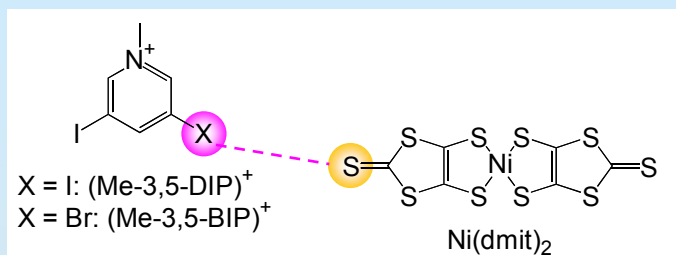


$Ni(dmit)_2$ Salts Having Conducting and Magnetic Electrons Based on Molecular π -Electrons

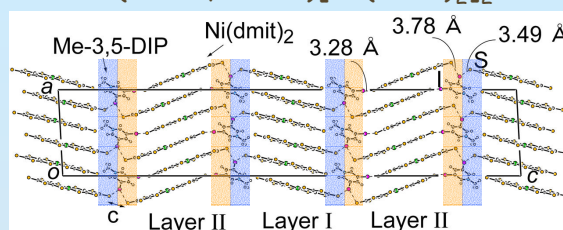
Y. Kosaka, H. M. Yamamoto, A. Nakao, A. Fukaya, M. Tamura and R. Kato

Supramolecular halogen interaction



$$r(I) + r(S) = 3.78 \text{ \AA}$$

$\alpha-(Me-3,5-XIP)[Ni(dmit)_2]_2$

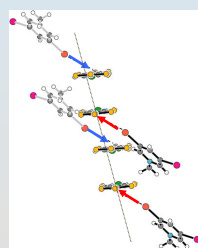


Crystal data: monoclinic, $C2/c$, $Z = 8$

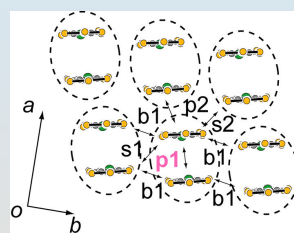
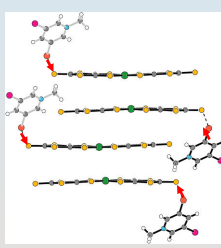
	a (Å)	b (Å)	c (Å)	β (°)	V (Å ³)
DIP	14.35(6)	6.47(3)	76.56(3)	92.99(3)	7098.24
BIP	14.22(4)	6.44(1)	76.15(2)	93.84(9)	6952.65

Y. Kosaka *et al.*, *J. Am. Chem. Soc.*, **2007**, *129*, 3054

Layer I



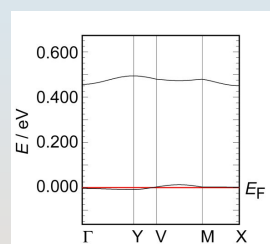
Strong dimerization



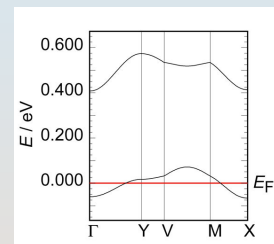
Overlap Integrals ($\times 10^{-3}$)

	p1	p2	s1	s2	b1
DIP	23.35	-0.38	-0.66	0.67	0.41
BIP	24.43	-1.52	-0.69	1.23	3.03

DIP salt

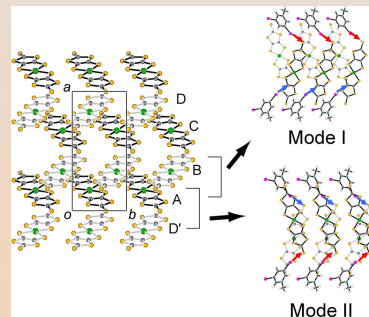


BIP salt

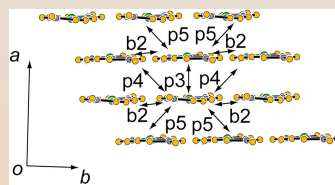


$U_{\text{eff}} \gg W$ Mott insulating state

Layer II

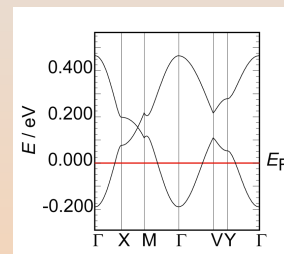
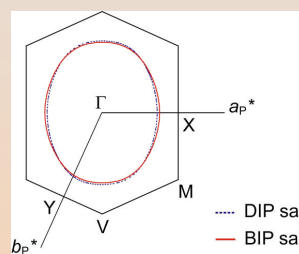


Spanning-overlap



Overlap Integrals ($\times 10^{-3}$)

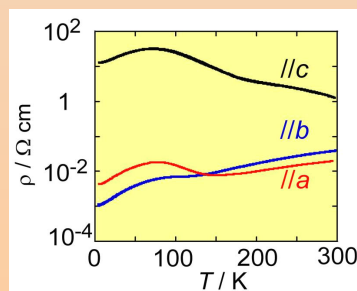
	p3	p4	p5	b2	c
DIP	-13.30	-0.50	-8.80	0.68	0.30
BIP	-12.29	-0.51	-9.69	0.74	0.18



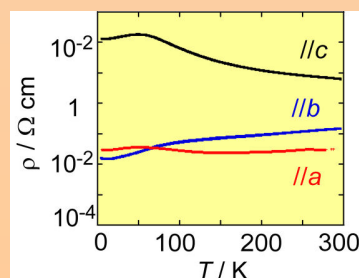
2D metallic state

Electrical Resistivity

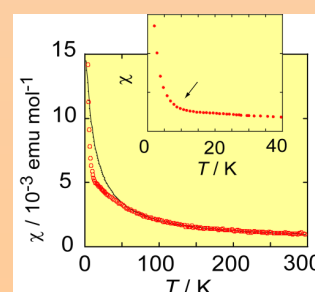
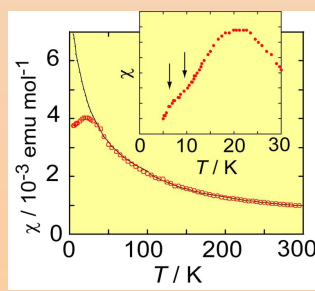
DIP salt



BIP salt



Magnetic Susceptibility



$$c_{\text{Total}} = (c_{\text{CW}} + c_{\text{Const.}})/2$$

c_{CW} : $C = 0.375 \text{ emu K mol}^{-1}$ (fixed)
 $\theta = -5.3 \text{ K}$
 $c_{\text{Const.}} = 7.2 \times 10^{-4} \text{ emu mol}^{-1}$

c_{CW} : $C = 0.375 \text{ emu K mol}^{-1}$ (fixed)
 $\theta = -10.7 \text{ K}$
 $c_{\text{Const.}} = 7.5 \times 10^{-4} \text{ emu mol}^{-1}$

→ 2D metallic conduction

→ Localized spins