**Supplementary Material**

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

ROAN FRASER, PETRUS H. VAN ROOYEN and MARILÉ LANDMAN\*

**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: R2= 0.99)

**Crystal data for complex 2**

Table 1. Crystal data and structure refinement for mo\_rf71x2\_0m\_5.

Identification code shelx

Empirical formula C18.31 H14.61 Mn2 O6

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 = 68.29(7)°.

 b = 9.913(8) Å = 80.74(6)°.

 c = 13.041(13) Å  = 67.54(6)°.

Volume 890.4(14) Å3

Z 2

Density (calculated) 1.643 Mg/m3

Absorption coefficient 1.450 mm-1

F(000) 445

Crystal size 0.099 x 0.085 x 0.057 mm3

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 F2

Data / restraints / parameters 4941 / 0 / 246

Goodness-of-fit on F2 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 104) and equivalent isotropic displacement parameters (Å2x 103)

for mo\_rf71x2\_0m\_5. U(eq) is defined as one third of the trace of the orthogonalized Uij 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)

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\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_

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 (Å2x 103)for mo\_rf71x2\_0m\_5. The anisotropic

displacement factor exponent takes the form: -22[ h2a\*2U11 + ... + 2 h k a\* b\* U12 ]

\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_

 U11 U22 U33 U23 U13 U12

\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_

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 104) and isotropic displacement parameters (Å2x 103)

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 C18 H14 O6 Re2

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 = 68.393(4)°.

 b = 9.9573(10) Å = 83.222(4)°.

 c = 13.1674(14) Å  = 66.777(4)°.

Volume 900.23(16) Å3

Z 2

Density (calculated) 2.578 Mg/m3

Absorption coefficient 13.466 mm-1

F(000) 640

Crystal size 0.192 x 0.082 x 0.071 mm3

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 F2

Data / restraints / parameters 3290 / 0 / 235

Goodness-of-fit on F2 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 104) and equivalent isotropic displacement parameters (Å2x 103)

for mo\_rf73\_0m. U(eq) is defined as one third of the trace of the orthogonalized Uij 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

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Symmetry transformations used to generate equivalent atoms:

Table 4. Anisotropic displacement parameters (Å2x 103)for mo\_rf73\_0m. The anisotropic

displacement factor exponent takes the form: -22[ h2a\*2U11 + ... + 2 h k a\* b\* U12 ]

\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_

 U11 U22 U33 U23 U13 U12

\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_

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 104) and isotropic displacement parameters (Å2x 103)

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 C18 H14 Mn O6 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 = 68.305(2)°.

 b = 9.7946(5) Å = 83.329(2)°.

 c = 13.0639(7) Å  = 67.577(2)°.

Volume 883.30(8) Å3

Z 2

Density (calculated) 2.133 Mg/m3

Absorption coefficient 7.592 mm-1

F(000) 540

Crystal size 0.231 x 0.148 x 0.137 mm3

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 F2

Data / restraints / parameters 3225 / 0 / 235

Goodness-of-fit on F2 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 104) and equivalent isotropic displacement parameters (Å2x 103)

for mo\_rf54x2\_0m\_a\_a. U(eq) is defined as one third of the trace of the orthogonalized Uij 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)

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Symmetry transformations used to generate equivalent atoms:

Table 4. Anisotropic displacement parameters (Å2x 103)for mo\_rf54x2\_0m\_a\_a. The anisotropic

displacement factor exponent takes the form: -22[ h2a\*2U11 + ... + 2 h k a\* b\* U12 ]

\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_

 U11 U22 U33 U23 U13 U12

\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_

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 104) and isotropic displacement parameters (Å2x 103)

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