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Systematic Coordination of Water-Soluble Monoand Bidentate Phosphine Ligands to the Organometallic Precursor fac-[ReBr₃(Co)₃]²⁻

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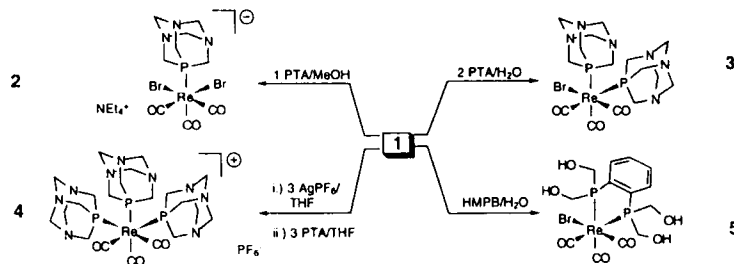
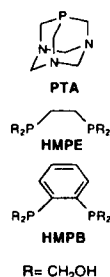
Systematic Coordination of Water-Soluble Mono- and Bidentate Phosphine Ligands to the Organometallic Precursor $fac-[ReBr_3(CO)_3]^{2-}$

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As part of our ongoing studies to develop new radiopharmaceuticals (and catalysts) based on water-soluble phosphines for diagnostic and therapeutic purposes, we are investigating the basic coordination behavior of mono- (PTA) and bidentate (HMPE, HMPB) ligand systems towards the low valent rhenium center $fac-[ReBr_3(CO)_3]^{2-}$ (1) in water and organic solvents at room temperature.

Depending on the reaction conditions we were able to quantitatively synthesize the mono- ($[ReBr_2PTA(CO)_3]^-$ 2), di- ($[ReBrPTA_2(CO)_3]$ 3) and tri-substituted ($[RePTA_3(CO)_3]^+$ 4) complexes as well as the neutral complexes $[ReBrL(CO)_3]$ (L = HMPE 5, HMPB 6).



Due to the mild reaction conditions (room temperature) we were able to elucidate the substitution mechanisms in the case of the neutral complexes 3, 5 and 6 by means of ^{31}P -NMR spectroscopy. Especially in the case of compound 3, we observed a strong influence of the coordination capacity of the solvent on the number of species during the substitution reaction and reaction kinetics. The presented complexes are the first examples of rhenium-carbonyl compounds with water-soluble phosphine ligand systems systematically investigated in respect to their substitution mechanism in aqueous and organic solutions under ambient conditions.