

Influence of geometry on positron binding to molecules

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Annihilation studies have established that positrons bind to most molecules. They also provide measurements of the positron-molecule binding energies, which are found to vary widely and depend upon molecular size and composition. Trends of binding energy with global parameters such as molecular polarizability and dipole moment have been discussed previously. Here, we present comparisons of positron binding energies to various pairs of isomers (i.e., having the same chemical composition but different arrangements of the atoms). A simple case is that of carbon chain isomers, where a particular atom (or group) is moved from the 1st carbon to the 2nd carbon in the chain (for example, 1-chloropropane vs 2-chloropropane). A key feature is that, since the atomic constituents do not change, the molecular parameters are approximately constant, and so any difference in binding energies appears to be due to the atomic arrangement. It is found that molecular geometry can play a significant role in determining the binding energies even for isomers with very similar polarizabilities (see Fig. 1) and dipole moments. The possible origins of this dependence are discussed.

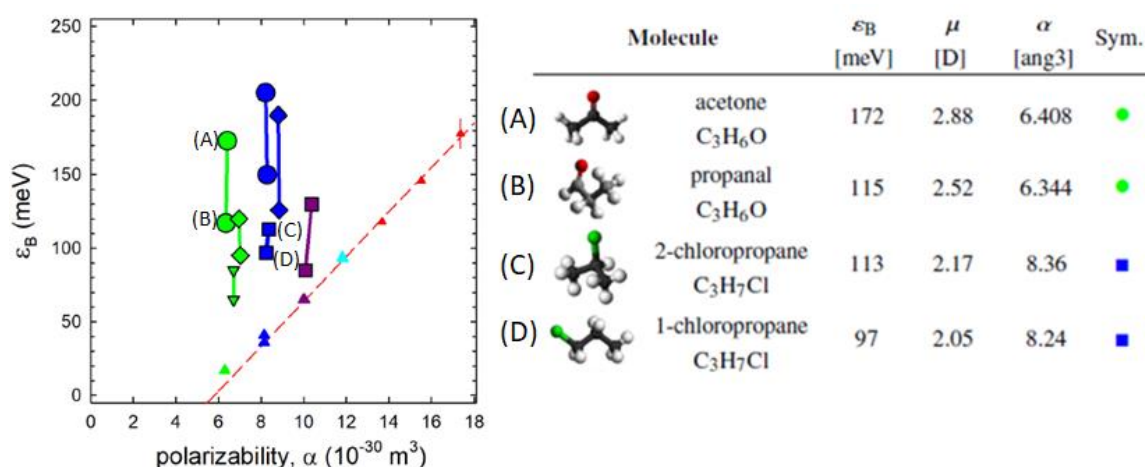


Fig.1. (left) Measured positron-molecule binding energy (ϵ_B) vs molecular polarizability (α) for isomer pairs, with each pair connected by a line. Table (right). Data for two isomer pairs are compared, with the symbols for them in Fig. 1 defined.

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