

Theoretical investigation of the binding of a positron to vibrational excited states of hydrogen cyanide molecule

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Positrons are widely used in both scientific and technological areas such as physics, chemistry, material science, medicine, and their interdisciplinary areas. A positron affinity (PA), which is a binding energy of a positron to an atom or molecule, have now been experimentally measured by Surko and co-workers for many molecular species such as some hydrocarbons (alkanes, alkenes, and aromatics), alcohols, and halogenated hydrocarbons [1-3]. Recently, Danielson *et al.* [4] have experimentally measured the binding of a positron to acetonitrile with the vibrational Feshbach resonance (VFR) technique and estimated its PA value as 180 meV. There is, however, no direct experimental evidence for the positron binding to hydrogen cyanide molecule (HCN) that is the simplest molecule including the nitrile (-CN) functional group. In this study, thus, we analyzed the characteristic features of the binding of a positron to HCN molecule with both quantum Monte Carlo (QMC) and *ab initio* molecular orbital calculations in order to theoretically predict the PA value of HCN molecule.

A positron should be able to form an infinite number of bound states with molecules if the molecule has a dipole moment with a value greater than 1.625 debye (the critical dipole moment). As is well known, nitrile molecules have strong dipole moments greater than 3 debye. Recently, we show that HCN molecule with a dipole moment of 3.3 debye, has a small PA value of 38 (5) meV at its equilibrium structure by the QMC calculation [5]. However, the effect of molecular vibrations must be taken into account for theoretically predicting an *observable* PA value, because the most of the experimental PA values are measured through the VFR, in which a positronic molecular complex can be formed at the molecular vibrational excited states. Thus, in this presentation, we will report the vibrational averaged PA values of HCN molecule for several vibrational excited states. In this analysis, the PA values at many molecular geometries are calculated with the configurations interaction (CI) calculation including electronic single excitation, positronic single excitation, and double excitations of single electronic - single positronic excitation configurations, and are averaged with a weight of vibrational probability density obtained with multi-dimensional unharmonic vibrational state analysis based on vibrational QMC technique.

References

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