

Ti^{IV} and Mo^V complexes with diesters. The crystal structure of [o-C₆H₄(CO₂CH₂CH₂Ph)₂Cl₄Ti], [C₂O₄(CH₂CH₂Ph)₂Cl₄Ti] and [o-C₆H₄(CO₂Et)₂Cl₃MoO]·C₆H₆.

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Streszczenie

The crystal structures of [o-C₆H₄(CO₂CH₂CH₂Ph)₂Cl₄Ti] (I), in the presence of activators a good catalyst for olefin polymerization, [C₂O₄(CH₂CH₂Ph)₂Cl₄Ti] (II) and [o-C₆H₄(CO₂Et)₂Cl₃MoO] (III), have been determined by X-ray diffraction methods and refined by a full-matrix least-squares technique to $R = 0.036$, 0.041 and 0.055 for 2775, 2437 and 2776 independent non-zero reflections for I, II and III, respectively. The crystals of I are triclinic, space group P with two molecules in a unit cell of dimensions $a = 10.475(8)$, $b = 10.078(9)$, $c = 13.683(9)$ Å, $\alpha = 88.75(7)$ °, $\beta = 72.65(6)$ °, $\gamma = 66.95(7)$ °. The crystals of II are monoclinic, space group $P2_1/c$, with four molecules in a cell with $a = 10.045(8)$, $b = 21.032(22)$, $c = 13.193(9)$ Å, $\beta = 128.91(6)$ °. The titanium atoms in I and II are octahedrally coordinated by four chlorine and two carbonyl oxygen atoms of coordinated *o*-diester molecules in the *cis* position. The crystals of III are triclinic, space group P , with two molecules in a unit cell of dimensions $a = 9.722(12)$, $b = 8.073(12)$, $c = 15.683(21)$ Å, $\alpha = 83.46(9)$ °, $\beta = 75.81(9)$ °, $\gamma = 67.74(9)$ °. Three Cl atoms, one oxo oxygen and two O atoms of the carbonyl groups form a distorted octahedron around the molybdenum atom. The chelate ligand atoms and the titanium atom in I or molybdenum atom in III form a seven-membered ring which is five-membered in II.

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