Electronic Supplementary Material (ESI) for Dalton Transactions

Synthesis and Property of *N*-Heterocyclic Carbene Rhenium(I) Carbonyl Complexes

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Supplementary

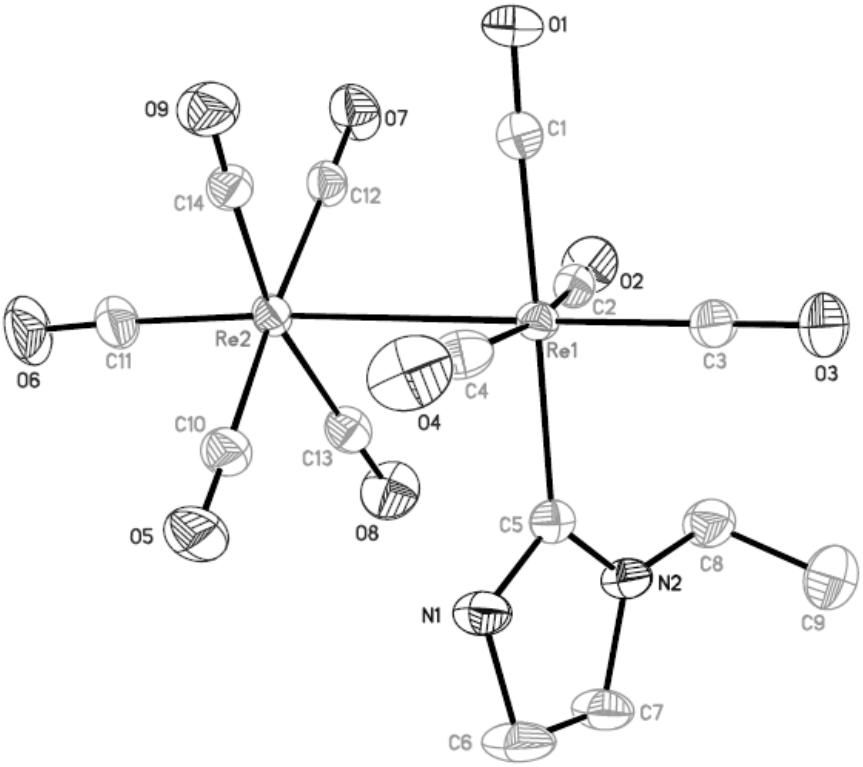

Figure S1 ORTEP Plot of **3b** (Drawn with 30 % probability ellipsoids)

Table S1. Bond lengths [Å] and angles [°] for **3b**.

Re(1)-C(3)	1.913(3)	O(4)-C(4)	1.141(4)
Re(1)-C(1)	1.967(4)	O(5)-C(10)	1.132(4)
Re(1)-C(4)	1.975(4)	O(6)-C(11)	1.153(4)
Re(1)-C(2)	1.979(4)	O(7)-C(12)	1.132(4)
Re(1)-C(5)	2.183(3)	O(8)-C(13)	1.130(4)
Re(1)-Re(2)	3.06893(19)	O(9)-C(14)	1.125(4)
Re(2)-C(11)	1.924(4)	N(1)-C(5)	1.338(4)
Re(2)-C(10)	1.973(4)	N(1)-C(6)	1.452(5)
Re(2)-C(13)	1.984(4)	N(2)-C(5)	1.331(4)
Re(2)-C(14)	1.990(4)	N(2)-C(8)	1.468(4)
Re(2)-C(12)	1.996(4)	N(2)-C(7)	1.465(4)
O(1)-C(1)	1.137(4)	C(6)-C(7)	1.508(5)
O(2)-C(2)	1.139(4)	C(8)-C(9)	1.493(5)
O(3)-C(3)	1.151(4)		

C(3)-Re(1)-C(1)	93.03(15)	C(13)-Re(2)-C(14)	166.18(14)
C(3)-Re(1)-C(4)	93.46(16)	C(11)-Re(2)-C(12)	94.10(15)
C(1)-Re(1)-C(4)	89.39(14)	C(10)-Re(2)-C(12)	174.11(14)
C(3)-Re(1)-C(2)	96.86(15)	C(13)-Re(2)-C(12)	90.49(14)
C(1)-Re(1)-C(2)	88.48(14)	C(14)-Re(2)-C(12)	88.30(14)
C(4)-Re(1)-C(2)	169.56(14)	C(11)-Re(2)-Re(1)	176.15(13)
C(3)-Re(1)-C(5)	87.99(13)	C(10)-Re(2)-Re(1)	86.75(11)
C(1)-Re(1)-C(5)	178.93(12)	C(13)-Re(2)-Re(1)	80.62(10)
C(4)-Re(1)-C(5)	90.22(13)	C(14)-Re(2)-Re(1)	85.58(10)
C(2)-Re(1)-C(5)	91.72(13)	C(12)-Re(2)-Re(1)	87.85(9)
C(3)-Re(1)-Re(2)	179.30(11)	C(5)-N(1)-C(6)	114.5(3)
C(1)-Re(1)-Re(2)	86.47(10)	C(5)-N(2)-C(8)	127.7(3)
C(4)-Re(1)-Re(2)	86.05(11)	C(5)-N(2)-C(7)	113.5(3)
C(2)-Re(1)-Re(2)	83.62(9)	C(8)-N(2)-C(7)	118.3(3)
C(5)-Re(1)-Re(2)	92.51(8)	O(1)-C(1)-Re(1)	178.0(3)
C(11)-Re(2)-C(10)	91.43(16)	O(2)-C(2)-Re(1)	177.4(3)
C(11)-Re(2)-C(13)	96.03(17)	O(3)-C(3)-Re(1)	179.6(4)
C(10)-Re(2)-C(13)	90.94(15)	O(4)-C(4)-Re(1)	177.9(3)
C(11)-Re(2)-C(14)	97.79(16)	N(1)-C(5)-N(2)	106.0(3)
C(10)-Re(2)-C(14)	88.95(14)	N(1)-C(5)-Re(1)	123.8(2)

N(2)-C(5)-Re(1)	130.2(2)	O(6)-C(11)-Re(2)	178.2(4)
N(1)-C(6)-C(7)	101.2(3)	O(7)-C(12)-Re(2)	178.7(3)
N(2)-C(7)-C(6)	102.1(3)	O(8)-C(13)-Re(2)	179.1(3)
N(2)-C(8)-C(9)	113.7(4)	O(9)-C(14)-Re(2)	177.6(3)
O(5)-C(10)-Re(2)	178.6(3)		

Symmetry transformations used to generate equivalent atoms: