

Analysis of hydrogen bond directionality in phosphoric triamides

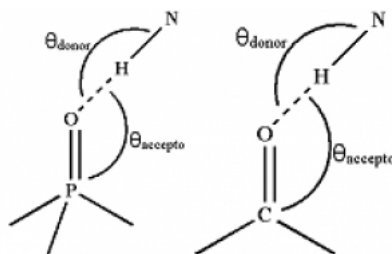
Maryam Taherzadeh¹, Mehrdad Pourayoubi¹, Marek Necas^{2,3}, Samad Shoghpour Bayraq¹, Hadi Amiri Rudbari⁴, Giuseppe Bruno⁵, Teresa Mancilla Percino⁶, Marco A. Leyva Ramírez⁶

¹Department of Chemistry, Faculty of Sciences, Ferdowsi University of Mashhad, Mashhad, Iran, ²Department of Chemistry, Masaryk University, Kotlarska 2, 61137 Brno, Czech Republic, ³CEITEC - Central European Institute of Technology, Masaryk University, Kamenice 5, 62500 Brno, Czech Republic, ⁴Department of Chemistry, University of Isfahan, Isfahan 81746-73441, Iran, ⁵Department of Chemical Sciences, University of Messina, Via F. Stagnod'Alcontres 31, 98166 Messina, Italy, ⁶Departamento de Química, Centro de Investigación y de Estudios Avanzados del Instituto Politécnico Nacional, Apartado Postal 14-740, México DF 07000, México
E-mail: taherzadehmaryam@yahoo.com

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.



Keywords: donor directionality, acceptor directionality, phosphoric triamide