Supporting Information for "Transformations of Group VII Carbonyl Complexes: Possible Intermediates in a Homogeneous Syngas Conversion Scheme"

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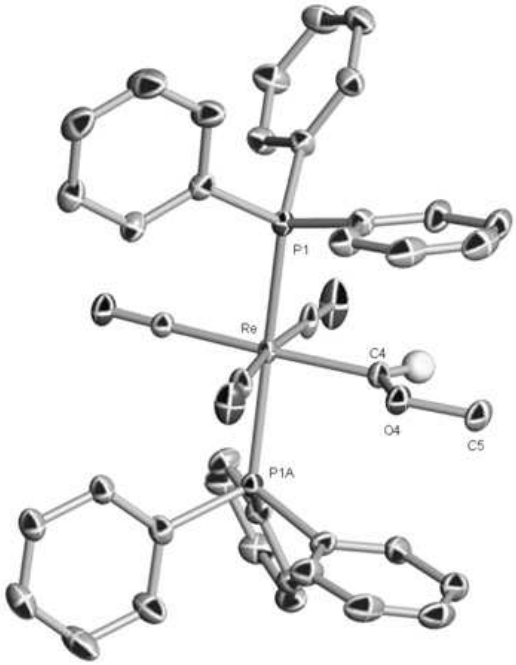
Contents

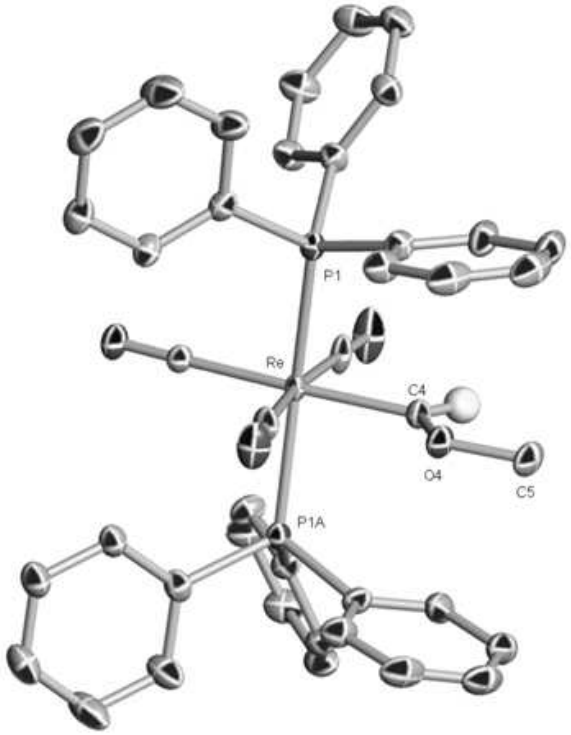
Thermal ellipsoid plot of $Re(PPh_3)_2(CO)_3(CHOMe)$ (3b).



Selected bond distances and angles for $Re(PPh_3)_2(CO)_3(CHOMe)$ (3b).

Re-C(1) 1.981(3)
Re-C(3) 1.993(2)
Re-C(2) 2.003(3)
Re-C(4) 2.064(3)
Re-P(1) 2.4387(4)
Re-P(1)#1 2.4388(4)
O(1)-C(1) 1.144(4)
O(2)-C(2) 1.148(3)
O(3)-C(3) 1.129(3)
O(4)-C(4) 1.290(4)
O(4)-C(5) 1.459(4)
C(4)-O(4)-C(5) 120.4(3)
O(4)-C(4)-Re 123.8(2)

Thermal ellipsoid plot of $Mn(PPh_3)_2(CO)_3(CH_2OMe)$ (5a).



Selected bond distances and angles for $Mn(PPh_3)_2(CO)_3(CH_2OMe)$ (5a).

Mn(1)-C(2) 1.794(3)
Mn(1)-C(1) 1.805(3)
Mn(1)-C(3) 1.846(3)
Mn(1)-C(4) 2.156(3)
Mn(1)-P(1) 2.2863(7)
Mn(1)-P(2) 2.2933(7)
O(1)-C(1) 1.169(3)
O(2)-C(2) 1.169(3)
O(3)-C(3) 1.145(3)
O(4)-C(5) 1.432(3)
O(4)-C(4) 1.455(3)
C(5)-O(4)-C(4) 111.2(2)
O(4)-C(4)-Mn(1) 113.35(16)

Structural parameters for 3b and 5a.

Complex	**3b** $[C_{41}H_{34}O_4P_2Re]^+[BC_{24}H_{20}]^-$	**5a**
Empirical Formula	• $0.5(CH_2Cl_2)$	$C_{41}H_{35}O_4P_2Mn$
Mol wt	1242.96	708.57
Temperature	100(2) K	100(2) K
Wavelength	0.71073 Å	0.71073 Å
Cryst Syst	Orthorhombic	Rhombohedral
Space Group	$Pmn2_1$	R-3
a, Å	20.2321(5)	43.9520(16)
b, Å	8.8558(2)	43.9520(16)
c, Å	15.6377(4)	11.9031(13)
α, deg	90	90
β, deg	90	90
γ, deg	90	120
Vol. Å3	2801.83(12)	19913.5(13)
Z	2	18
Density (calculated)	1.473 Mg/m^3	1.064 Mg/m^3
μ, mm^{-1}	2.370	0.403
F(000)	1256	6624
Crystal size	0.30 x 0.30 x 0.08 mm^3	0.41 x 0.08 x 0.03 mm^3
2θ range	1.65 to 40.56°	1.79 to 27.20°
Index Ranges	-36<=h<=36 -15<=k<=15 -28<=l<=26	-49<=h<=56 -56<=k<=32 -15<=l<=15
Reflections Collected	74440	46126
Independent reflections	16931 [R(int) = 0.0676]	9850 [R(int) = 0.0768]
Data/restraints/parameters	16931/1/371	9850/0/434
Goodness-of-fit on F^2	1.016	1.519
Final R indices[I>2sigma(I)]	R1 = 0.0316 wR2 = 0.0606	R1 = 0.0419 wR2 = 0.0766
R indices (all data)	R1 = 0.0404 wR2 = 0.0637	R1 = 0.0713 wR2 = 0.0783
Largest diff. peak and hole	2.141 and -1.452 e $Å^{-3}$	0.457 and -0.285 e $Å^{-3}$