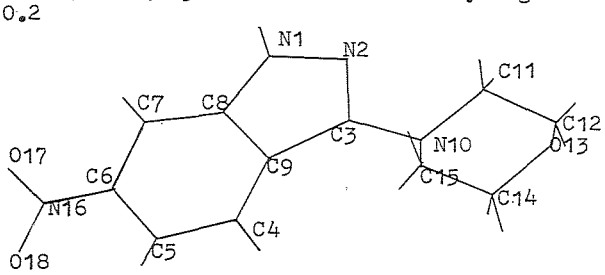
04.1–13 THE CRYSTAL AND MOLECULAR STRUCTURE OF 3-MORPHOLINE-6 NITRO-INDAZOLE. By Teresa Borowiak and Marian Gawron, Faculty of Chemistry, Adam Mickiewicz University, Grunwaldzka 6, 60-780 Poznań, Poland.

Some of the nitro-derivatives of 3-amino indazoles have been found to possess an antiinflamatory biological activity. The present work is a part of crystal structure determinations of a number compounds, where different amino-substituents are in the position 3 of indazole moiety and the nitro group occupies the position 4,5,6 or 7.

The crystals of the title compound are monoclinic, $P2_1/n$, Z=4; the structure was solved by direct methods and refined to a final R=0.054; the e.s.d.'s for the bond lenghts are 0.002-0.003 Å and for the valency angles 0.2



The distribution of long and short bonds in pyrazole moiety is the same as in pyrazole itself (T. La Cour, S.E. Rasmussen, Acta Chem. Scand. (1973),27, 1845). This indicates that the uncharged form of pyrazole contributes more to the resonance hybrid of five-membered ring than does the betaine form. The distortions of the benzo ring symmetry are quite marked and involve both: the bond lenghts and valency angles. They testify to the strong σ-electron withdrawing character of the NO_2 group; the NO_2 substituent angle is as large as 123.7(2)°. The overall pattern of bond lenghts in indazole moiety points to a conjugation of the molecule. However, the indazole is not perfectly planar, the angle between the benzo and pyrazole rings equals 3.03°.

The morpholine ring adopts a chair conformation and the orientation of this substituent towards the indazole moiety is described by the following torsion angles: C3-N10-C11-C12 and C3-N10-C15-C14, which are equal to 172.0(2)° and -171.7(2)°, respectively. Proton-donor center N1-H is involved in a hydrogen bond with the oxygen atom of morpholine-substituent what is in opposite to the crystal structure of pyrazole and indazole, where the molecules are connected by the N1···N2 intermolecular hydrogen bonds.

04.1–14 MORPHOLOGY OF ORGANIC CRYSTALS BY ENERGY CALCULATIONS. By Z. Berkovitch-Yellin, Structural Chemistry Dept., Weizmann Inst. of Science, Rehovot, 76 100, Israel

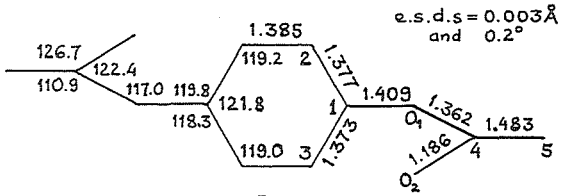
The morphology of a crystal is directly related to the relative growth rates of its faces with the general rule that those faces which grow slower appear as larger faces. It was demonstrated that there is a correlation between the growth velocity of a face and its attachment energy which is defined as the energy released per mole when a crystal slice is deposited on the face hkl (P. Hartman, J. Cryst. Growth (1980) 49, 157,166).

The theoretical form of organic crystals was studied by means of atom-atom potential energy calculations. The theoretical habits which are derived from the internal crystal structure, are best compared with the morphology of crystals obtained by sublimation. To derive the solution-grown habit of crystals solvent/solute and impurity/solute interactions at the various crystal faces were analyzed. Preferential adsorption of solvent molecules or impurity molecules on specific crystal faces cause delay in growth of these faces relative to other faces with a concomitant change in crystal habit.

The calculated morphologies are in good agreement with observed crystal habits.

04.1–15 THE STRUCTURE OF p-DIACETOXYBENZENE. By A. Roszak, Institute of Chemistry, Nicolaus Copernicus University, Gagarina 7, 87-100 Toruń, Poland and T. Borowiak and M. Gawron, Institute of Chemistry, Adam Mickiewicz University, Grunwaldzka 6, 60-780 Poznań, Poland.

The angular substituent parameters (Domenicano & Murray-Rust, Tetrahedron Lett.,2283,(1979)) for OAc group: $\Delta\alpha$=1.4, $\Delta\beta$=-1.1, $\Delta\gamma$=0.3, $\Delta\delta$=0.2 were found previously on the base of structure of 9-acetoxy-10-(2',4'-diacetoxyphenyl)anthracene (Roszak & Borowiak, Acta Cryst.,to be submitted). In order to prove these values the structure of p-diacetoxybenzene has been determined. The crystals are monoclinic, $P2_1/c$, Z=2; the final R is 0.051 for 907 reflexions.



The molecules are of $\bar{1}$ symmetry, however, the benzene ring has mmm symmetry within experimental error. The strong contraction of C1-C2, C1-C3 bonds and the increase of C2-C1-C3 angle in relation to unsubstituted benzene, is due to the σ-electron-withdrawing character of OAc group. The sums: $\Delta\alpha+\Delta\delta$=1.8 and $\Delta\beta+\Delta\gamma$=-0,9 are in good agreement with the expected values. The other confirmation of particular angular substituent parameters will be done by determination of other acetoxybenzene and 9-phenylanthracene derivatives.