Hexamethylphosphoramide Compounds: II. The Structure of a Complex Containing Two Different Coordination Polyhedra for Two Independent Neodymium(III) Ions

C. A. De Simone[a]; E. E. Castellano[a]; C. A. Fantin[b]; L. B. Zinner[b]; G. Vicentini[b]

[a] Instituto de Física e Química de São Carlos, Universidade de São Paulo, São Carlos, SP, Brazil [b] Instituto de Química, Universidade de São Paulo, São Paulo, SP, Brazil

PLEASE SCROLL DOWN FOR ARTICLE

Hexamethylphosphoramide Compounds: II. The Structure of a Complex Containing Two Different Coordination Polyhedra for Two Independent Neodymium(III) Ions

C.A. de Simone and E.E. Castellano, Instituto de Física e Química de São Carlos, Universidade de São Paulo, C.P. 369, 13.560, São Carlos, SP, Brazil.

C.A. Fantin, L.B. Zinner and G. Vicentini*, Instituto de Química , Universidade de São Paulo, C.P. 20.780, 01498, São Paulo, SP, Brazil.

The crystal structure of the complex of formula $\{|Nd(NCS)_3(HMPA)_3|$ $|Nd(NCS)_3(HMPA)_4|\}$ was determined by three-dimensional X-ray diffraction methods and refined anisotropically to a R = 0.040. The compound crystallizes in the trigonal system, space group R3 (N⁰ 146), with a = 19.947(3), b = 19.947(3), c = 20.106(3) Å, $\alpha = \beta =$ 90, γ = 120⁰, V = 6928(4) Å³, M = 1891.4, Z = 3, D_c = 1.360 g cm⁻³, λ(MoKα) = 0.71073 Å, μ = 1.4 cm⁻¹, F(000) = 2922.01. There are two independent Nd^{3+} ions located in the three fold axis. One of them, located at the origin (000) is coordinated to nitrogen atoms of three symmetry related NCS⁻ anions which are below the (x y) plane (negative z) and also to the oxygen atoms of three symmetry related HMPA groups above that plane. The coordination polyhedron is a slightly distorted octahedron. The other Nd^{3+} ion is located at (00,0.5025(1)). It is coordinated to the nitrogen atoms of three symmetry related NCS⁻ anions above the (xy $\frac{1}{2}$) plane and to oxygen atoms of three symmetry related HMPA groups below that plane. Another HMPA group has the O and P atoms located on the three-fold axis, above the (xy $\frac{1}{2}$) plane. The coordination number is in this case 7 and the polyhedron is a capped trigonal antiprism. The mean distances are: Nd-N = 2.44 Å, Nd-O = 2.35 Å and Nd-N = 2.52 Å, Nd-O = 2.36 Å for the octahedron and antiprism configurations , respectively. (CNPq, FAPESP, FINEP)