Ratifying the existence of pnicogen bonding from charge density analysis

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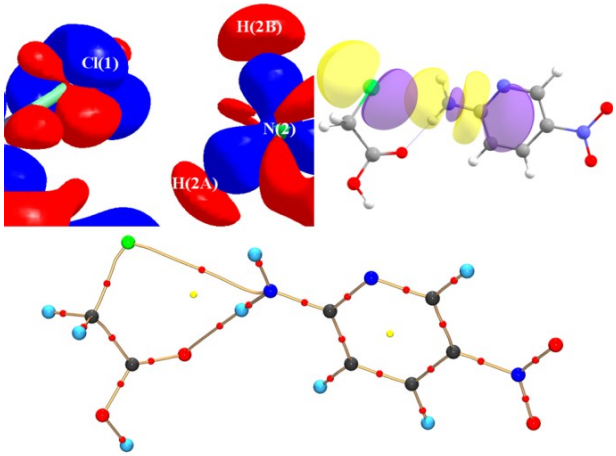
Pnicogen bond, a sparsely investigated and a least understood phenomenon, is a Lewis acid−Lewis base interaction involving elements of group 15 as an electron-pair acceptor.[1] In this experimental charge density study, pnicogen bonding has been analyzed for the first time both from qualitative and quantitative features derived based on Cambridge Structural Database, QTAIM topology, NBO and VSEPR theoretical analyses in molecular crystals.[2] The compounds studied are a) a co-crystal of 2-Amino-5-Nitropyridine and 2-chloroacetic acid and b) polymorphic forms of acetazolamide (API). The monoclinic form specifically depicts the pnicogen bond and both compounds provide the essential features of the nature of this bonding. In addition, a weak S...O contact is observed with the charge concentrated region (CC) of sulphur facing the charge depleted region (CD) of a sp^2-hybridized carbonyl oxygen, an example hitherto not discussed in terms of experimental charge density based on the deformation densities and the ESP maps.



References

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