Tricyclic ligands on cyclam core and X-ray crystallographic structure of hexachloro-(1,11:4,8-bis(pyridine-2,6-diyl-bis(2-(*N*-(2-formidoylethylene)carbamoyl)ethylene))-1,8-diazonia-4,11-diazacyclotetradecane)-dimanganese(II) dimethanol dihydrate solvate.

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Streszczenie

The synthesis of tricyclic compounds on functionalized cyclam core is described. The addition of four methyl acrylate molecules and consecutive condensation of this derivative with ethylenediamine resulted in formation of 1,4,8,11-tetrakis(2-(N-(2-aminoethyl)carbamoyl)ethyl)-1,4,8,11-tetraazacyclotetradecane (3). Compound 3 was the substrate for further condensation with dialdehydes: iso-phthaldialdehyde and 2,6-pyridinedicarbaldehyde, resulting in spontaneous macrocycle ring closure to give tricyclic derivatives: 1,11:4,8-bis(benzene-1,3-diyl-bis(2-(N-(2-formidoylethylene)carbamoyl)ethylene))-1,4,8,11-tetraazacyclotetradecane (4) in the reaction of 3 with iso-phthaldialdehyde and three isomers: 1,4:8,11-bis(pyridine-2,6-diyl-bis(2-(N-(2-formidoylethylene)carbamoyl)ethylene))-1,4,8,11-tetraazacyclotetradecane (5A), 1,11:4,8-bis(pyridine-2,6-diyl-bis(2-(N-(2-formidoylethylene)carbamoyl)ethylene))-1,4,8,11-tetraazacyclotetradecane (5B), and 1,8:4,11-bis(pyridine-2,6-diyl-bis(2-(N-(2-formidoylethylene)carbamoyl)ethylene))-1,4,8,11-tetraazacyclotetradecane (5C) when 2,6-pyridinedicarbaldehyde was used. The compounds 4, 5B, and 5C were identified crystallographically. The isolated 5A converted in solution into the mixture of 5B and 5C as monitored by the 1H NMR spectroscopy. The tricycle 5 is able to accept two manganese(II) metal ions by reacting with manganese(II) dichloride with simultaneous diprotonation of 5. Structure of the resulting Mn2(5BH2)Cl6·(CH3OH)2(H2O)2 was determined crystallographically.

Słowa kluczowe

Macrocycle, cyclam, Schiff-base, Isomers, Dimanganese(II) complex