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Bond metamorphosis between coordinate (dative) and single covalent bonds: BN-ethylamine molecule

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Abstract: The BN-ethylamine molecule ($NH_2BH_2NH_3$) [1] was studied in order to show the bond metamorphosis step-by-step between BN single (…H_2B-NH_2) and coordinate (dative) (…H_2B-NH_3) [2-4]. Analyzing the molecular orbitals, charges and bond order along the hydrogen tunneling process ($NH_3BH_2NH_2$ ↔ $NH_2BH_3NH_2$ ↔ $NH_2BH_2NH_3$), it is possible to follow the bond metamorphosis between single covalent and coordinate (dative) bonds. The bond metamorphosis can also be followed along the hydrogen transfer observing the three main molecular orbitals. The IRC profile and the HOMO are shown in Fig.1. The hydrogen tunneling potential and its two first states are shown in Fig.2.

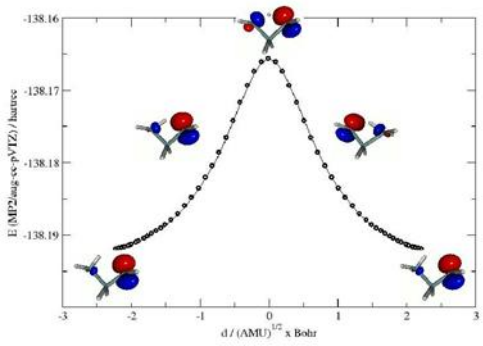

Fig.1

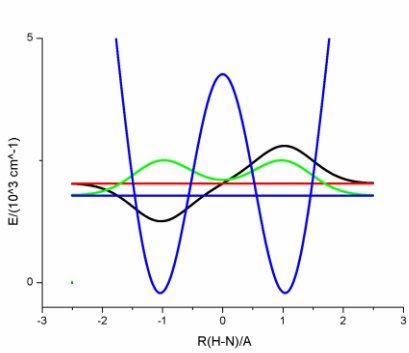

Fig.2

The molecular geometries, the harmonic vibrational analysis, and the IRC calculation were carried out at the MP2/aug-cc-pVDZ level of theory. MP2 and CCSD(T) single point energies were obtained using a larger aug-cc-pVTZ basis set. All calculations were performed with Gaussian09. The potential energy curve to dissociation limit of transferred hydrogen (H…$NH_2BH_2NH_2$ ↔ $NH_3BH_2NH_2$ ↔ $NH_2BH_3NH_2$ ↔ $NH_2BH_2NH_3$ ↔ $NH_2BH_2NH_2$…H), obtained by the methods previously described, was considered to solve the Schrödinger equation to find the eigenstates of the tunneling hydrogen process.

The main objective of this work was to illustrate the smooth modification between the two important different kinds of chemical bond. The technical analysis was presented

and the practical result was condensed in three most important MOs, which describe the metamorphosis process. These three MOs are shown in Fig.3 for the minimum of energy, intermediary geometry, and transition state. The charges, bond orders, and bond lengths were considered to study the bond transformation connected to tunneling transfer of hydrogen atom. This work can also contribute to educational issues, for example showing the difference between covalent and dative chemical bonds.

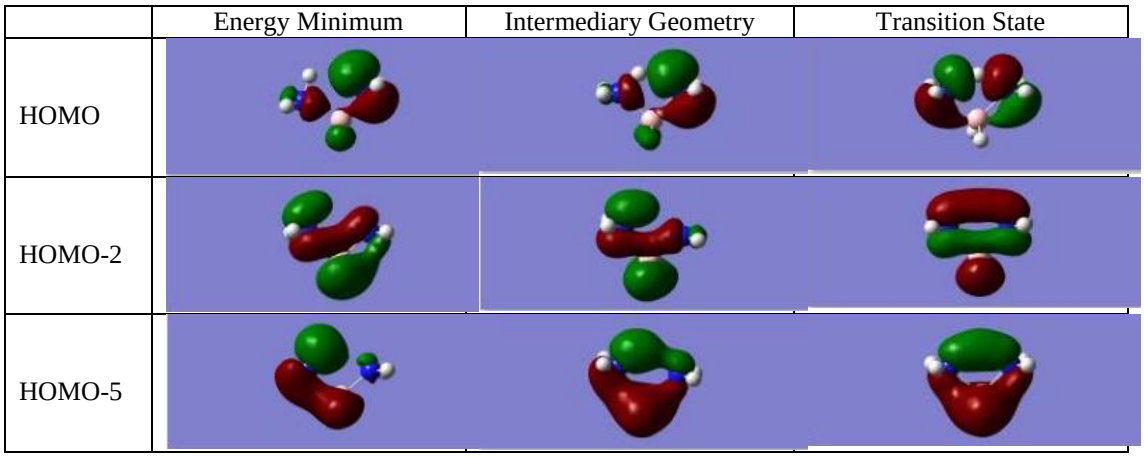

Fig.3

Key-words: **BN coordinate (dative) bond, BN covalente bond, hydrogen tunneling**

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