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The crystal structures of methyl 1,5-dithio-α-D-ribopyranoside quarterhydrate and methyl 1,5-dithio-β-D-ribopyranoside: errata.

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Errors are corrected in Tables 1 and 3 of Girling & Jeffrey [*Acta Cryst.* (1974), B30, 327–333].

In Table 1 of Girling & Jeffrey (1974), the atomic parameters given for methyl 1,5-dithio-α-D-ribopyranoside and methyl 1,5-dithio-β-D-ribopyranoside are those for the L enantiomers. The correct values are obtained by reversing the signs of the y coordinates. For methyl 1,5-dithio-α-D-ribopyranoside, molecule A, the following parameters for C(4) were omitted: x 4139, y −288, z 7182, β_{11} 9·9 (5), β_{22} 256 (19), β_{33} 56 (3), β_{12} 4 (3), β_{13} 7 (1), β_{23} 28 (7). For methyl 1,5-dithio-α-D-ribopyranoside, molecule B, the coordinates given for O(3) refer to O(4). The coordinates for O(3) were omitted; they are as follows: x 4990, y −6301, z 3321, β_{11} 8·7 (4), β_{22} 303 (14), β_{33} 63 (3), β_{12} −12 (2), β_{13} 0·4 (8), β_{23} 33 (5). These coordinates are for the D enantiomer.

In Table 3, the signs of the torsion angles for (IA) and (IB) refer to the L enantiomer. They have to be reversed for the D enantiomer.

Reference

GIRLING, R. L. & JEFFREY, G. A. (1974). *Acta Cryst.* B30, 327–333.

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Comment on *The crystal and molecular structure of phenothiazine*, by J. J. H. McDowell.

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There are strong indications that the data reported by McDowell [*Acta Cryst.* (1976), B32, 5–10] on the structure of phenothiazine are affected by disorder and that the precision of the molecular dimensions is overestimated.

A crystal structure investigation of phenothiazine was undertaken in this laboratory some years ago. The cell parameters measured by us were only slightly different from those recently reported by McDowell (1976) (see Table 1).

Moreover, the positional and thermal parameters we arrived at differ by no more than 1·5 s.d. from those reported by McDowell. The following observations led us to the conclusion that our results suffered from disorder and that no high accuracy could be claimed:

(1) Weissenberg photographs about the orthorhombic a axis reveal marked diffuse streaking parallel to $\mathbf{c}^*$. In addition, it was found that even after long exposures no reflexions could be recorded in large regions corresponding to $k \gtrsim 10$, indicating comparatively high values for anisotropic thermal parameters β_{22}.

(2) Refinement of the structure, with isotropic thermal parameters only, resulted in a residual R of $\simeq 0·25$. An electron density difference map at this stage clearly showed two phenothiazine molecules shifted by about 0·3 Å in opposite directions along a perpendicular to the plane $y = \frac{1}{4}$. There was a sharp drop in the residual to $R \simeq 0·08$ when anisotropic thermal parameters were included in the refinement.

Table 1. *Comparison of cell parameters*

	van de Waal & Feil	McDowell (1976)
a	7·918 (2) Å	7·916 (10) Å
b	20·945 (3)	20·974 (10)
c	5·882 (2)	5·894 (10)
Space group	*Pnma*	*Pnma*

(3) Low-temperature Weissenberg photographs (recorded at 120 K) revealed a number of features, not observed at room temperature: (*a*) $hk0$ reflexions with h odd, forbidden by *Pnma* space-group symmetry, were clearly present. The behaviour of the intensities of these reflexions with increasing temperature is strongly indicative of an order–disorder transition. At the transition point (224·6 K) these reflexions have completely disappeared. (*b*) No unusual 'black' regions. (*c*) Diffuse streaking [see (1) above] has disappeared. (*d*) All reflexions split into two components in a way which is consistent with the superposition of two reciprocal monoclinic lattices, related by a 180° rotation about the (monoclinic) c^* axis.

(4) The existence of an order–disorder transition at 224·6 K was confirmed by heat-capacity measurements with a powder specimen.

(5) Analysis of anisotropic β values showed them to be unacceptable as parameters describing thermal motion (a detailed discussion is given below).