Abstract

Title: Synthesis of a ferrocenyl-substituted bicyclic phosphite

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This thesis synthesis describes the of a novel bicyclic phosphite $\{N-(2,6,7-\text{trioxa-1-phosphabicyclo}[2.2.2]\text{oct-4-yl}\}$ ferrocene (3). This compound was obtained by the reaction of phosphorus trichloride with the appropriate tris(hydroxymethyl)methyl-amide in the presence of triethylamine or pyridine. The reaction conditions were optimized by varying the solvent, reaction temperature and the base to achive the highest possible yield of the product and to enable its easy and effective chromatographic purification. A new compound, 2-ferrocenyl-4,4-bis(chloromethyl)-4,5-dihydro-1,3-oxazol (4), was isolated as the by-product of this reaction. Compound 3 was further used to prepare the carbonyl complex cis-[W(CO)₄(3- κP)₂] (5). All the newly prepared compounds were characterized by NMR spectroscopy, mass spectrometry, infrared spectroscopy and by elemental analysis, and their molecular structures were determined by X-ray diffraction analysis. Hydrogen bonds are cooperating to form one-dimensional chains in the crystals of phosphite 3 and solvate $4 \times \frac{1}{2}$ H₂O or complicated three-dimensional assemblies in the case of solvate $5 \times \text{Me}_2\text{CO} \times \text{H}_2\text{O}$.

Keywords: phosphites; ferrocene ligands; complexes; structure elucidation