The Structure of Hexaaquo-tris(*N,N*-dimethylformamide)neodymium Trifluoromethanesulfonate

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Recently [1], a series of lanthanide compounds of the general formula $[Ln(DMF)_3(H_2O)_6](CF_3SO_3)_3$ (Ln = La, Ce, Pr, Nd, Sm, Eu, Tb and Dy) was synthesized and the structure of the neodymium compound was established by a single-crystal X-ray diffraction analysis. The crystals were reported to be triclinic, space group $P1$, with $a = 8.589(4)$, $b = 11.222(2)$, $c = 12.271(2)$ Å, $\alpha = 56.83(2)$, $\beta = 62.13(2)$, $\gamma = 75.14(2)^\circ$, $Z = 1$. The structure is properly described as rhombohedral, space group $R3m$. The vectors $[1,0,\bar{1}]$, $[0,1,0]$ and $[0,\bar{1},1]$ define, within experimental error, a rhombohedral cell with $a_r = 11.219(2)$ Å, $\alpha_r = 113.72(2)^\circ$, $Z = 1$. After suitable transformation and averaging, the atom coordinates in Table 1 result. The agreement among the coordinates that were averaged is approximately what would be expected from the esd's reported in Table III of ref. 1.

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TABLE 1. $[Nd(DMF)_3(H_2O)_6](CF_3SO_3)_3$; coordinates, space group $R3m$

Atom	Site	x	y	z
Nd	1(a)	0.0	0.0	0.0
OWA	3(b)	−0.257	−0.257	−0.091
OWB	3(b)	0.155	0.155	0.319
O1	3(b)	0.076	0.076	−0.145
C1	3(b)	0.120	0.120	−0.197
N(1)	3(b)	0.156	0.156	−0.277
C(11)	6(c)	0.251	0.124	−0.316
S	3(b)	−0.3856	−0.3856	0.3054
O(11)	6(c)	−0.347	−0.228	0.421
O(13)	3(b)	−0.534	−0.534	0.187
C(111)	3(b)	−0.343	−0.343	0.187
F(11)	3(b)	−0.198	−0.198	0.287
F(12)	6(c)	−0.355	−0.460	0.082

There are no significant changes in bond lengths or angles. The point symmetry of the coordination polyhedron is C_{3v}, as noted in ref. 1; in space group $R3m$ that symmetry is crystallographically exact rather than only approximate.

References

1 D. M. Araújo Melo, G. Vicentini, L. B. Zinner, C. A. de Simone and E. E. Castellano, *Inorg. Chim. Acta, 146* (1988) 123.

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