SHORT COMMUNICATIONS

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Acta Cryst. (1988). C**44**, 1866

Crown ether complexes of alkaline-earth metal ions. III. Structures of 1,4,7,10,13,16-hexaoxacyclooctadecane (18-crown-6) complexed with magnesium and barium thiocyanates. Erratum.

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Abstract

In the paper by Wei, Tinant, Declercq, Van Meerssche & Dale [*Acta Cryst.* (1988), C**44**, 77–80], the space group of compound (1) $C_{12}H_{24}O_6.Mg(SCN)_2.4H_2O$ was reported to be $Pna2_1$, with unit cell $a = 9{\cdot}225$ (2), $b = 19{\cdot}256$ (7), $c = 13{\cdot}267$ (4) Å. Further calculation revealed that the correct space group is *Pnam*. Refinement based on that space group gave an R value of 0·044 for 1279 observed reflections.

In the centrosymmetric model there is a mirror plane through the Mg cation, both SCN anions and two of the coordinated water molecules (O8*w* and O9*w*). A crystallographic center of symmetry is located at the center of the 18-crown-6 ring. The full-matrix least-squares refinement gave $R = 0{\cdot}044$, $wR = 0{\cdot}057$, $S = 0{\cdot}57$, $w = [\sigma^2(F) + 0{\cdot}0191F^2]^{-1}$, max. $\Delta/\sigma = 0{\cdot}24$, max. and min. $\Delta\rho$ in final difference map 0·20 and −0·35 e Å^{-3}. The atomic coordinates with the old and new labels correlated are given in Table 1.* There are no significant changes in bond lengths and angles but the e.s.d.'s are better than previously reported. This correction does not affect the description of the complex.

The authors are indebted to Dr Le Page of the Chemistry Division, NRC, Ottawa, for the correction of the space group.

Table 1. *Atomic coordinates* (× 10^4) *and equivalent isotropic temperature factors* (Å^2)

$B_{eq} = \frac{8}{3}\pi^2 \sum_i \sum_j U_{ij} a_i^* a_j^* \mathbf{a}_i.\mathbf{a}_j.$

	x	y	z	B_{eq}
Mg	11180 (1)	5218 (1)	2500	2·41 (2)
S1	14690 (2)	7139 (1)	2500	6·44 (3)
S2	14135 (2)	3118 (1)	2500	5·17 (2)
N1	12839 (5)	5994 (2)	2500	4·37 (5)
N2	12653 (4)	4381 (2)	2500	3·71 (4)
C13	13587 (5)	6473 (3)	2500	3·47 (5)
C14	13254 (5)	3854 (2)	2500	3·15 (5)
O1,O4	8395 (3)	3803 (1)	10680 (2)	3·56 (3)
O2,O5	6946 (2)	5097 (1)	10434 (2)	3·59 (3)
O3,O6	8856 (3)	6290 (1)	10357 (2)	3·68 (3)
C1,C7	6875 (4)	3855 (2)	10505 (3)	4·19 (4)
C2,C8	6326 (4)	4514 (2)	10959 (3)	4·12 (4)
C3,C9	6704 (4)	5725 (2)	10957 (3)	4·29 (4)
C4,C10	7293 (4)	6317 (2)	10363 (3)	4·12 (4)
C5,C11	9427 (5)	6820 (2)	9717 (3)	4·66 (4)
C6,C12	11042 (4)	6818 (2)	9777 (3)	4·57 (4)
O7*w*,O10*w*	10907 (2)	5196 (1)	966 (2)	3·09 (3)
O8*w*	9421 (4)	4513 (2)	2500	3·61 (4)
O9*w*	9673 (4)	6052 (2)	2500	3·94 (4)

* Lists of anisotropic thermal parameters, revised H-atom coordinates and all bond lengths and angles have been deposited with the British Library Document Supply Centre as Supplementary Publication No. SUP 51069 (3 pp.). Copies may be obtained through The Executive Secretary, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

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Complexes of cadmium(II) bromide and cadmium(II) iodide with 18-crown-6 ether. Erratum.

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In Table 1 of the paper by Hazell [*Acta Cryst.* (1988), C**44**, 88–92] the z coordinate for C(1) should be −147 (5). Bond distances and angles were calculated from the correct coordinates.

All relevant information is contained in the *Abstract*.

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