Electronic Supplementary Information for Dalton Transactions

A tetranuclear organorhenium(I) complex of the 2,3,5,6-tetrafluoro-7,7,8,8-tetracyano-*p*-quinodimethane radical anion, $TCNQF4^{\bullet-}$

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Electronic Supporting Information

Table S. Selected experimental and ADF/BP calculated bond lengths (Å) and angles (^{o}) for $\{(\mu_4\text{-TCNQF4})[Re(CO)_3(bpy)]_4\}(PF_6)_3$.

bond lengths	Exper.	Calc.	*bond lengths*	Exper.	Calc.
Re1-C1	1.923(18)	1.930	Re2-N4	2.128(12)	2.084
Re1-C2	2.00(3)	1.951	Re2-N5	2.153(18)	2.175
Re1-C3	1.99(2)	1.933	Re2-N6	2.158(12)	2.173
Re1-N1	2.122(11)	2.087	C7-C8	1.443(19)	1.417
Re1-N2	2.178(15)	2.174	C8-C10	1.40(2)	1.443
Re1-N3	2.195(13)	2.175	C8-C9	1.44(2)	1.416
Re2-C4	1.962(18)	1.934	C10-C12	1.437(18)	1.416
Re2-C5	1.95(3)	1.953	C10-C11	1.440(19)	1.415
Re2-C6	1.92(2)	1.931	C11-C12	1.31(2)	1.377
bond angles			*bond angles*		
C2-Re1-C3	85.2(9)	88.9	C6-Re2-C4	87.9(10)	89.9
C2-Re1-C1	88.2(10)	89.9	C6-Re2-C5	83.4(12)	89.0
C3-Re1-C1	89.3(8)	89.9	C4-Re2-C5	89.1(12)	90.5
C2-Re1-N1	94.5(8)	92.5	C6-Re2-N5	101.4(12)	97.9
C3-Re1-N1	90.8(6)	89.7	C4-Re2-N5	93.7(11)	93.0
C1-Re1-N1	177.3(8)	177.5	C5-Re2-N5	174.5(8)	172.4
C2-Re1-N2	174.4(8)	172.0	C6-Re2-N4	93.2(8)	90.5
C3-Re1-N2	100.2(7)	97.5	C4-Re2-N4	176.7(11)	178.0
C1-Re1-N2	93.4(8)	92.2	C5-Re2-N4	94.1(9)	91.9
N1-Re1-N2	83.9(6)	87.8	N5-Re2-N4	83.0(7)	85.0

C2-Re1-N3	99.5(8)	97.4	C6-Re2-N6	176.6(11)	172.4
C3-Re1-N3	174.7(7)	173.4	C4-Re2-N6	93.4(8)	93.1
C1-Re1-N3	93.5(7)	92.1	C5-Re2-N6	99.7(8)	98.0
N1-Re1-N3	86.1(5)	85.5	N5-Re2-N6	75.4(6)	74.9
N2-Re1-N3	75.1(6)	74.8	N4-Re2-N6	85.4(5)	86.6

Figure S1 Absorption spectrum of $\{(\mu_4\text{-TCNQF4})[Re(CO)_3(bpy)]_4\}(PF_6)_3$ in CH_2Cl_2