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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 $\{[\text{Nd}(\text{NCS})_3(\text{HMPA})_3][\text{Nd}(\text{NCS})_3(\text{HMPA})_4]\}$ 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 $R\bar{3}$ (No 146), with $a = 19.947(3)$, $b = 19.947(3)$, $c = 20.106(3)$ Å, $\alpha = \beta = 90^\circ$, $\gamma = 120^\circ$, $V = 6928(4)$ Å³, $M = 1891.4$, $Z = 3$, $D_c = 1.360$ g cm⁻³, $\lambda(\text{MoK}\alpha) = 0.71073$ Å, $\mu = 1.4$ 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 (xy) 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: $\text{Nd-N} = 2.44$ Å, $\text{Nd-O} = 2.35$ Å and $\text{Nd-N} = 2.52$ Å, $\text{Nd-O} = 2.36$ Å for the octahedron and antiprism configurations, respectively. (CNPq, FAPESP, FINEP)