THE IONIZATION ENERGY OF CYANO PHOSPHINOGEN (HPCN)

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Optimized structures and harmonic vibrational frequencies have been determined for cyano phosphinogen (HPCN) and the corresponding singly charged cation at the B3LYP/6-311++g(2df,p) level of theory. Total energies have also been determined at the G2 level of theory in order to predict the ionization energy of HPCN. In the ground state of $HPCN^+$, the molecule is bent (C_s symmetry) and the electronic state is of $^1A'$ symmetry. The lowest-lying triplet state of the cation ($^3A''$) lies approximately 1 eV above the singlet state and the molecule is also bent in this state (C_s symmetry). The energy ordering of states in the cation is unexpected by analogy to $HNCN^+$ whose ground state is of triplet spin degeneracy. Also, the triplet state of $HNCN^+$ is linear, unlike $HPCN^+$. Structures, harmonic frequencies and ionization energies will be presented for the cyano phosphinogen system and discussed in comparison the cyano amidogen system.