PS11.07.18 INFLUENCE OF INTERMOLECULAR INTERACTIONS IN THE CRYSTAL PHASE ON CONFORMATION OF FLEXIBLE DI-AND TETRAHYDROPYRIMIDINE RINGS. O.V.Shishkin, V.I.Shil'nikov, A.N.Nesmeyanov Institute of Organoelement Compounds, Russian Academy of Sciences, Moscow Russia

The molecular and crystal structures of derivatives of the 7-aryl-4,7-dihydro-1,2,3-triazolo[1,5-a]pyrimidine and 4-aryl-1,2,3,4-tetrahydro-2-thiopyrimidine which contain flexible six-membered rings have been studied. Results of calculations by AM1 method show that substituents in the phenyl rings do not influence on equilibrium conformation of the di- and tetrahydropyrimidine rings (boat and half-chair respectively). However, experimental data, especially for 4,7-dihydroazolopyrimidine derivatives, indicate considerable change of endocyclic torsion angles. In the case of the nitro group presence in the dihydropyrimidine ring a chair conformation of dihydrocycle has been found in the crystal phase unlike results of quantum-chemical calculations. All these effects can be explained only by differences of intermolecular interactions in the crystals. Analysis of the crystal packing showed that strenghthening of some non-bonded interactions in the crystal (for example, hydrogen bond) causes a decrease of puckering of the pyrimidine ring. Dependence between energy of intermolecular interactions calculated by atom-atom potential method and magnitudes of torsion angles has been investigated. Analysis of the non-bonded interaction potential gradient agrees well with molecules deformation in the crystals as compared with the gase phase.

PS11.07.19 A SEMIEMPIRICAL QUANTUM CHEMICAL METHOD TO CALCULATE THE LATTICE ENERGIES OF ORGANIC MOLECULAR CRYSTALS. By Gerhard Raabe, Institut für Organische Chemie, RWTH Aachen, Prof.-Pirlet-Str. 1, D-52056 Aachen, Germany

A semiempirical quantum chemical method based on a perturbative approach [1] is presented which retains the original meaning of the contributions (dispersion, electrostatic, induction, and repulsion energy) to the lattice energy. These components are obtained using the results of the semiempirical MINDO/3 method [2]. Thus the dispersion energy is calculated by means of the London formula employing MINDO/3-FP [3] atom-in-molecule polarizabilities and vertical (Koopmans) ionization potentials. Only the Coulomb part of the electrostatic energy is considered employing MINDO/3 atomic charges which are also used together with the polarizabilities to obtain the induction energy. An approximate method is used to calculate the exchange repulsion energy which includes the repulsive part of the lattice energy via MINDO/3 molecular orbitals and overlap integrals.

Results obtained for several organic compounds including some polymorphs are presented. The choice of the molecular model is discussed, emphasizing the importance of a correct positioning of the hydrogen atoms.

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PS11.07.20 OPTICAL RESOLUTION OF DL-HISTIDINE THROUGH INTERACTIONS WITH ACHIRAL GLYCOLIC ACID. Stephen Suresh and M. Vijayan, Molecular Biophysics Unit, Indian Institute of Science, Bangalore 560 012, India

As part of a programme aimed at studying biologically and evolutionarily important interaction and aggregation patterns, crystals of DL-histidine glycolate and L-histidine glycolate were prepared and analyzed. Crystallization experiments involving DL-histidine and glycolic acid yielded in addition to DL-histidine glycolate, a conglomerate containing crystals of L-histidine glycolate and D-histidine glycolate in an unusual process of chiral separation through interaction with an achiral molecule. The crystal structure of DL-histidine glycolate is made up of alternating layers of unlike molecules as in many other binary complexes involving amino acids. The arrangement of molecules in the structure of L-histidine glycolate is almost identical to that in one of the forms of L-histidine acetate, thus providing another example for the invariance of certain aggregation patterns with respect to changes in the molecules involved. The structure involves packing of columns containing L-histidine molecules and glycolate ions tightly hydrogen bonded to one another. In fact, among the six hydrogen bonds in the structure, five are between unlike molecules within the column. Thus, the histidine-glycolate interactions are much stronger than histidine-histidine interactions, while glycolate-glycolate interactions are non-existent. This points to the high propensity for the occurance of this type of aggregation involving chiral molecules in association with glycolate ions even in a solution containing molecules of both chiralities. Such aggregates might co-exist in high concentration with those involving both L and D histidine molecules and glycolate ions despite the entropic advantages the latter might have. The crystals obtained from the solution could then be those of L-histidine glycolate, D-histidine glycolate or DL-histidine glycolate, often leading to chiral separation. Thus the observed aggregation of molecules in the chiral complex also appears to provide a structural rationale for chiral separation of histidine in the presence of glycolic acid.

PS11.07.21 THE INFLUENCE OF CRYSTAL PACKING ON THE MOLECULAR STRUCTURE OF MAIN GROUP ELEMENT COMPOUNDS. Edward R.T. Tiekink and Mark A. Buntine Department of Chemistry, The University of Adelaide, Adelaide, S.A. 5005, AUSTRALIA

In a number of recent reviews it has been demonstrated that the molecular structure found in main group element compounds may be dependent on seemingly minor changes in chemistry [1]. Hence, different coordination geometries, coordination numbers or even stoichiometries may be found for compounds with very similar chemical formulae [1]. For example, consider the structures of $Hg(S_2COR)_2$ [2]: when R = Me, a three coordinate T-shaped geometry is found for Hg in a linear polymeric array; for R = nPr, the Hg atoms are tetrahedral and the structure is comprised of two-dimensional sheets; when R = iPr, the Hg atoms are again tetrahedral, however, the structure is now a three-dimensional polymer. In the absence of obvious steric and/or electronic effects, it may be concluded that this phenomenon occurs as a result of crystal packing effects. Polymorphs provide an ideal opportunity to examine 'crystal packing' effects on molecular structure. Several organotin systems, including $Ph_2Sn(bipy)Cl_2$ and $Ph_2Sn(S_2CNEt_2)_2$, which are known to crystallise as polymorphs have been subjected to *ab initio* molecular orbital calculations to investigate their preferred 'gas phase' geometries. Geometry optimisations at the Hartree Fock level of theory, using both the 3-21G and LanL2DZ basis sets, have shown that the distinct structural configurations exhibited by the crystalline polymorphs independently relax to an identical gas-phase geometry. It is