Synthesis and Structure of a Tetranuclear Nickel Complex of a 40-Membered Macrocyclic Octaamine-Tetrathiophenolate Ligand

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The syntheses and characterization of tetranuclear Ni complexes [(L²)Ni₄][ClO₄]₄ (3) and [(L²)Ni₄(NCS)₄] (4) of a 40-membered macrocyclic octaamine-tetrathiophenolate ligand (L²)₄ are described. Single-crystal X-ray structure analysis of 4 reveals well-separated molecules of the tetranuclear isothiocyanate complex [(L²)Ni⁴(μ²-NCS)]₄. The four Ni³⁺ centers are arranged in binuclear [Ni₂Ni(μ-SR)₂Ni₂(NCS)]₂ subunits containing distorted square-planar NiN₂S₂ and distorted octahedral NiN₂S₂(NCS)₂ sites. The fact that the two isothiocyanate groups at the octahedral Ni site are in trans positions can be ascribed to the large ring size of the macrocycle.