The *X*-Ray Crystal Structure of the Antimalarial and Antileprotic Drug, 4,4′-Diaminodiphenyl Sulphone[1]

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Summary The crystal structure of the important antimalarial and antileprotic drug, 4,4′-diaminodiphenyl sulphone ("Dapsone"), has been determined.

4,4′-DIAMINODIPHENYL SULPHONE has been known as an antileprotic drug for more than 30 years[2] and interest in it as an antimalarial has greatly increased in recent years with the appearance of chloroquine-resistant strains of malaria. Besides wishing to determine its structure as part of a long-term investigation of antimalarial drugs, we are also interested in the detailed molecular structure of sulphones as a means of studying the interaction of sulphur with adjacent unsaturated centres and as a probe into the general question of 3*d*-orbital participation in the bonding of third-row elements.

4,4′-Diaminodiphenyl sulphone crystallized as needles from warm benzene in space group $P2_12_12_1$ with $Z = 4$. The cell dimensions are: $a = 8{\cdot}065 \pm 0{\cdot}005$, $b = 25{\cdot}57 \pm 0{\cdot}02$, $c = 5{\cdot}760 \pm 0{\cdot}001$ Å. Three-dimensional data were collected on a Picker FACS-1 diffractometer using

graphite monochromatised Mo-K_α radiation and the 2θ scan technique to a maximum 2θ of 65°. This produced 1653 observed reflections out of 2127 measured unique data. The structure was solved using symbolic-addition[3] and tangent-refinement[4] techniques. The 376 phases obtained from the direct methods were used to calculate an F_0 Fourier in which all non-hydrogen atoms were located and which atomic positions yielded an initial R value of 0·24. Refinement was by full-matrix least-squares techniques. Individual isotropic temperature factors and unit weights were employed and all parameters except hydrogen temperature factors were refined. The final R value was 0·12.†

The bond lengths and angles are shown in the Figure.‡ The carbon–carbon distances show the variation normally found in aromatic compounds and the other lengths and angles are in accord with published values for these kinds of connections. The two benzene rings and their respective nitrogen atoms are coplanar; the sulphur is in the plane of ring 2 but deviates by 0·13 Å from ring 1. Rings 1 and 2 subtend angles of 75° and 85° respectively with the plane through atoms S, C(1′), C(1), C(4′), C(4), N(1′), and N(1). The formation of an intermolecular hydrogen-bond between molecules related by the unit translation in the a direction can be seen in the N · · · O and H · · · O distances of 2·95 and 2·13 Å and the N–H · · · O angle of 151°.

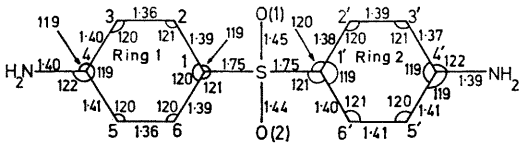

FIGURE. *Bond lengths* (Å) *and angles for* 4,4′-*diaminodiphenyl sulphone.* ∠O(1)–S–O(2) = 118°, ∠C(1)–S–C(1′) = 106°, ∠O(1)–S–C(1) = 108°, ∠O(1)–S–C(1′) = 107°, ∠O(2)–S–C(1) = 108°, ∠O(2)–S–C(1′) = 108°.

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†All calculations were performed using *X*-ray 67, Technical Report 67-58, Computer Science Center, University of Maryland, 1967.
‡ The average error in bond lengths is 0·01 Å and in angles is 0·8°.

[1] From a dissertation to be submitted by C. Dickinson to the Graduate School of the University of Maryland in partial fulfilment of the requirements for the Ph.D. degree.
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[3] J. Karle and I. L. Karle, *Acta Cryst.*, 1966, **21**, 849.
[4] J. Karle and H. Hauptman, *Acta Cryst.*, 1956, **9**, 635.