06-Crystallography of Organic Compounds

PS-06.02.10 The crystal and molecular structures of 2,6-bis-(N-methyl-N-ethylamino)-4-methylphenol and its bromo derivative. by C. Shambhugum, S. Shambhugum, Sundara Raj and M. N. Ponnuswamy, Department of Madras, Gandy Campus, Madras-600 925, India.

The crystal structures of 2,6-bis(N-methyl-N-ethylamino)-4-methylphenol (MMP) and its bromo derivative (MBP) have been determined by different authors since 1993 (García-Granda, S., Acta Cryst., 1993, C49, 000-000). The solid state conformations show a wide range of relative positions of the carboxylic groups partially affected by the molecular packing as the crystallographic data reveal.

The crystal structures of the two benzenecarboxylic acids were determined (García-Granda, S., Acta Cryst., 1993, C49, 000-000), in order to analyze their solid state preferred conformation and make a comparison between the X-Ray results and those in gas phase, semiempirical calculation has been performed on all members within the series.

Heat of formation is the criteria being used to make a difference among the conformers that belong to the same family and also intramolecular symmetry has been taken into account when possible. Both, AM1 and PM3 semiempirical methods have been used and the results are compared.

Methodology:

- Crystal Structure Determinations:
  Cad4, au29, Profile Analysis, Direct Methods, Dirif, Shelk76, Parst.

- Conformational Analysis:

PS-06.02.11 Diffuse scattering in p-chloro-N-(p-methylbenzylidene) aniline, C10H12ClN. by T.E. Welberry, B.M. Butler & A.P. Heerdigen, Research School of Chemistry, Australian National University, GPO Box 4, Canberra City, ACT 0200, Australia.

Detailed diffuse X-ray scattering measurements have been recorded from a sample of p-chloro-N-(p-methylbenzylidene) aniline, C10H12ClN (MeCl). The observed scattering has been interpreted by comparison with diffraction patterns of a model system obtained using Monte Carlo computer simulation. Strong diffuse scattering peaks originate from a type of disorder in which the molecule is flipped end-to-end, and indicate a tendency for the structure to form a super-lattice with local symmetry P2_1/n compared to the P2_1/a symmetry of the reported average structure. A second type of disorder involving side-to-side flipping of the molecules appears to occur randomly through the structure with no evidence for short-range ordering. Accompanying these two effects there is strong diffuse scattering which can be satisfactorily modelled assuming rigid-body molecular displacements. This scattering is largely temperature independent and must arise because local relaxational displacements accompany the main disorder.

PS-06.02.12 Crystal structures and conformational analysis of the twelve benzenecarboxylic acids. By S. García-Granda, B. Tujerena, and F. Gómez-Beltrán, Departamento de Química Física y Analítica, Universidad de Oviedo, Spain.

A family of novel antibacterial quinolones and naphthylides was prepared (J. Frigoza, J. Med. Chem., 1993, 36, 000). Within this series the usual piperazine or aminopyrindine groups were replaced by 7-azetidinyl substituents. Compounds with outstandingly broad-spectrum activity, particularly against Gram-positive organisms, improved in vitro efficacy in high blood levels were identified among these new azetidinylquinolones. In order to detect the structural trend responsible for the antibacterial activity of these compounds a QSAR study was performed (A. Cohen, Pharmacology Library, 1991, 16, 397-400).