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New bis-rhodium complex with a bidentate 3-phosphino-1,2,3,6-tetrahydrophosphinine P-ligand

Irina Odinets, Tamás Körtvélyesi, Réka Herbay, Péter Bagi and György Keglevich

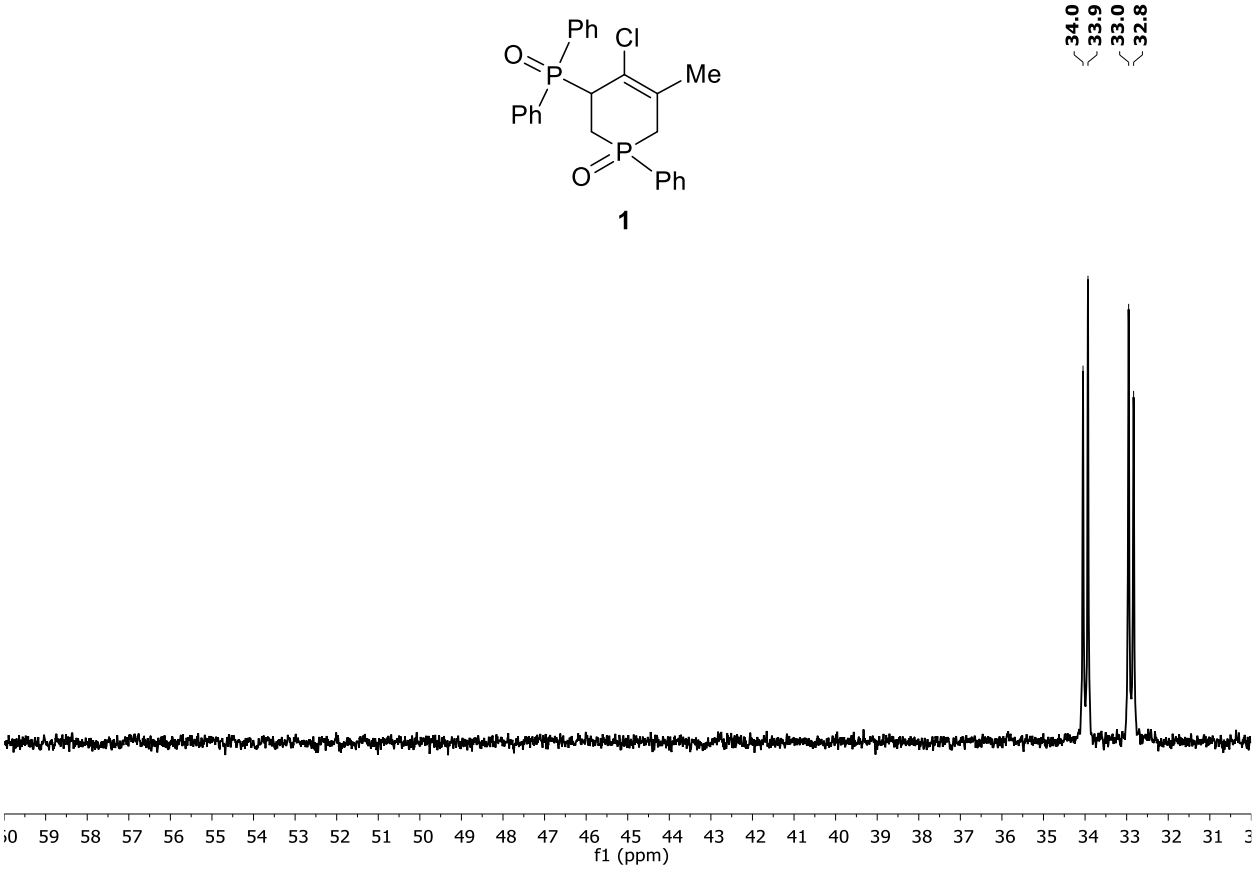

Figure S1. ^{31}P NMR spectrum of 4-chloro-3-diphenylphosphoryl-5-methyl-1-phenyl-1,2,3,6-tetrahydrophosphinine oxide **1.**

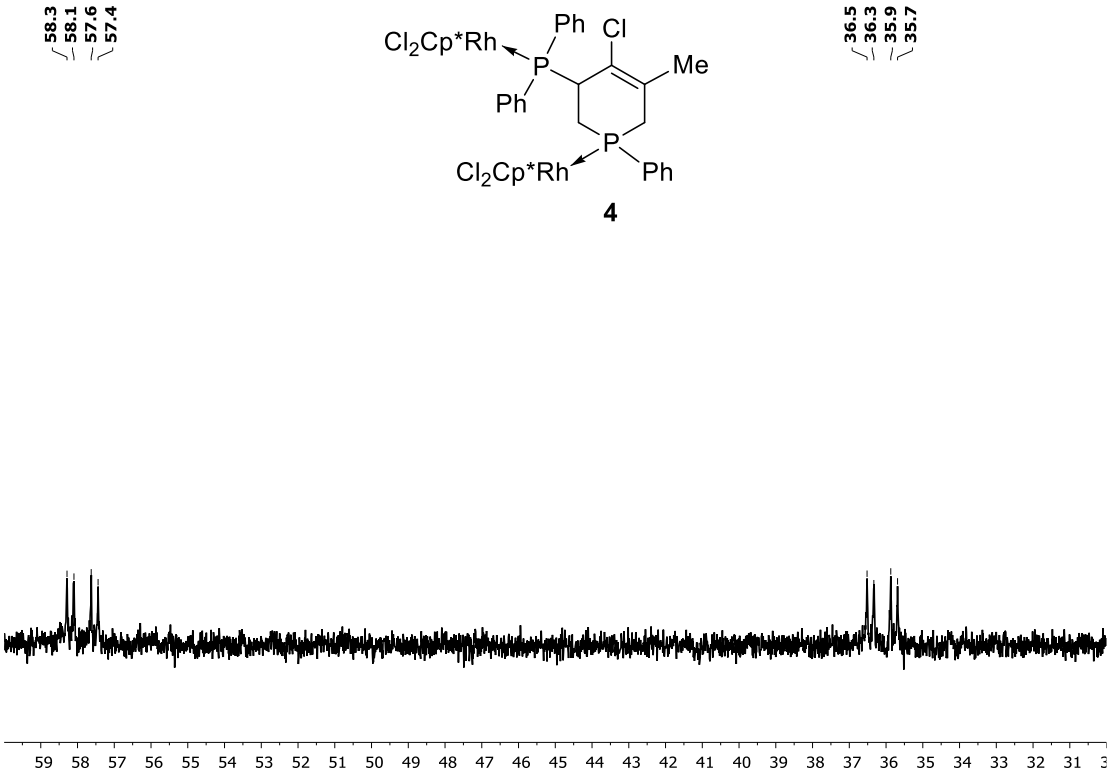

Figure S2. ^{31}P NMR spectrum of [4-chloro-3-diphenylphosphino-5-methyl-1-phenyl-1,2,3,6-tetrahydrophosphinine-P,P']bis[dichloro(pentamethylcyclopentadienyl)rhodium(III)] **4** with chemical shift values.

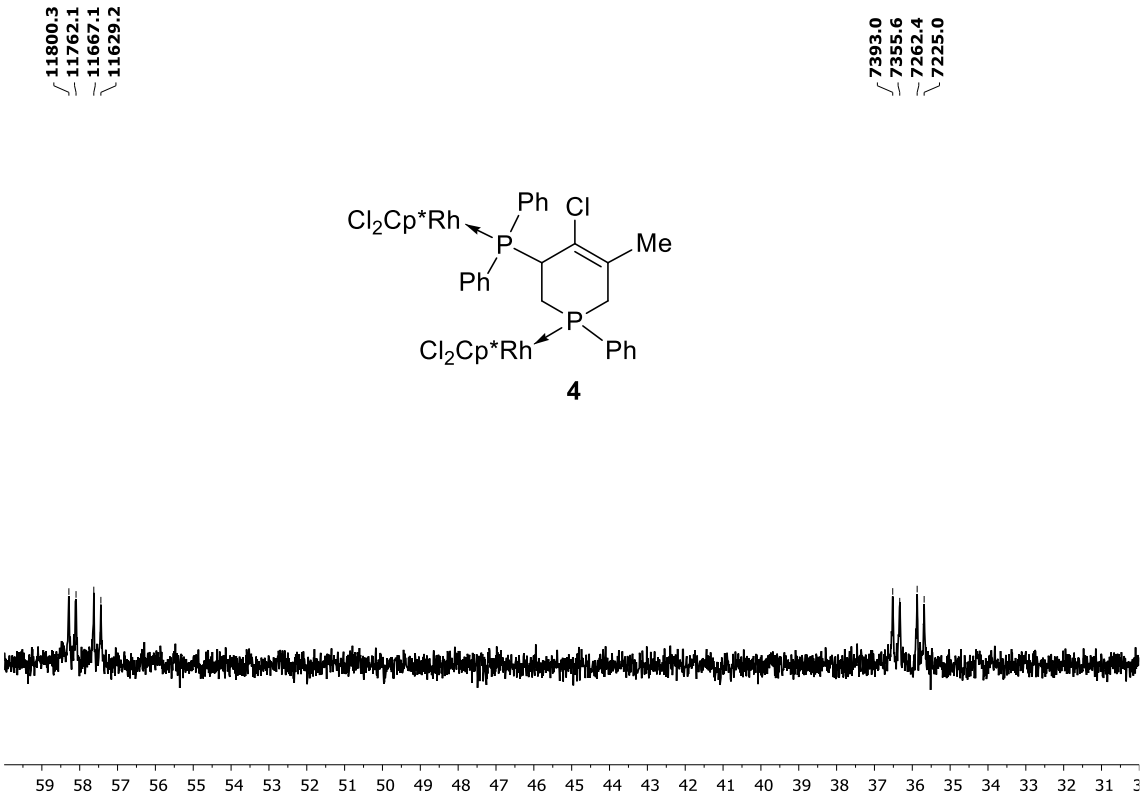

Figure S3. ^{31}P NMR spectrum of [4-chloro-3-diphenylphosphino-5-methyl-1-phenyl-1,2,3,6-tetrahydrophosphinine-P,P']bis[dichloro(pentamethylcyclopentadienyl)rhodium(III)] **4** with frequency values.

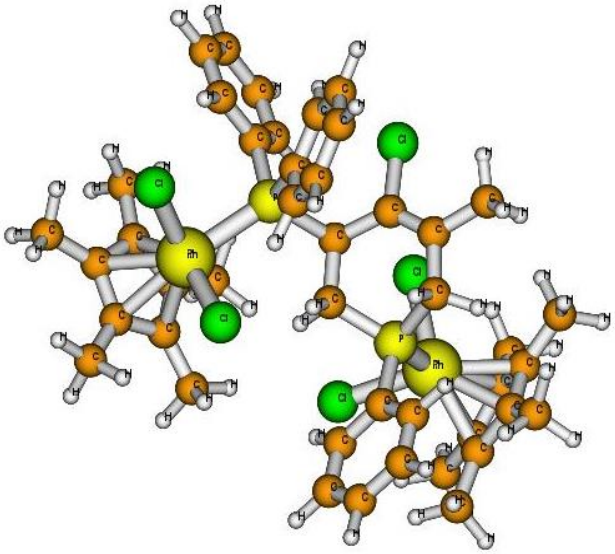

Figure S4 Stereostructure of bis-Rh(III) complex **4.** Selected bond lengths (Å), bond angles (°) and torsion angles (°) obtained by B3LYP/6-31G* and LANL2DZ ECP calculations:

Rh1-P1 2.355, Rh1-Cl 2.464, 2.444, Rh1-C 2.229, 2.314, 2.250, 2.216, 2.317, 2.250, P1-C2 1.845, C2-C3 1.550, C3-C4 1.516, C4-C5 1.344, C5-C6 1.517, C6-P1 1.853, P1-C1' 1.842, C3-P2 1.935, P2-C1" 1.846, 1.846, Rh2-P2 2.424, Rh2-Cl 2.482, 2.438, Rh2-C, 2.240, 2.287, 2.271, 2.260, 2.285, Cl-Rh1-Cl 91.004, Cl-Rh1-P1 92.77, P1-Rh1-C 149.33, 112.71, 98.75, 155.56, 118.02, Rh1-P1-C2 117.82, P1-C2-C3 114.91, C2-C3-C4 115.32, C3-C4-C5 128.75, C4-C5-C6 122.30, C5-C6-P1 112.11, C6-P1-C2 96.15, C2-P1-C1' 104.33, C1"-P2-C1" 105.24, Cl-Rh2-Cl 92.61, C3-P2-C1" 106.82, 103.50, P2-Rh2-C 142.32, 125.66, 162.51, 108.39, 101.49, P1-C2-C3-C4 –30.80, C2-C3-C4-C5 –3.35, C3-C4-C5-C6 1.41, C4-C5-C6-P1 33.57, C5-C6-P1-C2 –54.95, C6-P1-C2-C3 54.71, P1-C2-C3-P2 –159.42, C3-C2-P1-C1' 160.47, C2-C3-P2-C1" –151.76, P1-C6-C5-C(Me) –144.29, Cl-Rh-P1-C2 –47.19, C2-P1-Rh1-C –136.62, 141.63, 142.30, –147.17, 176.55, C3-P2-Rh2-C –116.34, –27.98, –42.33, –96.51, –58.46.

Numbering of the atoms is as follows: P1: cyclic P; P2: exocyclic P; Rh1: Rh complexed with the cyclic P atom; Rh2: Rh complexed with the exocyclic P atom; C2-C6: C atoms of heterocyclic ring; C1'-C6' C atoms of the phenyl ring attached to cyclic P atom. C1"-C6" C atoms of the exocyclic Ph_2P moiety.