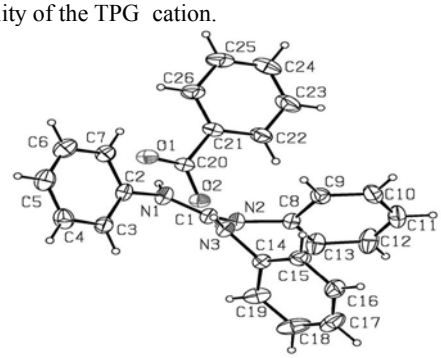
flexibility of the TPG^{+} cation.



We also performed density functional theory calculations within the local density approximation using the code Abinit [6].

[1] Kemme, A., Rutkis, M., Eiduss, J., *Latv. PSR Zinat. Akad. Vestis, Kim. Ser. 5*, 1988, 595.
[2]Klement, U., Range, K.-J., Hayessen, R., Heckmann, K.-D., *Z.Kristallogr*., 1995, 220, 611.
[3]Pereira Silva, P. S., Paixão, J. A., Ramos Silva, M., Matos Beja, A. *Acta Cryst*., 2006, E62, o3073.
[4]Pereira Silva, P. S., Cardoso, C., Ramos Silva, M., Paixão, J. A., *Acta Cryst*., 2007, E63, o501.
[5]Pereira Silva, P. S., Ramos Silva, M., Paixão, J. A., Matos Beja, A. *Acta Cryst. E, in print*.
[6] Gonze, X., Beuken, J.-M., Caracas, R., Detraux, F., Fuchs, M., Rignanese, G.-M,. Sindic, L., Verstraete, M., Zerah, G., Jollet, F. , Torrent, M., Roy, A., Mikami, M., Ghosez, Ph., Raty, J.-Y. , Allan, D.C., *Computational Materials Science,* 2002, 25, 478.

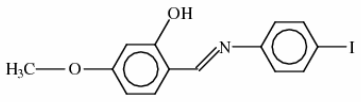
MS16 P09

Crystallographic and conformational analyses of (*E*) 2-[(4iodophenylimino)metyhl]-5-methoxyphenol

Onur Şahin[a], Orhan Büyükgüngör[a], Mustafa Odabaşoğlu[b], Çiğdem Albayrak[b] [a]*Ondokuz Mayıs Univ., Department of Physics, Samsun-Turkey.* [b]*Ondokuz Mayıs Univ., Department of Chemistry, Samsun-Turkey.*
E-mail: onurs@omu.edu.tr

Keywords: Crystal structure; PM3; Conformational analysis

(E)-2-[4iodophenylimino)methyl]-5-methoxyphenol ($C_{14}H_{12}INO_2$) was synthesized and its crystal structure determined. It crystallizes in the orthorhombic space group, $Pna2_1$, with a = 6.2833(4), b = 7.1334(4), c = 29.0321(14) Å, $R(F^2)$ = 0.0238 for 2560 independent reflections.



The intramolecular hydrogen bond occurs between the pairs of atom O1 and N1 [2.609(4)Å] and the hydrogen atom is essentially bonded to the oxygen atom. There are two intermolecular C-H· · ·O hydrogen bonds between neighbouring molecules. The aromatic phenyl rings are an acceptor of four intermolecular C-H· · ·Ph hydrogen bonds. Conformations of the title compound were investigated by semi-empirical quantum mechanical PM3 calculations.

MS16 P10

Comparison of ferredoxins from *Ps. aeruginosa, E. coli* and an *Al. vinosum* mutant E. Saridakis[a], P. Giastas[a], G. Efthymiou[c], J.-M. Moulis[b], P. Kyritsis[c], I. M. Mavridis[a], [a]*National Center for Scientific Research "Demokritos", Athens, Greece,* [b]*DRDC/BMC, CEA-GRENOBLE, France,* [c]*Department of Chemistry, University of Athens, Greece*
Email: esaridak@chem.demokritos.gr

Keywords: ferredoxins; redox proteins; electron transfer proteins

The 2[4Fe-4S] Ferredoxins (Fds) are a type of electron transfer proteins found in anaerobic microorganisms. Two main families can be distinguished: The first includes the clostridial Fds with two isopotential [4Fe-4S] clusters (~ –400 mV). The second includes Fds characterized by very negative and widely different reduction potentials of the two clusters (~ -670 to ~ -430 mV). The 2[4Fe-4S] *Allochromatium vinosum* ferredoxin (AlvinFd) is the prototype of the second family and its structure has already been solved to a resolution of 2.1Å [1]. A characteristic member of the AlvinFd family from *Pseudomonas aeruginosa* has recently been determined to 1.32Å resolution [2]. Presently, the V13G mutant AlvinFd crystal structure has been solved to 1.65Å. It was crystallized in space group $P3_12$, a = b = 51.42, c = 76.55Å. The structure of another member of the family, the *E. coli* 2[4Fe-4S] ferredoxin (EcFd), was also determined to a resolution of 1.65Å. The latter, which exhibits merohedral twinning, was crystallized in space group $P3_2$, a = b = 65.35, c = 132.34Å. The comparison of the three members of the Fd family (detailed structural information, precise geometry of the clusters, conformation around and between the two clusters) will be presented. The structural studies are expected to shed more light on the unusual redox properties of these ferredoxins.

[1] Moulis J.-M., Sieker L.C., Wilson K.S., Dauter Z. *Protein Sci.* 1996, 1765.
[2] Giastas P., Pinotsis, N., Efthymiou, G., Wilmanns M., Kyritsis P., Moulis J.-M., Mavridis I. M. *J. Biol. Inorg. Chem.* 2006, 445.

MS16 P11

Non-traditional Bonding Interactions via Experimental Charge Density Nav S. Dhaliwal[1], Lee M. Daniels[1], T. Stanley Cameron[2] and Joseph D. Ferrara[1], [1]Rigaku Americas Corp., 9009 New Trails Dr., The Woodlands, TX 77381 USA and [2]Department of Chemistry, Dalhousie University, Halifax, Nova Scotia, Canada B3H 4J3.

Years ago, crystallography revolutionized a lot of thought about Important Science, and provided perhaps the most powerful tool for the study of chemical bonding. Precise positional information giving exact bond distances became routine; more recently advances in charge density studies have provided extensive views of bonding once available only in theory. Direct observation of covalent bonding is now possible, and extension of the analysis provides detailed information about *intermolecular* interactions. Using the criteria proposed by Koch and Popelier, a "bond path" can be constructed between any two atoms or groups in a structure, allowing one to distinguish "bonding" interactions from van der Waals contacts. In this work interactions such as H-H bonding, F-F bonding, I-S bonding, P-N ring bonding, etc. are considered.