SHORT COMMUNICATION

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Structure of $C_{32}H_{34}N_2O_5S_2$: corrigendum.

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Abstract

The structure of this compound [Olszak, Stępień, Wajsman, Grabowski, Glinka & Lecocq (1987). *Acta Cryst.* C**43**, 2169–2171], which contains a 13-membered heterocyclic ring, was described as triclinic, space group $P\bar{1}$, with $a = 12{\cdot}756\ (3)$, $b = 9{\cdot}950\ (3)$, $c = 13{\cdot}566\ (3)$ Å, $\alpha = 90{\cdot}49\ (1)$, $\beta = 118{\cdot}04\ (1)$, $\gamma = 90{\cdot}04\ (1)°$, $Z = 2$. It should be described as monoclinic, space group $C2/c$, with $a' = 23{\cdot}947\ (6)$, $b' = 12{\cdot}756\ (3)$, $c' = 9{\cdot}950\ (3)$ Å, $\beta' = 90{\cdot}57\ (3)°$, $Z = 4$. The $C2/c$ coordinates are given. The molecule lies on an exact, rather than an approximate, twofold axis.

The vectors describing the new cell are [102], [100] and [010]. The corresponding coordinate transformations are: $x' = z/2 + 0{\cdot}25$, $y' = x - z/2 - 0{\cdot}25$, $z' = y$; the translations are needed to place the origin at the conventional center of symmetry in $C2/c$. After averaging the transformed coordinates over appropriate pairs of atoms, the $C2/c$ coordinates in Table 1 result.

The shifts in the original $P\bar{1}$ coordinates (Olszak *et al.*, 1987, Table 1) necessary to achieve the symmetry of $C2/c$ are slightly larger than usual: the maximum shift is 0·014 Å and the r.m.s. value of 'shift/σ' is 1·25 compared with the expectation value of 1·0. I suspect that this discrepancy is due to the original authors' failure to achieve the usual degree of convergence in their least-squares refinement; Olszak *et al.* (1987) quote a 'max. shift/e.s.d.' ratio of 0·996.

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Table 1. *Coordinates* ($\times 10^4$), *space group* $C2/c$

The atoms are numbered according to Table 1 of Olszak *et al.* (1987); the numbering in their Fig. 1 differs in some instances.

	x	*y*	*z*
O(8)	0·5000	0·0976	0·2500
S(1,2)	0·6523	0·3639	0·2306
N(1,6)	0·5952	0·3676	0·3206
O(1,4)	0·6411	0·4260	0·1144
O(2,3)	0·6662	0·2562	0·2182
C(2,5)	0·5712	0·4720	0·3465
C(3,4)	0·5080	0·4718	0·3244
C(9,7)	0·5494	0·1604	0·2532
C(11,21)	0·7053	0·4276	0·3240
C(12,22)	0·7398	0·3688	0·4065
C(13,23)	0·7796	0·4190	0·4847
C(14,24)	0·7856	0·5249	0·4820
C(15,25)	0·7517	0·5826	0·3968
C(16,26)	0·7118	0·5332	0·3174
C(141,241)	0·8278	0·5794	0·5715
C(31,41)	0·5883	0·2898	0·4251
C(32,46)	0·6036	0·3154	0·5571
C(33,45)	0·5938	0·2448	0·6594
C(34,44)	0·5693	0·1502	0·6322
C(35,43)	0·5554	0·1247	0·5013
C(36,42)	0·5643	0·1938	0·3949

The molecule lies on a crystallographically exact, rather than an approximate, twofold axis. Other details of the reported structure are little changed.

References

OLSZAK, T. A., STĘPIEŃ, A., WAJSMAN, E., GRABOWSKI, M. J., GLINKA, R. & LECOCQ, D. (1987). *Acta Cryst.* C**43**, 2169–2171.