Analysis of hydrogen bond directionality in phosphoric triamides

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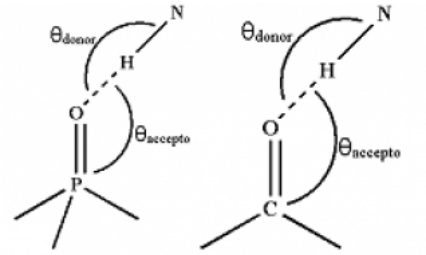
Six new crystal structures, [4-Cl-C6H4C(O)NH]P(O)[NR1R2]2 (NR1R2 = N(CH2C6H5)2 (1), NHCH2C6H5 (2), NHC6H4(4-CH3) (3)) and [RC(O)NH]P(O)[N(CH3)(CH2C6H5)]2 (R = 3-F-C6H4 (4), (3,5-F2)C6H3 (5)) and [(3,5-F2)C6H3C(O)NH]P(O)[NH]2C5H10 (6) are reported. The H…O=P and H…O=C angles were analyzed considering the new structures and their 156 analogous [RC(O)NH]P(O)[NR1R2]2 (R1 ≠ H, R2 = H or ≠ H) structures from the Cambridge Structural Database (CSD; Version 5.37, May 2016), in order to evaluate the acceptor directionality and nearly position of lone electron pair (LEP) at the oxygen atoms. The analyses were performed based on the original deposited structure and also after neutron-normalization of the N—H values. The H…O=C angles were found in a wider range with respect to the H…O=P angles which are more directional. Moreover, the maximum populations of H…O=P angles are within 135°–140°, while the two most populated ranges for H…O=C angles are within 150°–155° and then 140°–145°. The N—H…O angles were also analyzed to update a previous work for evaluation of the hydrogen bond angles (donor directionality) and to complete our discussion. The analysis of H…O=X (X = C, P) and N—H…O angles were also considered based on the hydrogen-bonded motifs including the noted angles to study the rigidity or flexibility of the motifs and the influence on the overall tendency of the angles.

[1] C. H. Görbitz (2016) Acta Crystallogr., Sect. B 72, 167–168.
[2] C. R. Groom et al. (2016) Acta Crystallogr., Sect. B 72, 171–179.



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