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Mono and dinuclear Re(V) complexes with a hydrospirophosphorane HP~O derived ligand: synthesis, structural analysis and molecular dynamics.

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Streszczenie

Two neutral mono and dinuclear rhenium(V) complexes, cis-ReOCl2(P~O)(pym) (1) and cis-[ReOCl2(P~O)]2(μ–pym) (2 · (CH3)2CO), with the hydrospirophosphorane ligand HP~O (HP~O = octamethyl-2,2,3,3,7,7,8,8-tetraoxa-5λ5 1,4,6,9-phosphaspiro-4,4-nonane) have been prepared. The coordination geometry of the complexes has been determined in solution by NMR and UV–Vis spectroscopy, as well as in the solid state by IR, FIR spectroscopy and single crystal X-ray diffraction. The complexes display distorted octahedral geometries. X-ray structures of 1 and 2 reveal that the ReCl2NP fragments are equatorially disposed and the oxygens, terminal oxo and alcoholato, lie in axial positions. The pyrimidine coordinates as a monodentate or bridging ligand. Detailed temperature dependent 1H NMR analysis for both 1 and 2 shows that in solution the diaza moiety exhibits hindered rotation about the Re–N bond. Furthermore two concomitant conformation changes, one in the metallacycle and the second in the phosphorus cycle, are also observed for dimer 2.

Słowa kluczowe

Oxo-rhenium(V) complexes, Hydrospirophosphorane ligand, Diaza ligand, Dinuclear compound

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