05. PHYSICAL PROPERTIES AND STRUCTURE

05.1-44 ALLAGES MOLECULAIRES - SYSTÈME p-DICHLORE-BENZENE/p-DINITROBENZENE par N.B. Chanh, M. Cuevas, H. Font-Altaba, Y. Haget

05.1-45 STUDIES OF THE POLYMORPHS OF 4-FLUORO-1-NITROBENZENE, 4-CHLORO-1,2-DINITROBENZENE AND 4-CHLORO-1,3-DINITROBENZENE. By A. Wilkins and R.W.H. Small, Chemistry Department, The University, Lancaster, England.

Halogenated derivatives of mono- and dinitrobenzenes have been reported to show an unusual degree of polymorphism. Two, and frequently more, melting points have been recorded for compounds of this type. Single crystals of the less stable forms of many of these compounds are difficult to obtain but in the case of each of the three title compounds the structures of two polymorphs have been determined. The purpose of the investigation has been to determine (i) the influence of the crystal environment on the molecular parameters, particularly torsion angles; (ii) any common features of intermolecular association and (iii) the relation between the structures of the polymorphs of each compound and, where appropriate, the mode of transformation. The six crystal structures will be described and discussed in these terms.

05.1-46 PHASE TRANSITIONS IN Azo Compounds. Molecular and Crystal Structures of the Low- and High-Temperature Forms of 2-Amino-3-hydroxy-6-methyl-4-chloro-1,3-dinitrobenzene. By Gautam R. Desiraju, School of Chemistry, University of Hyderabad, Hyderabad 500 134, India.

The title compound undergoes phase transitions at 393, 442 and 449 K. The low-temperature modification crystallizes in the space group Pbc a and the high temperature form in P2_1/c.

The structures of both forms have been solved from counter data (CAD-4) using the program MULTAN 78. The structures have been refined satisfactorily using full-matrix least-squares methods (ORFLS).

The notable features in both structures are the hydrogen bonding between amino and hydroxy groups of neighbouring molecules and the conformations of the six-membered rings about the central C=N=N=C linkage. The structural basis for the phase transitions can be rationalized and the relationship of these structures to those of the isoelectronic benzilidene anils understood, from the structures of the two polymorphs.