

PS06.00.08 AROMATIC-AROMATIC AND C-H...O INTERACTIONS IN THE CRYSTAL STRUCTURES OF O-SUBSTITUTED MYO-INOSITOLS. U. Samanta¹, D. Pal¹, V.G. Puranik¹, P. Chakrabarti¹, T.Das², T. Praveen², M.S. Shashidhar². ¹Division of Physical Chemistry, ²Division of Organic Chemistry (Synthesis), National Chemical Laboratory, Pune 411008, India.

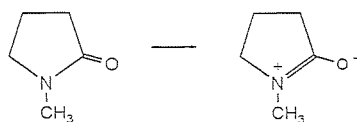
The crystal structure of DL-2,4-di-O-benzoyl-*myo*-inositol-1,3,5-orthoformate (I) and its 6-O-substituted (methyl and benzoyl) derivatives have been determined, and a few more are being investigated. These compounds crystallize with two molecules in the asymmetric unit, with the aromatic rings showing different geometries of interaction. The two molecules in (I) form a compact dimer such that the benzene rings in one are nearly perpendicular to those in the other. The orthoformate CH group takes part in a CH...O interaction. Another type of CH...O interaction that is observed in all these structures involves two adjacent aromatic CH groups and a carbonyl oxygen atom.

PS06.00.09 A CONFORMATION-DETERMINING INTERMOLECULAR C-H...O HYDROGEN BOND: STRUCTURE OF N-METHYL-2-PYRROLIDONE (NMP) Gerhard Müller, Martin Lutz, and Sjoerd Harder. *Fakultät für Chemie der Universität Konstanz, Universitätsstr. 10, D-78464 Konstanz, Germany.*

NMP (m.p. 249 K) was crystallized directly on the diffractometer with a modified zone-melting device using focussed light and its structure determined at 168 K. It adopts a slightly puckered ring conformation in the solid state which is intermediate between twist and envelope conformations.

The N-methyl group takes part in a nearly linear intermolecular C-H...O hydrogen bond to a neighboring keto group ($d(\text{H}\cdots\text{O}) = 2.57(2) \text{ \AA}$, $d(\text{C}\cdots\text{O}) = 3.552(2) \text{ \AA}$, angle (C-H...O) = $160(1)^\circ$). On the basis of all existing structural evidence and in agreement with the available energetic data, this C-H...O hydrogen bond clearly induces the methyl group to deviate from its usually preferred conformation with one C-H bond being nearly eclipsed to the adjacent N-C amide bond.

These findings are substantiated by molecular mechanics (MOMO) and highlevel *ab initio* calculations.



N-Methyl-2-Pyrrolidone

PS06.00.10 THE CRYSTAL STRUCTURES OF CONDENSATION PRODUCTS OF AMINO GUANYDINE NITRATE WITH ACETYLACETONE. Mirjalalov F.F., Khudayarov A.B., Sharipov Kh.T., Institute of Chemistry, RO"Spetsplav", Uzbekistan.

The X-ray diffraction studies of condensations products of aminoguanidine nitrate with acetylacetone obtained in aqueous-alcohol medium with pH=1 - 1-guanyl-3,5-dimethylpyrazole nitrate (I) and with pH=9 - 1-aminoguanidine-2-guanyl-1,4-dimethylpyrazoline nitrate (II) were carried out. The structure I crystallizes in the monoclini sp.gr. C2/c, $a=19.082(6)$, $b=7.096(2)$, $c=16.195(5) \text{ \AA}$, $b=121.64^\circ$, $d=1.43 \text{ g/cm}^3$, $Z=8$, $R=0.043$; II - in the rhombic sp.gr. P2₁2₁2₁, $a=7.500(1)$, $b=13.880(2)$, $c=14.276(2)$, $d=1.51 \text{ g/cm}^3$, $Z=4$, $R=0.064$. The structure I consist of planar positive $\text{C}_6\text{H}_{11}\text{N}_4^+$ ions hydrogen-bonded to NO_3^- . The conjugations of pi-orbitals of five-membered ring in I are observed. Unlike I, in five-membered ring of dipositive, nonplanar $\text{C}_7\text{H}_{18}\text{N}_8^{2+}$ ion conjugations of pi-orbital are absent. Both in I and II positive charges derived from protonisation delocalized in guanyl fragment of cations.

PS06.00.11 STRUCTURE OF 5 (4'-NN-DIMETHYL) BENZYLIDENE-2-PHENOLOXAZOLE-4-ONE, $\text{C}_{18}\text{H}_{16}\text{N}_2\text{O}_2$ S. Karmakar, A. N. Talukdar, Department of Physics, Gauhati University, Guwahati - 781014, India.

The benzylidene ring (A), the oxazolone ring system (B) and the attached phenyl ring (C) of the title compound (Fig 1) are almost planar having interplanar angles between A and B and that between B and C 4.3° and 2.5° respectively. The compound crystallises in monoclinic space group P2₁/c. Intensity data were collected on an Enraf-Nonius CAD-4 diffractometer using $\text{CuK}\alpha$ radiation. The structure was solved direct methods (SHELXS 86) and refined by full-matrix least squares methods (SHELX 90). The final R value is 0.068 for 1866 reflections. The N,N-dimethyl group is nearly coplanar with the benzylidene ring plane. There is no any hydrogen bonds and the structure is stabilised by van der Waals interaction in their crystalline space.

The crystal data are: $a = 12.177(4)$, $b = 3.966(1)$, $c = 30.944(8) \text{ \AA}$; $\beta = 101.17(1)^\circ$, $z = 4$, $D_x = 1.319 \text{ Mg m}^{-3}$, $D_m = 1.332 \text{ Mg m}^{-3}$.

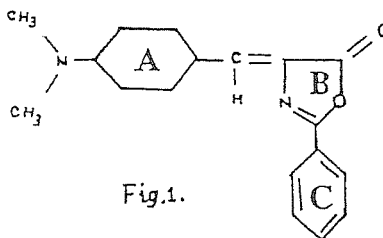


Fig.1.