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Synthesis and Crystal Structures of Phosphorusand Selenium-Containing Medium-Sized Heterocycles and Macrocycles

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New phosphorus- and selenium-containing heterocyclyes, 1,3,2,6-dioxaphosphaselenacyclooctanes (1a-1o), were synthesized in ca. 10% yields from 3-selena-1,5-penta-diol and $RP(X)Cl_2$ where R = alkoxyl, aroxyl, aryl and X = 0 or lone pair. Three macrocycles 3, 4 and 5, which were expected to be heterodinucleating ligands, were obtained in moderate yields (20-30%) from bis(o-bromomethylphenyl)phenylphosphine oxide 2 and corresponding selenium-containing materials.

These compounds formed complexes with heavy metals such as palladium(II) ion via their selenium atoms. The bioactivity of heterocycle 1c (X = O, R = 4-methylphenoxyl) was studied. The molecular structures of heterocycle 1c, macrocycle 3 and the complex $Pd(1c)_2Cl_2$ have been established by X-ray diffraction. It was found that the eight-membered ring of 1c and $Pd(1c)_2Cl$ existed in an unsymmetic boat-chair conformation in the solid state, and that there existed four pairs of two independent molecules in the unit cell of macrocycle 3.

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