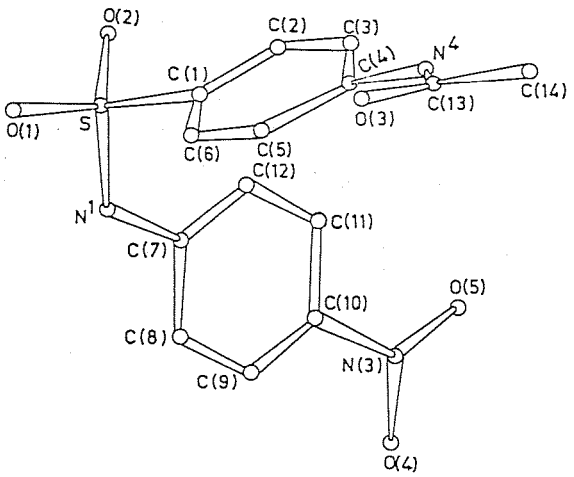
03.3-12 CRYSTAL AND MOLECULAR STRUCTURE OF N^4-ACETYL-N^1-(p-NITROPHENYL) SULPHANILAMIDE. By M. Ghosh, A.K. Basak, S.K. Mazumdar and B. Sheldrick*, Crystallography and Molecular Biology Division, Saha Institute of Nuclear Physics, Sector I, Block 'AF', Bidhannagar, Calcutta-700 064, India. *The Austbury Dept. of biophysics, University of Leeds, U.K.

Sulphonamides and its different derivatives are widely used as antibacterial drugs. The crystal structure analysis of the present compound, with p-nitrophenyl and acetyl substituent at the N^1- and N^4- position, has been determined as a part of continuing programme of structural studies of the substituted sulphonamides with the view to study the geometrical and conformational changes consequent to substituents which may in turn help to have a better insight into their biological activity.

Crystal data: Crystals from methanol, molecular formula $C_{14}H_{13}N_3O_5S$, M_r=335.34, space group = $P2_1/c$, with a=12.259(9), b=7.339(5), c=16.359(9) Å, β=98.84(4)°, V=1454(2)Å^3, Z=4, D_m=1.517 Mgm^{-3}, D_x=1.518 Mgm^{-3}, μ=2.22 mm^{-1}, F(000)=696. The structure was solved by direct methods and refined by full-matrix least-squares method to a final R=0.052 for 2532 'observed'[1≥2.5σ(I)] reflections. Both the phenyl rings almost planar, with slight distortion in bond lengths and angles, are folded towards each other making a dihedral angle of 88.6(1)°.

Sulphonyl nitrogen, N(1), is synclinal with respect to C(1)-C(6) bond. The torsion angles C(X)-C(1)-S-N(1) [X=2 and 6] [99.2(2)°, -80.9(2)°] and C(1)-S-N(1)-C(7)=-64.8(3)° are within the clustering range of $|\varepsilon_1|$ =70-120° and $|\varepsilon_2|$ =60-90° respectively. (Kalman et al, Acta Cryst. B37, 868-877, (1981)). In packing the molecules are found to be stabilised by the hydrogen bonding network of the type N-H...O.



03.4-1 CRYSTAL STRUCTURES OF MOLECULAR COMPLEXES INVOLVING SULFONAMIDES AND 9-AMINOACRIDINE. By C. Chakrabarti, S. Ghose and J.K. Dattagupta, Crystallography and Molecular Biology Division, Saha Institute of Nuclear Physics, 1/AF Bidhan Nagar, Calcutta 700 064, India.

A crystallographic study of molecular complexes of 9-aminoacridine with two different sulfa drugs sulfadimidine and sulfamethoxypyridazine, has been made with a view to study the nature of forces between the molecular species of the complexes and the corresponding structural changes of the individual molecules. Anisotropic refinement of the structures of 9-aminoacridine—sulfadimidine(I) and 9-aminoacridine—sulfamethoxypyridazine(II) have refined to R values of 0·063 and 0·046 respectively. Both the complexes are found to contain acridinium cations and sulfanilamidate anions which result from the transfer of a hydrogen ion to the nitrogen atom of the acridine ring from the sulfonamide nitrogen atom. As a result there are some small changes in the dimensions of the sulfonamide group. It is usually observed in sulfonamides that the dihedral angles between the two rings lie in the range 60 - 90°. Though in I this dihedral angle is 33·3°, in II this angle has a value of 83·9°. The conformation of the sulfonamide group is expressed by the torsion angles about the S-N bond and S-C(ring) bond, which fall in the ranges 60 - 90° and 70 - 120° respectively in a number of similar compounds. In the present study, these torsion angles are 73·0° and 102·6° for I and 60·1° and 68·1° for II lying well within their respective ranges. The acridine ring in both the structures is slightly non-planar, the dihedral angles between the two outer rings being 4·9° and 5·1° respectively. The nitrogen of the acridine ring forms H-bond with different nitrogen atoms of the sulfonamide anion in the two structures. In I it is bonded to the pyrimidine nitrogen atom while in II this nitrogen is H-bonded to the sulfonamide nitrogen.