31 level, and the MEP calculation, corresponding to the location of each non-bonded atomic contact, at the 6-311** level. The MEP was stored incrementally on a grid with its origin at the centroid of the solvent molecule. Computer programs were then used to analyze geometrical preferences and the correlation of the MEP with the directionality of the intermolecular interactions.

PS11.07.14 STRUCTURES OF SOME ANTHRAQUINONE DYES. E.S.Alekseyeva, A.V.Yatsenko,V.A.Tafeenko and L.A.Aslanov,Chemistry Dept., Moscow State University, 119899 Moscow, Russia.

The impact of crystal packing and specific intermolecular interactions on molecular structure has been illustrated by the example of five anthraquinone derivatives. Compounds 1 and 2 show analogous behaviour in solutions: in non-polar solvents the form A is a predominant one, whereas polar solvents displace the equilibrium towards ketoenamine form B.
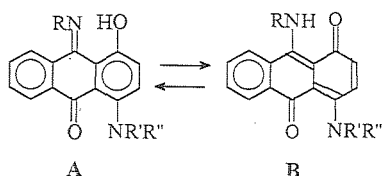
1: R = H, R' = Ac, R" =p-tolyl; 2: R = mesityl, R' = Ph, R" = H

The crystal structure of 1 is built up from centrosymmetric dimers (interplanar distance 3.43 Å), where two molecules are H-bonded in addition. As a result only form B takes place in crystal. No signs of H-bonding or other specific interactions are observed in the crystal structure of 2, hence the crystal surrounding displaces here the equilibrium towards form A like low-polar solvent.

Visible spectra of anthraquinone dyes are also related to the motif of crystal packing. The crystal structures of 1,4-bis(mesitylamino)anthraquinone(3),1,4-bis(phenylamino)anthraquinone (4) and 1-hydroxy-4-(p-tolylamino)anthraquinone (5) are built up from separated molecules, dimers and stacks with interplanar distance 3.35 and 3.50 Å respectively. As a result the maximum in reflection spectrum of 3 is blue shifted by 1000 cm-1 relative to the absorption spectrum in solutions, whereas 4 shows red shift by 700 cm-1 accompanied by the direct manifestation of vibrational structure.

PS11.07.15 ATTRACTIVE EDGE-TO-FACE AROMATIC INTERACTIONS IN A RANGE OF SIMPLE NITRONES, OXAZIRIDINES AND IMINES. By J.F. Malonea, D.R. Boyda, T.A. Evansa and A. Smitha, W.B. Jenningsb and W. O'Sullivanb, School of Chemistrya, The Queen's University of Belfast, Belfast, N. Ireland and Department of Chemistryb, University College, Cork, Republic of Ireland.

Attractive intramolecular edge-to-face type interactions between aromatic moieties have been identified by X-Ray studies and NMR in a range of simple nitrones, oxaziridines and imines. Intramolecular hydrogen to mid-aromatic ring distances of 2.60Å, 2.66Å, 2.70Å, 2.73Å and 2.78Å are observed. The Hunter-Sanders rules (C.A. Hunter and J.K. Sanders, *J. Am. Chem.* Soc., 1990, 112, 5525) are applied to the interactions and are found to be in agreement with the observations. Analysis of the crystal lattices have shown similar intermolecular interactions affecting the crystal packing, in some cases quite significantly. One case showed evidence in the NMR for an intramolecular edge-to-face type interaction which was not observed in the solid state where several intermolecular aromatic-aromatic interactions seemed to be controlling the geometry. The σ polarization of the atoms in the rings is proposed as being of importance in determining the type of interaction observed and hence the geometry.

PS11.07.16 ORIENTATIONAL DISORDER OF SOME ORGANIC MOLECULAR CRYSTALS STUDIED BY ATOM-ATOM POTENTIALS. Chitra Samanta, Dept. of Physics, Jadavpur University, Calcutta, India

Systematic analysis of molecular geometry and conformation were studied by atom-atom potential method.

The vander waal's inter molecular attraction concept leads to the pairwise nonbonded interaction potentials. Concerning the arrangements of atoms in a regular distribution the potential of Bucking ham's type -AA/r6+Be Alpha r/rm were applied to the study of organic molecular crystals.

The universal potential parameters, AA,B Alpha m are used from those of Giglio, E2.

The evaluation of lattice energies (Kcal/mol) with rotation of the molecules about an axis passing through the centre of gravity and normal to the molecular plan yields the interesting results regarding the confirmation of the molecular disorder.
The following crystals were studied:-

Crystals	Molecular Formula	Cell Parameters
1. 1,2 Dichloroethane	$C_2H_4Cl_2$	Ao=4.66° A
2. P- nitrobenzoic acid	$NO_2C_6H_4COOH$	AO=12.97° A
		BO=5.07° A
		CO=21.43° A
3. Pentaerythritol	$C(CH_2OH)_4$	AO=6.083° A
		CO=8.726° A

Ref:
1.Acta Cryst., Roychowdhury and Basak, B31, 1969.
2.Acta Cryst., Govezzotti, A and Simonetta, M, 17.559 1964.

PS11.07.17 C-H...π INTERACTION OBSERVED IN COMPLEXES OF SURFACTANT MOLECULES WITH AROMATIC COMPOUNDS. Keiju Sawada‡, Yuji Ohashi‡, Nahoko Iimura‡ and Hirotaka Hirata‡, "Department of Chemistry, Tokyo Institute of Technology, Japan and ‡Niigata College of Pharmacy, Japan

A C-H...π interaction has been found between surfactant molecules and aromatic compounds. Various complexes were obtained from an aqueous solution with cationic surfactants, such as cetyl-($C_{16}H_{33}N(CH_3)_3$,CTAB), myristil-(C_{14},MTAB), lauril(C_{12},LTAB) and decyl(C_{10},DTAB) trimethylammoniumbromide, and aromatic compounds. The griding of the two compounds in a mortar gave the same complexes as obtain in the solution.

In order to examine the interaction between surfactant molecules and aromatic compounds, we tried to form the complexes of CTAB, MTAB, LTAB, DTAB with biphenyl ($C_{10}H_8$) which has no functional groups. After many trials, all the complex crystals were successfully obtained. Moreover, the same complexes were formed by griding in a mortar. The analyzed structures of the complexes clearly suggest a special interaction, C-H..π, between the alkyl group and phenyl rings. This interaction should be a driving force of these formation.
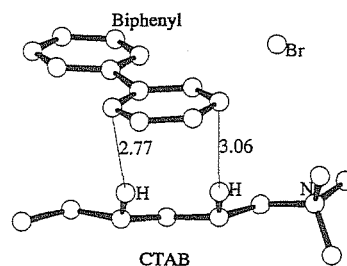

Fig.1 The Proposed C-H...π Interaction