

Analysis of S—P—N and N—P—N angles in phosphorothioic triamides

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The S—P—N and N—P—N bond angles have been analyzed in 30 phosphorothioic triamides structures (having a P(S)[N]₃ skeleton) deposited in the Cambridge Structural Database (CSD, version 5.34, May 2013 update [1]) and a new structure reported in the present work, P(S)[NHC₆H₄-4-CH₃]₃.2CH(CH₃)₂OH (**1**). The analysis shows the maximum S—P—N angle is 121.14° (in the structure with CSD refcode XIJVOB [2]) and the minimum value (106.78°) is shown in (**1**). Moreover, the maximum and minimum N—P—N angles are 114.89° (in XIJVOB) and 89.86° (in JEZWUG [3]), respectively. In each compound, the bond angle sum of the three S—P—N angles is more than the value related to the three N—P—N angles. The maximum deviation of the bond angle sum at the P atom (3 × S—P—N + 3 × N—P—N) is found for QOBDIU (654.14°).

The asymmetric unit of (**1**) contains two independent phosphorothioic triamide molecules and two molecules of 2-propanol. The phosphorus atom displays a distorted tetrahedral environment. The N atoms bonded to P atom have mainly *sp*² character and the environments of the nitrogen atoms are practically planar. In the crystal packing, the intermolecular O—H...S, N—H...S and [N—H...][N—H...]O hydrogen bonds form the octamers involving four phosphorothioic triamide molecules and four 2-propanol molecules. The spectroscopic features of (**1**) are also investigated.

References:

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