SHORT COMMUNICATIONS

Contributions intended for publication under this heading should be expressly so marked; they should not exceed about 1000 *words; they should be forwarded in the usual way to the appropriate Co-editor; they will be published as speedily as possible.*

Acta Cryst. (1984). C**40**, 1110

Diamminebis(dimethylglyoximato)cobalt(III) tetracyanonickelate(II) hexahydrate, $2C_8H_{20}CoN_6O_4^+.C_4N_4Ni^{2-}.6H_2O$: corrigendum.*

By RICHARD E. MARSH, *Arthur Amos Noyes Laboratory of Chemical Physics, California Institute of Technology, Pasadena, California* 91125, *USA*

(*Received* 19 *December* 1983; *accepted* 4 *April* 1984)

Abstract

The crystal structure of $(C_8H_{20}CoN_6O_4^+)_2(C_4N_4Ni^{2-}).6H_2O$ should be described in the orthorhombic space group *Immm* rather than the triclinic $P\bar{1}$ reported by Solans, Font-Altaba, Bermejo & Alvarez [*Acta Cryst.* (1983), C**39**, 1510–1512)].

The crystal structure of this compound was described as triclinic, space group $P\bar{1}$, with $a = 14{\cdot}496$ (4), $b = 10{\cdot}542$ (4), $c = 7{\cdot}069$ (3) Å, $\alpha = 90{\cdot}18$ (2), $\beta = 104{\cdot}05$ (2), $\gamma = 111{\cdot}56$ (2)°, $Z = 1$ (Solans, Font-Altaba, Bermejo & Alvarez, 1983; SFBA). The vectors [211], [010], [001] describe a body-centered cell with $a' = 26{\cdot}020$ (8), $b'(=b) = 10{\cdot}542$ (4), $c'(=c) = 7{\cdot}069$ (3) Å, $\alpha'(=\alpha) = 90{\cdot}18$ (2), $\beta' = 90{\cdot}01$ (2), $\gamma' = 90{\cdot}30$ (2)°. The corresponding transformations $x' = \frac{1}{2}x$, $y' = y - \frac{1}{2}x$, $z' = z - \frac{1}{2}x$ lead to atomic coordinates that are consistent with the symmetry of the orthorhombic space group *Immm* well within the reported uncertainties. The *Immm* coordinates are given in Table 1.

That the atomic arrangement conforms so closely to the symmetry of *Immm* is clear proof that the measured intensities conform to Laue symmetry *mmm* within their e.s.d.'s (a hemisphere of data, or four equivalent forms, was collected); yet the unit-cell angles α' and γ' appear to deviate from 90° by highly significant amounts. Almost certainly this is a manifestation of the well-known phenomenon that *precision* is not a valid measure of *accuracy*. Absorption, mis-centering of the crystal, misalignment of the diffractometer and other such effects can cause systematic errors in the orientation angles that, depending upon the region of reciprocal space in which the calibrating reflections lie, may result in unit-cell inaccuracies far larger than the derived precisions would suggest. The common practice of using precision indicators when specifying accuracies is a dangerous one.

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

Numbers in square brackets are coordinate shifts (averaged when two atoms are involved) necessary to achieve the symmetry of *Immm*; numbers in parentheses are e.s.d.'s (averaged where necessary) in a single parameter, obtained from Table 1 of SFBA.

	x	*y*	*z*
Ni	0	0	0
Co	2199 [–[(1)	0 [0] (2)	5000 [1] (2)
C(12)	0 [1] (6)	1745 [–] (20)	0 [27] (28)
N(12)	0 [4] (6)	2848 [–] (20)	0 [0] (39)
C(13)	728 [–] (6)	0 [5] (16)	0 [6] (20)
N(13)	1167 [–] (5)	0 [12] (15)	0 [9] (19)
O(21,26)	2676 [0] (4)	2442 [2] (11)	5000 [5] (13)
N(22,25)	2751 [0] (5)	1191 [7] (14)	5000 [7] (14)
C(23,24)	3210 [2] (5)	698 [8] (17)	5000 [1] (19)
C(27,28)	3678 [1] (6)	1484 [28] (21)	5000 [38] (29)
O(31,36)	1722 [0] (4)	2416 [8] (14)	5000 [2] (16)
N(32,35)	1645 [2] (4)	1170 [0] (14)	5000 [4] (15)
C(33,34)	1183 [1] (6)	713 [19] (20)	5000 [11] (19)
C(37,38)	709 [3] (7)	1482 [8] (24)	5000 [15] (29)
N(2,3)	2196 [5] (4)	0 [34] (16)	2252 [8] (16)
O(*W*1)	1779 [–] (4)	5000 [3] (12)	5000 [13] (16)
O(*W*2)	0 [12] (10)	5000 [0] (26)	2296 [–] (35)
O(*W*3)	708 [–] (8)	5000 [16] (27)	5000 [100] (61)

If preliminary photographs had been taken, it is very probable that the higher Laue symmetry would have been recognized and the unit-cell angles would have been constrained to 90°.

Editorial note: Authors informed a Co-editor that the possible higher symmetry was not overlooked by SFBA; space groups *Immm* and $P\bar{1}$ were both investigated by them before preparation of their paper. SFBA decided to consider space group $P\bar{1}$, according to e.s.d.'s and thermal coefficients obtained in the refinement in both space groups.

* Contribution No. 6960 from the Arthur Amos Noyes Laboratory of Chemical Physics. This work was supported in part by National Insitutes of Health Research Grant No. GM 16966.

0108-2701/84/061110-01$01.50

Reference

SOLANS, X., FONT-ALTABA, M., BERMEJO, M. J. & ALVAREZ, S. (1983). *Acta Cryst.* C**39**, 1510–1512.