Hexanuclear and octanuclear metal complexes of octadecaazamacrocycle based on diaminocyclohexane and pyridine units

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Streszczenie

An extended macrocyclic amine **L** derived from the [6+6] condensation of *trans-1,2*-diaminocyclohexane and 2,6-diformylpyridine contains 18 nitrogen atoms in its main cycle. All of these atoms can be engaged in the formation of polynuclear complexes with transition metal ions and the macrocycle **L** is able to bind six Cu(II), Ni(II) or Zn(II) ions within its interior. X-ray crystal structures of these complexes indicate variable coordination numbers of metal ions as well as various conformations adopted by the macrocyclic ligand. In the hexanuclear Cu(II) complex with coordinated nitrate anions Cu(II) ions are hexacoordinate and exhibit highly distorted octahedral geometry, while in analogous complexes with coordinated sulphate anions Cu(II) ions are pentacoordinate of distorted square pyramid geometry. Both complexes are relatively symmetric having (approximate) S_6 axis and adopt a circular doughnut shape with a central void not occupied by metal ions. The NMR spectrum of the zinc(II) derivative also reflects the symmetrical coordination. In contrast, the macrocycle **L** is squeezed and less symmetric in the octanuclear chloride derivative where two additional Cu(II) ions are linked to a hexanuclear macrocyclic unit via chloride bridges. The macrocycle is also squeezed in the hexanuclear Ni(II) complex containing metal ions of approximate octahedral geometry. In all three Cu(II) complexes the macrocycle provides N_3 donor set for each metal ion, while in the Ni(II) complex alternating N_3 and N_4 environments of the metal ions are observed.

Słowa kluczowe

Macrocyclic complexes, Polynuclear complexes, Nickel(II), Copper(II), Crystal structure