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# Quantum chemical study of Pnicogen bond based on point-of-charge and MEP

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*A pnicogen bond is a noncovalent bond between a pnicogen atom (X) and a Lewis base (Y). This type of bond is attributed to the anisotropic distribution of the charge density on the pnicogen atom, resulting in the formation of a positive cap (called the σ-hole)[1]. Pnicogen bond is similar to halogen and chalcogen[2] bond in that they contribute to the stabilization of macromolecules and inhibitor-receptor complexes. Pnicogen bond's characteristics are still unrevealed. For instance, the ability of PH3 molecule to form a dimmer via pnicogen bond was under debate. In current work, six molecules (XH3, XH2F and XF3; X = N and P) were studied using quantum mechanical calculations including point-of-charge (PoC), stabilization energy, natural bonding orbital (NBO) and Molecular electrostatic potential (MEP) calculations. Firstly, all molecules were fully optimized by the second-order Møller–Plesset (MP2) method with 6-311++G** basis set. MEPs were then generated for the molecules at B3LYP/6-311++G** level of theory. The stabilization energy of the studied molecules was calculated at MP2/aug-cc-pVTZ level with incorporation of a PoC at a distance ranging from 1.5 to 8.0Å. The results showed that the existence of a negative charge, i.e. Lewis base, causes destabilization in case of NH3 and PH3 molecules. In case of NH2F, NF3, PH2F and PF3, a PoC with a value of -0.25au enhances the stabilization of molecular energy with a value of ranging from -1.0 to -2.6 kcal/mol. Furthermore, quantum calculations including MEP and NBO showed that NH3 and PH3 molecules are not able to form pnicogen bond. The impact of Y-X···PoC angle and value of PoC on the stabilization energy was evaluated. The current study revealed the main pnicogen bond's characteristics which would serve as a framework for all future studies.*