angles in the heterocyclic ring.

Keywords: orgnophosphorus compounds, dioxaphosphepine rings, anticancer agents

P06.04.14

Acta Cryst. (2008). A**64**, C387

Crystal structure and quantum mechanical calculations of an oxime compound, $C_9H_{11}N_3O_2$

Arzu Ozek[1], Orhan Buyukgungor[1], Halil Ilkimen[2], Cengiz Yenikaya[2]
[1]Ondokuzmayis University, Physics, arzuozek@omu.edu.tr, Samsun, Kurupelit, 55139, Turkey, [2]Dumlipinar University, Department of Chemistry, Kutahya, Turkey, E-mail：arzuozek@omu.edu.tr

Oxime and dioxime derivatives are very important compounds in the chemical industry and medicine [1]. The oxime (-C=N-OH) moiety is potentially ambidentate, with possibilities of coordination through the N and/or O atoms. It is a functional group that has not been extensively explored in crystal engineering. In the solid state, oximes are usually associated via O-H...N hydrogen bonds of length 2.8 Å. Oxime groups posses stronger hydrogen-bonding capabilities than alcohols, phenols and carboxylic acids [2]. The hydrogen-bond systems in the crystals of oximes have been analysed and a correlation between a pattern of hydrogen bonding and N-O bond lengths has been suggested [3]. The configurational and/or conformational isomers of glyoxime derivatives (dioximes) have also been analysed [4]. The experimental geometry of $C_9H_{11}N_3O_2$ obtained from single-crystal X-ray diffraction was compared with those obtained from quantum-mechanical calculations. It is found that the bond lengths and angles obtained from two methods are in good agreement with each other.
[1] Sevagapandian, S., Rajagopal, G., Nehru, K. & Athappan, P. (2000). TransitionMet. Chem. 25, 388-393. [2] Marsman, A. W., Leussing, E. D., Zwikker, J. W. & Jenneskens, L. W. (1999). Chem. Mater. 11, 1484-1491. [3] Bertolasi, V., Gilli, G. & Veronese, A. C. (1982). Acta Cryst. B38, 502-511. [4] Chertanova, L., Pascard, C. & Sheremetev, A. (1994). Acta Cryst. B50, 708-716.

Keywords: oxime, X-ray diffraction, quantum mechanical methods

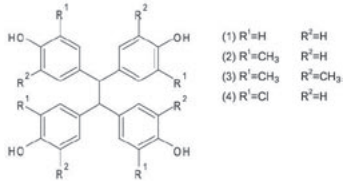
P06.06.15

Acta Cryst. (2008). A**64**, C387

Crystal structure analysis of inclusion crystals with tetrapodal host molecules

Kazuyuki Toyota[1], Hidehiro Uekusa[1], Natsuki Amanokura[2], Masami Kaneko[2], Hiroshi Suzuki[2]
[1]Tokyo Institute of Technology, Department of Chemistry and Materials Science, toyota.k.aa@m.titech.ac.jp, Tokyo, Meguro/Ookayama2-12-2, 152-8550, Japan, [2]Nippon Soda Co.Ltd, E-mail：toyota.k.aa@m.titech.ac.jp

Inclusion crystals have unique characteristics such as guest solubility or temperature dependent guest releasing, which is relevant to the structure of host framework enclosing guest molecules. Hence it is of great importance to investigate and develop host frame works to design new functional materials. 1,1,2,2-tetrakis (4-hydroxyphenyl) ethane, TEP (1), has four hydroxyl phenyl groups in different directions to build different types of hydrogen bonding host frameworks corresponding to guest molecule types. In our previous study, three types of host frameworks accommodating different kind of guest molecules via hydrogen bonds were analyzed to show TEP has well-qualified inclusion ability as an inclusion host molecule. By introducing one or two substituents next to hydroxyl group, (2)-(4), hydrogen bonding direction and pattern should be restricted and such TEP derivatives are expected to show different hydrogen bonding pattern which leads new host frameworks. In this study, inclusion crystals of TEP derivative are synthesized and their crystal structures are analyzed to compare the host framework structures.



Keywords: inclusion compounds, molecular interactions, crystal enjinnering

P06.06.16

Acta Cryst. (2008). A**64**, C387

A detailed study of the helical conformation in 2-aminothiazole derivatives

Vijay Thiruvenkatam[1], Guru Row N Tayur[2]
[1]Indian Institute of Science, Solid State and Structural Chemistry Unit, C/o Prof. T.N.Guru Row, Solid State and Structural Chemistry Unit, Indian Institute of Science, CV Raman Avenue,, Bangalore, Karnataka, 560012, India, [2]Solid State and Structural Chemistry Unit, Indian Institute of Science, CV Raman Avenue, Bangalore-560012, Karnataka, India, E-mail：vijay@sscu.iisc.ernet.in

Aminothiazoles have many applications such as antiviral, antimicrobial, bactericidal and fungicidal agents. Aminothiazoles metal complexes display anti cancer activity.[1] The crystal structures of 2-Aminothiazole N-Boc protected Leucine and Valine belongs to the space group $P\,2_12_12_1$ and $P\,4_12_12$ with cell dimensions a=10.5247(14)Å, b=11.2407(15) Å, c=30.3258(3) Å and a=9.2614(4)Å, b=9.2614(4)Å, c=36.6412(3)Å respectively. The molecules are packed via intermolecular N-H...O and N-H...N hydrogen bonds giving rise to the formation of helix like structure. The helical nature and the tilt associated with the title compounds compares well with those of the B-DNA. The pitch per one complete turn of the helix is 30.30Å and 36.64Å while the pitch in B-DNA is reported to be 34Å and this aspect might have consequences related to the activity profiles of this compound. The idea is to exploit the hydrogen bonding potential in the title compound to get the supramolecular assembly into a helix and examine its features with respect to DNA.
1. Lynch, D. E. *et al*, *Acta Cryst*, 1999, **B55**, 758


Valine Thiazole

Keywords: supramolecular assemblies, DNA, hydrogen bonding recognition