04.5-06 NUCLEIC ACID-DRUG INTERACTIONS: MODEL STUDIES. THE CRYSTAL STRUCTURES OF SALICYLIC ACID 9-ME-ADENINE, SALICYLIC ACID 2-AMINO-PYRIDINE AND SALICYLIC ACID-UREA COMPLEXES. By Robert W. Gellert and I-Nan Hsu, Department of Chemistry, California State University, Northridge, CA 91330

The crystal and molecular structures of complexes involving salicylic acid and a base (9-Me-adenine, 2-amino-pyridine or urea) have been determined by x-ray diffraction on an automated four-circle diffractometer, using CU K(α) radiation. The complexes between salicylic acid and the nucleoside analog (9-Me-adenine), or 2-amino-pyridine are acid-base adducts. The carboxylate anions [C-O=1.263(5) Å] interact with the bases through O...H-N hydrogen bonds [O(2)...H-N=2.851(5) Å, O(1)...H-N=2.652 (4) Å]. The aromatic bases are protonated at the N(1) positions respectively [H-N(1)=1.02(6) Å]. In contrast, a molecular adduct is found in the salicylic acid-urea complex. The carboxyl group, of the acid, is in the usual keto form [C=O(2)=1.234(4), C-O(1)=1.311(4) Å]. The linkage to urea is through O(1)-H...O(4)[2.540(4) Å] and O(2)...H-N [2.903(4) Å] hydrogen bonds. Crystallographic details: (1) Salicylic acid 2-Me-adenine, $C_{13}H_{13}N_5O_3$, crystallizes in the orthorhombic space group Pbcn Z=8. Unit cell parameters: a=25.296(5), b=8.055(1), c=12.918(4) Å. R=4.9%, R(w)=5.7% for 1069 nonzero reflections with I>2(σ)(I). (2) Salicylic acid 2-amino-pyridine, $C_{12}H_{12}N_2O_3$, crystals are orthrohombic, space group Pbca, Z=8. Unit cell parameters: a=15.928(5) b=11.830(5), c=11.768(6) Å. R(w)=5.5% for 1103 nonzero reflections with I>2(σ)(I). (3) Salicylic acid urea, $C_8H_{10}N_2O_4$, crystallizes in the monoclinic space group C2/c, Z=8. Unit cell parameters: a=22.206(3), b=5.108(1) c=17.177(2) Å, β=106.18(1) deg. R=5.7%, R(w)=5.0% for 1652 nonzero reflections with I>2(σ)(I).

04.5-07 OBSERVATION AND PREDICTION OF SHORT-RANGE ORDER IN DISORDERED MOLECULAR CRYSTALS. By T.R. Welberry and Joel Epstein, Research School of Chemistry, Australian National University, P.O. Box 4, Canberra, A.C.T. 2600, Australia.

We have developed a method of processing diffuse X-ray scattering data recorded on a conventional Weissenberg camera which facilitates the routine description of short-range order. The diffuse patterns are interpreted by comparison with optical diffraction analogues and computed patterns and with reference to the 'average' crystal structures determined by conventional methods.

We have investigated a number of disordered molecular crystals in which the disorder arises between substituent methyl- and halogen groups, due to the fact that both chloro- and bromo- have similar packing volumes to methyl-. We report on our analysis of two polymorphs of 9-bromo-10-methylanthracene, 2,3-dichloro-6,7-dimethylanthracene and two isomers of dibromodiethyl-dimethylbenzene. In all cases the diffuse X-ray pattern can be interpreted in terms of short-range correlations between a small number of neighbouring molecules.

While calculations using semi-empirical '6-exp' type intermolecular potentials can reasonably predict the 'average' structure of these compounds they fail to predict the short-range correlation effects that are observed. In order to account for these effects additional coulombic interaction terms must be included. It is found in all cases that the observed correlation between the orientation of neighbouring molecules is such that methyl-halogen contacts are preferred to either methyl-methyl or halogen-halogen. This information is only present in the diffuse scattering patterns.

04.5-08 THE INFLUENCE OF INTERMOLECULAR FORCES IN CRYSTAL LATTICE ON MOLECULAR STRUCTURE OF ORGANIC COMPOUNDS. By A. Katrusiak and Z. Kałuski, Institute of Chemistry, A. Mickiewicz University, Poznań, Poland.

The aim of this study was to determine the influence of intermolecular interactions of cyclic organic molecules in crystal lattices on their molecular structure. The problem is very important for comparing crystallographically determined molecular structures and when discussing the errors of molecular parameters obtained from X-ray analysis. All computations were based on comparison of molecular structures of two independent molecules in the asymmetric part of the unit-cell. The environments of the molecules differ and it is a suitable case for studying the influence of the crystal lattice forces on a molecule. Such parameters as torsion angles, valency angles and bond distances are discussed. It is possible to estimate for a certain class of compounds an "uncertainty of conformation", that is the mean changes of conformation caused by the intermolecular forces in a crystal lattice. The opinions concerning the influence of intermolecular forces on such parameters as bond distances and valency angles still differ. Very often it is believed that they are not influenced by these interactions. Small changes of bond distances C-C up to 0.05 Å cause the increase of the energy of the molecule up to 1 kcal/mol. This value is comparable with the energy of intermolecular forces and it was assumed that the strain caused by the latter may generate the changes in valency angles and bond distances. It was attempted to estimate the magnitudes of these changes.

04.5-09 PACKING ANALYSES ON ORGANOMETALLIC COMPOUNDS. By H. Preut and H.-J. Haupt, Anorganische Chemie II der Universität, Postfach 50 05 00, D-4600 Dortmund 50, FRG.

Structural information on molecules are largely the result of diffraction analyses on single crystals. The molecular geometries, thus obtained are influenced by the packing forces between the molecules. Bond angles and bond distances as well as the symmetry of the molecules are changed by this, deviating to a greater or lesser extent from the corresponding geometry in the free molecule.

On the organometallic compounds $ph_3M\text{-}Mph_3$ (ph = C_6H_5; M = Ge, Sn, Pb) packing analyses were carried out by the atom-atom potential method in order to obtain information on the influence of packing forces on the molecules.

Energies, based on the van der Waals interactions, were calculated for different geometries of the free molecules. By comparing these energies with the energies which correspond to the molecular geometries existing in the crystal the deformation energy which is brought about by the packing forces at the molecule, may be estimated.

The crystal structure of a hexagonal modification of $(C_6H_5)_3Ge\text{-}Ge(C_6H_5)_3$, which could not be solved with X-rays, was determined by packing analyses and by minimizing the lattice energy. The lattice energy calculations were carried out with the program PCK 6 (D. E. Williams (1972). Acta Cryst. A 28, 629).