Supplementary Material

Conformational preferences of heteronuclear Fischer carbene complexes of cymantrene and cyclopentadienyl rhenium tricarbonyl

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Optimized Cartesian coordinates (Å)

Density functional theory (DFT) calculations of this study were performed with the hybrid functional B3LYP as implemented in the Gaussian 09 program package. Geometries of the neutral complexes were optimized in gas phase with the triple-ζ basis set 6-311G(d,p) on all atoms except W, where def2-TZVPP was used. Energies reported are gas phase electronic energies.

Complex 1:

Mn	2.203808	-0.4333	-0.073403
Mn	-2.507092	-0.168895	0.015797
O	-1.856194	-1.782296	2.424897
O	0.42351	1.902802	-0.432603
O	-2.501489	2.414205	1.489397
O	4.069809	1.147198	-1.738803
O	-5.431892	-0.604892	0.300097
O	1.902206	-2.4405	-2.219503
C	-0.633892	0.045903	-1.105003
C	-1.054093	-1.323797	-1.151403
H	-0.505294	-2.158897	-0.746903
C	-4.303292	-0.430193	0.218697
C	-2.120693	-1.147696	1.507997
C	0.617809	0.589102	-0.545403
C	1.650306	-1.640399	1.692597
H	0.780706	-2.274299	1.774497
C	-1.680691	0.810604	-1.743903
H	-1.66579	1.879604	-1.886403
C	-2.688292	-0.072095	-2.170403
H	-3.592892	0.203306	-2.693803
C	-2.52459	1.410805	0.937797
C	3.309509	0.555199	-1.104403
C	1.734608	-0.2777	2.095397
H	0.921508	0.306201	2.503797
C	-2.307493	-1.399895	-1.791703
H	-2.872394	-2.301995	-1.975603
C	3.811207	-0.922802	1.356997
H	4.859207	-0.905103	1.094597
C	2.945506	-2.033401	1.245197
H	3.217505	-3.012101	0.876097
C	1.981506	-1.6307	-1.402603
C	3.060608	0.170099	1.891597
H	3.452909	1.148599	2.127797
C	1.428211	2.810001	0.078697
H	2.292111	2.7833	-0.584703

H	1.736511	2.4644	1.064297
C	0.801113	4.187901	0.132497
H	1.526313	4.908301	0.519797
H	0.494213	4.518802	-0.862203
H	-0.074187	4.197002	0.785097

Complex 2:

O	-1.886089	-1.872418	-2.407323
O	-2.742904	2.314812	-1.609216
O	-5.586733	-0.794444	-0.445138
O	0.147896	1.954873	0.422742
O	1.705108	-2.296889	2.377507
O	3.77361	1.355765	1.877095
C	-2.211791	-1.226969	-1.518212
C	-2.520279	-1.398975	1.781318
H	-3.06131	-2.314254	1.972002
C	-4.469966	-0.570123	-0.328185
C	-2.744088	1.3257	-1.031921
C	2.891304	-1.925977	-1.040001
H	3.212461	-2.875163	-0.632666
C	1.599646	-0.280803	-1.979635
H	0.764406	0.244261	-2.421993
C	1.583463	-1.627971	-1.527233
H	0.752941	-2.313746	-1.596641
C	-0.871769	0.082837	1.110597
C	0.381762	0.652362	0.581048
C	-1.965467	0.829194	1.689479
H	-1.991201	1.901709	1.800915
C	-1.247908	-1.298557	1.183431
H	-0.657394	-2.125517	0.823865
C	3.708326	-0.778403	-1.177852
C	-2.958381	-0.074665	2.106633
H	-3.88971	0.184735	2.589754
C	1.784587	-1.501899	1.545726
C	2.895425	0.246545	-1.763761
H	3.239832	1.234748	-2.035368
C	3.050809	0.721661	1.237941
C	0.467446	4.226104	-0.229197
H	1.18729	4.959792	-0.601427
H	-0.360567	4.166829	-0.938417
H	0.079169	4.587997	0.725544
C	1.145614	2.881165	-0.067354
H	1.534447	2.503893	-1.011604
H	1.962882	2.923159	0.65224
C	5.177193	-0.687083	-0.881121

H	5.767878	-0.890461	-1.7812
H	5.461274	0.304731	-0.522433
H	5.477024	-1.411778	-0.121104
Mn	2.017332	-0.329491	0.196708
Mn	-2.695015	-0.228085	-0.067788

Complex 3:

O	-1.685216	-2.341031	-1.644723
O	-3.088588	1.744313	-2.40484
O	-5.563334	-1.230875	-0.409263
O	0.346035	2.243097	0.157012
O	1.059086	-1.934332	2.498531
O	3.80058	1.132447	1.411177
C	-2.105953	-1.471913	-1.014552
C	-2.70468	-0.222229	2.343984
H	-3.238779	-0.8499	2.81672
C	-4.524366	-0.772169	-0.241197
C	-2.985624	1.049749	-1.509045
C	2.073229	-2.231276	-0.950401
H	2.228757	-3.056209	-0.506182
C	1.021757	-0.477865	-1.999494
H	0.347694	0.073407	-2.378277
C	0.812189	-1.734742	-1.37692
H	-0.026164	-2.168875	-1.263635
C	-0.946294	0.742354	1.179741
C	0.331765	0.949584	0.460985
C	-2.007496	1.712536	1.304899
H	-1.991425	2.599499	0.96642
C	-1.404386	-0.452643	1.841304
H	-0.912777	-1.26164	1.925848
C	3.050975	-1.284168	-1.304155
H	3.983586	-1.357933	-1.138743
C	-3.07716	1.121414	2.017511
H	-3.897861	1.54222	2.240787
C	1.275645	-1.296768	1.557579
C	2.398042	-0.184976	-1.9605
H	2.816624	0.594719	-2.304271
C	2.94019	0.553619	0.89235
C	1.131413	4.30364	-0.685657
H	1.795038	4.7447	-1.257957
H	0.231014	4.500955	-1.017287
H	1.222083	4.634296	0.232068
C	1.358905	2.8318	-0.707995
H	1.270274	2.482096	-1.630291
H	2.26604	2.616355	-0.374527

Mn	-2.775823	-0.051956	0.05418
Re	1.660321	-0.393592	0.085081

Complex 4:

Re	2.305628	-0.297367	-0.062687
O	4.133641	1.598556	-1.622748
C	3.405728	0.883497	-1.05356
O	0.400997	2.042943	-0.4242
C	0.658368	0.748463	-0.60034
Re	-2.47572	-0.136344	-0.024385
O	1.977998	-2.1817	-2.427734
C	2.084585	-1.439421	-1.552756
O	-1.504505	-1.470486	2.553532
C	-1.885185	-0.956844	1.581194
C	-2.831421	1.498204	0.924897
O	-3.038005	2.499478	1.434912
C	-4.237106	-0.757639	0.392987
O	-5.290427	-1.15006	0.643664
C	1.738349	-0.329318	2.197041
H	0.97343	0.123851	2.532655
C	3.102219	-1.946165	1.312717
H	3.414362	-2.769251	0.955237
C	1.764396	-1.670749	1.705506
H	1.025926	-2.266193	1.650952
C	3.88382	-0.80179	1.539144
H	4.810895	-0.71031	1.354088
C	3.030352	0.2035	2.099674
H	3.293205	1.078197	2.360208
C	-0.560972	0.208862	-1.254502
C	-0.944891	-1.173745	-1.385533
H	-0.439297	-1.920633	-1.08896
C	-2.204354	-1.228636	-2.032906
H	-2.689326	-2.017878	-2.242905
C	-2.618307	0.115947	-2.314287
H	-3.425663	0.373749	-2.744028
C	-1.625464	0.979366	-1.843889
H	-1.648364	1.926965	-1.903821
C	1.308979	2.897633	0.310826
H	2.190581	2.926879	-0.136773
H	1.434523	2.553594	1.231031
C	0.707075	4.248669	0.346827
H	-0.204246	4.190871	0.701218
H	0.681485	4.619367	-0.559653
H	1.244772	4.830223	0.923473

Complex 5:

Re	2.030577	-0.116775	-0.032728
Mn	-2.675939	-0.453311	-0.031972
O	1.182957	-1.323015	2.63974
O	2.466963	2.631486	1.24313
O	4.894913	-0.937478	0.672166
O	-0.934181	1.88355	-0.467869
O	-2.351604	-2.420463	-2.173286
O	-4.530667	1.191837	-1.619898
C	1.512631	-0.857975	1.637466
C	1.778707	-1.354054	-1.951832
H	2.298625	-2.131576	-2.118728
C	3.826864	-0.612384	0.4044
C	2.320648	1.594932	0.796345
C	-3.391123	-2.017336	1.257265
H	-3.685479	-2.862045	0.938115
C	-2.05468	-0.327056	2.05571
H	-1.295844	0.154105	2.362938
C	-2.062927	-1.680827	1.633224
H	-1.310582	-2.261634	1.605301
C	0.082172	0.04985	-1.224763
C	-1.14016	0.575114	-0.574385
C	1.086738	0.842912	-1.89182
H	1.060407	1.784231	-2.013287
C	0.535297	-1.31652	-1.281708
H	0.073676	-2.068015	-0.9275
C	-4.193225	-0.877028	1.442926
H	-5.125341	-0.817332	1.26925
C	2.118604	-0.017016	-2.335893
H	2.899282	0.246274	-2.806744
C	-2.454219	-1.620601	-1.343547
C	-3.361562	0.183434	1.942017
H	-3.640977	1.065266	2.155589
C	-3.779234	0.562071	-1.000836
C	-1.356609	4.150181	0.038774
H	-1.934214	4.777884	0.523358
H	-0.434815	4.241408	0.357526
H	-1.392683	4.348574	-0.919929
C	-1.830096	2.758025	0.276003
H	-1.799245	2.54211	1.242029
H	-2.761605	2.649991	-0.042005

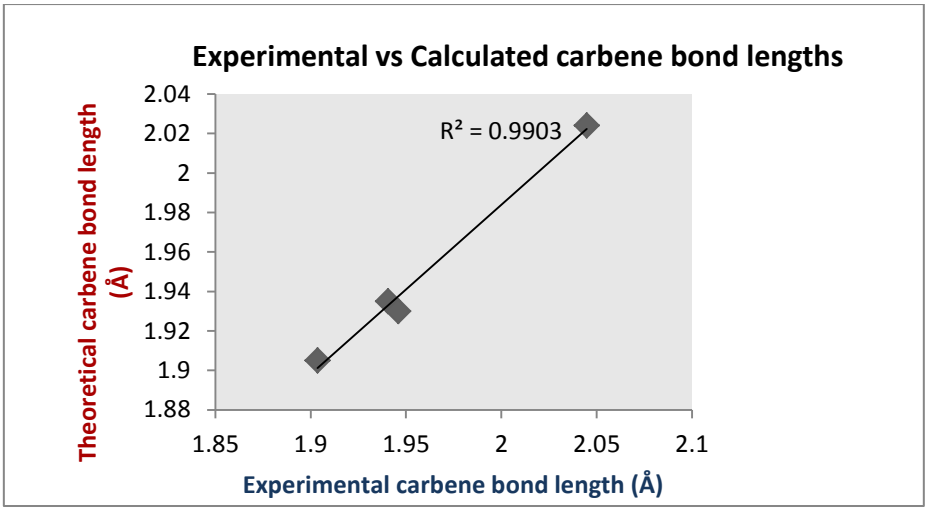

Figure S1: Plot of calculated M-carbene bond lengths for complexes 1, 2,4 and 5 vs experimentally determined values of related compounds (linear regression: R^2= 0.99)

Crystal data for complex 2

Table 1. Crystal data and structure refinement for mo_rf71x2_0m_5.

Identification code	shelx	
Empirical formula	$C_{18.31} H_{14.61} Mn_2 O_6$	
Formula weight	440.45	
Temperature	150(2) K	
Wavelength	0.71073 Å	
Crystal system	Triclinic	
Space group	P -1	
Unit cell dimensions	a = 8.024(6) Å	α= 68.29(7)°.
	b = 9.913(8) Å	β= 80.74(6)°.
	c = 13.041(13) Å	γ = 67.54(6)°.
Volume	890.4(14) $Å^3$	
Z	2	
Density (calculated)	1.643 Mg/m^3	
Absorption coefficient	1.450 mm^{-1}	
F(000)	445	
Crystal size	0.099 x 0.085 x 0.057 mm^3	
Theta range for data collection	2.362 to 25.344°.	
Index ranges	-9<=h<=9, -10<=k<=11, 0<=l<=15	
Reflections collected	18939	
Independent reflections	4941 [R(int) = 0.0867]	
Completeness to theta = 25.242°	99.8 %	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	4941 / 0 / 246	
Goodness-of-fit on F^2	1.041	
Final R indices [I>2sigma(I)]	R1 = 0.0548, wR2 = 0.0987	
R indices (all data)	R1 = 0.0853, wR2 = 0.1083	
Extinction coefficient	n/a	
Largest diff. peak and hole	0.576 and -0.464 e.$Å^{-3}$	

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for mo_rf71x2_0m_5. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
Mn(1)	3327(1)	2945(1)	4272(1)	21(1)
Mn(2)	2274(1)	7830(1)	1660(1)	25(1)
O(1)	2914(5)	5199(4)	5355(3)	33(1)
O(2)	3032(5)	716(5)	6457(3)	37(1)
O(3)	7302(5)	1797(5)	4304(3)	37(1)
O(9)	5261(5)	4861(4)	1874(3)	37(1)
O(12)	-1203(6)	7695(5)	1434(5)	67(2)
O(13)	3215(6)	8366(5)	-688(4)	58(1)
C(1)	3078(7)	4320(6)	4918(4)	23(1)
C(2)	3150(7)	1565(7)	5599(5)	28(1)
C(3)	5763(8)	2246(6)	4307(5)	27(1)
C(4)	1102(7)	4525(6)	3237(4)	24(1)
C(5)	945(7)	3058(7)	3660(4)	28(1)
C(6)	2449(7)	1992(7)	3302(4)	27(1)
C(7)	3569(7)	2800(6)	2660(4)	25(1)
C(8)	2748(7)	4395(6)	2602(4)	21(1)
C(9)	3527(7)	5634(6)	2047(4)	25(1)
C(10)	6567(7)	5630(7)	1421(6)	50(2)
C(11)	8234(8)	4466(8)	1169(6)	54(2)
C(12)	198(8)	7704(7)	1519(5)	41(2)
C(13)	2858(8)	8123(7)	245(5)	37(2)
C(14)	829(8)	9764(7)	2252(5)	34(2)
C(15)	1616(7)	8422(7)	3138(5)	33(2)
C(16)	3506(8)	7928(8)	2966(5)	41(2)
C(17)	3901(8)	8937(8)	1973(6)	43(2)
C(18)	2237(9)	10085(7)	1526(5)	41(2)
C(19)	2220(30)	11340(20)	692(14)	30(6)

Table 3. Bond lengths [Å] and angles [°] for mo_rf71x2_0m_5.

Mn(1)-C(1)	1.788(6)
Mn(1)-C(2)	1.790(7)
Mn(1)-C(3)	1.809(6)
Mn(1)-C(8)	2.128(6)
Mn(1)-C(4)	2.130(5)
Mn(1)-C(7)	2.133(6)
Mn(1)-C(5)	2.136(5)
Mn(1)-C(6)	2.160(5)
Mn(2)-C(12)	1.761(7)
Mn(2)-C(13)	1.772(7)
Mn(2)-C(9)	1.919(6)
Mn(2)-C(15)	2.147(6)
Mn(2)-C(16)	2.150(6)
Mn(2)-C(17)	2.161(6)
Mn(2)-C(18)	2.166(6)
Mn(2)-C(14)	2.173(6)
O(1)-C(1)	1.165(6)
O(2)-C(2)	1.139(6)
O(3)-C(3)	1.141(6)
O(9)-C(9)	1.336(6)
O(9)-C(10)	1.452(6)
O(12)-C(12)	1.151(7)
O(13)-C(13)	1.159(7)
C(4)-C(5)	1.399(7)
C(4)-C(8)	1.429(7)
C(4)-H(4)	0.9500
C(5)-C(6)	1.414(7)
C(5)-H(5)	0.9500
C(6)-C(7)	1.401(7)
C(6)-H(6)	0.9500
C(7)-C(8)	1.439(7)
C(7)-H(7)	0.9500
C(8)-C(9)	1.485(7)
C(10)-C(11)	1.479(8)
C(10)-H(10A)	0.9900
C(10)-H(10B)	0.9900

C(11)-H(11A)	0.9800
C(11)-H(11B)	0.9800
C(11)-H(11C)	0.9800
C(14)-C(15)	1.400(8)
C(14)-C(18)	1.407(8)
C(14)-H(14)	0.9500
C(15)-C(16)	1.412(8)
C(15)-H(15)	0.9500
C(16)-C(17)	1.388(9)
C(16)-H(16)	0.9500
C(17)-C(18)	1.420(8)
C(17)-H(17)	0.9500
C(18)-C(19)	1.315(17)
C(18)-H(18)	0.9500
C(19)-H(19A)	0.9800
C(19)-H(19B)	0.9800
C(19)-H(19C)	0.9800

C(1)-Mn(1)-C(2)	89.6(2)
C(1)-Mn(1)-C(3)	92.8(2)
C(2)-Mn(1)-C(3)	92.8(3)
C(1)-Mn(1)-C(8)	101.8(2)
C(2)-Mn(1)-C(8)	159.3(2)
C(3)-Mn(1)-C(8)	103.7(2)
C(1)-Mn(1)-C(4)	91.3(2)
C(2)-Mn(1)-C(4)	124.5(2)
C(3)-Mn(1)-C(4)	142.5(2)
C(8)-Mn(1)-C(4)	39.23(19)
C(1)-Mn(1)-C(7)	139.6(2)
C(2)-Mn(1)-C(7)	130.7(2)
C(3)-Mn(1)-C(7)	88.5(2)
C(8)-Mn(1)-C(7)	39.5(2)
C(4)-Mn(1)-C(7)	65.3(2)
C(1)-Mn(1)-C(5)	117.1(2)
C(2)-Mn(1)-C(5)	94.6(2)
C(3)-Mn(1)-C(5)	149.2(2)
C(8)-Mn(1)-C(5)	64.8(2)
C(4)-Mn(1)-C(5)	38.3(2)

C(7)-Mn(1)-C(5)	64.2(2)
C(1)-Mn(1)-C(6)	154.8(2)
C(2)-Mn(1)-C(6)	97.6(2)
C(3)-Mn(1)-C(6)	110.9(2)
C(8)-Mn(1)-C(6)	65.1(2)
C(4)-Mn(1)-C(6)	64.7(2)
C(7)-Mn(1)-C(6)	38.07(19)
C(5)-Mn(1)-C(6)	38.4(2)
C(12)-Mn(2)-C(13)	92.5(3)
C(12)-Mn(2)-C(9)	93.4(2)
C(13)-Mn(2)-C(9)	91.5(3)
C(12)-Mn(2)-C(15)	98.0(3)
C(13)-Mn(2)-C(15)	156.2(3)
C(9)-Mn(2)-C(15)	109.1(2)
C(12)-Mn(2)-C(16)	134.5(3)
C(13)-Mn(2)-C(16)	132.5(3)
C(9)-Mn(2)-C(16)	92.0(2)
C(15)-Mn(2)-C(16)	38.4(2)
C(12)-Mn(2)-C(17)	153.0(3)
C(13)-Mn(2)-C(17)	98.2(3)
C(9)-Mn(2)-C(17)	111.0(2)
C(15)-Mn(2)-C(17)	63.8(2)
C(16)-Mn(2)-C(17)	37.6(2)
C(12)-Mn(2)-C(18)	116.7(3)
C(13)-Mn(2)-C(18)	92.9(3)
C(9)-Mn(2)-C(18)	149.3(2)
C(15)-Mn(2)-C(18)	63.2(2)
C(16)-Mn(2)-C(18)	63.2(3)
C(17)-Mn(2)-C(18)	38.3(2)
C(12)-Mn(2)-C(14)	89.3(3)
C(13)-Mn(2)-C(14)	121.6(3)
C(9)-Mn(2)-C(14)	146.6(2)
C(15)-Mn(2)-C(14)	37.8(2)
C(16)-Mn(2)-C(14)	63.6(2)
C(17)-Mn(2)-C(14)	64.0(2)
C(18)-Mn(2)-C(14)	37.8(2)
C(9)-O(9)-C(10)	122.3(4)
O(1)-C(1)-Mn(1)	179.0(5)

O(2)-C(2)-Mn(1)	178.1(5)
O(3)-C(3)-Mn(1)	178.2(5)
C(5)-C(4)-C(8)	107.8(5)
C(5)-C(4)-Mn(1)	71.1(3)
C(8)-C(4)-Mn(1)	70.3(3)
C(5)-C(4)-H(4)	126.1
C(8)-C(4)-H(4)	126.1
Mn(1)-C(4)-H(4)	124.1
C(4)-C(5)-C(6)	109.4(5)
C(4)-C(5)-Mn(1)	70.6(3)
C(6)-C(5)-Mn(1)	71.7(3)
C(4)-C(5)-H(5)	125.3
C(6)-C(5)-H(5)	125.3
Mn(1)-C(5)-H(5)	124.0
C(7)-C(6)-C(5)	107.5(5)
C(7)-C(6)-Mn(1)	69.9(3)
C(5)-C(6)-Mn(1)	69.9(3)
C(7)-C(6)-H(6)	126.3
C(5)-C(6)-H(6)	126.3
Mn(1)-C(6)-H(6)	125.5
C(6)-C(7)-C(8)	108.7(5)
C(6)-C(7)-Mn(1)	72.0(3)
C(8)-C(7)-Mn(1)	70.1(3)
C(6)-C(7)-H(7)	125.7
C(8)-C(7)-H(7)	125.7
Mn(1)-C(7)-H(7)	123.9
C(4)-C(8)-C(7)	106.6(5)
C(4)-C(8)-C(9)	127.0(5)
C(7)-C(8)-C(9)	126.3(5)
C(4)-C(8)-Mn(1)	70.5(3)
C(7)-C(8)-Mn(1)	70.5(3)
C(9)-C(8)-Mn(1)	121.2(3)
O(9)-C(9)-C(8)	103.9(4)
O(9)-C(9)-Mn(2)	129.1(4)
C(8)-C(9)-Mn(2)	126.9(4)
O(9)-C(10)-C(11)	106.8(5)
O(9)-C(10)-H(10A)	110.4
C(11)-C(10)-H(10A)	110.4

O(9)-C(10)-H(10B)	110.4
C(11)-C(10)-H(10B)	110.4
H(10A)-C(10)-H(10B)	108.6
C(10)-C(11)-H(11A)	109.5
C(10)-C(11)-H(11B)	109.5
H(11A)-C(11)-H(11B)	109.5
C(10)-C(11)-H(11C)	109.5
H(11A)-C(11)-H(11C)	109.5
H(11B)-C(11)-H(11C)	109.5
O(12)-C(12)-Mn(2)	176.4(6)
O(13)-C(13)-Mn(2)	177.8(5)
C(15)-C(14)-C(18)	107.3(6)
C(15)-C(14)-Mn(2)	70.1(3)
C(18)-C(14)-Mn(2)	70.8(3)
C(15)-C(14)-H(14)	126.4
C(18)-C(14)-H(14)	126.4
Mn(2)-C(14)-H(14)	124.4
C(14)-C(15)-C(16)	108.3(6)
C(14)-C(15)-Mn(2)	72.1(3)
C(16)-C(15)-Mn(2)	70.9(3)
C(14)-C(15)-H(15)	125.9
C(16)-C(15)-H(15)	125.9
Mn(2)-C(15)-H(15)	122.8
C(17)-C(16)-C(15)	108.6(6)
C(17)-C(16)-Mn(2)	71.7(3)
C(15)-C(16)-Mn(2)	70.7(3)
C(17)-C(16)-H(16)	125.7
C(15)-C(16)-H(16)	125.7
Mn(2)-C(16)-H(16)	123.6
C(16)-C(17)-C(18)	107.2(6)
C(16)-C(17)-Mn(2)	70.8(3)
C(18)-C(17)-Mn(2)	71.0(3)
C(16)-C(17)-H(17)	126.4
C(18)-C(17)-H(17)	126.4
Mn(2)-C(17)-H(17)	123.5
C(19)-C(18)-C(14)	130.0(10)
C(19)-C(18)-C(17)	120.1(10)
C(14)-C(18)-C(17)	108.5(6)

C(19)-C(18)-Mn(2)	134.1(9)
C(14)-C(18)-Mn(2)	71.4(4)
C(17)-C(18)-Mn(2)	70.7(3)
C(14)-C(18)-H(18)	125.7
C(17)-C(18)-H(18)	125.7
Mn(2)-C(18)-H(18)	123.9
C(18)-C(19)-H(19A)	109.5
C(18)-C(19)-H(19B)	109.5
H(19A)-C(19)-H(19B)	109.5
C(18)-C(19)-H(19C)	109.5
H(19A)-C(19)-H(19C)	109.5
H(19B)-C(19)-H(19C)	109.5

Symmetry transformations used to generate equivalent atoms:

Table 4. Anisotropic displacement parameters ($Å^2 x\ 10^3$)for mo_rf71x2_0m_5. The anisotropic displacement factor exponent takes the form: $-2\pi^2[\ h^2 a^{*2} U^{11} + ... + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Mn(1)	19(1)	25(1)	26(1)	-12(1)	3(1)	-10(1)
Mn(2)	23(1)	25(1)	32(1)	-11(1)	-4(1)	-9(1)
O(1)	32(2)	33(2)	37(2)	-21(2)	-4(2)	-8(2)
O(2)	42(3)	33(3)	34(3)	-5(2)	3(2)	-16(2)
O(3)	18(2)	42(3)	60(3)	-28(2)	3(2)	-11(2)
O(9)	20(2)	30(2)	53(3)	-8(2)	10(2)	-12(2)
O(12)	33(3)	40(3)	126(5)	-12(3)	-30(3)	-16(2)
O(13)	69(3)	61(3)	31(3)	-16(2)	-7(2)	-8(3)
C(1)	17(3)	28(3)	23(3)	-7(3)	2(2)	-9(2)
C(2)	25(3)	27(3)	40(4)	-19(3)	-4(3)	-8(3)
C(3)	33(4)	27(3)	30(3)	-17(3)	3(3)	-15(3)
C(4)	16(3)	31(3)	29(3)	-12(3)	-5(2)	-7(2)
C(5)	26(3)	41(4)	28(3)	-12(3)	3(2)	-23(3)
C(6)	36(4)	31(3)	27(3)	-15(3)	-5(3)	-19(3)
C(7)	25(3)	32(3)	25(3)	-16(3)	0(2)	-12(3)
C(8)	19(3)	24(3)	23(3)	-8(2)	-2(2)	-9(2)
C(9)	19(3)	36(3)	23(3)	-12(3)	2(2)	-12(3)
C(10)	22(3)	37(4)	81(5)	-7(4)	12(3)	-17(3)

C(11)	38(4)	61(5)	73(5)	-32(4)	17(4)	-27(4)
C(12)	35(4)	27(4)	59(5)	-12(3)	-13(3)	-7(3)
C(13)	38(4)	32(4)	42(4)	-16(3)	-12(3)	-6(3)
C(14)	34(4)	32(4)	39(4)	-20(3)	0(3)	-8(3)
C(15)	30(4)	46(4)	29(4)	-21(3)	1(3)	-11(3)
C(16)	35(4)	54(4)	48(4)	-31(4)	-8(3)	-15(3)
C(17)	30(4)	60(5)	65(5)	-42(4)	12(3)	-29(3)
C(18)	51(4)	40(4)	47(4)	-27(3)	8(3)	-23(3)
C(19)	48(13)	16(11)	19(11)	6(8)	4(9)	-17(9)

Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for mo_rf71x2_0m_5.

	x	y	z	U(eq)
H(4)	265	5443	3351	29
H(5)	-22	2816	4117	34
H(6)	2661	924	3467	33
H(7)	4684	2367	2319	30
H(10A)	6807	6014	1963	60
H(10B)	6107	6523	741	60
H(11A)	9156	4941	860	81
H(11B)	8674	3591	1849	81
H(11C)	7977	4097	633	81
H(14)	-423	10350	2158	41
H(15)	986	7927	3750	40
H(16)	4364	7052	3448	49
H(17)	5067	8871	1653	51
H(18)	2097	10929	851	61
H(19A)	3434	11189	355	45
H(19B)	1372	11556	142	45
H(19C)	1851	12223	957	45

Table 6. Torsion angles [°] for mo_rf71x2_0m_5.

C(8)-C(4)-C(5)-C(6)	-0.5(6)
Mn(1)-C(4)-C(5)-C(6)	-61.5(4)
C(8)-C(4)-C(5)-Mn(1)	61.0(3)
C(4)-C(5)-C(6)-C(7)	0.8(6)
Mn(1)-C(5)-C(6)-C(7)	-60.1(4)
C(4)-C(5)-C(6)-Mn(1)	60.8(4)
C(5)-C(6)-C(7)-C(8)	-0.8(6)
Mn(1)-C(6)-C(7)-C(8)	-60.8(4)
C(5)-C(6)-C(7)-Mn(1)	60.0(4)
C(5)-C(4)-C(8)-C(7)	0.0(6)
Mn(1)-C(4)-C(8)-C(7)	61.5(3)
C(5)-C(4)-C(8)-C(9)	-176.4(5)
Mn(1)-C(4)-C(8)-C(9)	-114.9(5)
C(5)-C(4)-C(8)-Mn(1)	-61.5(4)
C(6)-C(7)-C(8)-C(4)	0.5(6)
Mn(1)-C(7)-C(8)-C(4)	-61.6(3)
C(6)-C(7)-C(8)-C(9)	176.9(5)
Mn(1)-C(7)-C(8)-C(9)	114.9(5)
C(6)-C(7)-C(8)-Mn(1)	62.0(4)
C(10)-O(9)-C(9)-C(8)	-175.0(5)
C(10)-O(9)-C(9)-Mn(2)	6.0(8)
C(4)-C(8)-C(9)-O(9)	161.2(5)
C(7)-C(8)-C(9)-O(9)	-14.5(7)
Mn(1)-C(8)-C(9)-O(9)	73.1(5)
C(4)-C(8)-C(9)-Mn(2)	-19.7(8)
C(7)-C(8)-C(9)-Mn(2)	164.5(4)
Mn(1)-C(8)-C(9)-Mn(2)	-107.8(4)
C(9)-O(9)-C(10)-C(11)	-170.4(5)
C(18)-C(14)-C(15)-C(16)	0.7(6)
Mn(2)-C(14)-C(15)-C(16)	62.1(4)
C(18)-C(14)-C(15)-Mn(2)	-61.4(4)
C(14)-C(15)-C(16)-C(17)	-0.9(6)
Mn(2)-C(15)-C(16)-C(17)	62.0(4)
C(14)-C(15)-C(16)-Mn(2)	-62.8(4)
C(15)-C(16)-C(17)-C(18)	0.7(6)
Mn(2)-C(16)-C(17)-C(18)	62.0(4)

C(15)-C(16)-C(17)-Mn(2)	-61.4(4)
C(15)-C(14)-C(18)-C(19)	-166.7(12)
Mn(2)-C(14)-C(18)-C(19)	132.5(13)
C(15)-C(14)-C(18)-C(17)	-0.3(7)
Mn(2)-C(14)-C(18)-C(17)	-61.2(4)
C(15)-C(14)-C(18)-Mn(2)	60.9(4)
C(16)-C(17)-C(18)-C(19)	167.7(11)
Mn(2)-C(17)-C(18)-C(19)	-130.4(11)
C(16)-C(17)-C(18)-C(14)	-0.2(7)
Mn(2)-C(17)-C(18)-C(14)	61.6(4)
C(16)-C(17)-C(18)-Mn(2)	-61.9(4)

Symmetry transformations used to generate equivalent atoms:

Table 7. Hydrogen bonds for mo_rf71x2_0m_5 [Å and °].

D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)
C(10)-H(10A)...O(12)#1	0.99	2.58	3.198(8)	120.8

Symmetry transformations used to generate equivalent atoms:

#1 x+1,y,z

Crystal data for complex 4

Table 1. Crystal data and structure refinement for mo_rf73_0m.

Identification code	shelx	
Empirical formula	$C_{18}\ H_{14}\ O_6\ Re_2$	
Formula weight	698.69	
Temperature	150(2) K	
Wavelength	0.71073 Å	
Crystal system	Triclinic	
Space group	P -1	
Unit cell dimensions	a = 8.0402(8) Å	α= 68.393(4)°.
	b = 9.9573(10) Å	β= 83.222(4)°.
	c = 13.1674(14) Å	γ = 66.777(4)°.
Volume	900.23(16) $Å^3$	
Z	2	
Density (calculated)	2.578 Mg/m^3	
Absorption coefficient	13.466 mm^{-1}	
F(000)	640	
Crystal size	0.192 x 0.082 x 0.071 mm^3	
Theta range for data collection	2.374 to 25.348°.	
Index ranges	-9<=h<=9, -11<=k<=11, -15<=l<=15	
Reflections collected	25343	
Independent reflections	3290 [R(int) = 0.0698]	
Completeness to theta = 25.242°	100.0 %	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	3290 / 0 / 235	
Goodness-of-fit on F^2	1.068	
Final R indices [I>2sigma(I)]	R1 = 0.0211, wR2 = 0.0525	
R indices (all data)	R1 = 0.0242, wR2 = 0.0537	
Extinction coefficient	n/a	
Largest diff. peak and hole	1.252 and -1.261 $e.Å^{-3}$	

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for mo_rf73_0m. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
Re(1)	6691(1)	7776(1)	4314(1)	11(1)
Re(2)	7821(1)	5560(1)	1516(1)	12(1)
O(1)	7029(5)	4377(4)	5350(3)	26(1)
O(2)	7005(5)	7736(4)	6625(3)	28(1)
O(3)	2551(4)	8978(4)	4426(3)	26(1)
O(9)	4821(4)	8493(4)	1701(3)	29(1)
O(12)	11390(4)	6019(4)	1269(3)	26(1)
O(13)	6753(5)	7393(4)	-908(3)	33(1)
C(1)	6890(6)	5673(6)	4963(4)	16(1)
C(2)	6867(6)	7768(5)	5751(4)	16(1)
C(3)	4096(7)	8490(5)	4408(4)	19(1)
C(4)	9017(6)	7314(5)	3137(4)	16(1)
C(5)	9206(6)	8317(6)	3607(4)	17(1)
C(6)	7656(6)	9753(6)	3276(4)	17(1)
C(7)	6535(7)	9630(6)	2617(4)	17(1)
C(8)	7332(6)	8119(5)	2505(4)	14(1)
C(9)	6545(6)	7506(5)	1897(4)	16(1)
C(10)	3538(7)	8203(8)	1212(6)	46(2)
C(11)	1764(7)	9490(7)	1132(5)	34(1)
C(12)	10015(7)	5888(6)	1353(4)	20(1)
C(13)	7156(7)	6735(6)	22(4)	20(1)
C(14)	9198(7)	2889(5)	2219(4)	21(1)
C(15)	8378(7)	3409(6)	3093(4)	24(1)
C(16)	6469(7)	4093(6)	2885(4)	25(1)
C(17)	6127(7)	4000(6)	1899(5)	26(1)
C(18)	7823(7)	3268(6)	1473(4)	23(1)

Table 3. Bond lengths [Å] and angles [°] for mo_rf73_0m.

Re(1)-C(1)	1.896(5)
Re(1)-C(2)	1.911(5)
Re(1)-C(3)	1.925(5)
Re(1)-C(7)	2.294(5)
Re(1)-C(4)	2.297(5)
Re(1)-C(5)	2.300(5)
Re(1)-C(8)	2.304(5)
Re(1)-C(6)	2.306(5)
Re(2)-C(12)	1.892(5)
Re(2)-C(13)	1.894(5)
Re(2)-C(9)	2.022(5)
Re(2)-C(14)	2.294(5)
Re(2)-C(15)	2.300(5)
Re(2)-C(18)	2.303(5)
Re(2)-C(16)	2.326(5)
Re(2)-C(17)	2.334(5)
O(1)-C(1)	1.163(6)
O(2)-C(2)	1.156(6)
O(3)-C(3)	1.143(6)
O(9)-C(9)	1.333(5)
O(9)-C(10)	1.446(6)
O(12)-C(12)	1.152(6)
O(13)-C(13)	1.170(6)
C(4)-C(5)	1.414(6)
C(4)-C(8)	1.445(6)
C(4)-H(4)	0.9500
C(5)-C(6)	1.432(7)
C(5)-H(5)	0.9500
C(6)-C(7)	1.390(7)
C(6)-H(6)	0.9500
C(7)-C(8)	1.440(6)
C(7)-H(7)	0.9500
C(8)-C(9)	1.483(6)
C(10)-C(11)	1.477(7)
C(10)-H(10A)	0.9900
C(10)-H(10B)	0.9900

C(11)-H(11A)	0.9800
C(11)-H(11B)	0.9800
C(11)-H(11C)	0.9800
C(14)-C(18)	1.408(7)
C(14)-C(15)	1.421(7)
C(14)-H(14)	0.9500
C(15)-C(16)	1.426(7)
C(15)-H(15)	0.9500
C(16)-C(17)	1.400(8)
C(16)-H(16)	0.9500
C(17)-C(18)	1.429(7)
C(17)-H(17)	0.9500
C(18)-H(18)	0.9500

C(1)-Re(1)-C(2)	87.98(19)
C(1)-Re(1)-C(3)	90.45(19)
C(2)-Re(1)-C(3)	89.87(19)
C(1)-Re(1)-C(7)	139.89(18)
C(2)-Re(1)-C(7)	131.97(18)
C(3)-Re(1)-C(7)	92.70(19)
C(1)-Re(1)-C(4)	95.60(18)
C(2)-Re(1)-C(4)	126.67(17)
C(3)-Re(1)-C(4)	143.05(18)
C(7)-Re(1)-C(4)	60.18(17)
C(1)-Re(1)-C(5)	119.72(18)
C(2)-Re(1)-C(5)	98.42(18)
C(3)-Re(1)-C(5)	148.79(18)
C(7)-Re(1)-C(5)	59.59(17)
C(4)-Re(1)-C(5)	35.84(16)
C(1)-Re(1)-C(8)	104.88(18)
C(2)-Re(1)-C(8)	158.63(18)
C(3)-Re(1)-C(8)	106.72(18)
C(7)-Re(1)-C(8)	36.51(16)
C(4)-Re(1)-C(8)	36.60(15)
C(5)-Re(1)-C(8)	60.46(16)
C(1)-Re(1)-C(6)	154.87(18)
C(2)-Re(1)-C(6)	101.25(18)
C(3)-Re(1)-C(6)	112.67(18)

C(7)-Re(1)-C(6)	35.18(17)
C(4)-Re(1)-C(6)	60.11(17)
C(5)-Re(1)-C(6)	36.23(16)
C(8)-Re(1)-C(6)	60.28(16)
C(12)-Re(2)-C(13)	91.9(2)
C(12)-Re(2)-C(9)	90.5(2)
C(13)-Re(2)-C(9)	90.50(19)
C(12)-Re(2)-C(14)	94.4(2)
C(13)-Re(2)-C(14)	124.23(19)
C(9)-Re(2)-C(14)	144.63(18)
C(12)-Re(2)-C(15)	102.6(2)
C(13)-Re(2)-C(15)	155.5(2)
C(9)-Re(2)-C(15)	108.80(19)
C(14)-Re(2)-C(15)	36.04(18)
C(12)-Re(2)-C(18)	119.6(2)
C(13)-Re(2)-C(18)	95.87(19)
C(9)-Re(2)-C(18)	148.85(19)
C(14)-Re(2)-C(18)	35.68(18)
C(15)-Re(2)-C(18)	59.83(18)
C(12)-Re(2)-C(16)	136.7(2)
C(13)-Re(2)-C(16)	131.1(2)
C(9)-Re(2)-C(16)	93.87(19)
C(14)-Re(2)-C(16)	59.55(18)
C(15)-Re(2)-C(16)	35.89(18)
C(18)-Re(2)-C(16)	59.39(18)
C(12)-Re(2)-C(17)	153.5(2)
C(13)-Re(2)-C(17)	99.9(2)
C(9)-Re(2)-C(17)	112.96(19)
C(14)-Re(2)-C(17)	59.31(19)
C(15)-Re(2)-C(17)	59.23(19)
C(18)-Re(2)-C(17)	35.90(18)
C(16)-Re(2)-C(17)	34.98(19)
C(9)-O(9)-C(10)	121.3(4)
O(1)-C(1)-Re(1)	179.0(4)
O(2)-C(2)-Re(1)	178.6(4)
O(3)-C(3)-Re(1)	176.8(4)
C(5)-C(4)-C(8)	108.3(4)
C(5)-C(4)-Re(1)	72.2(3)

C(8)-C(4)-Re(1)	71.9(3)
C(5)-C(4)-H(4)	125.9
C(8)-C(4)-H(4)	125.9
Re(1)-C(4)-H(4)	121.7
C(4)-C(5)-C(6)	108.2(4)
C(4)-C(5)-Re(1)	72.0(3)
C(6)-C(5)-Re(1)	72.1(3)
C(4)-C(5)-H(5)	125.9
C(6)-C(5)-H(5)	125.9
Re(1)-C(5)-H(5)	121.7
C(7)-C(6)-C(5)	107.9(4)
C(7)-C(6)-Re(1)	71.9(3)
C(5)-C(6)-Re(1)	71.6(3)
C(7)-C(6)-H(6)	126.0
C(5)-C(6)-H(6)	126.0
Re(1)-C(6)-H(6)	122.1
C(6)-C(7)-C(8)	109.7(4)
C(6)-C(7)-Re(1)	72.9(3)
C(8)-C(7)-Re(1)	72.1(3)
C(6)-C(7)-H(7)	125.1
C(8)-C(7)-H(7)	125.1
Re(1)-C(7)-H(7)	121.5
C(7)-C(8)-C(4)	105.9(4)
C(7)-C(8)-C(9)	126.7(4)
C(4)-C(8)-C(9)	127.4(4)
C(7)-C(8)-Re(1)	71.4(3)
C(4)-C(8)-Re(1)	71.5(3)
C(9)-C(8)-Re(1)	120.4(3)
O(9)-C(9)-C(8)	104.4(4)
O(9)-C(9)-Re(2)	128.7(3)
C(8)-C(9)-Re(2)	126.8(3)
O(9)-C(10)-C(11)	107.4(4)
O(9)-C(10)-H(10A)	110.2
C(11)-C(10)-H(10A)	110.2
O(9)-C(10)-H(10B)	110.2
C(11)-C(10)-H(10B)	110.2
H(10A)-C(10)-H(10B)	108.5
C(10)-C(11)-H(11A)	109.5

C(10)-C(11)-H(11B)	109.5
H(11A)-C(11)-H(11B)	109.5
C(10)-C(11)-H(11C)	109.5
H(11A)-C(11)-H(11C)	109.5
H(11B)-C(11)-H(11C)	109.5
O(12)-C(12)-Re(2)	177.1(4)
O(13)-C(13)-Re(2)	176.6(4)
C(18)-C(14)-C(15)	108.4(4)
C(18)-C(14)-Re(2)	72.5(3)
C(15)-C(14)-Re(2)	72.2(3)
C(18)-C(14)-H(14)	125.8
C(15)-C(14)-H(14)	125.8
Re(2)-C(14)-H(14)	121.2
C(14)-C(15)-C(16)	107.4(5)
C(14)-C(15)-Re(2)	71.8(3)
C(16)-C(15)-Re(2)	73.1(3)
C(14)-C(15)-H(15)	126.3
C(16)-C(15)-H(15)	126.3
Re(2)-C(15)-H(15)	120.7
C(17)-C(16)-C(15)	108.3(5)
C(17)-C(16)-Re(2)	72.8(3)
C(15)-C(16)-Re(2)	71.0(3)
C(17)-C(16)-H(16)	125.9
C(15)-C(16)-H(16)	125.9
Re(2)-C(16)-H(16)	122.0
C(16)-C(17)-C(18)	108.3(5)
C(16)-C(17)-Re(2)	72.2(3)
C(18)-C(17)-Re(2)	70.9(3)
C(16)-C(17)-H(17)	125.9
C(18)-C(17)-H(17)	125.9
Re(2)-C(17)-H(17)	122.7
C(14)-C(18)-C(17)	107.6(4)
C(14)-C(18)-Re(2)	71.8(3)
C(17)-C(18)-Re(2)	73.2(3)
C(14)-C(18)-H(18)	126.2
C(17)-C(18)-H(18)	126.2
Re(2)-C(18)-H(18)	120.6

Symmetry transformations used to generate equivalent atoms:

Table 4. Anisotropic displacement parameters ($Å^2 x\ 10^3$)for mo_rf73_0m. The anisotropic displacement factor exponent takes the form: $-2\pi^2[\ h^2 a^{*2} U^{11} + ... + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Re(1)	11(1)	11(1)	13(1)	-5(1)	0(1)	-4(1)
Re(2)	12(1)	13(1)	14(1)	-7(1)	2(1)	-5(1)
O(1)	26(2)	13(2)	32(2)	-5(2)	-2(2)	-4(2)
O(2)	32(2)	33(2)	21(2)	-12(2)	-3(2)	-12(2)
O(3)	13(2)	23(2)	46(2)	-16(2)	1(2)	-7(2)
O(9)	14(2)	31(2)	47(2)	-30(2)	-10(2)	3(2)
O(12)	17(2)	38(2)	37(2)	-25(2)	11(2)	-14(2)
O(13)	32(2)	33(2)	19(2)	-6(2)	-4(2)	-1(2)
C(1)	13(2)	17(3)	18(2)	-9(2)	2(2)	-4(2)
C(2)	14(2)	12(2)	21(3)	-7(2)	2(2)	-5(2)
C(3)	31(3)	13(2)	17(3)	-5(2)	0(2)	-14(2)
C(4)	12(2)	17(2)	17(2)	-6(2)	1(2)	-5(2)
C(5)	21(2)	23(3)	13(2)	-8(2)	1(2)	-13(2)
C(6)	21(2)	15(2)	21(3)	-11(2)	5(2)	-10(2)
C(7)	21(2)	13(2)	15(2)	-4(2)	1(2)	-5(2)
C(8)	11(2)	16(2)	14(2)	-5(2)	1(2)	-4(2)
C(9)	15(2)	18(3)	14(2)	-9(2)	2(2)	-5(2)
C(10)	22(3)	55(4)	81(5)	-54(4)	-17(3)	0(3)
C(11)	18(3)	32(3)	47(4)	-10(3)	-9(3)	-6(2)
C(12)	20(3)	22(3)	19(3)	-11(2)	1(2)	-6(2)
C(13)	24(3)	15(3)	22(3)	-9(2)	2(2)	-6(2)
C(14)	21(3)	9(2)	28(3)	-5(2)	4(2)	-4(2)
C(15)	28(3)	24(3)	17(3)	-4(2)	2(2)	-11(2)
C(16)	24(3)	21(3)	26(3)	-7(2)	11(2)	-10(2)
C(17)	22(3)	21(3)	37(3)	-6(2)	1(2)	-13(2)
C(18)	33(3)	20(3)	22(3)	-9(2)	3(2)	-17(2)

Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for mo_rf73_0m.

	x	y	z	U(eq)
H(4)	9855	6287	3221	19
H(5)	10189	8078	4064	21
H(6)	7434	10635	3473	20
H(7)	5413	10422	2290	20
H(10A)	3457	7190	1669	56
H(10B)	3926	8170	476	56
H(11A)	860	9328	802	51
H(11B)	1394	9509	1864	51
H(11C)	1861	10486	677	51
H(14)	10459	2373	2149	25
H(15)	8990	3317	3705	29
H(16)	5582	4536	3337	30
H(17)	4967	4362	1570	31
H(18)	7993	3073	807	27

Table 6. Torsion angles [°] for mo_rf73_0m.

C(8)-C(4)-C(5)-C(6)	-0.2(5)
Re(1)-C(4)-C(5)-C(6)	-63.5(3)
C(8)-C(4)-C(5)-Re(1)	63.3(3)
C(4)-C(5)-C(6)-C(7)	0.2(5)
Re(1)-C(5)-C(6)-C(7)	-63.2(3)
C(4)-C(5)-C(6)-Re(1)	63.4(3)
C(5)-C(6)-C(7)-C(8)	-0.1(5)
Re(1)-C(6)-C(7)-C(8)	-63.1(3)
C(5)-C(6)-C(7)-Re(1)	63.0(3)
C(6)-C(7)-C(8)-C(4)	0.0(5)
Re(1)-C(7)-C(8)-C(4)	-63.6(3)
C(6)-C(7)-C(8)-C(9)	178.1(4)
Re(1)-C(7)-C(8)-C(9)	114.5(5)
C(6)-C(7)-C(8)-Re(1)	63.6(3)
C(5)-C(4)-C(8)-C(7)	0.1(5)
Re(1)-C(4)-C(8)-C(7)	63.6(3)
C(5)-C(4)-C(8)-C(9)	-177.9(4)
Re(1)-C(4)-C(8)-C(9)	-114.5(5)
C(5)-C(4)-C(8)-Re(1)	-63.5(3)
C(10)-O(9)-C(9)-C(8)	-173.8(5)
C(10)-O(9)-C(9)-Re(2)	4.1(8)
C(7)-C(8)-C(9)-O(9)	-13.5(7)
C(4)-C(8)-C(9)-O(9)	164.2(5)
Re(1)-C(8)-C(9)-O(9)	75.1(4)
C(7)-C(8)-C(9)-Re(2)	168.6(4)
C(4)-C(8)-C(9)-Re(2)	-13.8(7)
Re(1)-C(8)-C(9)-Re(2)	-102.8(4)
C(9)-O(9)-C(10)-C(11)	178.8(5)
C(18)-C(14)-C(15)-C(16)	1.0(6)
Re(2)-C(14)-C(15)-C(16)	64.9(4)
C(18)-C(14)-C(15)-Re(2)	-63.9(3)
C(14)-C(15)-C(16)-C(17)	-0.3(6)
Re(2)-C(15)-C(16)-C(17)	63.7(4)
C(14)-C(15)-C(16)-Re(2)	-64.0(3)
C(15)-C(16)-C(17)-C(18)	-0.5(6)
Re(2)-C(16)-C(17)-C(18)	62.1(3)

C(15)-C(16)-C(17)-Re(2)	-62.6(4)
C(15)-C(14)-C(18)-C(17)	-1.3(5)
Re(2)-C(14)-C(18)-C(17)	-65.0(3)
C(15)-C(14)-C(18)-Re(2)	63.7(3)
C(16)-C(17)-C(18)-C(14)	1.1(5)
Re(2)-C(17)-C(18)-C(14)	64.1(3)
C(16)-C(17)-C(18)-Re(2)	-62.9(4)

Symmetry transformations used to generate equivalent atoms:

Table 7. Hydrogen bonds for mo_rf73_0m [Å and °].

D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)
C(10)-H(10A)...O(12)#1	0.99	2.57	3.245(7)	125.7
C(10)-H(10A)...O(12)#1	0.99	2.57	3.245(7)	125.7

Symmetry transformations used to generate equivalent atoms:

#1 x-1,y,z

Crystal data for complex 5

Table 1. Crystal data and structure refinement for mo_rf54x2_0m_a_a.

Identification code	shelx	
Empirical formula	C_{18} H_{14} Mn O_6 Re	
Formula weight	567.43	
Temperature	150(2) K	
Wavelength	0.71073 Å	
Crystal system	Triclinic	
Space group	P -1	
Unit cell dimensions	a = 8.0405(4) Å	α= 68.305(2)°.
	b = 9.7946(5) Å	β= 83.329(2)°.
	c = 13.0639(7) Å	γ = 67.577(2)°.
Volume	883.30(8) $Å^3$	
Z	2	
Density (calculated)	2.133 Mg/m^3	
Absorption coefficient	7.592 mm^{-1}	
F(000)	540	
Crystal size	0.231 x 0.148 x 0.137 mm^3	
Theta range for data collection	2.396 to 25.350°.	
Index ranges	-9<=h<=9, -11<=k<=11, -15<=l<=15	
Reflections collected	23313	
Independent reflections	3225 [R(int) = 0.0499]	
Completeness to theta = 25.242°	100.0 %	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	3225 / 0 / 235	
Goodness-of-fit on F^2	1.132	
Final R indices [I>2sigma(I)]	R1 = 0.0267, wR2 = 0.0754	
R indices (all data)	R1 = 0.0272, wR2 = 0.0757	
Extinction coefficient	n/a	
Largest diff. peak and hole	2.907 and -0.574 e.$Å^{-3}$	

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for mo_rf54x2_0m_a_a. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
Re(1)	6701(1)	7769(1)	4331(1)	14(1)
Mn(1)	7731(1)	5580(1)	1544(1)	4(1)
O(1)	7035(5)	4327(4)	5424(3)	24(1)
O(2)	7016(6)	7757(5)	6645(3)	27(1)
O(3)	2598(5)	8933(5)	4458(4)	27(1)
O(9)	4792(5)	8391(5)	1756(4)	29(1)
O(12)	11179(6)	6024(6)	1254(4)	31(1)
O(13)	6680(6)	7338(6)	-800(3)	35(1)
C(1)	6894(7)	5622(6)	5017(4)	17(1)
C(2)	6874(7)	7779(6)	5782(5)	18(1)
C(3)	4129(7)	8472(6)	4435(4)	17(1)
C(4)	8989(7)	7292(6)	3146(4)	16(1)
C(5)	9201(7)	8333(6)	3594(4)	18(1)
C(6)	7671(7)	9775(6)	3252(4)	19(1)
C(7)	6523(7)	9619(6)	2602(4)	17(1)
C(8)	7321(7)	8072(6)	2523(4)	15(1)
C(9)	6512(7)	7412(6)	1941(4)	17(1)
C(10)	3461(8)	8063(9)	1321(7)	42(2)
C(11)	1779(9)	9479(8)	1118(7)	38(2)
C(12)	9786(7)	5888(6)	1371(4)	20(1)
C(13)	7070(7)	6674(6)	125(5)	21(1)
C(14)	9159(8)	3063(7)	2152(5)	23(1)
C(15)	8389(8)	3552(7)	3053(5)	23(1)
C(16)	6494(8)	4210(7)	2893(5)	23(1)
C(17)	6074(8)	4136(7)	1896(5)	24(1)
C(18)	7746(8)	3432(7)	1437(5)	23(1)

Table 3. Bond lengths [Å] and angles [°] for mo_rf54x2_0m_a_a.

Re(1)-C(1)	1.907(5)
Re(1)-C(3)	1.921(5)
Re(1)-C(2)	1.920(6)
Re(1)-C(4)	2.284(5)
Re(1)-C(8)	2.289(5)
Re(1)-C(7)	2.293(5)
Re(1)-C(5)	2.297(5)
Re(1)-C(6)	2.307(5)
Mn(1)-C(12)	1.765(6)
Mn(1)-C(13)	1.786(6)
Mn(1)-C(9)	1.918(6)
Mn(1)-C(14)	2.152(6)
Mn(1)-C(18)	2.154(6)
Mn(1)-C(15)	2.158(6)
Mn(1)-C(16)	2.181(5)
Mn(1)-C(17)	2.191(6)
O(1)-C(1)	1.145(7)
O(2)-C(2)	1.138(7)
O(3)-C(3)	1.138(7)
O(9)-C(9)	1.336(7)
O(9)-C(10)	1.453(7)
O(12)-C(12)	1.163(7)
O(13)-C(13)	1.155(7)
C(4)-C(5)	1.417(7)
C(4)-C(8)	1.434(7)
C(5)-C(6)	1.429(8)
C(6)-C(7)	1.408(8)
C(7)-C(8)	1.441(7)
C(8)-C(9)	1.489(7)
C(10)-C(11)	1.485(9)
C(14)-C(18)	1.407(8)
C(14)-C(15)	1.420(8)
C(15)-C(16)	1.416(8)
C(16)-C(17)	1.416(8)
C(17)-C(18)	1.433(8)

C(1)-Re(1)-C(3)	90.6(2)
C(1)-Re(1)-C(2)	87.4(2)
C(3)-Re(1)-C(2)	89.4(2)
C(1)-Re(1)-C(4)	95.4(2)
C(3)-Re(1)-C(4)	143.0(2)
C(2)-Re(1)-C(4)	127.2(2)
C(1)-Re(1)-C(8)	104.6(2)
C(3)-Re(1)-C(8)	106.7(2)
C(2)-Re(1)-C(8)	159.5(2)
C(4)-Re(1)-C(8)	36.55(18)
C(1)-Re(1)-C(7)	139.7(2)
C(3)-Re(1)-C(7)	92.3(2)
C(2)-Re(1)-C(7)	132.8(2)
C(4)-Re(1)-C(7)	60.47(19)
C(8)-Re(1)-C(7)	36.67(18)
C(1)-Re(1)-C(5)	119.7(2)
C(3)-Re(1)-C(5)	148.7(2)
C(2)-Re(1)-C(5)	99.0(2)
C(4)-Re(1)-C(5)	36.04(18)
C(8)-Re(1)-C(5)	60.64(18)
C(7)-Re(1)-C(5)	60.04(19)
C(1)-Re(1)-C(6)	154.8(2)
C(3)-Re(1)-C(6)	112.6(2)
C(2)-Re(1)-C(6)	101.9(2)
C(4)-Re(1)-C(6)	60.23(19)
C(8)-Re(1)-C(6)	60.54(19)
C(7)-Re(1)-C(6)	35.65(19)
C(5)-Re(1)-C(6)	36.17(19)
C(12)-Mn(1)-C(13)	92.9(3)
C(12)-Mn(1)-C(9)	92.4(2)
C(13)-Mn(1)-C(9)	92.1(2)
C(12)-Mn(1)-C(14)	90.5(2)
C(13)-Mn(1)-C(14)	122.2(2)
C(9)-Mn(1)-C(14)	145.4(2)
C(12)-Mn(1)-C(18)	117.8(2)
C(13)-Mn(1)-C(18)	92.7(2)
C(9)-Mn(1)-C(18)	149.0(2)
C(14)-Mn(1)-C(18)	38.1(2)

C(12)-Mn(1)-C(15)	99.2(2)
C(13)-Mn(1)-C(15)	156.6(2)
C(9)-Mn(1)-C(15)	107.2(2)
C(14)-Mn(1)-C(15)	38.5(2)
C(18)-Mn(1)-C(15)	64.0(2)
C(12)-Mn(1)-C(16)	135.2(2)
C(13)-Mn(1)-C(16)	131.6(2)
C(9)-Mn(1)-C(16)	90.6(2)
C(14)-Mn(1)-C(16)	64.0(2)
C(18)-Mn(1)-C(16)	63.8(2)
C(15)-Mn(1)-C(16)	38.1(2)
C(12)-Mn(1)-C(17)	154.3(2)
C(13)-Mn(1)-C(17)	97.5(2)
C(9)-Mn(1)-C(17)	110.5(2)
C(14)-Mn(1)-C(17)	64.1(2)
C(18)-Mn(1)-C(17)	38.5(2)
C(15)-Mn(1)-C(17)	63.8(2)
C(16)-Mn(1)-C(17)	37.8(2)
C(9)-O(9)-C(10)	122.3(5)
O(1)-C(1)-Re(1)	179.0(5)
O(2)-C(2)-Re(1)	178.4(5)
O(3)-C(3)-Re(1)	177.4(5)
C(5)-C(4)-C(8)	108.6(5)
C(5)-C(4)-Re(1)	72.5(3)
C(8)-C(4)-Re(1)	71.9(3)
C(4)-C(5)-C(6)	108.0(5)
C(4)-C(5)-Re(1)	71.5(3)
C(6)-C(5)-Re(1)	72.3(3)
C(7)-C(6)-C(5)	108.0(5)
C(7)-C(6)-Re(1)	71.6(3)
C(5)-C(6)-Re(1)	71.5(3)
C(6)-C(7)-C(8)	108.8(5)
C(6)-C(7)-Re(1)	72.7(3)
C(8)-C(7)-Re(1)	71.5(3)
C(4)-C(8)-C(7)	106.6(4)
C(4)-C(8)-C(9)	127.4(5)
C(7)-C(8)-C(9)	126.0(5)
C(4)-C(8)-Re(1)	71.5(3)

C(7)-C(8)-Re(1)	71.8(3)
C(9)-C(8)-Re(1)	119.9(3)
O(9)-C(9)-C(8)	104.4(4)
O(9)-C(9)-Mn(1)	129.0(4)
C(8)-C(9)-Mn(1)	126.6(4)
O(9)-C(10)-C(11)	106.6(5)
O(12)-C(12)-Mn(1)	177.0(5)
O(13)-C(13)-Mn(1)	177.7(5)
C(18)-C(14)-C(15)	107.8(5)
C(18)-C(14)-Mn(1)	71.0(3)
C(15)-C(14)-Mn(1)	71.0(3)
C(16)-C(15)-C(14)	108.2(5)
C(16)-C(15)-Mn(1)	71.9(3)
C(14)-C(15)-Mn(1)	70.5(3)
C(17)-C(16)-C(15)	108.4(5)
C(17)-C(16)-Mn(1)	71.5(3)
C(15)-C(16)-Mn(1)	70.0(3)
C(16)-C(17)-C(18)	107.1(5)
C(16)-C(17)-Mn(1)	70.7(3)
C(18)-C(17)-Mn(1)	69.4(3)
C(14)-C(18)-C(17)	108.5(5)
C(14)-C(18)-Mn(1)	70.8(3)
C(17)-C(18)-Mn(1)	72.1(3)

Symmetry transformations used to generate equivalent atoms:

Table 4. Anisotropic displacement parameters ($Å^2 x\ 10^3$)for mo_rf54x2_0m_a_a. The anisotropic displacement factor exponent takes the form: $-2\pi^2[\ h^2 a^{*2} U^{11} + ... + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Re(1)	16(1)	14(1)	15(1)	-6(1)	0(1)	-7(1)
Mn(1)	7(1)	6(1)	4(1)	-3(1)	2(1)	-5(1)
O(1)	25(2)	15(2)	30(2)	-6(2)	2(2)	-7(2)
O(2)	36(2)	32(2)	19(2)	-13(2)	-3(2)	-12(2)
O(3)	18(2)	24(2)	42(3)	-14(2)	0(2)	-9(2)
O(9)	17(2)	34(2)	45(3)	-27(2)	-10(2)	-2(2)
O(12)	27(2)	45(3)	39(3)	-27(2)	13(2)	-22(2)
O(13)	40(3)	36(2)	19(2)	-4(2)	-4(2)	-7(2)
C(1)	14(2)	21(3)	19(3)	-9(2)	3(2)	-6(2)
C(2)	17(3)	13(3)	27(3)	-8(2)	1(2)	-6(2)
C(3)	19(3)	14(2)	19(3)	-5(2)	-1(2)	-9(2)
C(4)	17(2)	17(3)	17(2)	-8(2)	3(2)	-7(2)
C(5)	19(3)	24(3)	17(3)	-8(2)	0(2)	-13(2)
C(6)	26(3)	17(3)	20(3)	-7(2)	3(2)	-12(2)
C(7)	21(3)	14(2)	15(2)	-3(2)	0(2)	-7(2)
C(8)	16(2)	16(2)	13(2)	-5(2)	2(2)	-7(2)
C(9)	15(2)	23(3)	12(2)	-4(2)	0(2)	-8(2)
C(10)	18(3)	51(4)	70(5)	-43(4)	-13(3)	-3(3)
C(11)	24(3)	32(4)	55(4)	-10(3)	-13(3)	-9(3)
C(12)	24(3)	18(3)	20(3)	-12(2)	6(2)	-8(2)
C(13)	23(3)	19(3)	24(3)	-10(2)	3(2)	-8(2)
C(14)	24(3)	18(3)	26(3)	-6(2)	6(2)	-11(2)
C(15)	30(3)	25(3)	17(3)	-7(2)	1(2)	-14(2)
C(16)	28(3)	24(3)	20(3)	-8(2)	8(2)	-14(2)
C(17)	25(3)	20(3)	29(3)	-5(2)	-1(2)	-13(2)
C(18)	36(3)	22(3)	20(3)	-10(2)	5(2)	-18(2)

Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for mo_rf54x2_0m_a_a.

	x	y	z	U(eq)
H(4)	9813	6252	3242	19
H(5)	10187	8111	4043	22
H(6)	7465	10680	3432	23
H(7)	5407	10404	2270	20
H(10A)	3261	7120	1858	50
H(10B)	3872	7867	626	50
H(11A)	837	9311	822	57
H(11B)	1390	9659	1812	57
H(11C)	1999	10402	586	57
H(14)	10407	2573	2051	27
H(15)	9033	3454	3657	28
H(16)	5648	4630	3373	28
H(17)	4904	4487	1590	29
H(18)	7877	3247	762	28

Table 6. Torsion angles [°] for mo_rf54x2_0m_a_a.

C(8)-C(4)-C(5)-C(6)	-0.2(6)
Re(1)-C(4)-C(5)-C(6)	-63.5(4)
C(8)-C(4)-C(5)-Re(1)	63.3(4)
C(4)-C(5)-C(6)-C(7)	0.2(6)
Re(1)-C(5)-C(6)-C(7)	-62.7(4)
C(4)-C(5)-C(6)-Re(1)	63.0(4)
C(5)-C(6)-C(7)-C(8)	-0.2(6)
Re(1)-C(6)-C(7)-C(8)	-62.8(4)
C(5)-C(6)-C(7)-Re(1)	62.7(4)
C(5)-C(4)-C(8)-C(7)	0.1(6)
Re(1)-C(4)-C(8)-C(7)	63.8(3)
C(5)-C(4)-C(8)-C(9)	-177.6(5)
Re(1)-C(4)-C(8)-C(9)	-114.0(5)
C(5)-C(4)-C(8)-Re(1)	-63.7(4)
C(6)-C(7)-C(8)-C(4)	0.0(6)
Re(1)-C(7)-C(8)-C(4)	-63.6(3)
C(6)-C(7)-C(8)-C(9)	177.8(5)
Re(1)-C(7)-C(8)-C(9)	114.2(5)
C(6)-C(7)-C(8)-Re(1)	63.6(4)
C(10)-O(9)-C(9)-C(8)	-172.3(6)
C(10)-O(9)-C(9)-Mn(1)	8.6(9)
C(4)-C(8)-C(9)-O(9)	163.3(5)
C(7)-C(8)-C(9)-O(9)	-13.9(7)
Re(1)-C(8)-C(9)-O(9)	74.5(5)
C(4)-C(8)-C(9)-Mn(1)	-17.5(8)
C(7)-C(8)-C(9)-Mn(1)	165.2(4)
Re(1)-C(8)-C(9)-Mn(1)	-106.3(4)
C(9)-O(9)-C(10)-C(11)	-174.1(6)
C(18)-C(14)-C(15)-C(16)	0.6(6)
Mn(1)-C(14)-C(15)-C(16)	62.4(4)
C(18)-C(14)-C(15)-Mn(1)	-61.8(4)
C(14)-C(15)-C(16)-C(17)	0.0(6)
Mn(1)-C(15)-C(16)-C(17)	61.5(4)
C(14)-C(15)-C(16)-Mn(1)	-61.6(4)
C(15)-C(16)-C(17)-C(18)	-0.5(6)
Mn(1)-C(16)-C(17)-C(18)	60.1(4)

C(15)-C(16)-C(17)-Mn(1)	-60.6(4)
C(15)-C(14)-C(18)-C(17)	-0.9(6)
Mn(1)-C(14)-C(18)-C(17)	-62.7(4)
C(15)-C(14)-C(18)-Mn(1)	61.8(4)
C(16)-C(17)-C(18)-C(14)	0.9(6)
Mn(1)-C(17)-C(18)-C(14)	61.9(4)
C(16)-C(17)-C(18)-Mn(1)	-61.0(4)

Symmetry transformations used to generate equivalent atoms:

Table 7. Hydrogen bonds for mo_rf54x2_0m_a_a [Å and °].

D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)
C(10)-H(10A)...O(12)#1	0.99	2.62	3.214(8)	118.4

Symmetry transformations used to generate equivalent atoms:

#1 x-1,y,z