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Positron binding by molecules ☆

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An infinite number of stable electronic bound states is known to be formed, in the Born–Oppenheimer approximation, around polar molecules having a dipole moment D larger than $D_c = 1.625$ Debye [1]. This is a consequence of the long-range dipole interaction (behaving as $\sim r^{-2}$ at large r) between the electron and the polar molecule, and does not depend on the nature of the short-range interactions. Even if $D < D_c$, or no dipole moment at all, electronic bound states may still be formed around a molecule because of the short-range interactions, but only a finite number of them is possible.

These facts do not depend on the sign of the dipole interaction. Hence, a positron is expected to have an infinite number of bound states around a molecule with $D > D_c$ at the equilibrium nuclear position. It may have a finite number of bound states if $D < D_c$.

There have been some theoretical attempts to find out stable states of a positron bound by molecules [2–4] using the Hartree–Fock (HF), quantum Monte Carlo, and other approaches. Most of these calculations suggest a positronic bound state if D exceeds a threshold of 3–4 Debye.

We have recently carried out extensive HF calculations of positronic states formed by a variety of polar molecules and have discussed the characteristic features of positron binding [5]. The classes of molecules we have dealt with are:

1. alkali hydrides,
2. diatomics consisting of two different alkali atoms,
3. diatomics of an alkaline-earth atom and an atom in the (16) group,
4. alkali hydroxides,
5. other organic polyatomics.

We have clearly found that D is a critical quantity for determining the positron binding energy E_b. Within each particular series of molecules, E_b is a monotonically and smoothly increasing function of D in the HF approximation. For nearly the same D, E_b is larger for molecules having a more electronegative atom or more tightly bound electrons. Thus, E_b is larger for oxides than for hydrides. The positron cloud is found to be concentrated on the side of and behind the more electronegative atom in the molecule.

Only one positron bound state has been found for each of the highly polar molecules calculated in this work. No bound state has been found for molecules with $D < 4$ Debye. This is partly because of the lack of positron correlations with the electrons in the HF approximation, and partly

☆ This work has been recently published elsewhere. Please consult [5] for details.

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because of the missing long-range dipole interaction. A project taking account of these two kinds of effect is in progress.

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