SHORT COMMUNICATIONS

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The crystal structure of $(+)_{589}$-tris[(−)-*trans*-1,2-diaminocyclohexane]cobalt(III) chloride monohydrate* ('*ob*' isomer): errata.

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Abstract

The space group of the title compound [Kobayashi, Marumo & Saito (1972). *Acta Cryst.* B**28**, 2709–2715] is not $C2$ but $R32$. The $[10\bar{1}]$ zone axis of the $C2$ cell is the c axis of a trigonal cell with dimensions $a = 10{\cdot}714\ (4)$, $c = 18{\cdot}701\ (1)$ Å, $Z = 3$. The complex ion is thus required to have a rigorous D_3 symmetry. Refinement based on the correct space group gave an R value of 0·025 for 797 observed independent reflections.

The final atomic coordinates are given in Table 1 and relevant interatomic distances and bond angles are listed in Table 2¶ within a complex ion, which are close to the mean values of the previously reported values averaged by assuming D_3 symmetry.

The Miller indices and the fractional atomic coordinates for the $R32$ structure are related to those of the previous $C2$ structure by the following matrices:

(i) *Fractional atomic coordinates*

$$\begin{pmatrix} x \\ y \\ z \end{pmatrix} = \begin{pmatrix} 1/3 & 1 & 1/3 \\ 2/3 & 0 & 2/3 \\ 2/3 & 0 & -1/3 \end{pmatrix} \begin{pmatrix} x' \\ y' \\ z' \end{pmatrix} + \begin{pmatrix} -5/6 \\ -2/3 \\ -1/6 \end{pmatrix},$$

where x, y, z and x', y', z' are the $R32$ and $C2$ coordinates, respectively and the translation $(-5/6, -2/3, -1/6)$ moves the origin of coordinates of the $C2$ structure to that required for the standard setting of $R32$.

(ii) *Miller indices*

$$\begin{pmatrix} h \\ k \\ l \end{pmatrix} = \begin{pmatrix} 0 & 1 & 0 \\ 1/2 & -1/2 & 1 \\ 1 & 0 & -1 \end{pmatrix} \begin{pmatrix} h' \\ k' \\ l' \end{pmatrix},$$

where hkl are $R32$ indices and $h'k'l'$ are $C2$ indices.

The general structural features including absolute configuration are the same as for the previous paper.

The authors would like to thank Dr J. E. Davies of the University Chemical Laboratory, Cambridge, for pointing out this error.

Reference

KOBAYASHI, A., MARUMO, F. & SAITO, Y. (1972). *Acta Cryst.* B**28**, 2709–2715.

Table 1. *Positional and isotropic thermal parameters* ($\times 10^4$ *for non-hydrogen atoms,* $\times 10^3$ *for hydrogen atoms and* U_{eq})

	x	y	z	U_{eq}/U_{iso}* (Å²)
Co(1)	0	0	0	21
Cl(1)	5634 (1)	0	5000 (1)	56
N(1)	9002 (3)	8253 (2)	9396 (1)	27
C(1)	7781 (2)	7075 (2)	9797 (1)	24
C(3)	5866 (3)	6686 (3)	676 (1)	33
C(4)	4751 (3)	5434 (4)	221 (1)	44
O(1)†	0	0	7968 (4)	85
H(1)	849 (3)	863 (3)	101 (2)	9 (7)
H(2)	797 (3)	952 (3)	76 (1)	9 (7)
H(3)	668 (3)	821 (3)	−13 (1)	13 (7)
H(4)	544 (3)	716 (3)	92 (2)	19 (9)
H(5)	623 (3)	633 (3)	103 (1)	11 (8)
H(6)	427 (5)	577 (5)	−9 (2)	24 (8)
H(7)	401 (3)	476 (3)	51 (1)	10 (7)

* $U_{eq} = \frac{1}{3}\sum_i\sum_j U_{ij}a_i^*a_j^*\mathbf{a}_i.\mathbf{a}_j$.
† Population: 0·5.

Table 2. *Interatomic distances* (Å) *and bond angles* (°) *within the complex ion*

Co(1)–N(1)	1·980 (3)	N(1)–Co(1)–N(1′)	84·1 (1)
N(1)–C(1)	1·488 (4)	Co(1)–N(1)–C(1′)	110·2 (2)
C(1)–C(3)	1·522 (4)	N(1)–C(1)–C(1′)	106·0 (2)
C(1)–C(1′)	1·516 (4)	C(3)–C(1)–C(1′)	110·6 (2)
C(3)–C(4)	1·532 (5)	C(4)–C(3)–C(1)	110·1 (3)
C(4)–C(4′)	1·513 (6)	C(3)–C(4)–C(4′)	111·9 (3)
		N(1)–C(1)–C(3)	114·0 (2)

* IUPAC name: $(+)_{589}$-tris[(−)-*trans*-1,2-cyclohexanediamine]-cobalt(III) chloride monohydrate.

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¶ Lists of structure factors, anisotropic thermal parameters and interatomic distances and bond angles involving H atoms within a complex ion have been deposited with the British Library Lending Division as Supplementary Publication No. SUP 38321 (9 pp). Copies may be obtained through The Executive Secretary, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

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