σ-Hole Interactions of Trivalent Group V Atoms

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Abstract

From some recent papers, it could be inferred that noncovalent interactions between covalently-bonded Groups IV – VI atoms and negative sites (e.g. Lewis bases) are a recent discovery. In reality, many such interactions have been known experimentally for decades. What is new is the recognition, since 2007, that most of these (as well as Group VII) fit under the umbrella of σ-hole interactions, as recently reviewed [1,2]. In this presentation we focus upon Group V. We have made a survey of the crystal structures in the Cambridge Structural Database, looking for close contacts between trivalent nitrogen, phosphorus and arsenic atoms and the electronegative atoms nitrogen, oxygen and fluorine [3]. The interatomic separations were to be no more than 4.0 Å and the interactions were to be near-linear (as is characteristic of σ-hole interactions). A total of 285 such close contacts was found. Some specific examples will be discussed in terms of their computed electrostatic potentials.

[1] P. Politzer and J. S. Murray, *ChemPhysChem* 2013, **14**, 278-294.

[2] P. Politzer, J. S. Murray and T. Clark, *Phys. Chem. Chem. Phys*. 2013, **15**, 11178-11189.

[3] P. Politzer, J. S. Murray, S. D. Zarić and G. V. Janjić, *Crystals*, 2014, in press.