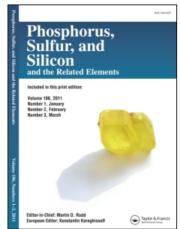
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Hexamethylphosphoramide Compounds: II. The Structure of a Complex Containing Two Different Coordination Polyhedra for Two Independent Neodymium(III) Ions

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

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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. compound crystallizes in the trigonal system, space group R3 146), with a = 19.947(3), b = 19.947(3), c = 20.106(3) Å, $\alpha = \beta =$ 90, $\gamma = 120^{\circ}$, V = 6928(4) Å³, M = 1891.4, Z = 3, $D_c = 1.360 \text{ g cm}^{-3}$, $\lambda \, (\text{MoK}\alpha) = 0.71073 \, \text{Å}, \, \mu = 1.4 \, \text{cm}^{-1}, \, F(000) = 2922.01.$ There are two independent Nd3+ ions located in the three fold axis. One of them, located at the origin (000) is coordinated to nitrogen atoms three symmetry related NCS anions which are below the (x y) plane (negative z) and also to the oxygen atoms of three symmetry lated HMPA groups above that plane. The coordination polyhedron is a slightly distorted octahedron. The other Nd³⁺ ion is located at (00,0.5025(1)). It is coordinated to the nitrogen atoms of 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: $Nd-N = 2.44 \stackrel{\circ}{A}$, $Nd-0 = 2.35 \stackrel{\circ}{A}$ and $Nd-N = 2.52 \stackrel{\circ}{A}$. Nd-O = 2.36 Å for the octahedron and antiprism configurations , respectively. (CNPq, FAPESP, FINEP)