Oxo-entity-controlled diastereomer peculiarity of rhenium(V) complexes $ReOX_2(P{\sim}O)py$ [X=Cl, Br, I; P~O = $(OCMe_2CMe_2O)POCMe_2CMe_2O(1–)$;py = pyridine]: synthesis and molecular and crystal structural characterization.

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Streszczenie

The stability of diastereomers of ReOX2(P~O)py complexes determined by the arrangement of the oxo-entity O=Re-(–O~P) is manifested in molecular recognition and crystallization behavior [X = Cl, Br, I; P~O = (OCMe2CMe2O)POCMe2CMe2O(
1–); py = pyridine]. With X = Cl and Br both chiral cis [OC-6–52] and achiral trans [OC-6–15] complexes can be obtained concomitantly, while for X = I only a trans complex can be afforded. Molecular structures were characterized using NMR IR and UV/Vis spectroscopic methods with the aid of DFT computational analysis and were ultimately corroborated by the single-crystal X-ray diffraction method. These analyses revealed that the most stable diastereomers involve an O=Re(–O~P) oxo arrangement in an
axial disposition reinforced with a phosphorus ligating atom mutually cis due to extensive π-bonding both for chiral cisand achiral trans complexes, regardless of whether X = Cl, Br, or I. However, the disparate intramolecular geometry
either cis or trans in the solid state results in enantiomorphic crystals related to space group P212121 (X = Cl, Br) or crystals pertinent to the centrosymmetric framework P21/c (X = Cl, Br, I), respectively. Thoughtful analysis of crystal structures
reveals a supramolecular architecture due to intermolecular forces involving hydrogen bonding and electric dipole–dipole
interactions (among other contact interactions). Thus, chiral cis complexes (X = Cl, Br) show helical crystal packing that succeeds in spontaneous resolution, while trans stereoisomers (X = Cl, Br, I) do not and rather exhibit a zig-zag supramolecular framework

Słowa kluczowe

Noncovalent interactions, Crystal engineering, Rhenium complexes, P, O ligand, Density functional calculations

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