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The synthesis and structural comparison of $fac-[Re(CO)_3]^+$ containing complexes with altered β -diketone and phosphine ligands

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Abstract

Six rhenium(I) complexes are structurally compared, with regards to steric and electronic influences induced by the different β -diketone (benzoylacetone – Benzac, trifluoroacetylacetone – Tfaa and hexafluoroacetylacetone – Hfaa) and phosphine ligands (cyclohexyldiphenyl phosphine - PPh_2Cy and dicyclohexylphenyl phosphine - $PPhCy_2$). The complexes $fac-[Re(Benzac)(CO)_3(PPh_2Cy)]$ (**2**), $fac-[Re(Benzac)(CO)_3(PPhCy_2)]$ (**3**), $fac-[Re(Tfaa)(CO)_3(PPh_2Cy)]$ (**5**), $fac-[Re(Tfaa)(CO)_3(PPhCy_2)]$ (**6**), $fac-[Re(Hfaa)(CO)_3(PPh_2Cy)]$ (**8**) and $fac-[Re(Hfaa)(CO)_3(PPhCy_2)]$ (**9**) were synthesized by using the '2+1' mixed ligand approach and characterized by means of IR, UV/Vis, 1H -, ^{13}C - and ^{31}P NMR and also X-ray diffraction, clearly showing the increase in the carbonyl stretching frequencies and downfield shifts in the ^{31}P NMR as the fluoro atoms on the ligand backbone increases. The Tolman angles for the coordinated phosphine ligands are: **2** = 134.77° ; **3** molecule A = 146.81° ; **5** = 134.46° ; **6** = 146.05° ; **8** = 136.68° and **9** = 146.22° , illustrating the change in steric bulk as the cyclohexyl ligands on the phosphine ligands increase. A direct link is noted between the Re-P distances ($2.4906(6)$ Å for **2**, $2.5213(17)$ Å for **3** molecule A, $2.4865(16)$ Å for **5**, $2.5372(15)$ Å for **6**, $2.4906(14)$ Å for **8** and $2.5365(16)$ Å for **9**), O,O'-bidentate ligand bite angles, O4-Re-O5, ($85.12(6)^\circ$ for **2**, $83.34(13)^\circ$ for **3** molecule A, $84.91(12)^\circ$ for **5**, $83.53(12)^\circ$ for **6**, $84.54(11)^\circ$ for **8** and $83.7(2)^\circ$ for **9**) and the calculated dihedral angles ($3.677(1)^\circ$ for **2**, $12.521(1)^\circ$ for **3** molecule A, $1.489(7)^\circ$ for **5**, $12.463(11)^\circ$ for **6**, $2.940(7)^\circ$ for **8** and $11.747(6)^\circ$ for **9**). The dihedral angle is calculated between the equatorial plane (Re1,C1,O1,C2,O2,O4,C5,C6,C7,O5) and the plane through Re1,O4,C5,C6,C7,O5. Dihedral angles of approximately four times larger are observed in complexes with coordinated $PPhCy_2$ ligands compared to the PPh_2Cy containing analogues, indicating the steric effect induced on the bidentate ligand by the extra cyclohexyl substituent on the $PPhCy_2$ ligand.

1. Introduction

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