Additions and Corrections

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S. Chandrasekhar, D. G. Fortier, and A. McAuley*: Syntheses of Chromium and Copper Complexes of Hexaazamacrocycles. Crystal Structures of Chromium(III) Complexes of 1,4,7,10,13,16-Hexaazacyclooctadecane and 1,4,7,11,14,17-Hexaazacycloeicosane.

Pages 1424−1429. In the original paper, we presented data for the synthesis and crystal structure of [Cr(1,4,7,10,13,16-hexaazacyclooctadecane)]Br_3 together with other macrocyclic species. However, following further spectroscopic studies, it became clear that the wrong space group I_12/m_1 (No. 12) was used for this complex. The data have been re-examined and have been found to conform to the space group $R\bar{3}m$ (trigonal, No. 166). The pertinent data are as follows: $a = b = c =$ 8.038(3) Å, $\alpha = \beta = \gamma = 72.83(3)°$, 1 molecule/unit cell, cell volume 463 Å^3. Refinement of the structure in the new unit cell leads to an asymmetric unit that is one-twelfth of the complex cation with the following fractional atomic coordinates and temperature factors:

atom	*x/a*	*y/b*	*z/c*	U_{eq}, Å^2
Cr	0(1)	0(1)	0(1)	178(5)
Br(1)	22055(8)	22055(8)	22055(8)	325(4)
Br(2)	50000(1)	50000(1)	50000(1)	381(5)
N(1)	1691(5)	−1619(8)	1691(5)	28(3)
C(1)	3242(9)	−2711(11)	686(9)	69(4)

Estimated standard deviations are given in parentheses; coordinates × 10^n, $n = 5, 5, 4, 4$ for Cr, Br, N, C; temperature parameters × 10^n, $n = 4, 4, 3, 3$ for Cr, Br, N, C. U_{eq} = the equivalent isotropic temperature parameter = $^1/_3\sum_i\sum_j U_{ij}a_i^*a_j^*(\mathbf{a}_i\cdot\mathbf{a}_j)$. The number of reflections used was 751 ($I > 2\sigma_I$) out of a total of 872, with 23 parameters to be refined in the cycle. Refinement converged at $R = 0.067$ and $R_w = 0.076$, where R and R_w are defined in the paper and $w = 4.3/(\sigma_F^2 + 0.001F^2)$. The overall structural form of the cation is that depicted in the paper, but several of the bond angles and interatomic distances differ. All Cr−N distances are identical at 2.092(6) Å. The N(1)−C(1) bond distance is 1.468(7) Å, and C(1)−C(1)′ is 1.497(16) Å. Bond angles are C(1)−N(1)−Cr = 110.0(4)°, C(1)−N(1)−C(1)′ = 112.3(8)°, the open-faced angle N(1)−Cr−N(1)′ = 97.9(2)°, and the internal chelating angle N(1)−Cr−N(1)″ = 82.1(2)°. As a result, the trigonal twist angle is now 60°.

Supplementary Material Available: Listings of anisotropic temperature factors and selected intermolecular distances (1 page). Ordering information is given on any current masthead page.

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