



Differences in the geometries of compounds with $[O]_nP(O)[N]_{3-n}$, $[O]_nP(S)[N]_{3-n}$ and $[C]_mP(O)[N]_{3-m}$ ($n = 0, 1, 2, 3$; $m = 1, 2, 3$) segments: A Cambridge Structural Database analysis completed with fourteen new structures

Mehrdad Pourayoubi^{a*}, Mozghan Abrishami^b, Marjan Narghani^a, Marek Nečas^{c,d}, Banafsheh Vahdani Alviri^a, Farahnaz Hamzehee^a, Amir Shokooch Saljooghi^a, Mahmoud Delavar^b, Teresa Mancilla Percino^e, Marco A. Leyva Ramírez^e, Michal Dušek^f, Margarida S. Henriques^f, Aurelien Crochet^g, Monika Kučeraková^f, Václav Eigner^f

^aDepartment of Chemistry, Faculty of Sciences, Ferdowsi University of Mashhad, Mashhad, Iran, ^bDepartment of Chemistry, Payame Noor University, 19395-4697 Tehran, I.R. Iran, ^cDepartment of Chemistry, Masaryk University, Kotlarska 2, 61137 Brno, Czech Republic, ^dCEITEC - Central European Institute of Technology, Masaryk University, Kamenice 5, 62500 Brno, Czech Republic, ^eDepartamento de Química, Centro de Investigación y de Estudios Avanzados del Instituto Politécnico Nacional, Apartado Postal 14-740, México DF 07000, México, ^fInstitute of Physics ASCR, v.v.i., Na Slovance 2, 182 21 Prague 8, Czech Republic, ^gFribourg Centre for Nanomaterial's, FriMat, University of Fribourg, Chemin du Musée 3, CH-1700 Fribourg, Switzerland, (e-mail: pourayoubi@um.ac.ir)

Recently, we reported on the analysis of hydrogen bond pattern in different families of phosphorous(V) compounds, considering the structure determination of some derivatives and the study of analogous structures deposited in the Cambridge Structural Database.^{1,2} These efforts led to find some “empirical rules” which are benefit to prediction of hydrogen bond patterns for such molecules with limited numbers of H-bond donor and H-bond acceptor sites. In continuing, we are interesting to study of the geometry at the P, N, C, O and S atoms in structures with $[O]_nP(O)[N]_{3-n}$, $[O]_nP(S)[N]_{3-n}$ and $[C]_mP(O)[N]_{3-m}$ ($n = 0, 1, 2, 3$; $m = 1, 2, 3$) segments. This survey on the CSD was completed with reporting of fourteen new structures belonging to different families of P(V) compounds within a tetrahedral environment and updated our previous studies. The new structures are $[CH_2FC(O)NH]P(O)[NHC_6H_4-4-CH_3]_2$ (1), $[C_6H_5]P(O)[NHCH_2C_6H_4-4-CH_3]_2$ (2), $[C_6H_5]P(O)[NHC_6H_4-4-CH_3][NHCH_2C_6H_5]$ (3), $[4-Cl-C_6H_4NH]P(O)[N(CH_3)(C_6H_{11})]_2$ (4), $[4-Cl-C_6H_4NH]P(O)[NC_4H_8O]_2$ (5), $[4-Cl-C_6H_4NH]P(O)[NC_5H_9-4-CH_3]_2$ (6), $[4-CH_3-C_6H_4NH]P(O)[NC_5H_9-4-CH_3]_2$ (7), $[4-Cl-C_6H_4NH]_3P(O)$ (8), $P(S)[NH^tBu]_3$ (9), $[CH_3O]_2P(S)[NHNHC_6H_5]$ (10), $[4-Cl-C_6H_4O]P(O)[NHC_6H_{11}]_2$ (11), $[4-Cl-C_6H_4O]P(O)[NHC_6H_5]_2$ (12), $[4-Cl-C_6H_4O]P(O)[N(CH_3)(C_6H_{11})]_2$ (13) and $[4-Cl-C_6H_4O]P(O)[NHC_6H_4-4-CH_3]_2$ (14). The main topics of investigation are as follows: (i) the study of histograms of $P=X$ ($X = O$ & S) and $P-Y$ ($Y = O, N$ & C) bond lengths in order to a comparison of each bond length in different families of structures involving it, (ii) the analysis of bond-angle sums at the nitrogen atoms bonded to phosphorous in a three-coordinated $[P]N[Z][W]$ environment [Z and W atoms are any atoms from CSD, including H and C] and a comparison between different families including nitrogen atoms, (iii) the analysis of the vector of lone electron pair (LEP) located at the non-planar nitrogen atoms with respect to the $P=X$ bond vector and (iv) evaluation of the acceptor directionalities in $N-H...X=P$ ($X = O$ & S) hydrogen bonds with considering the $H...X=P$ angles.

References

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