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References

BROWN, D. S., EINSTEIN, F. W. B. & TUCK, D. B. (1969). *Inorg. Chem.* **8**, 14–18.

GRANT, D. F. & GABE, E. J. (1974). NRC Report 14325, National Research Council of Canada, Ottawa, Canada.

PREWITT, C. T., SHANNON, R. D., ROGERS, D. B. & SLEIGHT, A. W. (1969). *Inorg. Chem.* **8**, 1985–1993.

VEIDIS, M. V. & PALENIK, G. (1969). *Chem. Commun.* pp. 586–587.

X-RAY System (1972). Tech. Rep. TR-192, Comput. Sci. Center, Univ. of Maryland, U.S.A.

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Dimethyl Sulfone Diimine, a Neutron Study

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Abstract. $(CH_3)_2S(NH)_2$, orthorhombic, *F*2*dd* (No. 43), $a=5{\cdot}44$, $b=10{\cdot}59$, $c=16{\cdot}13$ Å, $Z=8$. The structure was refined from neutron diffraction data. The molecules lie on twofold axes, and are linked together by a three-dimensional network of N–H···N hydrogen bonds. The methyl groups are in an eclipsed conformation.

Introduction. A single crystal about 2 mm in diameter, kindly provided by Dr A. J. Mabis, was mounted on a four-circle neutron diffractometer at the National Bureau of Standards reactor. Of 262 reflections measured ($\lambda=1{\cdot}00$ Å) 206 had intensities significantly above background. Unit-cell dimensions and a trial set of phases were obtained from the X-ray structure deter-

Table 1. *Final refined atomic parameters for dimethyl sulfone diimine*

Temperature factors are given as the coefficients of the expression $\exp[-(h^2\beta_{11}+k^2\beta_{22}+l^2\beta_{33}+2hk\beta_{12}+2hl\beta_{13}+2kl\beta_{23})]$. Values are $\times 10^4$.

	x	y	z	β_{11}	β_{22}	β_{33}	β_{12}	β_{13}	β_{23}
S	0	0	0	193 (39)	58 (7)	20 (3)	0	0	−5 (4)
C	−2058 (22)	1266 (5)	211 (3)	422 (23)	82 (5)	34 (2)	78 (8)	37 (6)	−2 (3)
N	1339 (22)	−456 (3)	783 (2)	309 (12)	88 (3)	24 (1)	5 (6)	−25 (3)	6 (2)
H(1)	2414 (27)	246 (12)	998 (6)	458 (42)	144 (12)	40 (4)	2 (22)	−33 (10)	4 (6)
H(2)	−3112 (40)	1450 (18)	−324 (7)	1056 (108)	302 (26)	51 (6)	435 (27)	−33 (17)	5 (8)
H(3)	−3297 (39)	1001 (11)	696 (8)	567 (50)	157 (10)	66 (6)	64 (23)	74 (16)	0 (7)
H(4)	−1074 (48)	2037 (12)	390 (8)	886 (77)	86 (9)	126 (10)	−31 (28)	87 (28)	−41 (7)

Table 2. *Interatomic distances and angles in dimethyl sulfone diimine*

Distances marked with an asterisk are involved in hydrogen bonds.

i	j	k	D_{ij}	D_{jk}	D_{ik}	$\angle ijk$
C	S	C′	1·780 (8)	1·780 (8)	2·767 (10)	102·0 (7)
C	S	N	1·780 (8)	1·536 (6)	2·593 (6)	102·6 (3)
C	S	N′	1·780 (8)	1·536 (6)	2·756 (6)	112·2 (2)
N	S	N′	1·536 (6)	1·536 (6)	2·706 (6)	123·4 (8)
S	N	H(1)	1·536 (6)	1·008 (17)*	2·094 (13)	109·0 (5)
N	H(1)	N″	1·008 (17)*	2·359 (16)*	3·335 (3)*	162·8 (9)
S	C	H(2)	1·780 (8)	1·056 (15)	2·345 (14)	108·9 (8)
S	C	H(3)	1·780 (8)	1·070 (16)	2·366 (16)	109·8 (8)
S	C	H(4)	1·780 (8)	1·018 (18)	2·322 (13)	109·1 (1·1)
H(2)	C	H(3)	1·056 (15)	1·070 (16)	1·717 (16)	107·8 (1·6)
H(2)	C	H(4)	1·056 (15)	1·018 (18)	1·715 (25)	111·7 (1·6)
H(3)	C	H(4)	1·070 (16)	1·018 (18)	1·705 (22)	109·6 (1·1)

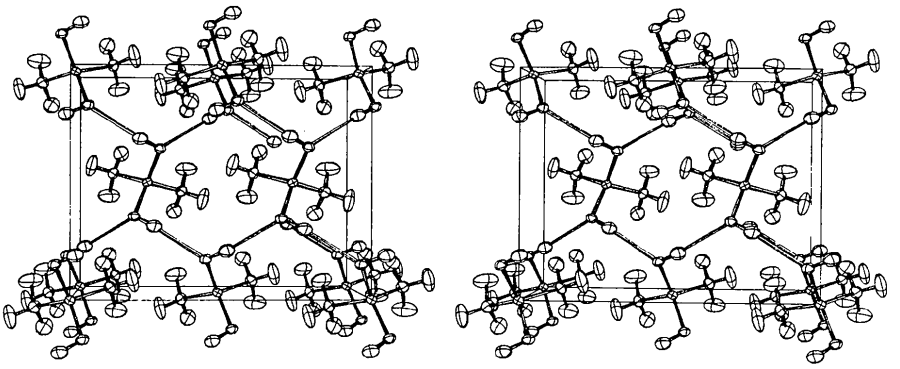

Fig. 1. Stereoscopic view of the structure of dimethyl sulfone diimine, looking down the *a* axis. Half of the unit cell is shown, from $z=0$ to $z=\frac{1}{2}$.

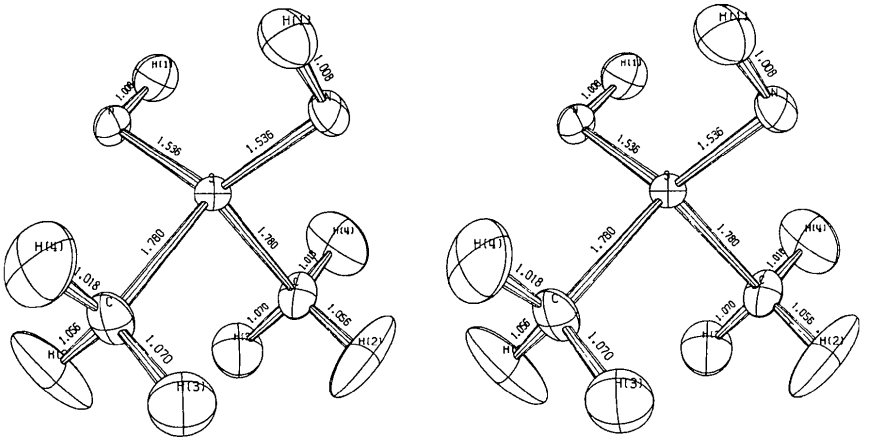

Fig. 2. Stereoscopic view of the dimethyl sulfone diimine molecule.

mination of Webb & Gloss (1967), and a Fourier map was calculated using the observed values of the structure amplitudes. Trial positions for the four hydrogen atoms were readily found in this map, and the structure was refined by least squares, using the program *RFINE* (Finger & Prince, 1975). With anisotropic temperature factors, an isotropic secondary extinction parameter (Zachariasen, 1968), and weights assigned by $w=[\sigma_s^2+(0{\cdot}015F)^2]^{-1}$, where σ_s is a standard deviation computed from counting statistics, the final weighted R was 0·041.* The final atomic parameters are given in Table 1.

Discussion. Table 2 is a summary of interatomic distances and angles, while Fig. 1 is a stereoscopic view (Johnson, 1965) of one half of the unit cell viewed down the *a* axis. Fig. 2 is a stereoscopic view of the molecule. Each nitrogen atom participates in two N–H···N hydrogen bonds, resulting in an arrangement of zigzag chains which form a three-dimensional network. The average C–H bond distance in the methyl group, uncorrected for thermal motion, is 1·048 Å, and all bond angles in the methyl group are within 2 e.s.d.'s of the tetrahedral angle, 109·5°. One hydrogen atom in the methyl group is very close to the C–S–C plane, so that the two methyl groups in the molecule are eclipsed. The shortest intermolecular distance outside of a hydrogen bond is 2·28 (2) Å between H(2) on one molecule and H(4) on the other.

* A table of observed and calculated structure factors has been deposited with the British Library Lending Division as Supplementary Publication No. SUP 31157 (3 pp.). Copies may be obtained through The Executive Secretary, International Union of Crystallography, 13 White Friars, Chester CH1 1NZ, England.

References

FINGER, L. W. & PRINCE, E. (1975). *RFINE*, NBS Tech. Note 854, National Bureau of Standards, Washington, D.C.

JOHNSON, C. K. (1965). *ORTEP*. Oak Ridge National Laboratory Report ORNL-3794.

WEBB, N. C. & GLOSS, R. A. (1967). *Tetrahedron Lett.* **11**, 1043–1047.

ZACHARIASEN, W. H. (1968). *Acta Cryst.* A**24**, 421–424.