01	-0.0000018	0.0003002	-0.0001746	0.0005422	0.0512626	-0.9214893	-0.3421791
S	3.5406466D-01	0.0000005	-0.0000792	0.0000495	-0.0000887	-0.0108537	-0.4446392	-0.3438672
S	8.0534945D-02	-0.0000001	0.0000154	-0.0000092	0.0000190	0.0017859	-0.0125330	0.5650010
S	3.0590075D-02	0.0000000	-0.0000058	0.0000035	-0.0000069	-0.0006596	0.0028707	0.6387444
P		2P	3P	4P	5P	6P		
BASIS/ORB. ENERGY		-829.7556400	-215.1205700	-55.7496340	-11.7170340	-1.1773022		
P	4.9077226D+08	0.0000104	-0.0000056	-0.0000030	-0.0000015	0.0000006		
P	6.8890516D+07	0.0000327	-0.0000175	-0.0000094	-0.0000047	0.0000018		

P	1.3876032D+07	0.0000885	-0.0000476	-0.0000254	-0.0000127	0.0000049
P	3.4272603D+06	0.0002189	-0.0001178	-0.0000629	-0.0000314	0.0000121
P	9.8297792D+05	0.0005105	-0.0002752	-0.0001470	-0.0000735	0.0000282
P	3.1715758D+05	0.0011591	-0.0006268	-0.0003350	-0.0001676	0.0000644
P	1.1216313D+05	0.0026201	-0.0014235	-0.0007617	-0.0003813	0.0001465
P	4.2913817D+04	0.0059434	-0.0032492	-0.0017412	-0.0008717	0.0003348
P	1.7553818D+04	0.0136571	-0.0075329	-0.0040465	-0.0020282	0.0007798
P	7.6006329D+03	0.0315511	-0.0176323	-0.0095025	-0.0047636	0.0018299
P	3.4613852D+03	0.0712829	-0.0406470	-0.0220245	-0.0110678	0.0042594
P	1.6517901D+03	0.1480806	-0.0869706	-0.0474879	-0.0238838	0.0091779
P	8.2288824D+02	0.2581841	-0.1574202	-0.0868868	-0.0439123	0.0169351
P	4.2628720D+02	0.3299796	-0.2024935	-0.1117066	-0.0562359	0.0215678
P	2.2760085D+02	0.2564529	-0.0853752	-0.0307586	-0.0133526	0.0051074
P	1.2323017D+02	0.0915711	0.2603896	0.2294139	0.1313014	-0.0524022
P	6.8713254D+01	0.0078324	0.5053078	0.4609889	0.2639935	-0.1037153
P	3.8458084D+01	0.0011258	0.3109313	0.1350279	0.0486481	-0.0183530
P	2.1147372D+01	-0.0007429	0.0590438	-0.5271830	-0.4694562	0.2094700
P	1.1904852D+01	0.0003835	0.0009725	-0.5643221	-0.5499961	0.2394771
P	6.5032997D+00	-0.0002304	0.0004776	-0.1438941	0.3095273	-0.2015380
P	3.4980348D+00	0.0001330	-0.0003566	-0.0051472	0.7274441	-0.4907717
P	1.8099932D+00	-0.0000566	0.0000842	-0.0011680	0.2836677	-0.0693426
P	8.3313924D-01	0.0000230	-0.0000382	0.0003350	0.0221372	0.5401279
P	3.7574708D-01	-0.0000089	0.0000144	-0.0001123	0.0003154	0.5411884
P	1.5315832D-01	0.0000022	-0.0000038	0.0000241	-0.0000278	0.1234321
	D	3D	4D	5D		
BASIS/ORB. ENERGY	-171.0635200	-38.8653770	-5.7923404			
D	3.8263672D+04	0.0001496	0.0000868	-0.0000406		
D	9.7013351D+03	0.0009121	0.0005308	-0.0002486		
D	3.3897795D+03	0.0044158	0.0025839	-0.0012127		
D	1.3961871D+03	0.0179966	0.0106107	-0.0049860		
D	6.3880729D+02	0.0597185	0.0356879	-0.0168378		
D	3.1529081D+02	0.1540893	0.0936860	-0.0443526		
D	1.6450727D+02	0.2859949	0.1732167	-0.0820409		
D	8.9573353D+01	0.3511610	0.1922728	-0.0878408		
D	5.0105075D+01	0.2476392	0.0089520	0.0187311		

D	2.8145921D+01	0.0852334	-0.3146950	0.2070246
D	1.5965204D+01	0.0090351	-0.4630815	0.2953455
D	9.1001525D+00	0.0012891	-0.2628534	0.0270959
D	5.3442793D+00	-0.0009785	-0.0544599	-0.3273769
D	3.5379889D+00	0.0008749	-0.0091837	-0.2450014
D	2.4822445D+00	-0.0005151	0.0000627	-0.3466603
D	1.3940717D+00	0.0001017	-0.0005219	-0.2038656
D	6.9236582D-01	-0.0000297	0.0000606	-0.0397631
D	2.4252270D-01	0.0000032	-0.0000179	-0.0017582
	F	4F	5F	
BASIS/ORB. ENERGY		-22.3053860	-0.4674206	
F	2.1069211D+03	-0.0003253	0.0001195	
F	7.0664432D+02	-0.0028766	0.0010528	
F	3.0080396D+02	-0.0157443	0.0058128	
F	1.4554316D+02	-0.0569498	0.0209840	
F	7.5301026D+01	-0.1490519	0.0554238	
F	4.0200965D+01	-0.2825179	0.1009316	
F	2.1409036D+01	-0.3684956	0.1174898	
F	1.1324544D+01	-0.2845698	0.0171883	
F	5.8348691D+00	-0.1023105	-0.2164675	
F	2.8692829D+00	-0.0111785	-0.3894480	
F	1.3303068D+00	-0.0006774	-0.3698164	
F	5.6756884D-01	-0.0001604	-0.2314568	
F	2.1186365D-01	-0.0000857	-0.0823569	

MENDELEVIUM [RN]7S(2)5F(13), 2F

CHARGE =101.000000

SYMMETRY SPECIES	S	P	D	F
NUMBER OF BASIS FUNCTIONS	35	26	18	13
NUMBER OF CLOSED SHELLS	7	5	3	1
NUMBER OF OPEN SHELLS	0	0	0	1
OPEN SHELL OCCUPATION NUMBER	0	0	0	13

*** FINAL SCF RESULTS ***

E =-35703.431489770

ORBITAL ENERGIES AND EXPANSION COEFFICIENTS

S	1S	2S	3S	4S	5S	6S	7S
BASIS/ORB. ENERGY	-5403.0511000	-1054.9704000	-277.4667400	-76.1701920	-18.1795560	-2.7202485	-0.2047874
S 3.3197211D+12	0.0000044	-0.0000020	0.0000010	0.0000005	-0.0000003	-0.0000001	0.0000000
S 3.0854929D+11	0.0000168	-0.0000075	0.0000037	0.0000020	-0.0000010	-0.0000005	0.0000001
S 4.5944571D+10	0.0000474	-0.0000211	0.0000104	0.0000055	-0.0000029	-0.0000013	0.0000003
S 9.3100875D+09	0.0001113	-0.0000493	0.0000244	0.0000129	-0.0000067	-0.0000030	0.0000007
S 2.3140966D+09	0.0002317	-0.0001024	0.0000506	0.0000268	-0.0000138	-0.0000062	0.0000015
S 6.8587039D+08	0.0004269	-0.0001882	0.0000929	0.0000492	-0.0000254	-0.0000113	0.0000028
S 2.3728454D+08	0.0007139	-0.0003141	0.0001551	0.0000821	-0.0000425	-0.0000189	0.0000047
S 8.9612632D+07	0.0012702	-0.0005582	0.0002755	0.0001458	-0.0000754	-0.0000335	0.0000083
S 3.2313443D+07	0.0025145	-0.0011041	0.0005449	0.0002883	-0.0001492	-0.0000663	0.0000165
S 1.1045240D+07	0.0049099	-0.0021558	0.0010639	0.0005629	-0.0002913	-0.0001294	0.0000322
S 3.7425115D+06	0.0092345	-0.0040605	0.0020046	0.0010607	-0.0005488	-0.0002438	0.0000607
S 1.3047393D+06	0.0165790	-0.0073190	0.0036159	0.0019135	-0.0009902	-0.0004400	0.0001095
S 4.7664120D+05	0.0286763	-0.0127564	0.0063116	0.0033414	-0.0017293	-0.0007683	0.0001913
S 1.8330298D+05	0.0477903	-0.0215411	0.0106824	0.0056585	-0.0029291	-0.0013016	0.0003241
S 7.4811442D+04	0.0757263	-0.0348457	0.0173503	0.0092006	-0.0047636	-0.0021167	0.0005269
S 3.2628115D+04	0.1135417	-0.0539066	0.0269840	0.0143275	-0.0074225	-0.0032991	0.0008216
S 1.5097301D+04	0.1629683	-0.0808874	0.0408701	0.0217576	-0.0112754	-0.0050109	0.0012471
S 7.2556421D+03	0.2196353	-0.1161210	0.0592984	0.0316430	-0.0164217	-0.0073032	0.0018197
S 3.5843132D+03	0.2534494	-0.1433106	0.0743788	0.0398914	-0.0207040	-0.0092027	0.0022890
S 1.8092426D+03	0.2174126	-0.1142312	0.0566937	0.0299122	-0.0155047	-0.0068978	0.0017221
S 9.2241675D+02	0.1034329	0.0677863	-0.0629083	-0.0382957	0.0207032	0.0093142	-0.0023309
S 4.7297762D+02	0.0150623	0.3986396	-0.3542975	-0.2193299	0.1184935	0.0532171	-0.0132582
S 2.4424373D+02	0.0006792	0.4929244	-0.5346859	-0.3516860	0.1945621	0.0880201	-0.0219915
S 1.2110738D+02	-0.0004610	0.1775667	0.0099877	0.0475010	-0.0347219	-0.0169347	0.0043085
S 7.0362870D+01	0.0004182	-0.0120969	0.7478239	0.9020099	-0.5934917	-0.2801274	0.0703107
S 3.9040334D+01	-0.0003416	0.0121835	0.4791530	0.6651691	-0.4643194	-0.2263880	0.0572155
S 2.1309149D+01	0.0002508	-0.0072983	0.0664368	-0.6872699	0.7208969	0.3884570	-0.0996184
S 1.2041802D+01	-0.0001566	0.0041899	0.0001531	-0.8443461	1.3062050	0.7915480	-0.2061263
S 6.4452989D+00	0.0000811	-0.0020842	0.0005084	-0.1382321	-0.4695591	-0.4554154	0.1252037
S 3.3239828D+00	-0.0000363	0.0009122	-0.0003633	-0.0008155	-1.1292176	-1.1321274	0.3220702
S 1.3208760D+00	0.0000189	-0.0004710	0.0001084	-0.0008780	-0.1794788	0.0944095	-0.0366343
S 7.6624688D-01	-0.0000121	0.0003011	-0.0000660	0.0004204	0.0423744	0.8966061	-0.3509755
S 3.5405327D-01	0.0000032	-0.0000796	0.0000206	-0.0000630	-0.0087857	0.4112662	-0.3120927

S	8.0536328D-02	-0.0000006	0.0000158	-0.0000037	0.0000141	0.0014471	0.0089995	0.5701885
S	3.1438162D-02	0.0000002	-0.0000061	0.0000014	-0.0000052	-0.0005449	-0.0018604	0.6269606
	P	2P	3P	4P	5P	6P		
BASIS/ORB. ENERGY	-850.5392300	-221.2740500	-57.6146270	-12.1337720	-1.1977328			
P	4.8748560D+08	0.0000111	-0.0000059	-0.0000032	-0.0000016	0.0000006		
P	6.8680830D+07	0.0000347	-0.0000187	-0.0000100	-0.0000050	0.0000019		
P	1.3811438D+07	0.0000941	-0.0000507	-0.0000271	-0.0000136	0.0000052		
P	3.4160163D+06	0.0002313	-0.0001247	-0.0000667	-0.0000335	0.0000128		
P	9.8188399D+05	0.0005389	-0.0002911	-0.0001559	-0.0000783	0.0000300		
P	3.1654442D+05	0.0012211	-0.0006617	-0.0003546	-0.0001782	0.0000683		
P	1.1212377D+05	0.0027493	-0.0014968	-0.0008030	-0.0004038	0.0001547		
P	4.2903566D+04	0.0062243	-0.0034105	-0.0018326	-0.0009215	0.0003530		
P	1.7559440D+04	0.0142484	-0.0078776	-0.0042431	-0.0021362	0.0008191		
P	7.6007778D+03	0.0328338	-0.0183983	-0.0099433	-0.0050065	0.0019180		
P	3.4614931D+03	0.0737489	-0.0421710	-0.0229158	-0.0115678	0.0044395		
P	1.6517102D+03	0.1523311	-0.0897503	-0.0491524	-0.0248304	0.0095156		
P	8.2257095D+02	0.2627051	-0.1605882	-0.0888928	-0.0451357	0.0173593		
P	4.2645901D+02	0.3299111	-0.2019019	-0.1114652	-0.0563080	0.0215307		
P	2.2771622D+02	0.2507902	-0.0747135	-0.0231686	-0.0093163	0.0035191		
P	1.2310140D+02	0.0858913	0.2784510	0.2455496	0.1414096	-0.0562846		
P	6.8712400D+01	0.0066635	0.5042391	0.4615944	0.2652210	-0.1038931		
P	3.8504653D+01	0.0010544	0.2968215	0.1060471	0.0292633	-0.0103432		
P	2.1160114D+01	-0.0007031	0.0531713	-0.5522408	-0.4998147	0.2231262		
P	1.1922490D+01	0.0003571	0.0006674	-0.5448321	-0.5264423	0.2269863		
P	6.5134234D+00	-0.0002096	0.0003899	-0.1293153	0.3623645	-0.2319050		
P	3.4979269D+00	0.0001209	-0.0003148	-0.0040877	0.7166811	-0.4842809		
P	1.8082522D+00	-0.0000513	0.0000705	-0.0010627	0.2572817	-0.0336551		
P	8.3298031D-01	0.0000208	-0.0000320	0.0003064	0.0187548	0.5524350		
P	3.7506513D-01	-0.0000080	0.0000120	-0.0001034	0.0003350	0.5241599		
P	1.5245873D-01	0.0000020	-0.0000032	0.0000219	-0.0000414	0.1139358		
	D	3D	4D	5D				
BASIS/ORB. ENERGY	-175.8632100	-40.2170150	-6.0160077					
D	3.8539209D+04	0.0001572	0.0000916	-0.0000432				
D	9.6431755D+03	0.0009849	0.0005755	-0.0002712				
D	3.3228183D+03	0.0048512	0.0028517	-0.0013469				

D	1.3645113D+03	0.0195417	0.0115731	-0.0054708
D	6.2803495D+02	0.0631208	0.0379232	-0.0180125
D	3.1270424D+02	0.1589550	0.0970537	-0.0462162
D	1.6378220D+02	0.2927623	0.1779005	-0.0848120
D	8.8714393D+01	0.3566807	0.1922102	-0.0874898
D	4.9013840D+01	0.2392393	-0.0155796	0.0336759
D	2.7359405D+01	0.0732026	-0.3453459	0.2281205
D	1.5604610D+01	0.0072275	-0.4498662	0.2856488
D	9.0416825D+00	0.0006167	-0.2352950	-0.0063225
D	5.4718791D+00	-0.0002833	-0.0491004	-0.2999511
D	3.7119397D+00	0.0001262	-0.0089536	-0.2881490
D	2.4441302D+00	-0.0000946	-0.0005909	-0.3431305
D	1.3967653D+00	0.0000038	-0.0003476	-0.1780763
D	7.3719247D-01	-0.0000085	0.0000295	-0.0381959
D	3.0859683D-01	-0.0000005	-0.0000166	-0.0028055

	F	4F	5F
BASIS/ORB. ENERGY		-23.2933530	-0.4881710
F	2.1091038D+03	-0.0003455	0.0001290
F	7.0804495D+02	-0.0030744	0.0011454
F	3.0016793D+02	-0.0168129	0.0063130
F	1.4541138D+02	-0.0598134	0.0224355
F	7.5355015D+01	-0.1550036	0.0586030
F	4.0217323D+01	-0.2895853	0.1049305
F	2.1415664D+01	-0.3699927	0.1182387
F	1.1331146D+01	-0.2750585	0.0061803
F	5.8433329D+00	-0.0934759	-0.2336967
F	2.8704904D+00	-0.0095960	-0.3953494
F	1.3291926D+00	-0.0007219	-0.3603107
F	5.6835306D-01	-0.0002228	-0.2181243
F	2.1330351D-01	-0.0001012	-0.0748662

NOBELIUM [RN]7S(2)5F(14), 1S

CHARGE =102.000000

SYMMETRY SPECIES	S	P	D	F
NUMBER OF BASIS FUNCTIONS	35	26	18	13

NUMBER OF CLOSED SHELLS	7	5	3	2
NUMBER OF OPEN SHELLS	0	0	0	0
OPEN SHELL OCCUPATION NUMBER	0	0	0	0

*** FINAL SCF RESULTS ***

E = -36645.981043563

ORBITAL ENERGIES AND EXPANSION COEFFICIENTS

	S	1S	2S	3S	4S	5S	6S	7S
BASIS/ORB. ENERGY	-5541.5645000	-1086.3249000	-286.3938300	-78.9256290	-18.8873100	-2.8023278	-0.2073940	
S 3.2489842D+12	0.0000049	-0.0000022	0.0000011	0.0000006	-0.0000003	-0.0000001	0.0000000	
S 3.0419762D+11	0.0000186	-0.0000083	0.0000041	0.0000022	-0.0000011	-0.0000005	0.0000001	
S 4.5797007D+10	0.0000524	-0.0000234	0.0000116	0.0000062	-0.0000032	-0.0000014	0.0000004	
S 9.0175846D+09	0.0001257	-0.0000560	0.0000277	0.0000147	-0.0000076	-0.0000034	0.0000008	
S 2.2175415D+09	0.0002562	-0.0001139	0.0000563	0.0000299	-0.0000155	-0.0000069	0.0000017	
S 6.6548830D+08	0.0004614	-0.0002047	0.0001012	0.0000536	-0.0000279	-0.0000124	0.0000031	
S 2.3511209D+08	0.0007416	-0.0003284	0.0001623	0.0000860	-0.0000447	-0.0000199	0.0000049	
S 9.3565629D+07	0.0012502	-0.0005530	0.0002732	0.0001448	-0.0000752	-0.0000335	0.0000082	
S 3.4428209D+07	0.0026051	-0.0011512	0.0005687	0.0003014	-0.0001566	-0.0000696	0.0000172	
S 1.1470997D+07	0.0052117	-0.0023028	0.0011376	0.0006030	-0.0003132	-0.0001393	0.0000343	
S 3.8000470D+06	0.0098060	-0.0043390	0.0021443	0.0011366	-0.0005904	-0.0002626	0.0000647	
S 1.3034368D+06	0.0176393	-0.0078365	0.0038756	0.0020546	-0.0010674	-0.0004747	0.0001170	
S 4.7067372D+05	0.0304036	-0.0136127	0.0067424	0.0035759	-0.0018578	-0.0008263	0.0002037	
S 1.8044847D+05	0.0499418	-0.0226636	0.0112519	0.0059711	-0.0031030	-0.0013803	0.0003402	
S 7.4289263D+04	0.0773401	-0.0358287	0.0178599	0.0094880	-0.0049311	-0.0021934	0.0005406	
S 3.2768456D+04	0.1153996	-0.0551528	0.0276408	0.0147037	-0.0076480	-0.0034029	0.0008390	
S 1.5141261D+04	0.1672644	-0.0835411	0.0422543	0.0225343	-0.0117202	-0.0052139	0.0012847	
S 7.2414792D+03	0.2222269	-0.1182372	0.0604588	0.0323260	-0.0168497	-0.0075016	0.0018503	
S 3.5859565D+03	0.2511668	-0.1420297	0.0736682	0.0395581	-0.0205869	-0.0091592	0.0022556	
S 1.8122793D+03	0.2135407	-0.1087861	0.0532849	0.0280494	-0.0146263	-0.0065137	0.0016094	
S 9.1843375D+02	0.0984049	0.0850400	-0.0760530	-0.0462174	0.0251551	0.0113264	-0.0028022	
S 4.7184691D+02	0.0126782	0.4078644	-0.3663495	-0.2278336	0.1234459	0.0555095	-0.0136966	
S 2.4587404D+02	0.0010171	0.4792996	-0.5210840	-0.3441637	0.1919365	0.0869841	-0.0215056	
S 1.2100148D+02	-0.0007776	0.1707142	0.0504091	0.0868262	-0.0610406	-0.0293154	0.0073064	
S 7.0281008D+01	0.0007035	-0.0180056	0.7613261	0.9324645	-0.6154391	-0.2911202	0.0724253	
S 3.8977150D+01	-0.0005438	0.0150418	0.4456182	0.6044373	-0.4304336	-0.2112785	0.0527611	
S 2.1318029D+01	0.0003920	-0.0093647	0.0582993	-0.7518474	0.8211697	0.4477376	-0.1135367	

S	1.2028101D+01	-0.0002453	0.0055057	-0.0010630	-0.8032014	1.2495880	0.7618933	-0.1969406
S	6.4154817D+00	0.0001277	-0.0027921	0.0010739	-0.1146105	-0.5770524	-0.5508870	0.1504703
S	3.3461427D+00	-0.0000573	0.0012405	-0.0006487	-0.0011442	-1.0741209	-1.0809896	0.3040047
S	1.3207744D+00	0.0000295	-0.0006360	0.0002737	-0.0003584	-0.1596401	0.1792798	-0.0620240
S	7.6640180D-01	-0.0000192	0.0004126	-0.0001764	0.0000964	0.0400530	0.8553697	-0.3397984
S	3.6074458D-01	0.0000051	-0.0001109	0.0000508	0.0000204	-0.0085133	0.3883299	-0.2948199
S	8.0611525D-02	-0.0000010	0.0000209	-0.0000093	-0.0000031	0.0013394	0.0086320	0.5963374
S	3.1110764D-02	0.0000004	-0.0000080	0.0000036	0.0000015	-0.0005029	-0.0018653	0.5986619
	P	2P	3P	4P	5P	6P		
BASIS/ORB. ENERGY	-871.6405500	-227.5264900	-59.5057070	-12.5515400	-1.2163888			
P	4.8036783D+08	0.0000119	-0.0000064	-0.0000034	-0.0000017	0.0000007		
P	6.7913052D+07	0.0000370	-0.0000199	-0.0000107	-0.0000054	0.0000021		
P	1.3747703D+07	0.0001000	-0.0000539	-0.0000289	-0.0000146	0.0000056		
P	3.3758987D+06	0.0002482	-0.0001340	-0.0000719	-0.0000363	0.0000138		
P	9.6669786D+05	0.0005737	-0.0003105	-0.0001667	-0.0000841	0.0000321		
P	3.1408191D+05	0.0012816	-0.0006960	-0.0003739	-0.0001887	0.0000720		
P	1.1204526D+05	0.0028770	-0.0015697	-0.0008443	-0.0004263	0.0001628		
P	4.2893582D+04	0.0065295	-0.0035855	-0.0019316	-0.0009753	0.0003724		
P	1.7545411D+04	0.0148568	-0.0082341	-0.0044473	-0.0022482	0.0008591		
P	7.6096362D+03	0.0340581	-0.0191319	-0.0103670	-0.0052416	0.0020016		
P	3.4612270D+03	0.0765432	-0.0438994	-0.0239253	-0.0121283	0.0046388		
P	1.6497869D+03	0.1564957	-0.0924706	-0.0507798	-0.0257609	0.0098409		
P	8.2307748D+02	0.2664190	-0.1633283	-0.0906937	-0.0462478	0.0177256		
P	4.2658298D+02	0.3312263	-0.2017494	-0.1113252	-0.0564195	0.0215043		
P	2.2712643D+02	0.2447435	-0.0632823	-0.0150644	-0.0049108	0.0017741		
P	1.2297752D+02	0.0793134	0.2965162	0.2620545	0.1516975	-0.0601375		
P	6.8659038D+01	0.0062039	0.5029246	0.4608707	0.2657189	-0.1038179		
P	3.8491088D+01	0.0006280	0.2820459	0.0765676	0.0086530	-0.0016413		
P	2.1202050D+01	-0.0004311	0.0473504	-0.5751273	-0.5273190	0.2349473		
P	1.1948102D+01	0.0001795	0.0006729	-0.5242062	-0.5034150	0.2153425		
P	6.5742798D+00	-0.0001008	0.0002063	-0.1159481	0.4098443	-0.2598486		
P	3.4965427D+00	0.0000603	-0.0002246	-0.0045792	0.7136836	-0.4794968		
P	1.7776097D+00	-0.0000240	0.0000359	-0.0004938	0.2293275	0.0056331		
P	8.2803544D-01	0.0000102	-0.0000183	0.0001111	0.0131860	0.5623282		
P	3.7302744D-01	-0.0000039	0.0000067	-0.0000309	0.0010092	0.5061029		

P	1.5022828D-01	0.0000010	-0.0000018	0.0000036	-0.0002087	0.1040648
	D	3D	4D	5D		
BASIS/ORB. ENERGY	-180.7206400	-41.5806400	-6.2372830			
D	3.6197145D+04	0.0001829	-0.0001070	0.0000507		
D	9.0682083D+03	0.0011410	-0.0006693	0.0003173		
D	3.1480221D+03	0.0055690	-0.0032899	0.0015624		
D	1.2939016D+03	0.0224704	-0.0133675	0.0063591		
D	5.9147639D+02	0.0731241	-0.0442250	0.0211273		
D	2.9134083D+02	0.1816550	-0.1114098	0.0534036		
D	1.5177063D+02	0.3137096	-0.1904862	0.0911139		
D	8.3258294D+01	0.3378728	-0.1719420	0.0769061		
D	4.7915869D+01	0.2024587	0.0388483	-0.0463550		
D	2.8754443D+01	0.0677533	0.2863682	-0.1886539		
D	1.7661784D+01	0.0103179	0.4099714	-0.2733449		
D	1.0635773D+01	0.0011411	0.2900444	-0.0765050		
D	6.1604910D+00	-0.0003578	0.0849132	0.3001137		
D	3.7437625D+00	0.0001926	0.0060721	0.3817096		
D	2.4013063D+00	-0.0001635	0.0021584	0.3017591		
D	1.3837302D+00	0.0000289	-0.0001789	0.1726080		
D	6.5282376D-01	-0.0000129	0.0000855	0.0293887		
D	1.3445144D-01	0.0000004	-0.0000027	0.0005581		
	F	4F	5F			
BASIS/ORB. ENERGY	-24.2892590	-0.5128740				
F	2.1168731D+03	-0.0003698	0.0001395			
F	7.0922986D+02	-0.0032552	0.0012284			
F	3.0051677D+02	-0.0179667	0.0068189			
F	1.4377918D+02	-0.0654865	0.0248876			
F	7.3806840D+01	-0.1663928	0.0635424			
F	3.9667554D+01	-0.2910990	0.1062272			
F	2.1672925D+01	-0.3521264	0.1125517			
F	1.1902688D+01	-0.2620128	0.0087871			
F	6.4125625D+00	-0.0990163	-0.2049442			
F	3.3025908D+00	-0.0131514	-0.3678172			
F	1.5892106D+00	-0.0004210	-0.3702317			
F	6.8635396D-01	-0.0000199	-0.2471784			

F 2.5311325D-01 -0.0000015 -0.0921750

LAWRENCIUM [RN]7S(2)6D(1)5F(14), 2D

CHARGE =103.000000

SYMMETRY SPECIES	S	P	D	F
NUMBER OF BASIS FUNCTIONS	35	26	18	13
NUMBER OF CLOSED SHELLS	7	5	3	2
NUMBER OF OPEN SHELLS	0	0	1	0
OPEN SHELL OCCUPATION NUMBER	0	0	1	0

*** FINAL SCF RESULTS ***

E =-37607.117579940

ORBITAL ENERGIES AND EXPANSION COEFFICIENTS

	S	1S	2S	3S	4S	5S	6S	7S
BASIS/ORB. ENERGY	-5683.4666000	-1118.8066000	-295.8351800	-82.0268870	-19.8827970	-3.0852902	-0.2459073	
S 3.9674449D+12	0.0000051	-0.0000023	0.0000011	0.0000006	-0.0000003	-0.0000001	0.0000000	
S 3.0998446D+11	0.0000212	-0.0000096	0.0000048	0.0000025	-0.0000013	-0.0000006	0.0000002	
S 4.4219987D+10	0.0000595	-0.0000268	0.0000133	0.0000071	-0.0000037	-0.0000017	0.0000005	
S 8.6642089D+09	0.0001383	-0.0000621	0.0000307	0.0000163	-0.0000085	-0.0000038	0.0000010	
S 2.1905312D+09	0.0002758	-0.0001234	0.0000611	0.0000324	-0.0000169	-0.0000076	0.0000021	
S 6.5291003D+08	0.0005098	-0.0002277	0.0001126	0.0000598	-0.0000312	-0.0000141	0.0000038	
S 2.3171930D+08	0.0007760	-0.0003459	0.0001711	0.0000909	-0.0000474	-0.0000214	0.0000058	
S 9.5239269D+07	0.0012952	-0.0005767	0.0002852	0.0001514	-0.0000790	-0.0000356	0.0000097	
S 3.5362672D+07	0.0027056	-0.0012034	0.0005951	0.0003160	-0.0001648	-0.0000743	0.0000203	
S 1.1834136D+07	0.0054416	-0.0024198	0.0011966	0.0006353	-0.0003314	-0.0001493	0.0000407	
S 3.8675549D+06	0.0103962	-0.0046294	0.0022901	0.0012161	-0.0006343	-0.0002859	0.0000780	
S 1.3033025D+06	0.0187975	-0.0084044	0.0041604	0.0022095	-0.0011527	-0.0005195	0.0001417	
S 4.6460724D+05	0.0321745	-0.0145008	0.0071902	0.0038204	-0.0019932	-0.0008983	0.0002451	
S 1.7850768D+05	0.0516680	-0.0236033	0.0117296	0.0062353	-0.0032538	-0.0014666	0.0004001	
S 7.4219301D+04	0.0791841	-0.0369316	0.0184338	0.0098126	-0.0051218	-0.0023084	0.0006299	
S 3.2794928D+04	0.1189414	-0.0572136	0.0286937	0.0152859	-0.0079828	-0.0035991	0.0009818	
S 1.5070360D+04	0.1716991	-0.0863852	0.0437782	0.0234061	-0.0122296	-0.0055122	0.0015046	
S 7.2199568D+03	0.2220187	-0.1187167	0.0606750	0.0324568	-0.0169780	-0.0076607	0.0020885	
S 3.6051838D+03	0.2484202	-0.1406792	0.0731483	0.0394380	-0.0206365	-0.0092987	0.0025422	
S 1.8136838D+03	0.2126191	-0.1032805	0.0490489	0.0254313	-0.0132272	-0.0059752	0.0016175	
S 9.0344198D+02	0.0926437	0.1062352	-0.0913669	-0.0549621	0.0298572	0.0136423	-0.0036958	

S	4.6813900D+02	0.0094178	0.4161545	-0.3814195	-0.2397262	0.1309320	0.0596309	-0.0163779
S	2.4541320D+02	0.0016116	0.4697817	-0.5032400	-0.3307498	0.1847871	0.0850121	-0.0230887
S	1.1580165D+02	-0.0013311	0.1644112	0.1145041	0.1464545	-0.0982251	-0.0479190	0.0126422
S	6.9777657D+01	0.0012599	-0.0354239	0.7475454	0.9455283	-0.6328902	-0.3028999	0.0847295
S	3.9119662D+01	-0.0008821	0.0220608	0.4170598	0.5134510	-0.3594900	-0.1813011	0.0480434
S	2.0896731D+01	0.0006217	-0.0136871	0.0515353	-0.8015280	0.9033038	0.5104528	-0.1398640
S	1.2138201D+01	-0.0003993	0.0083794	-0.0029390	-0.7329301	1.1565940	0.7094710	-0.2098505
S	6.3765371D+00	0.0001963	-0.0040337	0.0014400	-0.1143952	-0.6668407	-0.6348242	0.2018824
S	3.3353146D+00	-0.0000884	0.0018057	-0.0007683	0.0063186	-1.0191810	-1.0695968	0.3262351
S	1.3405308D+00	0.0000422	-0.0008602	0.0003081	-0.0035258	-0.1195572	0.3647951	-0.1128564
S	7.2285688D-01	-0.0000271	0.0005520	-0.0001934	0.0021639	0.0231658	0.8213579	-0.4568829
S	3.6247974D-01	0.0000088	-0.0001803	0.0000659	-0.0006705	-0.0057110	0.2899926	-0.2001377
S	8.5177924D-02	-0.0000016	0.0000323	-0.0000116	0.0001224	0.0007900	0.0084372	0.7816438
S	3.1672413D-02	0.0000006	-0.0000115	0.0000042	-0.0000438	-0.0002741	-0.0019186	0.4267255
	P	2P	3P	4P	5P	6P		
BASIS/ORB. ENERGY	-893.3238800	-234.1531200	-61.6977700	-13.2351450	-1.3907309			
P	3.7082389D+08	0.0000149	-0.0000080	-0.0000043	-0.0000022	0.0000009		
P	5.5960854D+07	0.0000432	-0.0000233	-0.0000125	-0.0000064	0.0000025		
P	1.2078576D+07	0.0001116	-0.0000603	-0.0000324	-0.0000164	0.0000064		
P	3.1161045D+06	0.0002701	-0.0001461	-0.0000786	-0.0000398	0.0000156		
P	3.0663962D+05	0.0013478	-0.0007334	-0.0003950	-0.0002003	0.0000782		
P	9.2071816D+05	0.0006136	-0.0003328	-0.0001791	-0.0000908	0.0000355		
P	1.1134365D+05	0.0029900	-0.0016349	-0.0008816	-0.0004473	0.0001747		
P	4.3139101D+04	0.0067395	-0.0037084	-0.0020032	-0.0010165	0.0003968		
P	1.7688129D+04	0.0154085	-0.0085605	-0.0046349	-0.0023548	0.0009200		
P	7.6444766D+03	0.0353691	-0.0199135	-0.0108222	-0.0054993	0.0021474		
P	3.4684548D+03	0.0791925	-0.0455582	-0.0248900	-0.0126816	0.0049585		
P	1.6475737D+03	0.1620285	-0.0959885	-0.0528878	-0.0269665	0.0105359		
P	8.1737833D+02	0.2740289	-0.1685891	-0.0938159	-0.0480902	0.0188394		
P	4.2257661D+02	0.3308159	-0.1998000	-0.1103189	-0.0561043	0.0218726		
P	2.2598536D+02	0.2338110	-0.0498431	-0.0052023	0.0003953	-0.0003320		
P	1.2410979D+02	0.0734748	0.3020465	0.2657667	0.1549321	-0.0627582		
P	7.0043697D+01	0.0065318	0.4923785	0.4570145	0.2648072	-0.1060374		
P	3.9661712D+01	0.0002507	0.2821623	0.0663690	0.0019663	0.0016800		
P	2.1342733D+01	-0.0001875	0.0495309	-0.6026288	-0.5647143	0.2574318		

P	1.1896995D+01	0.0000292	-0.0018687	-0.5091093	-0.4716903	0.2049053
P	6.4622849D+00	-0.0000139	0.0012889	-0.0982267	0.4836823	-0.3154239
P	3.4133231D+00	0.0000162	-0.0007687	-0.0032145	0.6934292	-0.4751643
P	1.7052642D+00	-0.0000047	0.0003090	-0.0003530	0.1878976	0.0663569
P	8.2660041D-01	0.0000024	-0.0001454	0.0000825	0.0064133	0.5843690
P	3.8674833D-01	-0.0000009	0.0000564	-0.0000179	0.0017111	0.4640145
P	1.6221806D-01	0.0000002	-0.0000140	0.0000002	-0.0004010	0.0935939
	D	3D	4D	5D	6D	
BASIS/ORB. ENERGY	-185.9085000	-43.2300790	-6.7027483	-0.1489716		
D	3.3883219D+04	0.0002137	0.0001256	0.0000600	-0.0000116	
D	8.4622061D+03	0.0013466	0.0007936	0.0003792	-0.0000737	
D	2.9454143D+03	0.0065288	0.0038728	0.0018550	-0.0003592	
D	1.2165807D+03	0.0259096	0.0155003	0.0074336	-0.0014459	
D	5.6042849D+02	0.0812883	0.0494247	0.0238260	-0.0046158	
D	2.8051156D+02	0.1897276	0.1169663	0.0564986	-0.0110198	
D	1.4961578D+02	0.3080649	0.1869001	0.0901688	-0.0173963	
D	8.4181768D+01	0.3249765	0.1649748	0.0736073	-0.0143832	
D	4.8470185D+01	0.2099833	-0.0513135	-0.0544220	0.0121681	
D	2.7105659D+01	0.0649045	-0.3857388	-0.2600051	0.0521909	
D	1.5063187D+01	0.0036298	-0.4663556	-0.2864395	0.0590150	
D	8.2071522D+00	0.0009501	-0.1930718	0.1558441	-0.0484733	
D	4.3572264D+00	-0.0005286	-0.0216994	0.5390371	-0.1301160	
D	2.2265941D+00	0.0001700	-0.0010543	0.3945681	-0.0898195	
D	1.0648062D+00	-0.0000865	0.0000320	0.1011806	0.1313288	
D	3.9734160D-01	0.0000223	-0.0000431	0.0051765	0.3838320	
D	1.3720912D-01	-0.0000085	0.0000136	-0.0000880	0.4862047	
D	4.3347259D-02	0.0000026	-0.0000038	0.0000499	0.3031453	
	F	4F	5F			
BASIS/ORB. ENERGY	-25.5654800	-0.7656116				
F	2.1242808D+03	-0.0003941	-0.0001541			
F	7.0941607D+02	-0.0034698	-0.0013592			
F	3.0046753D+02	-0.0190554	-0.0074978			
F	1.4366872D+02	-0.0688755	-0.0271752			
F	7.3742902D+01	-0.1731135	-0.0684943			
F	3.9627640D+01	-0.2972964	-0.1121598			

F	2.1694527D+01	-0.3512684	-0.1142564
F	1.1940555D+01	-0.2532281	0.0014132
F	6.4417387D+00	-0.0916219	0.2254609
F	3.3092089D+00	-0.0113389	0.3830287
F	1.6026906D+00	-0.0003066	0.3597547
F	7.1663710D-01	-0.0000201	0.2181153
F	2.8133596D-01	0.0000014	0.0684116