2nd Iranian Student Chemistry Conference
University of Guilan, Rasht, 6-8 Oct. 2015

A new solvated thiophosphoramide: single crystal X-ray diffraction, NMR study and Hirshfeld surface analysis

Elham Torabi Farkhani[a], Mehrdad Pourayoubi[a]*, Pavel V. Andreev[b], Ekaterina S. Shegravina[c]

[a]*Department of Chemistry, Faculty of Sciences, Ferdowsi University of Mashhad, Mashhad, Iran*
[b]*Department of Physics, N. I. Lobachevsky State University of Nizhni Novgorod, pr.Gagarina, 23-3, Nizhni Novgorod, Russia*
[c]*Department of Chemistry, UNN Lobachevsky State Universityof Nizhny Novgorod, Gagarin avenue, 23, Nizhni Novgorod, Russia*
torabielham2010@gmail.com
pourayoubi@um.ac.ir

Abstract:

Hirshfeld surfaces and two-dimensional fingerprint plots are used to study short intermolecular contacts in of phosphoramides,[1] and also in organotin (IV)-phosphoramide complexe.[2] In this study we present the crystal structure analysis complemented with the investigation of the molecular interactions in this compound.

The asymmetric unit of $[(cyclo\ C_6H_{11})(CH_3)N]P(S)[NC_4H_8O]_2.0.412CH_3OH$ is composed of two crystallographically independent phosphorothioic triamide molecules with together of methanol solvated molecule. The phosphorus atoms display a distorted tetrahedral environment with the maximum and minimum values of angles at the P atom for one of the N—P═S and one of the N—P—N angles, respectively. The environments at the nitrogen atoms are practically non-planar.

In this structure, the phosphorothioic triamide and methanol molecules are linked by some different intermolecular C—H…S and C—H…O interactions. The intermolecular interactions have been studied by Hirshfeld surface analysis and fingerprint plots, by using the program Crystal Explorer 3.1.[3]

These analyses reveal that H…H interactions of 78.3% and 77.7% for the two symmetry-independent phosphorothioic triamide molecules. Furthermore, the C—H…O interaction in one of the symmetry independent molecule and the C—H…S═P interaction in the other molecule are the characteristic interactions, appearing as very large red spots in the related Hirshfeld surface maps. The characterization of compound was also performed by $^{31}P\{^1H\}$, ^1H and ^{13}C NMR and mass spectroscopy.

Keywords: Thiophosphoramide, Hirshfeld surface, Crystal structure, NMR.

References

[1] K. Gholivand, F. Molaei and M. Hosseini., *Acta Cryst. B* **2015**, *71*, 176.

[2] M. Pourayoubi, S. S. Bayraq, A. Tarahhomi, M. Necas, K. Fejfarová, M. Dušek, *J. Organomet. Chem*. **2014**, *751*, 508.

[3] S. K. Wolff, D. J. Grimwood., J. J. McKinnon., M. J. Turner., D. Jayatilaka., M. A. Spackman, *CrystalExplorer version 3.1*, Univ.Western Australia: Perth**, 2013**.