

A database analysis of P—O—C bond angles in the structures with P(O)[O—C]₂[N] and P(S)[O—C]₂[N] segments: a comparison with P—S—C bond angles and completed with three new structures

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In the previous published papers, some structural features of phosphoramides^{1,2} and thiophosphoramides^{3,4} were considered through diffraction study of some derivatives and also analysis of analogous structures deposited in the Cambridge Structural Database.⁵ Among these systematic studies, some of them concern the analysis related to the nitrogen atom (s) bonded to phosphorous, in compounds containing N—P(=O) and N—P(=S) segments. Here, we focus on the oxygen atom (s) bonded to phosphorous, considering the structures with P(O)[O—C]₂[N] and P(S)[O—C]₂[N] segments deposited in the CSD and two new structures reported here: P(O)[OC₆H₅]₂[NHNHC₆H₅] and P(S)[OCH₃]₂[NHCH(CH₃)₂]. So, the histograms of P—O—C bond angles were considered in the noted structures. The result of this analysis for the structures with a P(S)[O—C]₂[N] segment is given in Fig. 1. Moreover, for a comparison of the geometry at the oxygen atom bonded to phosphorous atom with the geometry of the sulfur atom bonded to phosphorous, one novel salt structure is studied: [2-Cl-C₆H₄CH₂NH₃]₂ [(CH₃S)P(O)—O—P(O)(SCH₃)] and compared with a few analogous structures deposited in the CSD.

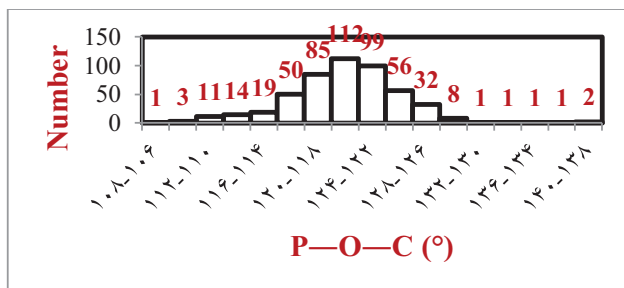


Fig. 1. A histogram of P—O—C bond angles (°) is given for the structures with a P(S)[O—C]₂[N] segments deposited in the CSD.

References

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