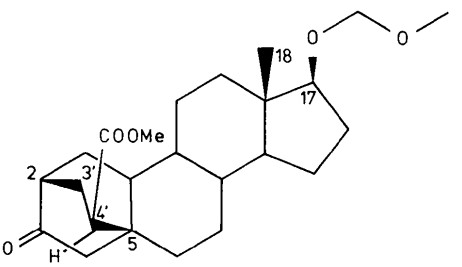
& Walliser, 1976; Schomburg, Thielmann & Winterfeldt, 1985, 1986; Chowdhury, Prelle, Schomburg, Thielmann & Winterfeldt, 1987).



(1)

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SHORT COMMUNICATION

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Acta Cryst. (1989). C**45**, 173–174

The space group of bis(1,3-propanediamine)mercury(II) sulfate dihydrate.

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Abstract

The structure of bis(1,3-propanediamine)mercury(II) sulfate dihydrate was originally presented in space group *P*2 [Kamenar, Grdenić & Hergold-Brundić (1984). *Acta Cryst.* C**40**, 1836–1838]; a more appropriate space group is *P*2/*n*.

Introduction

During the preparation of a brief review (Jones, 1986) of noncentrosymmetric structures published in *Acta Crystallographica,* Section C, 1984, it was noticed that some structures were in fact probably centrosymmetric. One such case is presented here.

Bis(1,3-propanediamine)mercury(II) sulfate dihydrate, $[Hg(C_3H_{10}N_2)_2]SO_4.2H_2O$ (Kamenar, Grdenić & Hergold-Brundić, 1984; henceforth KGH), was described in space group *P*2, with $a = 13{\cdot}830$, $b = 6{\cdot}023$, $c = 8{\cdot}250$ Å, $\beta = 97{\cdot}45°$, $Z = 2$; two independent Hg and two independent S atoms lay on twofold axes. Inspection of the atomic coordinates of KGH shows that the structure is to a good approximation centrosymmetric; a coordinate shift of *ca* 0·25, 0·48, 0·25 leads to atom positions corresponding closely to space group *P*2/*n*. Refinement on *F* of the *P*2/*n* structure using the deposited structure factors (1893 reflections, unit weights, Hg and S anisotropic) gives an *R* value of 0·038 for 43 parameters (*cf.* KGH: $R = 0{\cdot}033$ for a weighted refinement, all atoms anisotropic, 164 parameters). The reflections *h*0*l*, $h + l$ odd, are required to be systematically absent in *P*2/*n*; 20 such reflections are present in the list of observed structure factors, but all are weak. The max. Δ/σ in the final cycle was 0·001.

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Table 1. *Atom coordinates* ($\times 10^4$) *and isotropic temperature factors* ($Å^2 \times 10^3$)

	x	*y*	*z*	*U*	From
Hg	2500	4801 (1)	2500	22 (1)*	Hg(1,2)
N(1)	1286 (4)	7468 (11)	1520 (8)	19 (1)	N(1,4)
N(2)	1711 (5)	3476 (11)	4451 (8)	18 (1)	N(2,3)
C(1)	1228 (5)	9050 (13)	2884 (9)	20 (1)	C(1,4)
C(2)	622 (6)	11141 (13)	2433 (9)	21 (1)	C(2,5)
C(3)	689 (6)	2729 (13)	3894 (10)	22 (1)	C(3,6)
S	2500	8532 (4)	7500	13 (1)*	S(1,2)
O(2)	2138 (4)	9951 (10)	8771 (7)	24 (1)	O(1,3)
O(3)	3310 (4)	7133 (10)	8261 (7)	25 (1)	O(2,4)
O(1)	916 (5)	3752 (12)	−1442 (8)	35 (1)	O(5,6)

* Equivalent isotropic *U* calculated from anisotropic *U*.

Table 2. *Bond lengths* (Å) *and angles* (°)

Hg–N(1)	2·388 (7)	Hg–N(2)	2·208 (8)
C(1)–N(1)	1·484 (11)	C(1)–C(2)	1·531 (12)
C(2)–C(3^{iii})	1·531 (12)	C(3)–N(2)	1·497 (11)
O(2)–S	1·489 (7)	O(3)–S	1·475 (7)
N(1)–Hg–N(2)	95·6 (3)	N(1)–Hg–N(1^{i})	95·4 (4)
N(2)–Hg–N(1^{i})	112·9 (3)	N(2)–Hg–N(2^{i})	137·6 (4)
Hg–N(1)–C(1)	106·3 (5)	Hg–N(2)–C(3)	114·9 (6)
N(1)–C(1)–C(2)	115·2 (7)	C(1)–C(2)–C(3^{iii})	110·3 (7)
N(2)–C(3)–C(2^{ii})	112·8 (7)	O(2)–S–O(3)	109·5 (4)
O(2)–S–O(2^{iv})	110·0 (6)	O(3)–S–O(2^{iv})	108·7 (4)
O(3)–S–O(3^{iv})	110·3 (6)		

Symmetry operators: (i) 0·5−*x*, *y*, 0·5−*z*; (ii) *x*, −1+*y*, *z*; (iii) *x*, 1+*y*, *z*; (iv) 0·5−*x*, *y*, 1·5−*z*.

The newly refined structure shows the same qualitative features described by KGH. The Hg and S atoms lie on twofold axes 0·25, *y*, 0·25, and 0·25, *y*, 0·75 respectively (Table 1).* The coordination at the metal atom remains irregular tetrahedral, although the range of Hg–N bond lengths is somewhat reduced. A marked improvement in the geometry of the sulfate ion is notable; the spread of bond lengths and angles is reduced from 1·466–1·510 Å, 101·2–116·7° to 1·475, 1·489 Å, 108·7–110·3°. Similar changes can be seen in the light-atom bond lengths and angles (see Table 2).

The irregularities in geometry of the KGH structure are typical of the problems arising when a centrosymmetric structure is refined in a noncentrosymmetric space group; it is remarkable that such problems, including slow and erratic refinement, were apparently not noticed by KGH.

I thank the Verband der Chemischen Industrie for financial support.

* Lists of structure factors, anisotropic thermal parameters and H-atom parameters have been deposited with the British Library Document Supply Centre as Supplementary Publication No. SUP 51366 (15 pp.). Copies may be obtained through The Executive Secretary, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

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