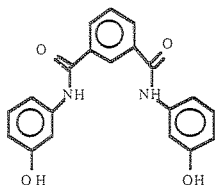


pyrrole NH, and bioactivity (including bioaffinity for some of them, Klaebmt, 1996). The 3D structure of the receptor has not been characterized yet. However, systematic analysis of a large number of substrates and inhibitors can provide information about the protein active site.

**PS11.01.11  $\pi$ - $\pi$  STACKING IN MODEL DYE HOSTS.** C.M. Murray, J.F. Malone, R. Docherty, A.J. Lavery, G. Stewart.

Weak hydrogen bonds e.g. C-H...O and weak interactions e.g.  $\pi$ - $\pi$  stacking and T-bonding have been shown to have a role within crystal structure<sup>1</sup>. The  $\pi$ - $\pi$  stacking interaction, though weak, is significant in the structure of 1,3 Bis(((3-hydroxyphenyl)amino)carbonyl)benzene which is reported.



This interaction has been quantified using the HABIT program<sup>2</sup>. Semi-empirical calculations of the heat of formation show agreement between the preferred conformation in the gas phase and the single crystal X-Ray diffraction structure. Similar structures retrieved from the Cambridge Structural Database confirm the importance of the  $\pi$ - $\pi$  interaction for not only single molecule asymmetric units of this type but also asymmetric units which contain hydrated species or co-crystals. Quantification of the values is reported and the conformational preference is also investigated.

1 G.R. Desiraju *Acc. Chem. Res.* 1991, 24, 290-296. A.D. Hamilton et al *J. Am. Chem. Soc.* 1988, 110, 6561-6562. D.R. Boyd et al *J. Am. Chem. Soc.* 1996 in press.

2 G. Clydesdale, R. Docherty, K.J. Roberts *Computer Physics Communications* 64 (1991) 311-328.

**PS11.01.12 STRUCTURE OF THE LEAD PICRATE COMPLEXES WITH 18-MEMBERED CROWN ETHERS IN THE CRYSTAL STATE AND IN ORGANIC SOLVENTS.** N. K. Dalley<sup>1</sup>, J. D. Lamb<sup>1</sup>, A. Y. Nazarenko<sup>2</sup>, E. B. Rusanov<sup>3</sup>. <sup>1</sup>Department of Chemistry and Biochemistry, Brigham Young University, Provo, Utah 84602, USA, <sup>2</sup>Analytical Chemistry Department, Taras Shevchenko University, Kiev 252033, Ukraine, <sup>3</sup>Institute of Organic Chemistry, NAS of Ukraine, Kiev, Ukraine

Despite the wide use of metal picrates for ion recognition studies, no structural data concerning lead picrate complexes with crown ethers have yet been published. Here we report molecular structures of Pb(18-crown-6)Picr<sub>2</sub> x CH<sub>2</sub>Cl<sub>2</sub> (I) and Pb(cis-syn-cis-dicyclohexano-18-crown-6)Picr<sub>2</sub> (II). In both complexes Pb<sup>2+</sup> is coordinated six O atoms of macrocycle, which has a distorted D<sub>3d</sub> geometry (Pb...O separations are 2.64-2.84 Å). Both picrate anions in (I) and only one in (II) are monodentate with Pb...O = 2.47-2.48 Å, while the second one in (II) is bidentate (Pb...O = 2.56 and 2.88 Å). This correlates with the existence of different types of picrate - Pb<sup>2+</sup> ion pairs in organic solvents in the presence of crown ethers, observed from spectral studies. The structural data together with our previously obtained structures of lead macrocyclic complexes enable us to discuss the features of ion recognition of Pb<sup>2+</sup> by crown ethers.

## Chemical Crystallography of the Future Open Commission

**MS11.02.01 BEYOND ROUTINE STRUCTURE DETERMINATION - THE RENAISSANCE OF SMALL MOIETY CRYSTALLOGRAPHY.** A. Alan Pinkerton, Department of Chemistry, University of Toledo, Toledo, OH 43606, USA

The introduction of area detectors, especially the CCD detector, into small moiety crystallography coupled with the availability of powerful, low cost workstations will have as large an impact on the discipline as that made by the introduction of automated diffractometers a quarter of a century ago. In the short term this will lead to a quantum jump in the number of routine structures determined each year. In the long term, crystallographers will devise new experiments and directions to take advantage of this technological advance. A number of potential new directions will be presented. This discussion will be based in part on experiences in my own laboratory and in part by gazing into a crystal ball (pun intended).

**MS11.02.02 TIME-RESOLVED STRUCTURE ANALYSIS OF CRYSTALLINE-STATE REACTION BY A NEW DIFFRACTOMETER DESIGNED FOR RAPID DATA COLLECTION.** Yuji Ohashi, Department of Chemistry, Tokyo Institute of Chemistry, Ookayama, Meguro-ku, Tokyo 152, Japan

The structural change of the reactant molecules can be directly observed by stepwise structure analysis using a new diffractometer in the process of the reaction. Since we found that the chiral cyanoethyl group bonded to the cobalt atom in a cobaloxime complex crystal was racemized by X-ray exposure without degradation of the single crystal form<sup>[1]</sup>, many solid-state reactions with retaining the single crystal form, crystalline-state reaction, have been observed<sup>[2]</sup>. Recently several crystalline-state reactions which proceeds within ten hours have been found<sup>[3]</sup>. In order to analyze the structural changes in such reactions, we have designed and constructed a new diffractometer for rapid data collection<sup>[4]</sup>. The diffractometer, which has two imaging plates as detectors, enables us to collect the three-dimensional intensity data within two hours. Several examples of the direct observation of the structural changes by stepwise crystal structure analyses using the diffractometer will be shown and a new crystal chemistry based on the time-resolved structure analysis will be proposed.

[1] Y. Ohashi and Y. Sasada, *Nature*, 267, 142 (1977)

[2] "Reactivity in Molecular Crystals", Ed. by Y. Ohashi, VCH (1993)

[3] Y. Ohashi et al., *Bull. Chem. Soc. Jpn.*, 68, 2517 (1995)

[4] Y. Ohashi and H. Uekusa, *J. Mol. Struct.*, (1995) in press.

**MS11.02.03 EXPERIMENTAL X-RAY DIFFRACTION EVIDENCE OF THE UNUSUAL BOND BENDING IN SMALL MOLECULES.** M. Antipin\*, and R. Boese,\*\* Institute of Organoelement Compounds, Moscow, Russia.\* Institute of Inorganic Chemistry, University of Essen, Germany\*\*

Molecular structure and geometry are often the only kind of information that many chemists are interested in as a final result of the X-ray analysis. Meanwhile, much more information may be extracted now from X-ray diffraction data using modern opportunities of this method. Thus, multipole representation of the electron density distributions and its topological analysis allow to describe the nature of some chemical bonds in new terms of the bond paths, critical point positions etc. This approach was found to be very fruitful for description bonding in small cyclic or strained cage molecules, where so called bent bonds are present.

In the deformation electron density (DED) maps the bending