Crystal Structure of Octahedral Nickel(II) Complex of Hexaazamacrotetracycle Containing Axial Azido Ligand

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The complex $[NiL(N_3)_2]_2 \cdot 5H_2O$ (1) (L = 1,3,10,12,15,18-hexaazatetracyclo[16.2.1.1^{12,15}.0^{4,9}] docosane) has been synthesized and structurally characterized. 1 crystallizes in the triclinic space group $P\overline{1}$, a = 8.6881(52)Å, b = 15.6997(19)Å, c = 17.4574((22)Å, α = 109.2728(104)°, β = 90.8492(220)°, γ = 93.5914(213)°, V = 2242(1), Z = 2 with two molecules in an asymmetric unit. The complex (1) contains two 1,3-diazacyclopentane subunits in the six-membered chelate rings and one cyclohexane subunit in the five-membered chelate ring. The nickel(II) ion is coordinated to the two tertiary and two secondary nitrogen atoms in a basal plane and two axial azido ligands with a distorted octahedral geometry.

