Electronic Supplementary Material (ESI) for Dalton Transactions.

Supplementary Information

The Pyrrole Ring η^2-Hapticity Bridged Binuclear Tricarbonyl Mo and W Complexes: Catalysis of Regioselective Hydroamination Reactions and DFT Calculations

Vikesh Kumar Jha, Ganesan Mani[*,a], Yogeswara Rao Davuluri and Anakuthil Anoop*

Department of Chemistry, Indian Institute of Technology – Kharagpur, Kharagpur, West Bengal, India 721 302, Fax: +91 3222 282252, E-mail: gmani@chem.iitkgp.ernet.in

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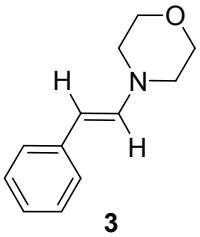
Experimental procedure for hydroamination reactions

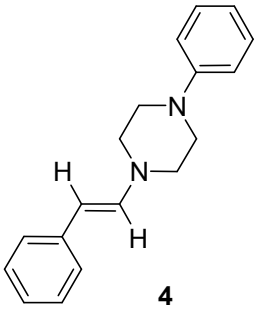
4-[(E)-2-phenylethenyl]morpholine, 3



3

Phenylacetylene (0.39 mL, 3.48 mmol), morpholine (0.15 mL, 1.74 mmol), and complex **1** (0.007 g, 0.007 mmol, 0.40 mol%) were taken in a 250 mL Schlenk flask and stirred at 25 °C. After 4 h the reaction mixture turned to a homogeneous oily solution and the stirring was continued for 96 h. The volatiles were removed under vacuum for 30 min to give **3a** as light yellow oily solid (0.305 g, 1.61 mmol, 92%). ^{1}H NMR (400 MHz, $CDCl_3$): δ = 7.26−7.22 (m, 4H, C_6H_5), 7.06 (m, 1H, C_6H_5), 6.63 (d, ^{3}J = 16, 1H, C*H*), 5.45 (d, ^{3}J =16, 1H, C*H*), 3.78 (br s, 4H, CH_2), 3.04 (br s, 4H, CH_2). GC-MS: $C_{12}H_{15}NO$, *M*r = 189.35.

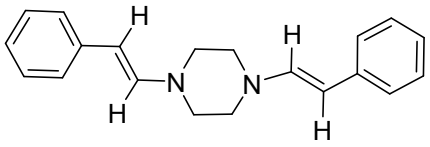
1-[(E)-2-phenylethenyl]N-phenylpiperazine, 4



4

Phenylacetylene (0.28 mL, 2.50 mmol), N-phenylpiperazine (0.2 mL, 1.26 mmol) and complex **1** (0.005, 0.005 mmol 0.40 mol %) were taken in a Schlenk flask and stirred at room temperature. After 4 h light yellow precipitate was formed and the stirring was continued for 96 h. The volatiles were removed under vacuum to give **3b** as slightly yellow oily solid (0.300 g, 1.13 mmol, 90%). ^{1}H NMR (400 MHz, $CDCl_3$): δ = 7.33-7.24 (m, 6H, Ph), 7.07−6.90 (m, 4H, Ph), 6.72 (d, ^{3}J =16, 1H, C*H*), 5.49 (d, ^{3}J = 12.0, 1H, C*H*), 3.26 (br s, 2H, CH_2), 3.23 (br s, 2H, CH_2). GC-MS: $C_{18}H_{20}N_2$, *M*r = 264.3.

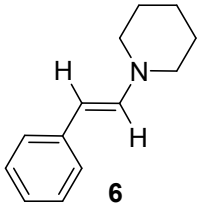
1-[(E)-2-phenylethenyl]piperazine, 5



5

Phenylacetylene (0.52 ml, 4.64 mmol), piperazine (0.10 g, 1.16 mmol), and complex **1** (0.005 g, 0.005 mmol, 0.43 mol %) were taken in a Schlenk flask and stirred at room temperature. After 4 h light yellow precipitate was formed and the stirring was continued for 96 h. The volatiles were removed under vacuum to give **3c** as slightly yellow oily solid (0.300 g, 1.03 mmol, 89%). ^{1}H NMR (400 MHz, $CDCl_3$): δ = 7.26−7.23 (m, 8H, Ph), 7.06 (m, 2H, Ph), 6.67 (d, ^{3}J = 14.4, 2H, CH), 5.47 (d, ^{3}J = 14.4, 2H, CH), 3.13 (s, 8H, NCH_2). GC-MS: $C_{20}H_{22}N_2$, *M*r = 290.3.

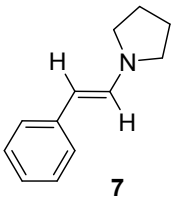
1-[(E)-2-phenylethenyl]piperidine, 6



6

Phenylacetylene (0.2 mL, 1.78 mmol), piperidine (0.17 mL, 1.72 mmol), and complex **1** (0.007 g, 0.007 mmol, 0.41 mol %) were taken in a Schlenk flask equipped with water condenser and refluxed at 80 °C for 5 h with its stopcock closed to ensure the volatile phenylacetylene not evaporated out. A homogeneous reaction mixture was obtained and cooled to room temperature. The volatiles were removed under vacuum to give **3d** as light brown oily compound (0.225 g, 1.20 mmol, 70%). ^{1}H NMR (400 MHz, $CDCl_3$): δ = 7.22 (br s, 4H, Ph), 7.03 (br s, 1H, Ph), 6.69 (d, ^{3}J = 14.0,1H, CH), 5.39 (d, ^{3}J =14.0, 1H, CH), 3.05 (br s, 4H, CH_2), 1.64 (br s, 4H, CH_2), GC-MS: $C_{13}H_{17}N$, *M*r = 187.3.

1-[(E)-2-phenylethenyl]pyrrolidine, 7



7

Phenylacetylene (0.39 mL, 3.6 mmol), pyrrolidine (0.15 mL, 1.8 mmol), and complex **1** (0.007 g, 0.007 mmol, 0.42 mol %) were taken in a Schlenk flask equipped with water condenser and refluxed at 80 °C for 3 h with its stopcock closed to ensure the volatile phenylacetylene not evaporated out. The homogeneous reaction mixture was cooled to room temperature and the volatiles were removed under vacuum to give an oily residue which contains the anti-Markovnikov product as the major component, as shown by ^{1}H NMR (0.113 g, 0.65 mmol, 36%). ^{1}H NMR (400 MHz, $CDCl_3$): δ = 7.19 (br m, 4H, Ph), 7.06 (d, ^{3}J = 14.0, 1H, C*H*), 6.95 (br m, 1H, Ph), 5.10 (d, ^{3}J = 14.0, 1H, C*H*), 3.23 (br m, 4H, CH_2), 1.92 (br m, 4H, CH_2). GC-MS: $C_{13}H_{17}N$, *M*r = 173.3.

NMR, HRMS and IR spectra

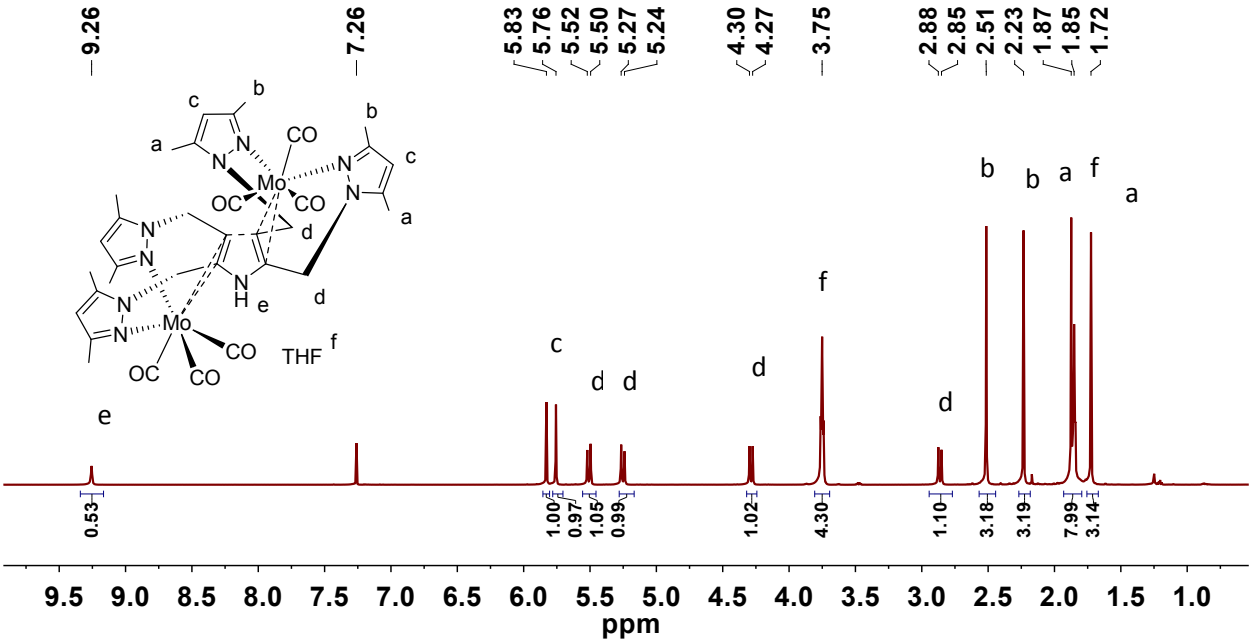


Figure S1: ^{1}H NMR (600 MHz, 22 °C) spectrum of complex **1** in $CDCl_3$.

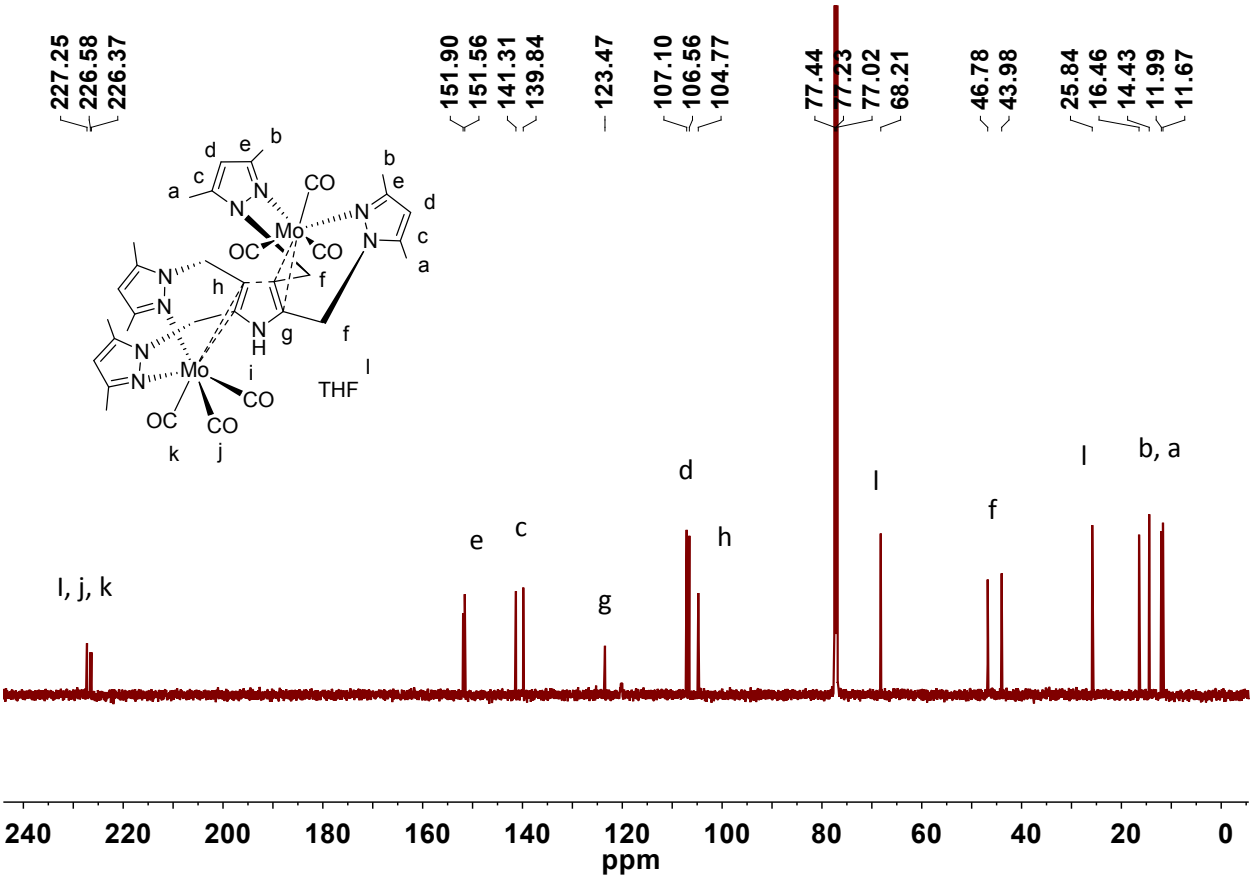


Figure S2: $^{13}C\{^{1}H\}$ NMR (153.9 MHz, 22 °C) spectrum of complex **1** in $CDCl_3$.

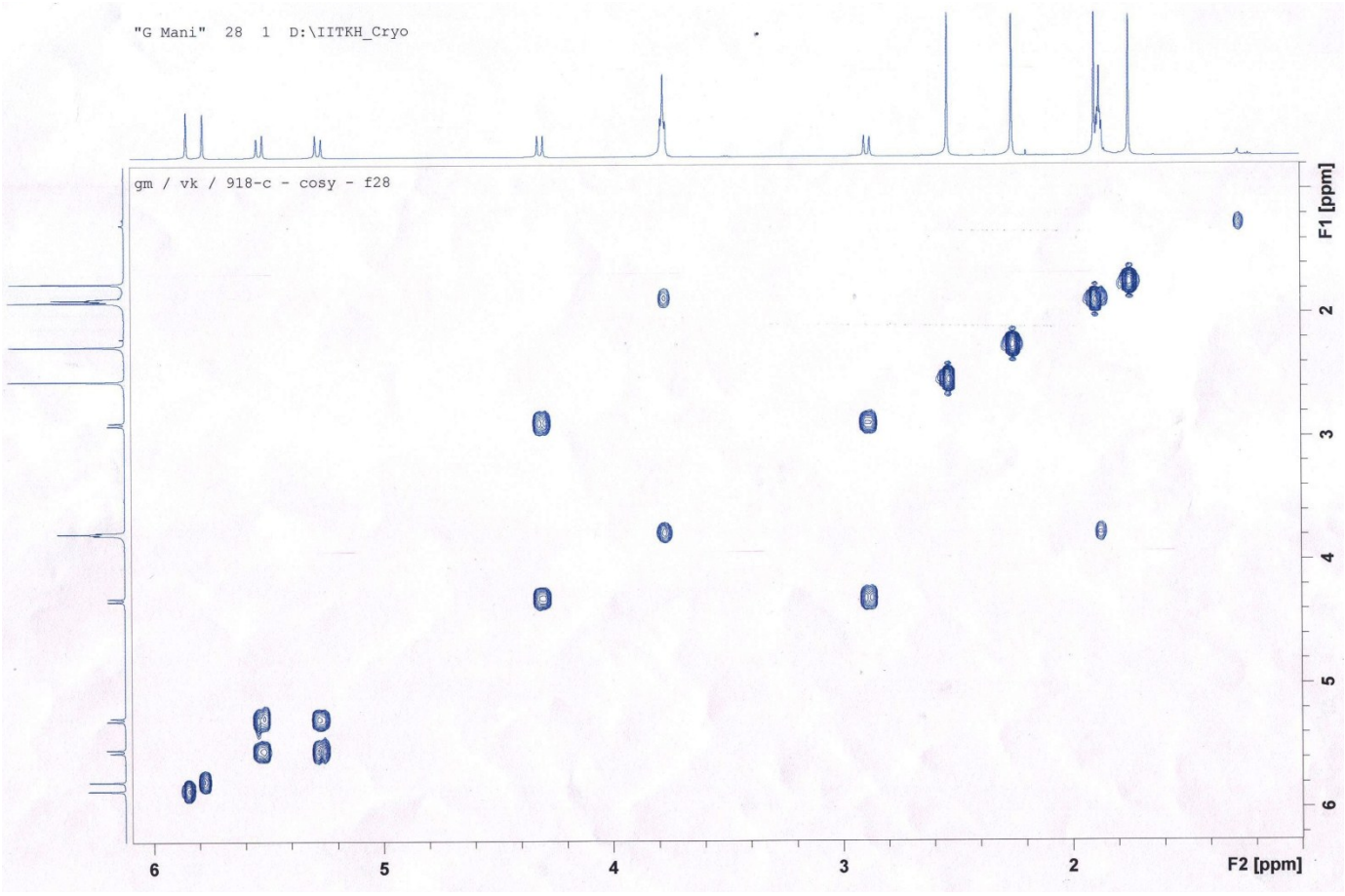


Figure S3: COSY NMR (600 MHz, 22 °C) spectrum of complex **1** in $CDCl_3$.

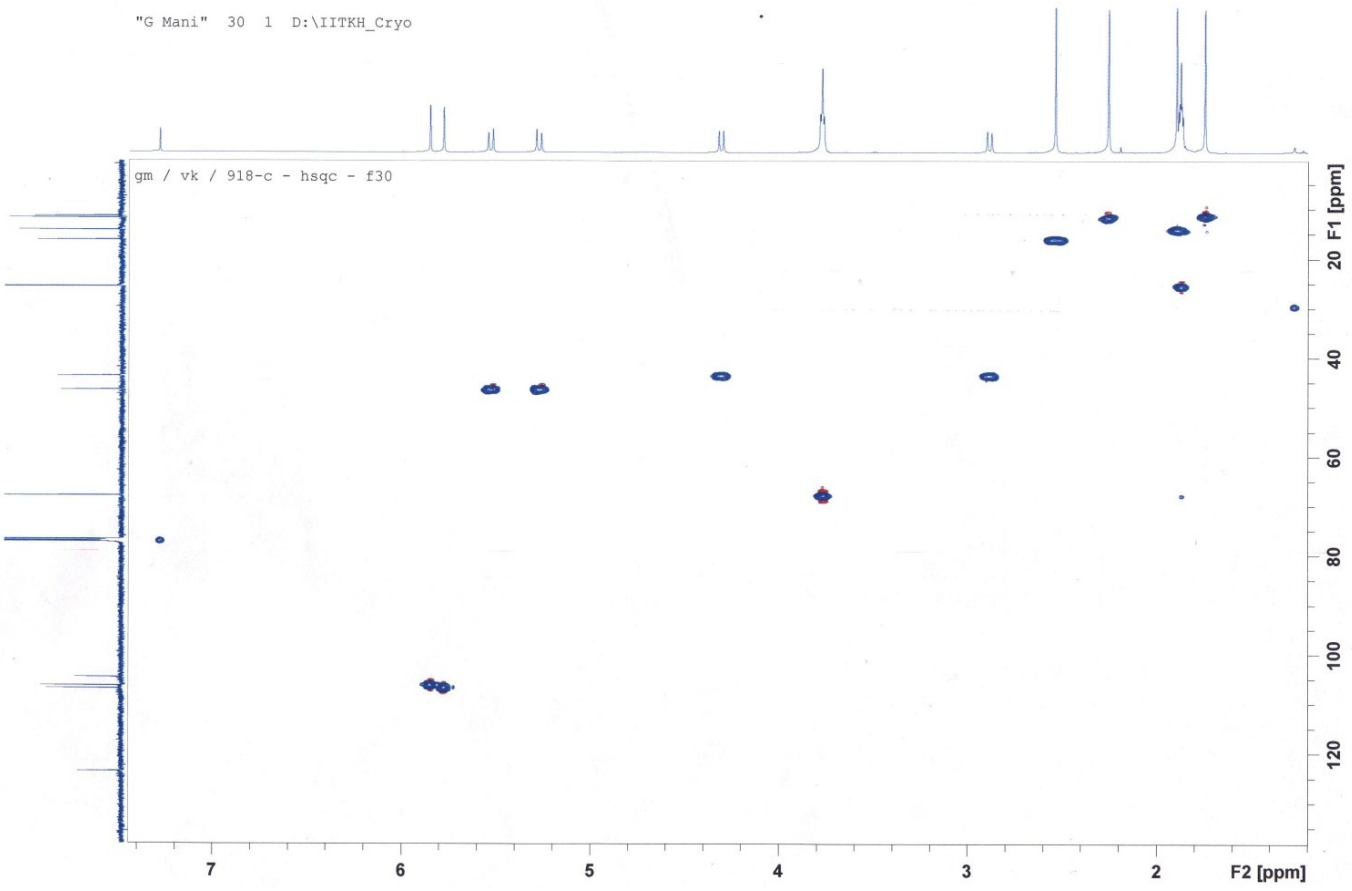


Figure S4: HSQC NMR (153.9 MHz, 22 °C) spectrum of complex **1** in $CDCl_3$.

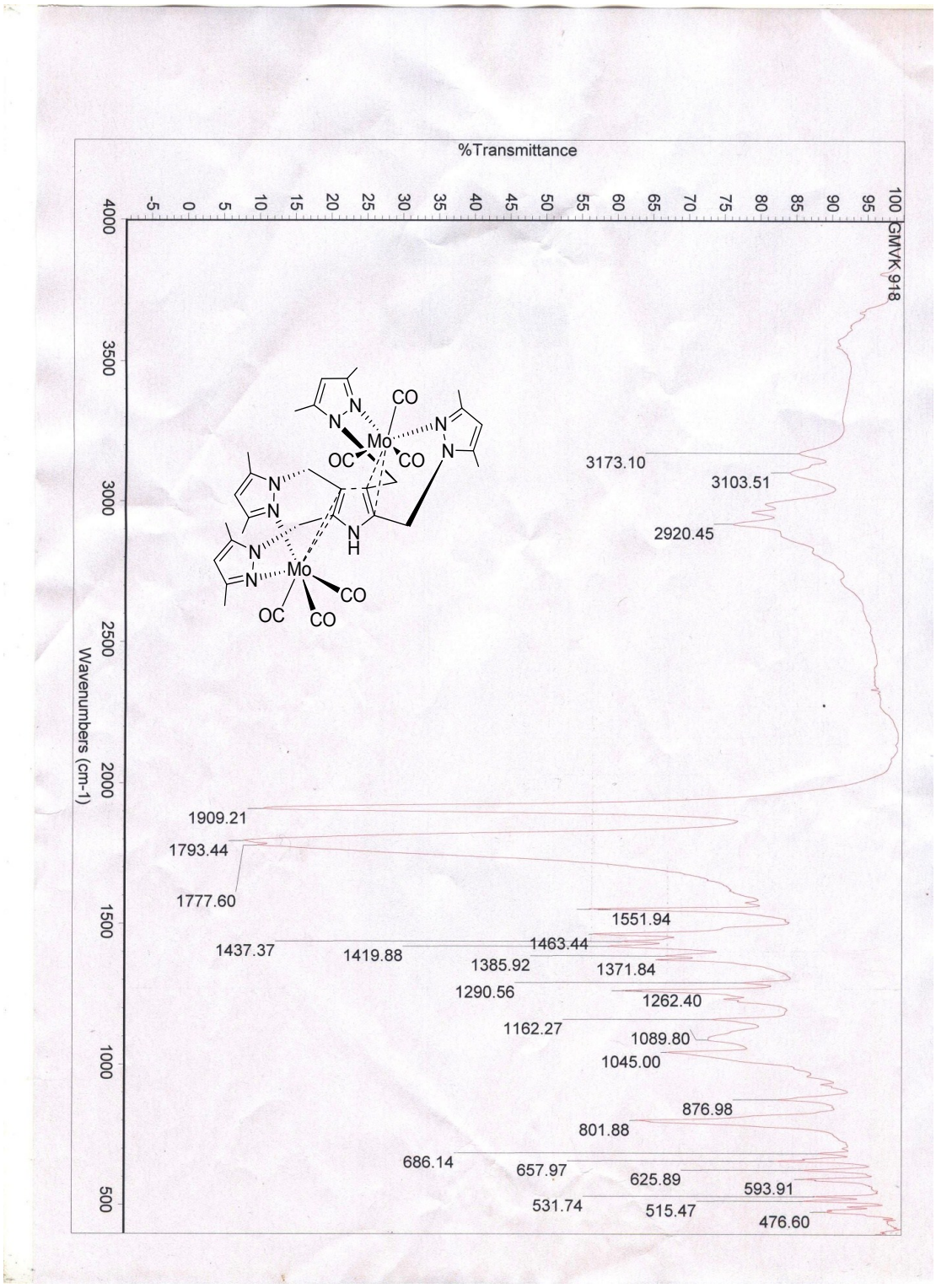


Figure S5: IR spectrum of complex **1** recorded as a KBr disc.

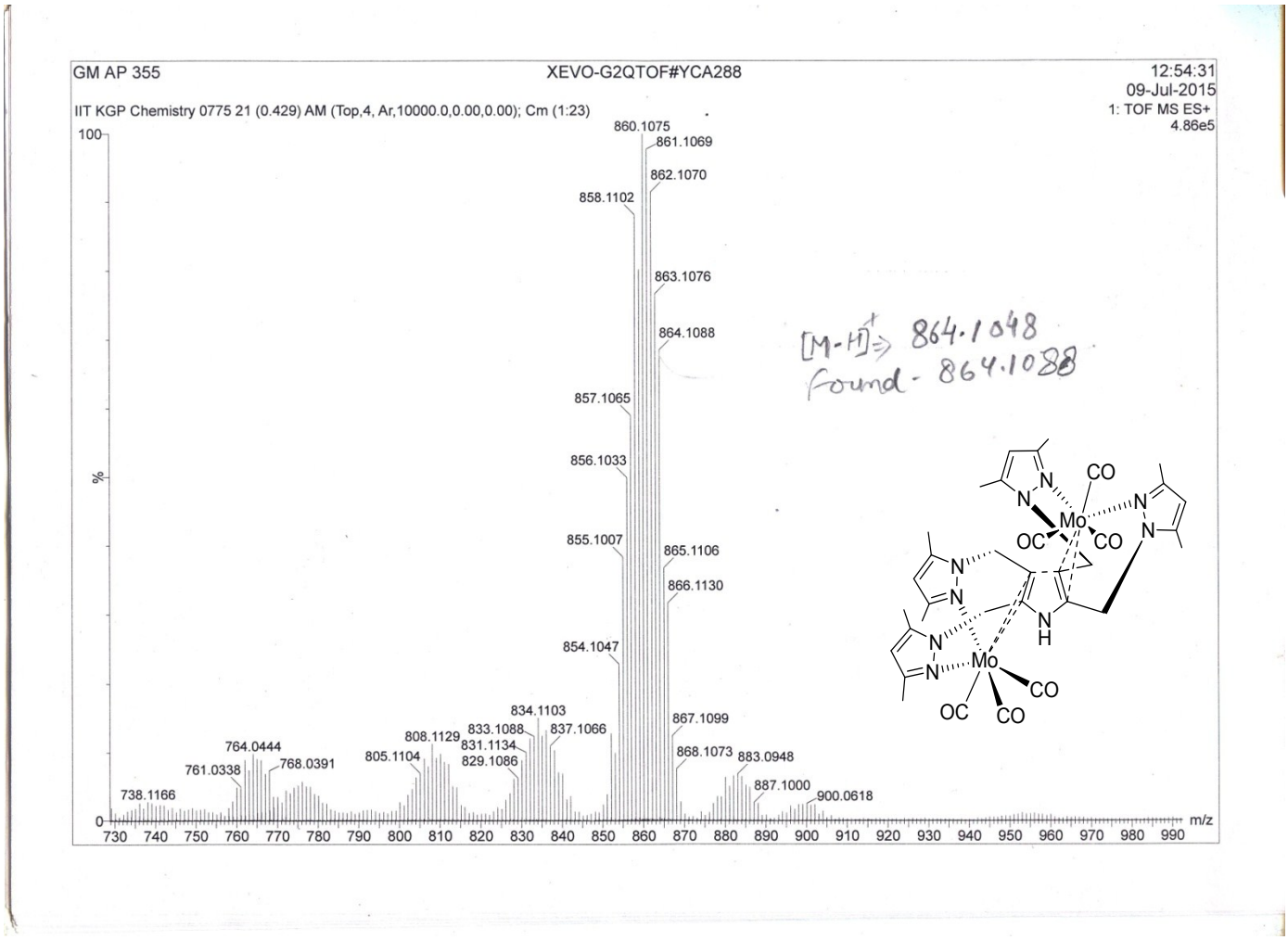


Figure S6: HRMS spectrum of complex **1**.

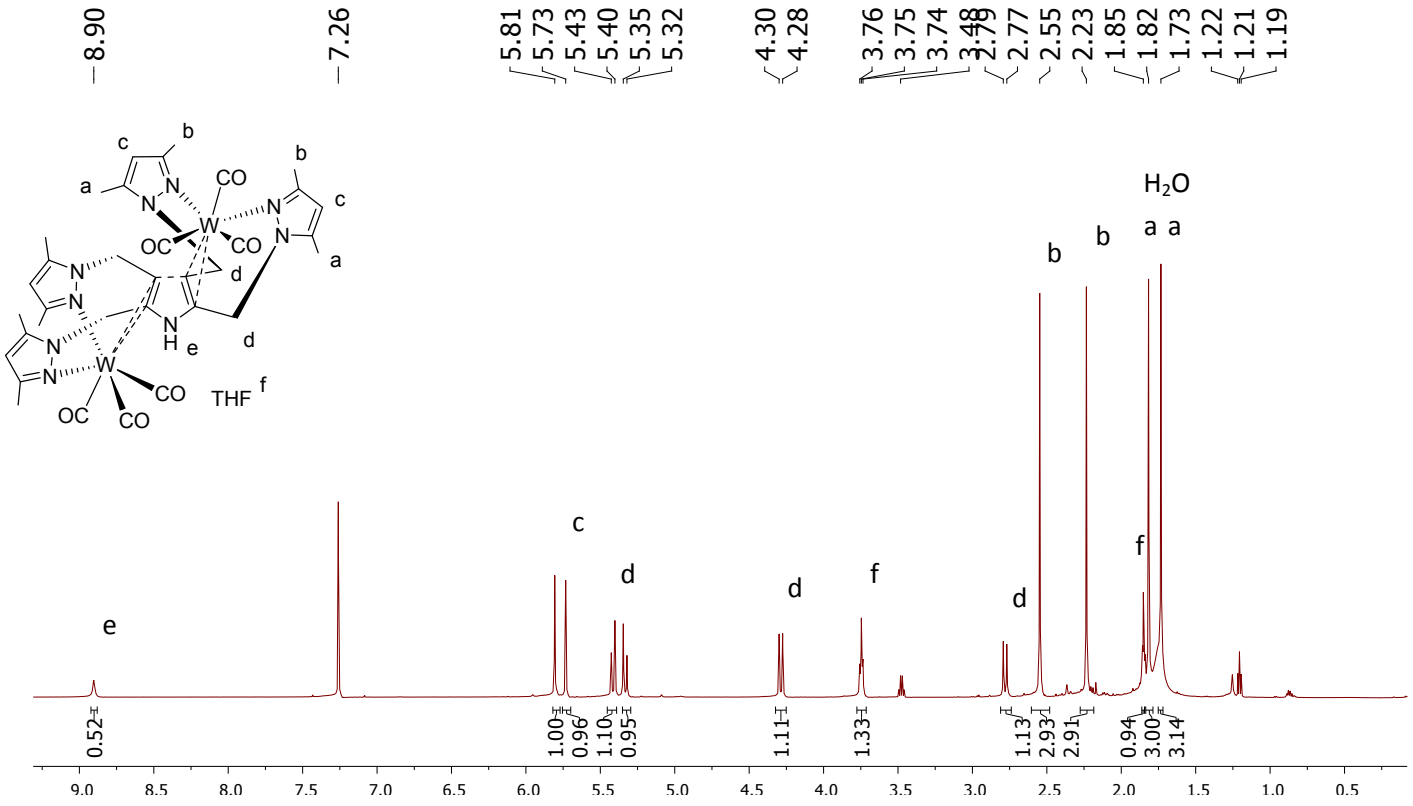


Figure S7: ^{1}H NMR (600 MHz, 22 °C) spectrum of complex **2** in $CDCl_3$.

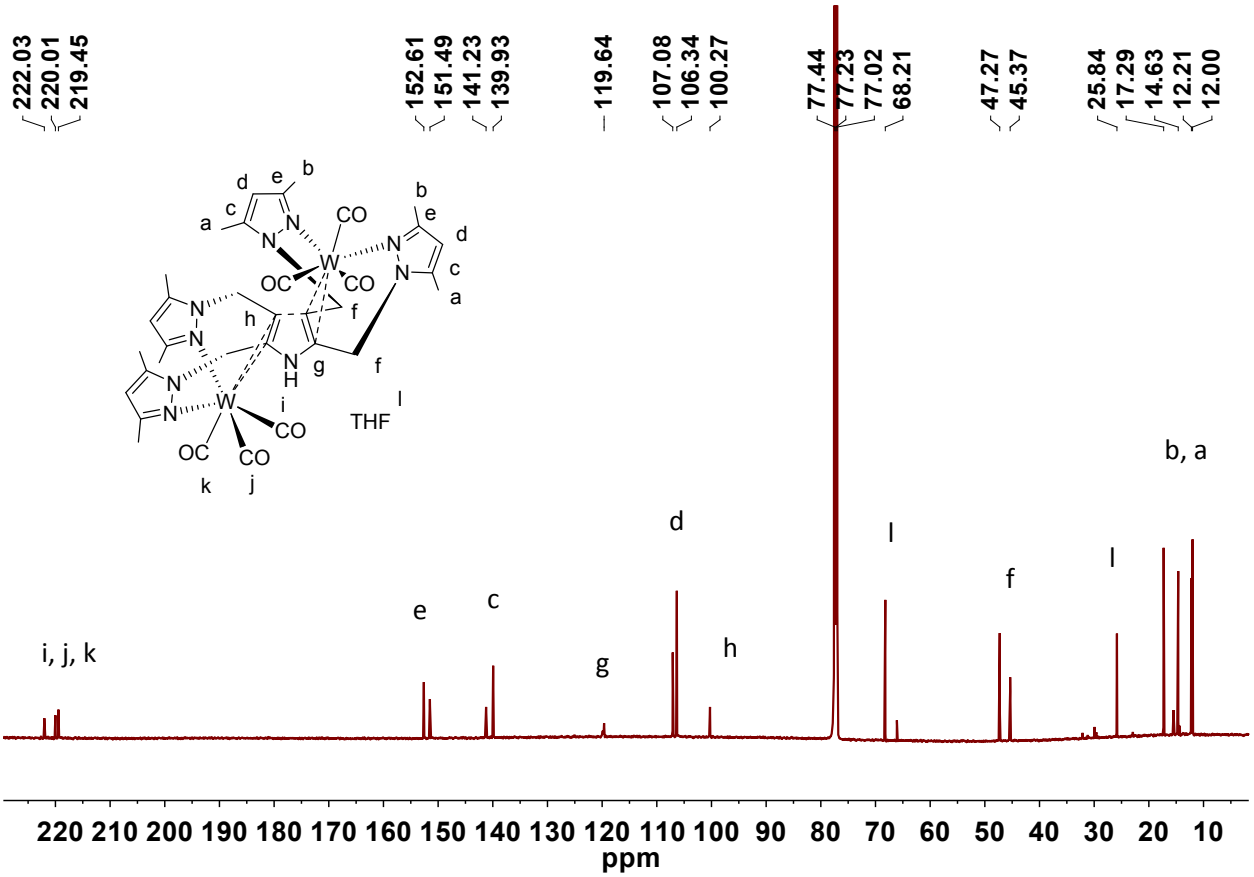


Figure S8: $^{13}C\{^{1}H\}$ NMR (153.9 MHz, 22 °C) spectrum of complex **2** in $CDCl_3$.

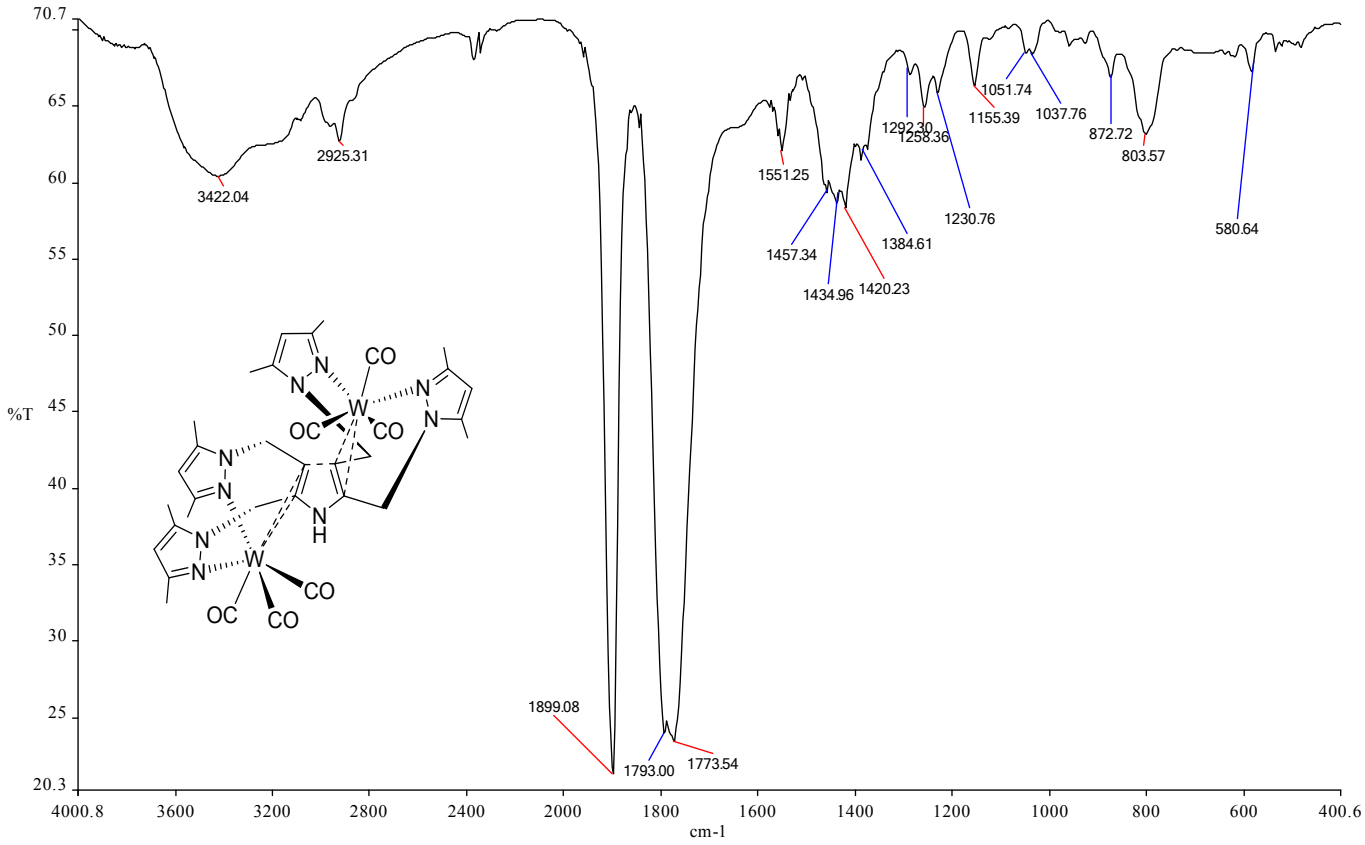


Figure S9: IR spectrum of complex **2** recorded as a KBr disc.

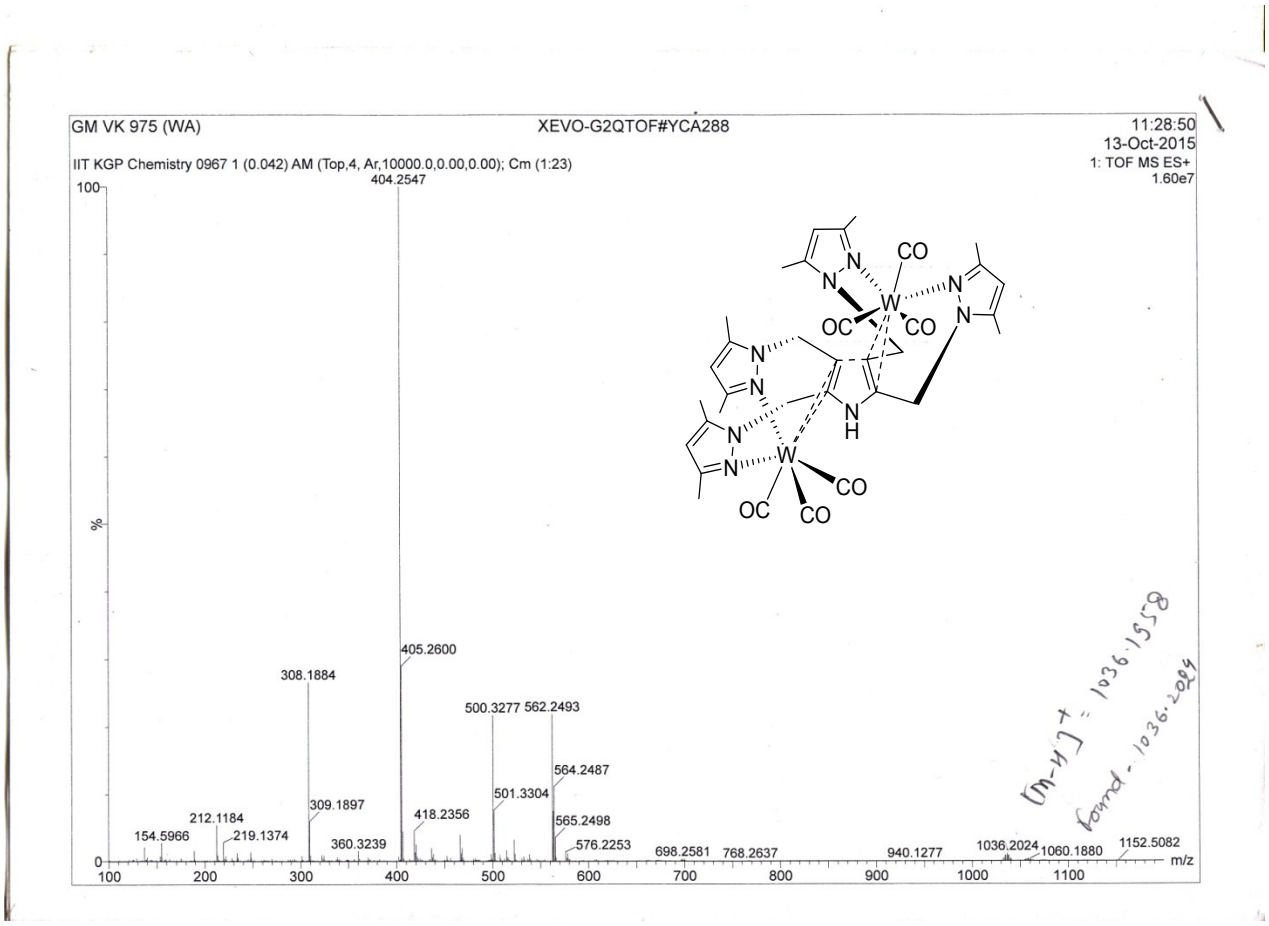


Figure S10: HRMS spectrum of complex **2**.

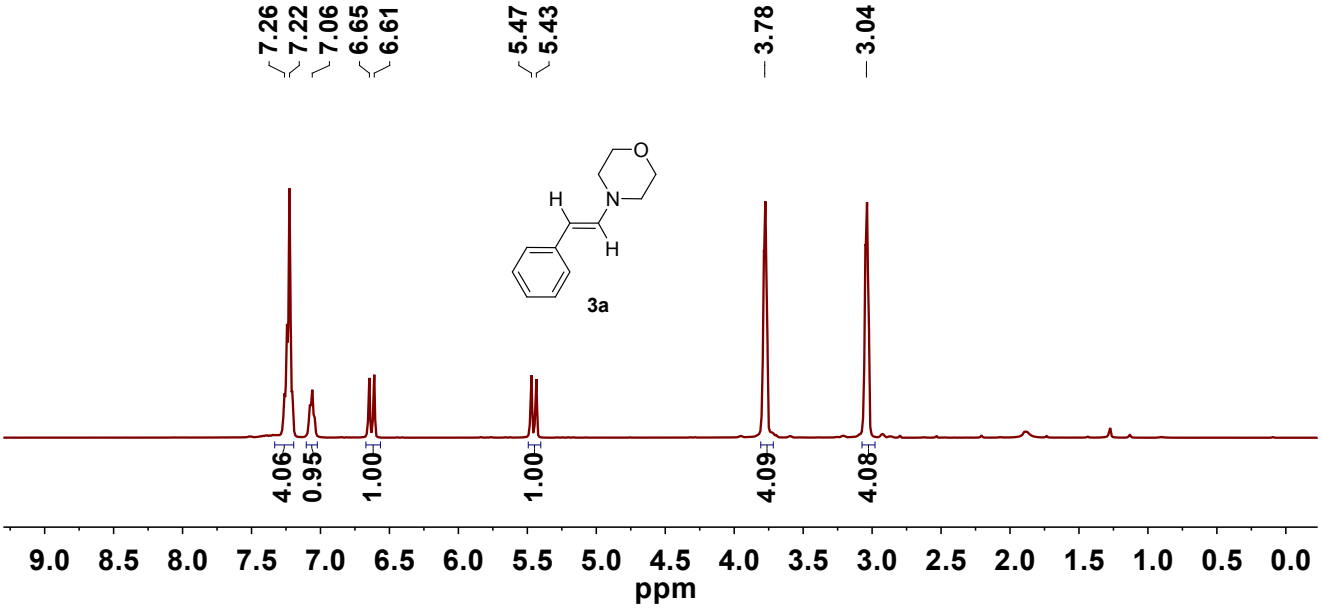


Figure S11: ^{1}H NMR (400 MHz, 22 °C) spectrum of 4-[(*E*)-2-phenylethenyl]morpholine **3** in $CDCl_3$.

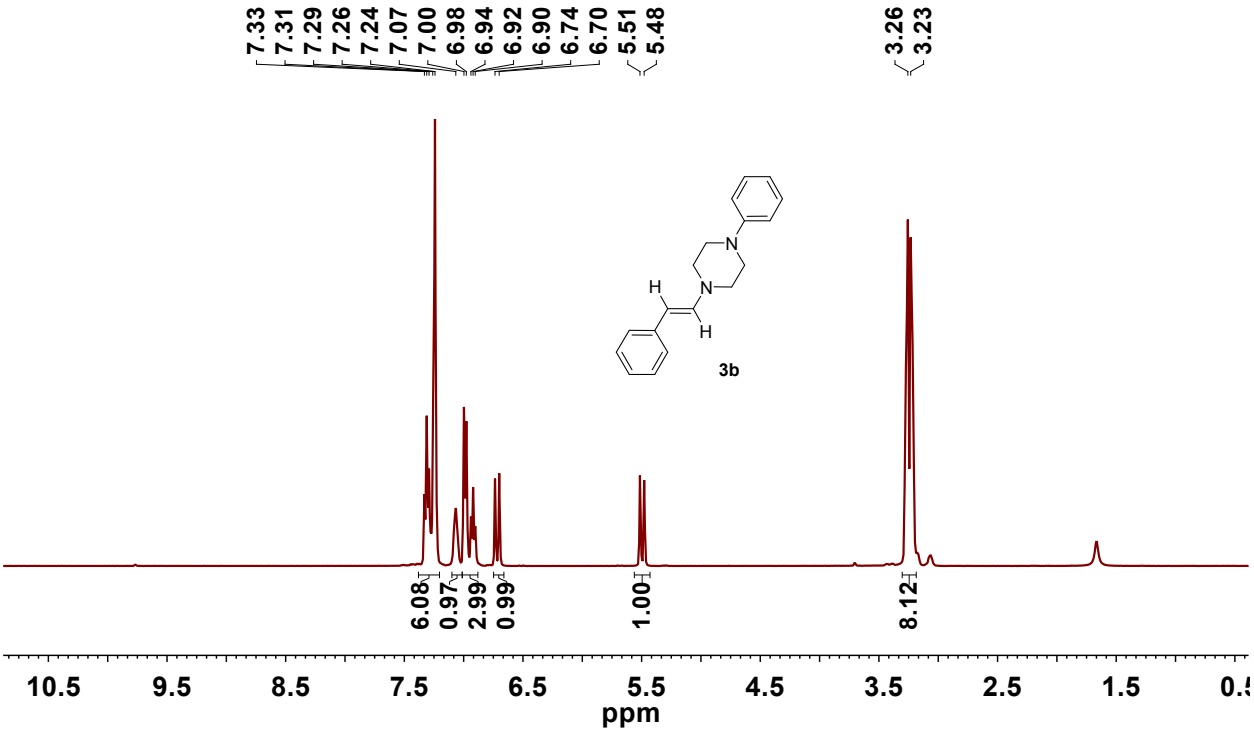


Figure S12: ^{1}H NMR (400 MHz, 22 °C) spectrum of 1-[(*E*)-2-phenylethenyl]-4-phenylpiperazine **4** in $CDCl_3$.

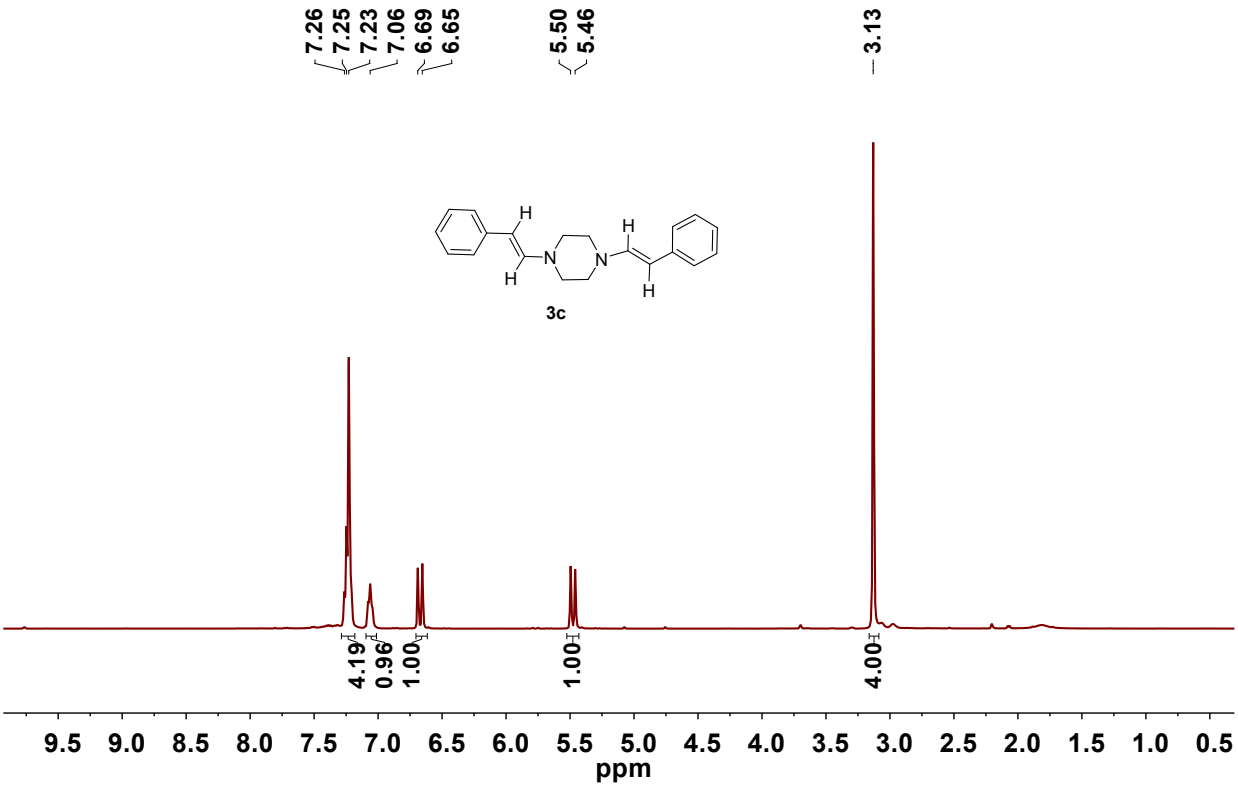


Figure S13: ^{1}H NMR (400 MHz, 22 °C) spectrum of 1,4-bis[(*E*)-2-phenylethenyl]piperazine **5** in $CDCl_3$.

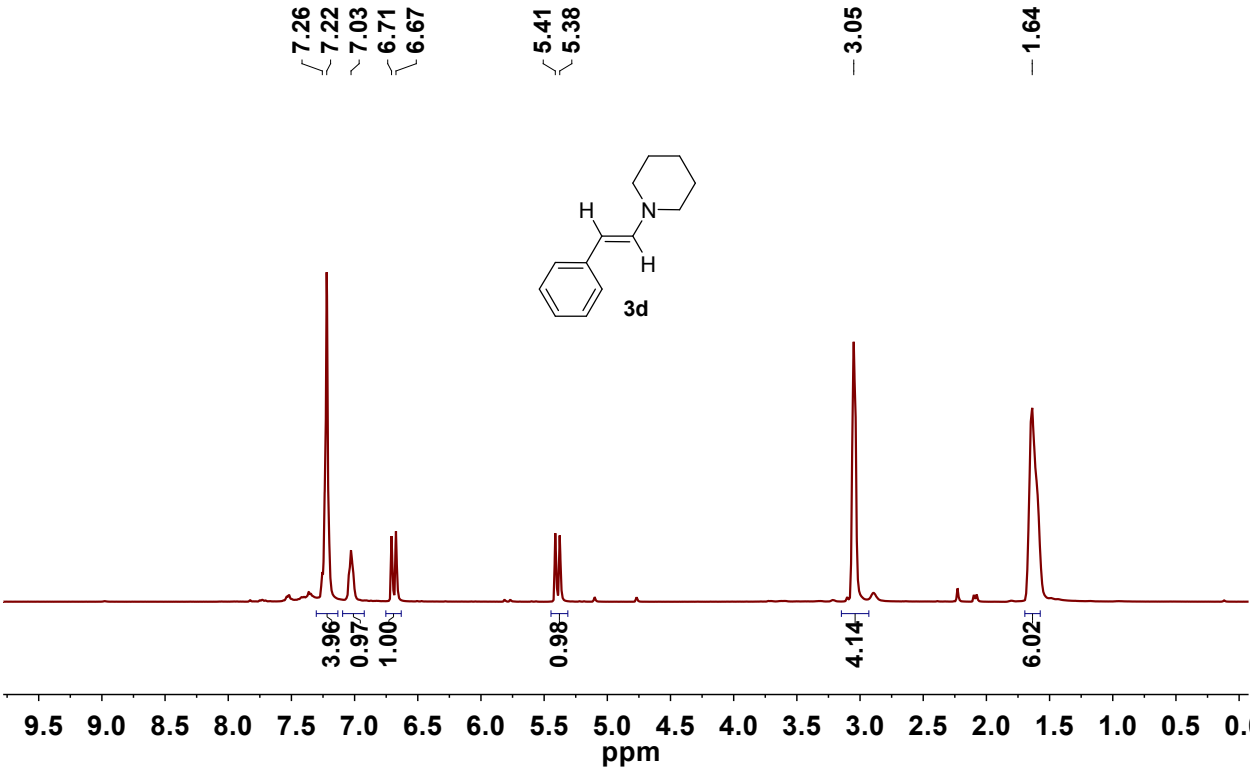


Figure S14: ^{1}H NMR (400 MHz, 22 °C) spectrum of 1-[(*E*)-2-phenylethenyl]piperidine **6** in $CDCl_3$.

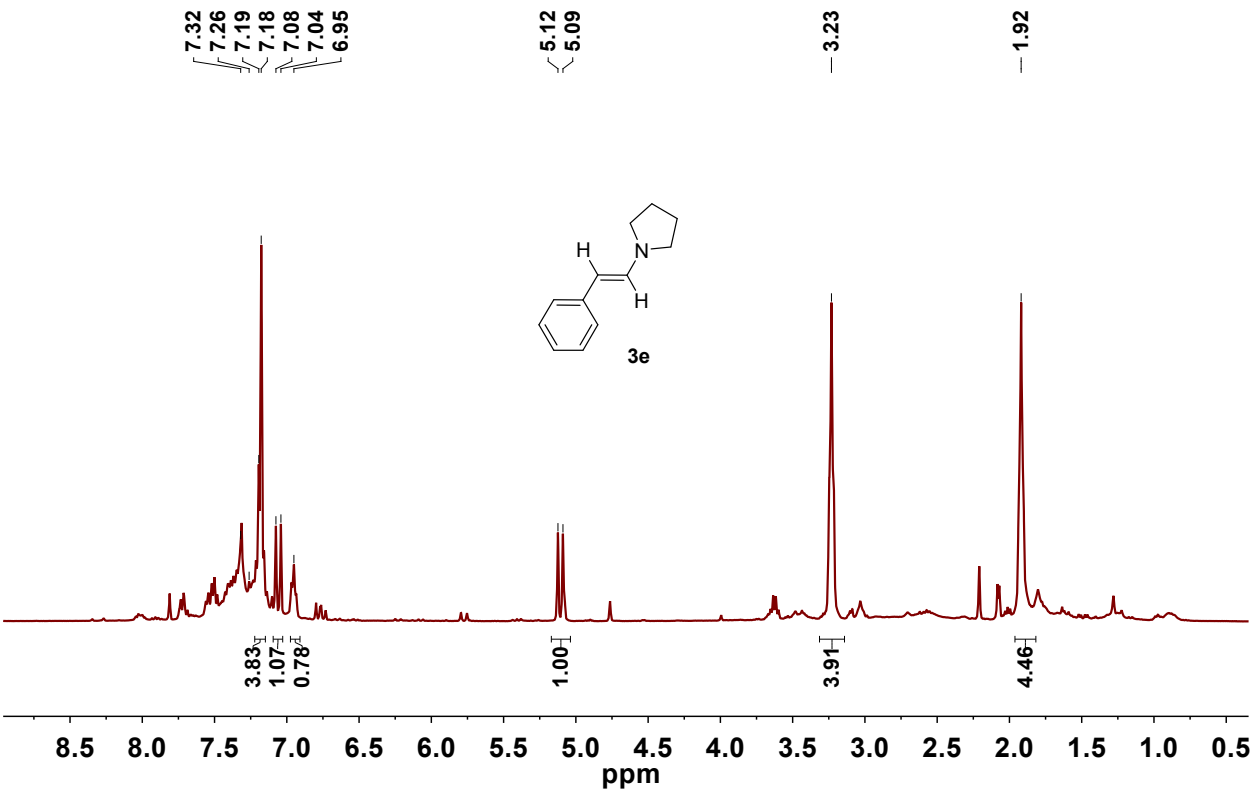


Figure S15: ^{1}H NMR (400 MHz, 22 °C) spectrum of 1-[(*E*)-2-phenylethenyl]pyrrolidine **7** in $CDCl_3$.

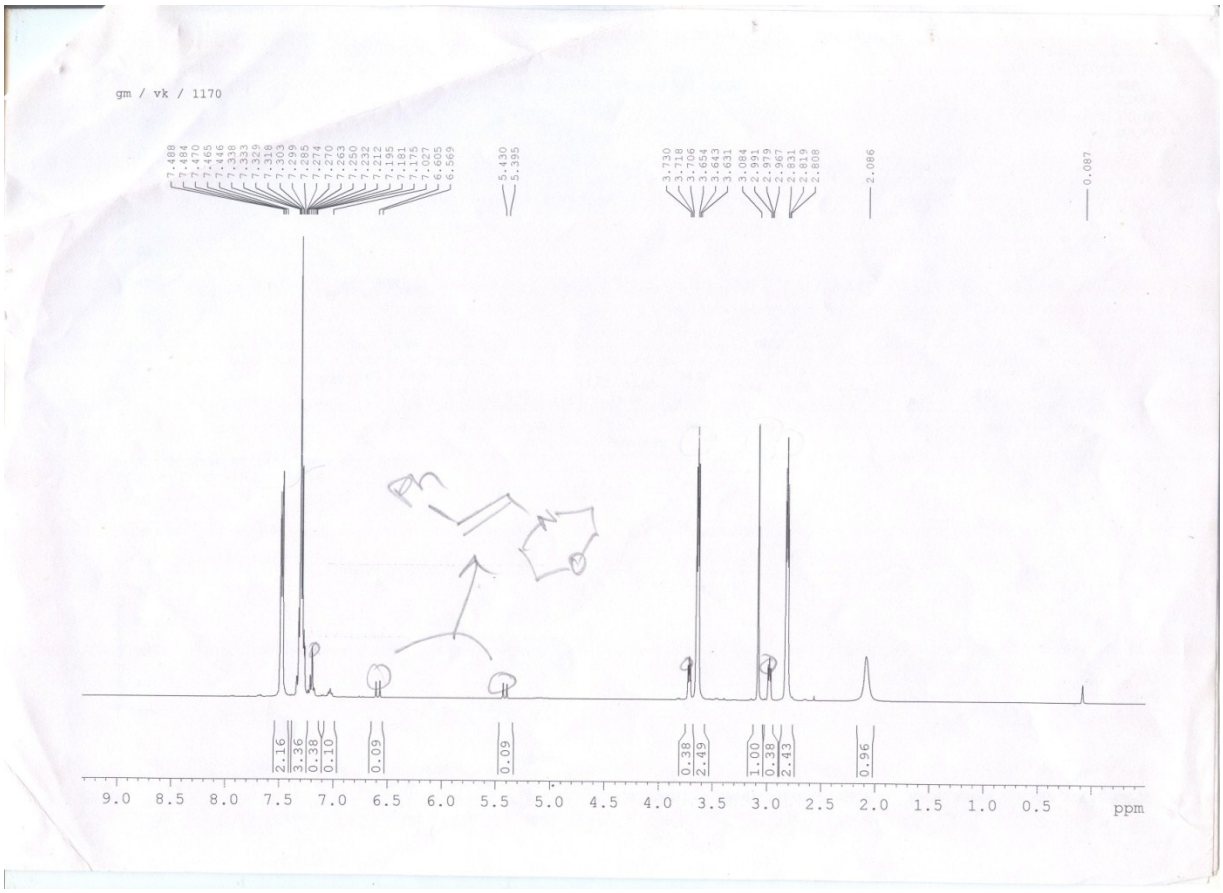


Figure S16: ^{1}H NMR (400 MHz, 22 °C) spectrum of the reaction mixture of PhCCH (2 equiv) and morpholine (1 equiv) in the presence of 1 mol% of $Mo(CO)_6$ in $CDCl_3$, showing the formation of 4-[(*E*)-2-phenylethenyl]morpholine and the starting compounds.

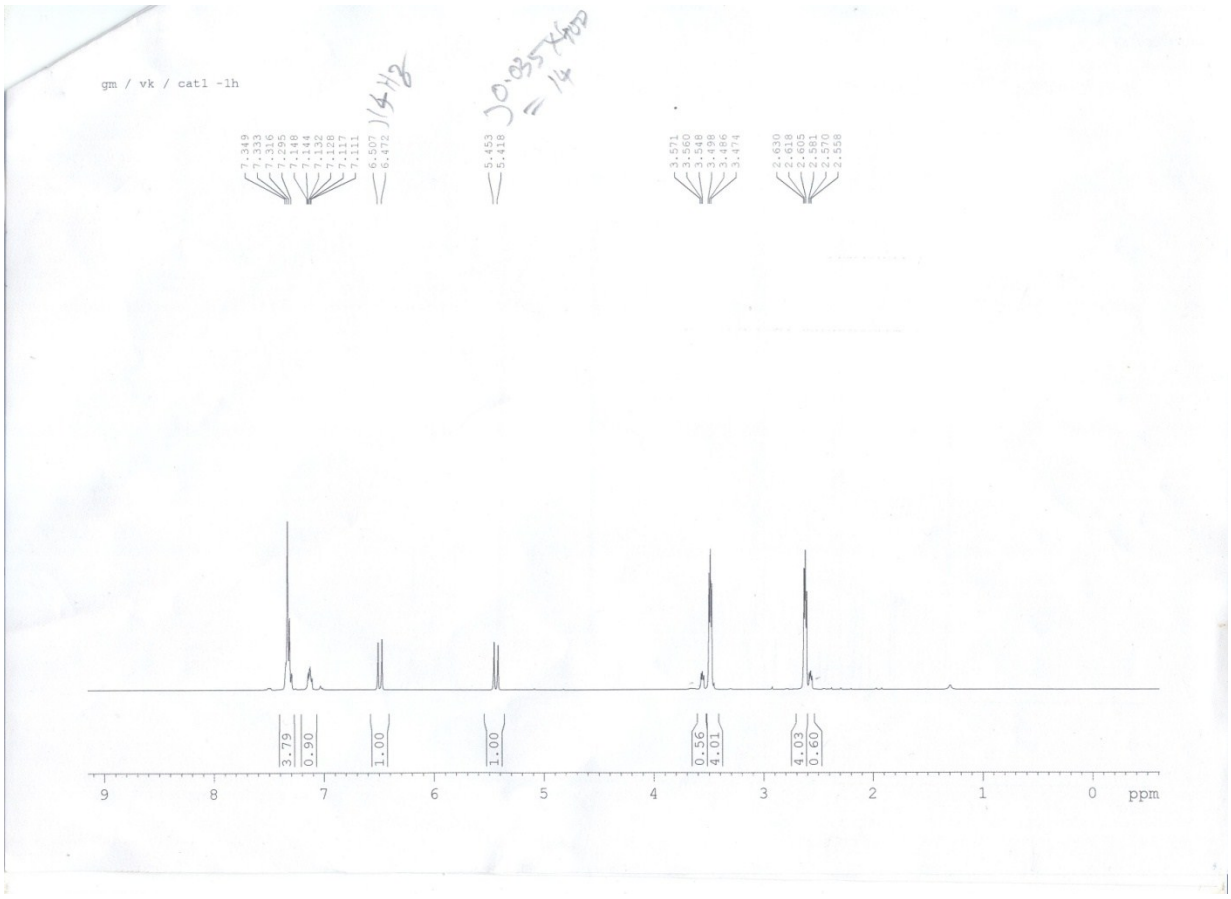


Figure S17. The ^{1}H NMR spectrum (400 MHz, 22 °C) recorded for a mixture of PhCCH (0.048 mL, 0.4 mmol), morpholine (0.048 mL, 0.4 mmol) and **1** (0.003 g, 0.003 mmol) kept at room temp for 3 days, giving solid and then dissolved in C_6D_6, showing disappearance of starting materials and formation of the anti-Markovnikov product.

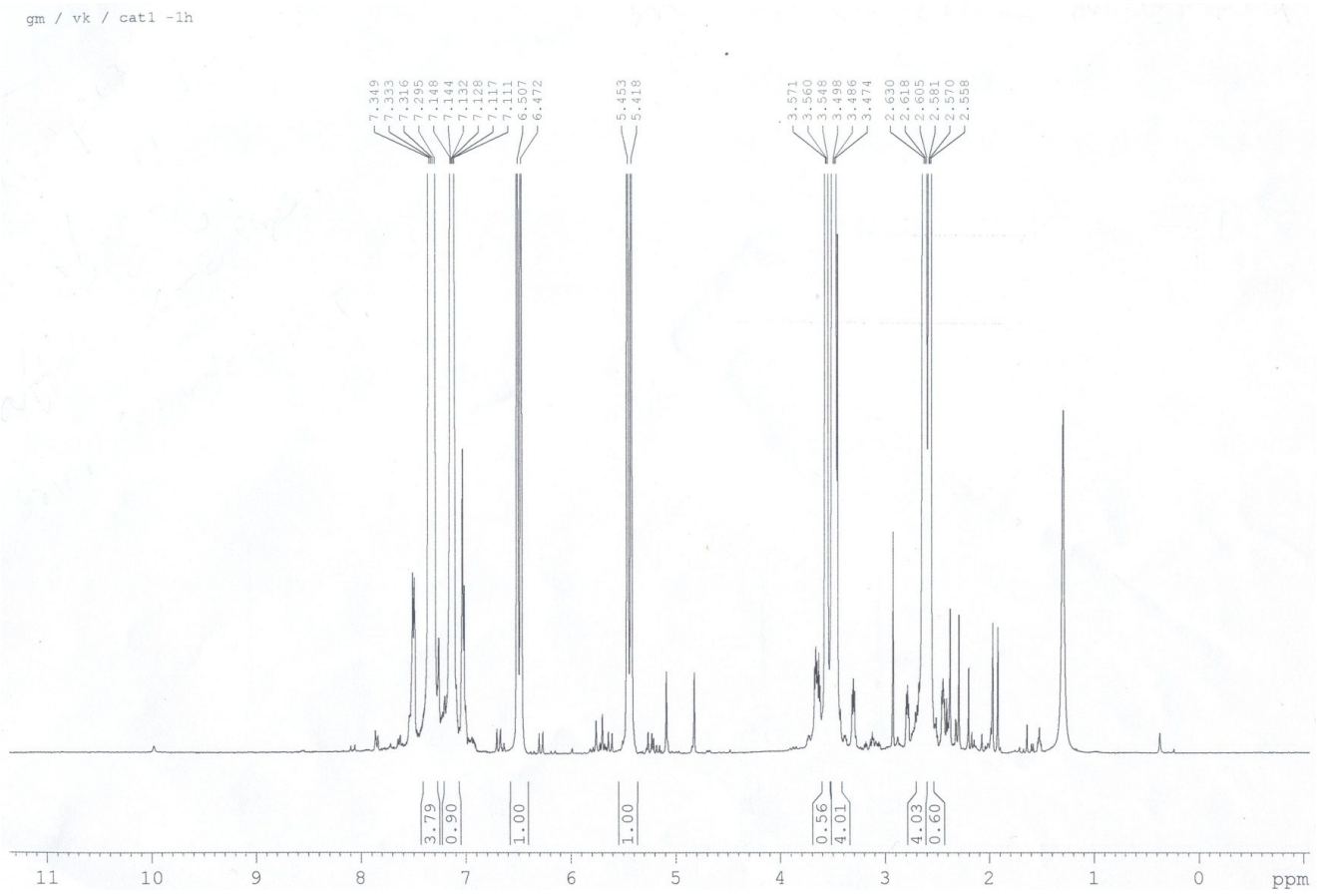


Figure S18. The expanded ^{1}H NMR spectrum(400 MHz, 22 °C) recorded for a mixture of PhCCH (0.048 mL, 0.4 mmol), morpholine (0.048 mL, 0.4 mmol) and **1** (0.003 g, 0.003 mmol) kept at room temp for 3 days, giving solid and dissolved in C_6D_6, showing disappearance of starting materials and formation of the anti-Markovnikov product. In addition, it shows the formation of different complex having attributes such as shifted AB quartets and NH resonance similar to complex **1**. The free ligand is also present. The absence of peaks around 4.33 ppm (s) and 4.19 ppm (s) for the methylene group protons present in the Markovnikov product shows that the Markovnikov product is not formed. (for the Markovnikov product ^{1}H NMR spectrum, see reference: B. Hu, H. Chen, Y. Liu, W. Dong, K. Ren, X. Xie, H. Xu and Z. Zhang, Chem. Commun., 2014, 50, 13547).

Computational details

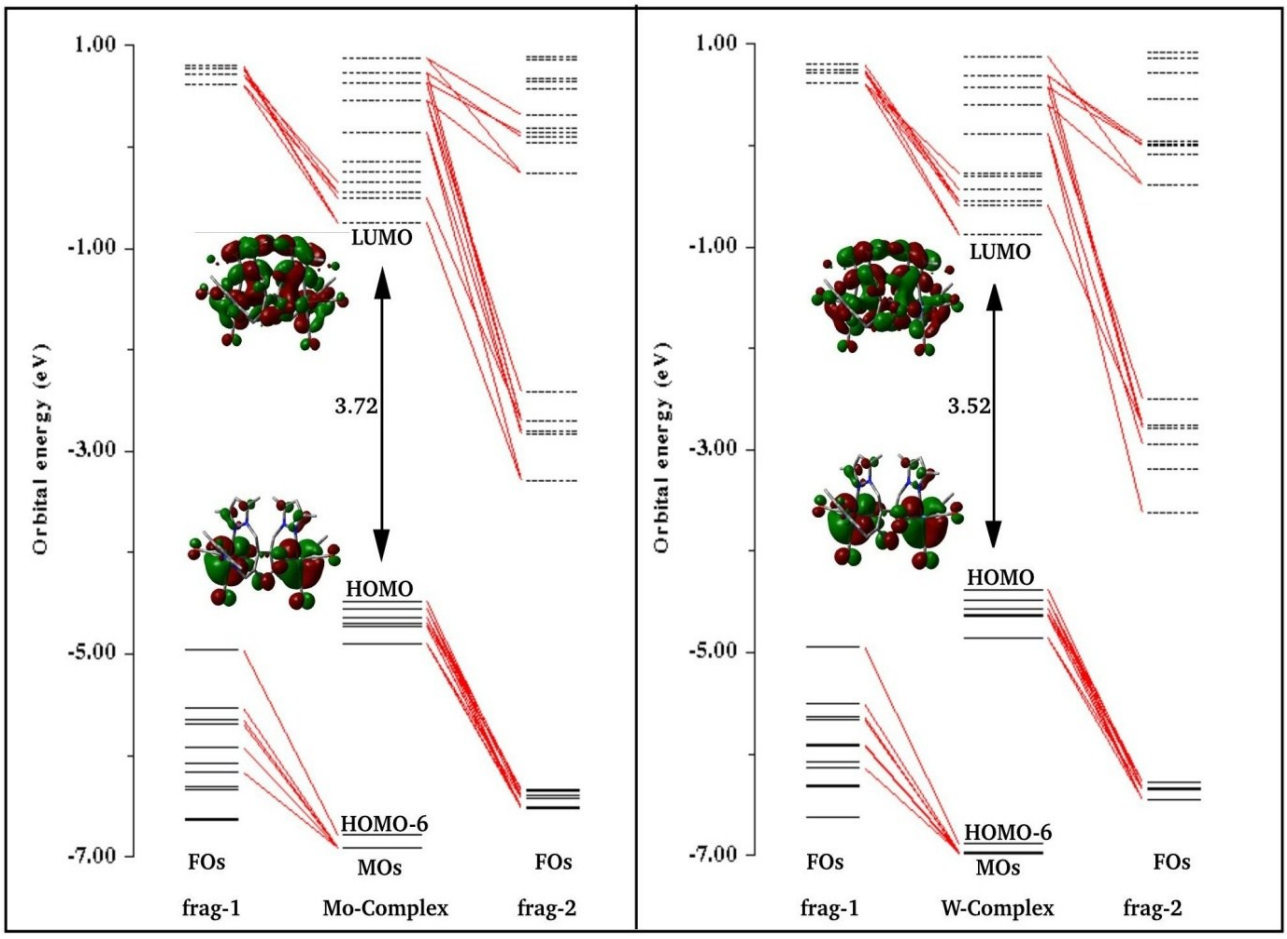


Figure S19. Molecular orbital energy diagram for fragment analysis of the free pyrrole ligand **LH** as a fragment 1 and metal carbonyl the fragment 2 for the Mo complex **1** and W complex **2**. (B3LYP)

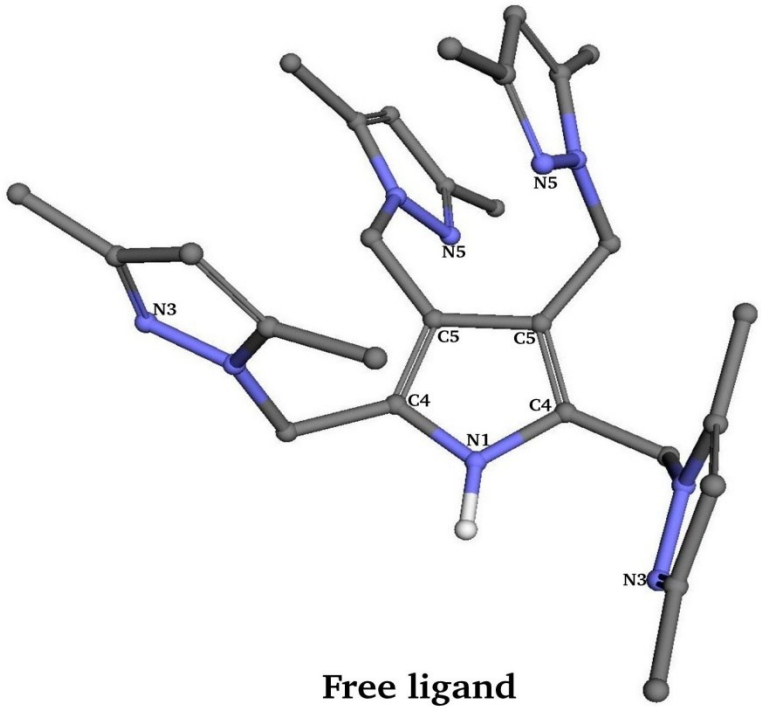


Figure S20. The optimized geometry of the free ligand **LH**. THF and hydrogen atoms are removed for clarity.

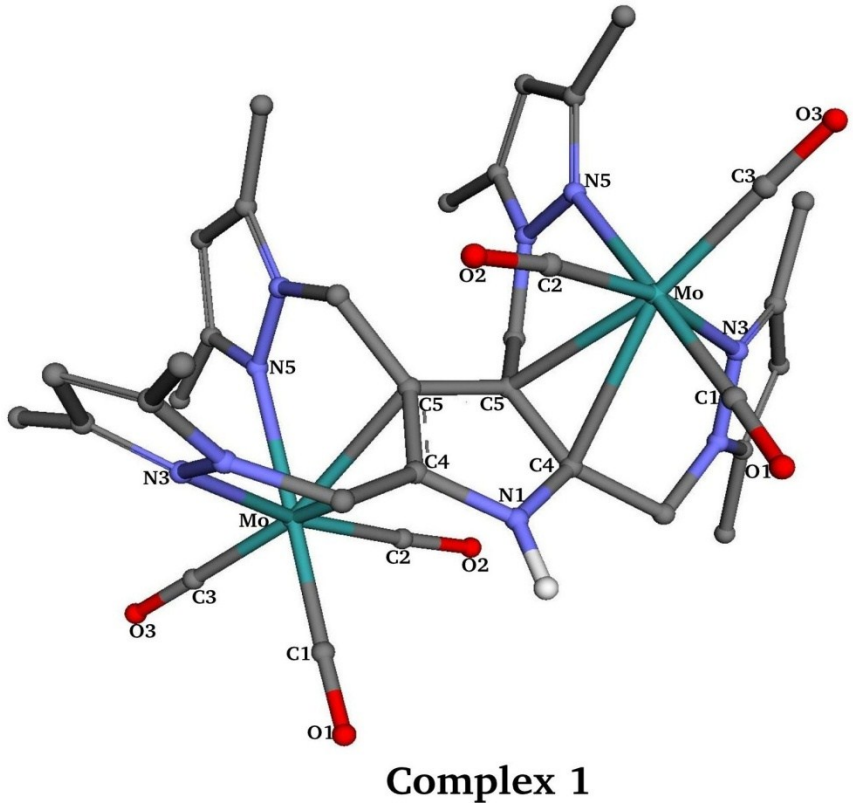
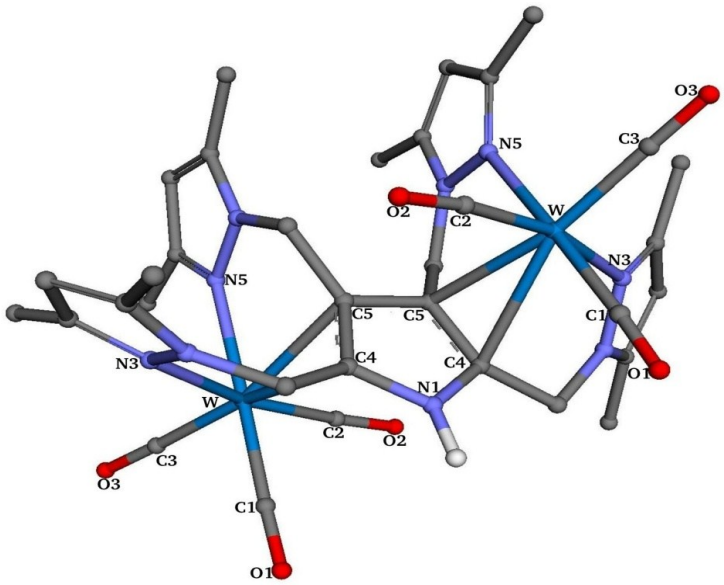


Figure S21. The optimized geometry of the Mo complex **1**. THF and hydrogen atoms are removed for clarity.



Complex 2

Figure S22. The optimized geometry of the W complex **2**. THF and hydrogen atoms are removed for clarity.

Table T1. Selected bond lengths (Å) of the optimized geometries (B3LYP, BP86 and M06) of **1** and **2** complexes.

For complex **1**

Bond Type	**B3LYP**	**BP86**	**M06**
C_4-C_5	1.401	1.418	1.398
C_1-O_1	1.170	1.183	1.167
C_2-O_2	1.177	1.189	1.175
C_3-O_3	1.166	1.179	1.163
Mo-C_4C_5	2.616	2.556	2.555
Mo-C_5C_4	2.553	2.482	2.485
Mo-C_1	1.955	1.952	1.949
Mo-C_2	1.946	1.945	1.937
Mo-C_3	1.956	1.958	1.961
Mo-N_3	2.287	2.260	2.273
Mo-N_5	2.279	2.254	2.269

For complex **2**

Bond Type	**B3LYP**	**BP86**	**M06**
C_4-C_5	1.404	1.421	1.403
C_1-O_1	1.172	1.183	1.169
C_2-O_2	1.180	1.192	1.179
C_3-O_3	1.169	1.181	1.165
W-C_4C_5	2.623	2.554	2.552
W-C_5C_4	2.543	2.483	2.471
W-C_1	1.973	1.978	1.967
W-C_2	1.961	1.964	1.952
W-C_3	1.972	1.977	1.979
W-N_3	2.301	2.275	2.290
W-N_5	2.289	2.264	2.279

Table T2. Selected Wiberg bond indices (**WBIs**) (B3LYP)

Mo Complex 1		**Bond Type**	**W Complex 2**	
1.3576	C_4-C_5	C=C	C_4-C_5	1.3535
1.9762	C_1-O_1	CO(trans-N_{meta})	C_1-O_1	1.9450
1.9248	C_2-O_2	CO(trans-N_{ortho})	C_2-O_2	1.8825
2.0079	C_3-O_3	CO(trans-CC)	C_3-O_3	1.9750
0.1736	Mo_1-C_4C_5	M-CC	W_1-C_4C_5	0.1758
0.2079	Mo_1-C_5C_4	M-CC	W_1-C_5C_4	0.2153
1.3487	Mo_1-C_1	M-CO(trans-N_{meta})	W_1-C_1	1.3298
1.4160	Mo_1-C_2	M-CO(trans-N_{ortho})	W_1-C_2	1.4147
1.3527	Mo_1-C_3	M-CO(trans-CC)	W_1-C_3	1.3532
0.4215	Mo_1-N_3	M-N(N_{ortho})	W_1-N_3	0.3783
0.4209	Mo_1-N_5	M-N(N_{meta})	W_1-N_5	0.3792

Table T3: Natural atomic charges of the metal coordinated atoms (B3LYP)

Atom Type	Mo Complex **1**	W Complex **2**
Metal	-1.116	-0.681
C1	0.711	0.600
C2	0.690	0.568
C3	0.710	0.601
C4	-0.127	-0.155
C5	0.202	0.191
N3	-0.272	-0.315
N5	-0.270	-0.314

Table T4: Electron density descriptors data (atomic units) for the selected bonds in Mo complex **1** and W complex **2**. $\rho(r_c)$, $\nabla^2\rho(r_c)$ and $H(r_c)$ data are at the bond critical point (BCP). (B3LYP)

BCP(Mo-Complex)	$\rho(r_c)$	$\nabla^2\rho(r_c)$	$G(r_c)$	$V(r_c)$	$H(r_c)$	E
C_4-C_5	0.3035	-0.7226	0.1058	-0.3923	-0.2865	-514.9
Mo_1-C_4C_5	0.0362	0.1016	0.0277	-0.0301	-0.0023	-39.5
Mo_1-C_5C_4	0.0402	0.1116	0.0313	-0.0347	-0.0034	-45.5
Mo_1-C_1	0.1333	0.4345	0.1695	-0.2303	-0.0608	-302.3
Mo_1-C_2	0.1369	0.4086	0.1671	-0.2322	-0.0650	-304.8
Mo_1-C_3	0.1340	0.4149	0.1654	-0.2270	-0.0616	-297.9
Mo_1-N_3	0.0594	0.2806	0.0713	-0.0725	-0.0012	-95.1
Mo_1-N_5	0.0593	0.2993	0.0751	-0.0754	-0.0003	-98.9

BCP(W-complex)	$\rho(r_c)$	$\nabla^2\rho(r_c)$	$G(r_c)$	$V(r_c)$	$H(r_c)$	E

C_4-C_5	0.3016	-0.7155	0.1045	-0.3879	-0.2833	-509.2
W_1-C_4C_5	0.0382	0.1006	0.0286	-0.0322	-0.0035	-42.2
W_1-C_5C_4	0.0440	0.1075	0.0329	-0.0389	-0.0060	-51.0
W_1-C_1	0.1316	0.4391	0.1697	-0.2296	-0.0599	-301.4
W_1-C_2	0.1363	0.4124	0.1685	-0.2340	-0.0654	-307.1
W_1-C_3	0.1330	0.4235	0.1671	-0.2284	-0.0612	-299.8
W_1-N_3	0.0612	0.2637	0.0707	-0.0755	-0.0048	-99.1
W_1-N_5	0.0616	0.2847	0.0751	-0.0790	-0.0039	-103.7

Table T5: Comparison of the pyrrole ring bond distances in the optimized free ligand **LH** with those in the optimized geometry for complexes **1** and **2** using three DFs, B3LYP, BP86 and M06, at basis set def2-SVP.

Bond Type	Free ligand (**LH**)			Complex **1**			Complex **2**		
	B3LYP	BP86	M06	B3LYP	BP86	M06	B3LYP	BP86	M06
C4-C5	1.387	1.394	1.376	1.401	1.418	1.398	1.404	1.421	1.403
C5-C5	1.427	1.432	1.421	1.456	1.466	1.455	1.462	1.470	1.460
N1-C4	1.370	1.379	1.372	1.370	1.381	1.369	1.370	1.382	1.369
N1-C4	1.367	1.376	1.367	1.370	1.379	1.368	1.370	1.380	1.368
N1-H5	1.028	1.028	1.017	1.035	1.051	1.033	1.036	1.051	1.032

Table T6: The metal d orbitals occupancies and their energies (a.u). (B3LYP)

Mo complex			
Atomic type		Occupancy	Energy (a.u)
t_{2g}	$4d_{xy}$	1.3960	-0.1042
	$4d_{xz}$	1.0054	-0.1109
	$4d_{yz}$	1.3871	-0.1060
e_g	$4d_{x^2-y^2}$	1.1127	-0.1101
	$4d_{z^2}$	1.2181	-0.1076
W complex			
t_{2g}	$5d_{xy}$	1.3322	-0.0884
	$5d_{xz}$	1.0179	-0.0612
	$5d_{yz}$	1.3231	-0.0885
e_g	$5d_{x^2-y^2}$	1.0271	-0.0819
	$5d_{z^2}$	1.1066	-0.0880

Table T7. The calculated net charge transfer for the fragments of complex **1** and **2** using the extended charge decomposition analysis (ECDA). (B3LYP)

Fragment 1[a]	Mo-Complex **1**	W-Complex **2**
C_1O_1	0.0640	0.3765
C_2O_2	0.0612	0.5286
C_3O_3	0.1519	0.3621
LH	0.8840	0.9215

[a] Fragment 2 is the rest of the molecule.

Table T8: The ν(CO) stretching frequencies for complex **1** and **2** (corrected with 0.96 frequency scaling factor) (B3LYP). The experimentally observed values are given in parenthesis.

Bond type	Mo complex (cm^{-1})	W complex (cm^{-1})
$\nu(C_4C_5)$	1499.1	1494.3
$\nu(C_1O_1)$	1861.5(1793)	1858.6(1793)
$\nu(C_2O_2)$	1813.2 (1778)	1809.4 (1773)
$\nu(C_3O_3)$	1930.2 (1909)	1927.5 (1899)

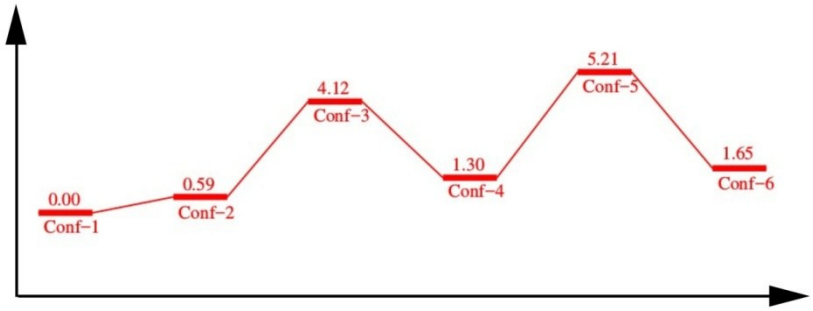


Figure S23. Conformational potential energy diagram for the optimized conformers of **LH**. (the y axis is for energy in kcal/mol). (B3LYP)

Coordinates of the optimized Mo and W complexes (B3LYP)

The coordinates for the Mo complex 1

C 1.51053 5.31813 0.27817
H 2.32740 4.83506 -0.27670
H 1.70542 5.22832 1.36477
C 1.27415 6.77807 -0.11152
H 1.48062 6.92210 -1.18530
H 1.90490 7.47602 0.45997
O 0.28186 4.64270 -0.03430
C -0.77014 5.58415 -0.30431
H -1.67752 5.25502 0.22133
H -0.96816 5.59987 -1.39375
C -0.22726 6.93357 0.16768
H -0.40442 7.05770 1.24931
H -0.68867 7.78281 -0.35911
C 2.96142 1.87133 -1.36641
C 1.49152 -0.00598 -2.64027
C 4.23713 -0.40781 -2.10302
C 3.53568 -3.48471 -2.22653
H 3.13969 -2.83142 -3.01885
H 3.57344 -4.52361 -2.58786
H 4.56458 -3.14679 -2.02422
C 2.68493 -3.39163 -1.00333
C 2.22934 -4.43291 -0.16411
H 2.41997 -5.49810 -0.27449
C 1.46972 -3.82016 0.82820
C 0.71248 -4.37523 1.98855
H 1.06787 -3.94624 2.94100
H 0.83866 -5.46663 2.03037
H -0.36473 -4.15407 1.89919
C 0.86946 -1.41028 1.30513
H 1.50452 -1.13241 2.15510
H -0.07369 -1.79835 1.71584
C 0.55699 -0.23510 0.42145
C 0.94009 1.10180 0.58929
C 1.84898 1.71385 1.61299
H 2.28793 2.64146 1.20925
H 1.27457 1.96018 2.51931
C 3.27336 0.42864 3.25257

C 2.69423 1.06385 4.47411
H 1.59839 0.93133 4.49773
H 2.90559 2.14633 4.50989
H 3.12479 0.59955 5.37268
C 4.19914 -0.59589 3.10239
H 4.72963 -1.11290 3.89879
C 4.30884 -0.82214 1.71092
C 5.12706 -1.84691 0.99389
H 5.43070 -1.47378 0.00530
H 4.54406 -2.77014 0.83638
H 6.02336 -2.10198 1.57991
N 3.50358 0.01608 1.05202
N 2.89137 0.77887 1.99556
N 2.24121 -2.21509 -0.54156
N 1.49693 -2.49361 0.55505
N 0.07630 1.89988 -0.11312
H 0.12057 2.93396 -0.12934
O 0.70041 0.07025 -3.50784
O 3.12480 3.01712 -1.53540
O 5.21281 -0.62632 -2.70332
Mo 2.62656 -0.02993 -1.05951
Mo -2.63985 0.31706 0.99300
C -3.84634 -2.91206 2.48456
H -3.38679 -2.22572 3.21219
H -3.97481 -3.90446 2.94280
H -4.84219 -2.50312 2.25080
C -2.99985 -3.01344 1.25886
C -2.63892 -4.16886 0.53048
H -2.91897 -5.19740 0.74686
C -1.83486 -3.72621 -0.51572
C -1.13315 -4.45753 -1.61139
H -1.45972 -4.10137 -2.60341
H -1.34658 -5.53372 -1.54061
H -0.04109 -4.31605 -1.54383
C -1.03022 -1.43715 -1.22844
H -1.64482 -1.18321 -2.10096
H -0.12970 -1.94748 -1.59956
C -0.60418 -0.21911 -0.45735
C -0.86246 1.12735 -0.74511
C -1.71508 1.72544 -1.82408

H -2.06415 2.72301 -1.50709
H -1.12537 1.83114 -2.74765
C -3.26594 0.43678 -3.34218
C -2.63561 0.89740 -4.61557
H -1.55727 0.66064 -4.62206
H -2.74438 1.98687 -4.75345
H -3.11219 0.39357 -5.46846
C -4.28730 -0.47311 -3.10007
H -4.87190 -1.00631 -3.84633
C -4.40949 -0.55813 -1.69402
C -5.32283 -1.42376 -0.88723
H -5.62259 -0.91140 0.03868
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H -6.22100 -1.68030 -1.46951
N -3.52025 0.25273 -1.11361
N -2.84287 0.86163 -2.12195
N -2.46066 -1.93113 0.68209
N -1.74852 -2.38127 -0.37828
C -2.79669 2.26278 1.11423
C -1.50147 0.37538 2.57078
C -4.27412 0.18626 2.05771
O -0.70332 0.44915 3.43219
O -2.85518 3.42989 1.16259
O -5.26442 0.11315 2.66951

The coordinates for the W-complex 2

C 0.86571 1.12749 0.67481
C 1.66988 1.75529 1.77437
H 2.10974 2.70023 1.41348
H 1.01867 1.96673 2.63615
C 3.01766 0.49069 3.49480
C 2.33840 1.09441 4.67978
H 2.72111 0.63359 5.60144
H 2.51320 2.18234 4.73876
H 1.24844 0.92739 4.62543
C 3.98039 -0.50654 3.39705
H 4.47048 -1.01728 4.22274
C 4.18848 -0.71492 2.01522
C 5.07663 -1.70588 1.33652
H 5.97840 -1.89396 1.93944

H 4.55176 -2.66566 1.19385
H 5.36861 -1.33639 0.34347
C 0.54779 -0.22372 0.46510
C 0.80711 -1.39398 1.37477
H 1.35806 -1.10637 2.27831
H -0.16037 -1.80334 1.69755
C 1.52005 -3.78269 0.93881
C 0.69341 -4.36518 2.03624
H 0.85199 -5.45174 2.09006
H 0.95668 -3.92408 3.01267
H -0.37954 -4.17934 1.85943
C 2.37015 -4.36623 0.00289
H 2.60144 -5.42439 -0.09638
C 2.85276 -3.30811 -0.79716
C 3.79243 -3.35813 -1.95496
H 3.88870 -4.38922 -2.32745
H 3.43611 -2.70110 -2.76299
H 4.79233 -2.99168 -1.67308
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C 2.98444 1.99019 -1.12751
N 0.02040 1.90435 -0.07303
N 2.70966 0.84554 2.22013
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N 1.52462 -2.45539 0.67483
N 2.33809 -2.14749 -0.36522
O 5.41747 -0.48673 -2.33630
O 0.90796 0.11448 -3.45339
O 3.11326 3.14978 -1.23758
W 2.69057 0.05565 -0.87532
W -2.69976 0.18711 0.83765
H 0.02987 2.94009 -0.08479
C -0.84714 1.10731 -0.77352
C -1.63418 1.68841 -1.91030
H -2.04708 2.66577 -1.60804
H -0.97872 1.82700 -2.78345
C -3.01949 0.35808 -3.55014
C -2.32332 0.86512 -4.77009
H -2.72153 0.35979 -5.66136
H -2.46430 1.95214 -4.89707

H -1.23900 0.66782 -4.70502
C -4.01236 -0.60111 -3.39099
H -4.51865 -1.14759 -4.18336
C -4.22592 -0.71559 -1.99907
C -5.14410 -1.63396 -1.26056
H -6.04044 -1.85027 -1.86197
H -4.64119 -2.58976 -1.03577
H -5.44333 -1.18398 -0.30333
C -0.56501 -0.23701 -0.48247
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H -1.40845 -1.21179 -2.23347
H 0.09531 -1.90954 -1.61619
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C -3.89328 -3.12180 2.13086
H -4.03136 -4.12808 2.55440
H -3.51119 -2.44067 2.90661
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N -3.41594 0.12635 -1.34760
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C -1.66152 0.27062 2.49934
C -2.94270 2.14145 0.96339
O -5.43675 -0.18513 2.33218
O -0.91196 0.36091 3.40683
O -3.04277 3.30863 0.99230
C -0.98434 5.51767 -0.39835
H -1.91093 5.14554 0.06076
H -1.09310 5.50244 -1.50039
C -0.55796 6.90430 0.08532
H -1.02159 7.71606 -0.49579
H -0.82939 7.03705 1.14612

O	0.09288	4.64383	-0.02295
C	1.25338	5.39367	0.37072
H	2.13682	4.94728	-0.10728
H	1.36454	5.33390	1.47110
C	0.96767	6.83035	-0.06885
H	1.50962	7.57345	0.53586
H	1.25257	6.96736	-1.12550

The coordinates for the free ligand LH

C	0.30550	0.83584	1.19428
C	0.49246	2.32179	1.18318
H	-0.07880	2.82812	1.97489
H	1.55959	2.55543	1.32955
C	0.24167	2.46361	-1.34141
C	1.13573	1.31025	-1.67191
H	1.40454	1.34448	-2.73842
H	2.06239	1.32282	-1.07706
H	0.62470	0.35134	-1.47598
C	-0.54370	3.25969	-2.16470
H	-0.59828	3.20889	-3.25085
C	-1.23965	4.13601	-1.29159
C	-2.23032	5.20667	-1.63751
H	-1.76732	6.00327	-2.24618
H	-3.07488	4.79908	-2.22005
H	-2.62489	5.65985	-0.71541
C	-0.82769	0.10372	0.88910
C	-2.15535	0.70369	0.55801
H	-2.13434	1.78669	0.75611
H	-2.36044	0.58542	-0.51843
C	-4.59356	0.44318	1.02855
C	-4.98416	1.30463	-0.12716
H	-6.07328	1.45688	-0.13719
H	-4.49242	2.29193	-0.07801
H	-4.68219	0.83577	-1.08032
C	-5.33898	-0.18796	2.01487
H	-6.42129	-0.16502	2.12916
C	-4.38698	-0.86299	2.82106
C	-4.62565	-1.72936	4.02096
H	-5.16697	-2.65430	3.75247
H	-3.66260	-2.01007	4.47375

H -5.23126 -1.20442 4.77941
N 1.36818 -0.02145 1.25971
H 2.33448 0.30602 1.38413
N -0.00304 2.89525 -0.06904
N -0.90494 3.89894 -0.02528
N -3.29241 0.12766 1.27995
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C 1.92646 -2.42469 0.88681
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H 1.38247 -3.36225 0.70672
C 2.73665 -2.51882 -1.50266
C 1.49381 -3.13987 -2.04744
H 1.64430 -3.40776 -3.10349
H 1.23027 -4.06028 -1.49697
H 0.63507 -2.44844 -1.98506
C 3.90182 -2.09644 -2.12765
H 4.13610 -2.17399 -3.18764
C 4.71482 -1.57337 -1.09175
C 6.08783 -0.98349 -1.21095
H 6.69773 -1.55245 -1.93112
H 6.04971 0.06181 -1.56646
H 6.59711 -0.99156 -0.23630
C -0.41325 -1.25271 0.73264
C -1.30011 -2.36177 0.26455
H -0.71698 -3.27602 0.06259
H -2.06289 -2.59000 1.02297
C -3.35505 -2.04213 -1.19102
C -4.31051 -2.73510 -0.27678
H -5.33672 -2.60954 -0.64985
H -4.09503 -3.81646 -0.21504
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C -3.56446 -1.39560 -2.40299
H -4.51591 -1.27425 -2.91736
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C -1.91418 -0.14240 -4.02461
H -1.98969 0.93843 -3.80800
H -0.87398 -0.34929 -4.32043
H -2.57902 -0.36654 -4.87395
N 2.90741 -2.24747 -0.17841

N	4.09454	-1.66267	0.08593
N	-2.01762	-1.95621	-0.94726
N	-1.35970	-1.30195	-1.92714
C	4.60525	1.69635	0.65634
H	4.41537	2.72122	0.29752
H	4.40564	0.98139	-0.15902
C	6.01133	1.50378	1.23070
H	6.73935	1.20841	0.46199
H	6.36411	2.43448	1.70637
O	3.70338	1.41329	1.74066
C	4.41605	0.85269	2.85318
H	3.81983	0.01873	3.25872
H	4.52856	1.62233	3.64025
C	5.76785	0.41940	2.28959
H	6.55430	0.36925	3.05823
H	5.65511	-0.56201	1.80414

Coordinates for the optimized conformers of LH (B3LYP)

Conf-1

C	0.0754304	0.5928562	1.3865256
C	0.2752279	2.0626864	1.5603726
H	-0.1801932	2.4449115	2.4955915
H	1.3632746	2.2895341	1.6159139
C	-0.3416841	2.6254291	-0.8642276
C	0.2492822	1.4263665	-1.5353151
H	0.2482749	1.5857696	-2.6297885
H	1.2922918	1.2181037	-1.2244399
H	-0.3535189	0.5168788	-1.3290030
C	-1.0328703	3.7070425	-1.4133312
H	-1.2423195	3.8640411	-2.4768964
C	-1.4296213	4.5187874	-0.3151503
C	-2.2546512	5.7688654	-0.3239882
H	-1.8556455	6.5191251	-1.0368445
H	-3.3018223	5.5542327	-0.6268827
H	-2.2728266	6.2199016	0.6863598
C	-1.1110517	-0.1452875	1.2912158
C	-2.4869071	0.3992966	1.5290561
H	-3.1733999	-0.4172114	1.8469404
H	-2.4721861	1.1406899	2.3507135
C	-3.8258564	2.2139368	0.3443074
C	-4.1082089	3.0347984	1.5609038
H	-4.7820514	3.8710658	1.2976050

H	-4.5976327	2.4502636	2.3681265
H	-3.1674173	3.4750647	1.9567731
C	-4.1819295	2.4004805	-0.9933883
H	-4.7784428	3.2262534	-1.3962399
C	-3.5758217	1.3282795	-1.7064817
C	-3.5653359	1.0605520	-3.1797367
H	-2.9991309	1.8458019	-3.7243429
H	-3.0818011	0.0844863	-3.3736248
H	-4.5904925	1.0421002	-3.6037180
N	1.1158868	-0.2527738	1.0858984
H	2.0815283	-0.0032822	0.8123248
N	-0.3555347	2.8439047	0.4970389
N	-1.0052459	3.9864154	0.8435767
N	-3.0560007	1.0752496	0.3616967
N	-2.9049336	0.5220212	-0.8649871
C	0.6403108	-1.4958420	0.7429726
C	1.5893411	-2.5636976	0.2957547
H	2.2288641	-2.9147763	1.1373568
H	1.0134315	-3.4224346	-0.0866608
C	2.7101929	-2.7159687	-1.9884692
C	2.1202310	-4.0353588	-2.3658793
H	2.3482897	-4.2628188	-3.4232733
H	2.5303172	-4.8620528	-1.7471823
H	1.0179510	-4.0146585	-2.2385932
C	3.5941771	-1.8688188	-2.6650102
H	4.0148788	-2.0324199	-3.6629265
C	3.8304276	-0.7745298	-1.7876693
C	4.6800602	0.4408203	-2.0040815
H	5.7052022	0.1685316	-2.3277808
H	4.2522456	1.0995075	-2.7887958
H	4.7542576	1.0266317	-1.0682735
C	-0.7535028	-1.4702110	0.8647622
C	-1.6829956	-2.5757196	0.4592436
H	-1.2816421	-3.5661164	0.7641151
H	-2.6666525	-2.4646296	0.9509626
C	-3.1279362	-2.5431566	-1.6435059
C	-4.4468668	-2.4473152	-0.9497570
H	-5.2635761	-2.4680770	-1.6947322
H	-4.6192829	-3.2809952	-0.2373088
H	-4.5234967	-1.4874380	-0.3975988
C	-2.8113736	-2.5270090	-3.0050512
H	-3.5226590	-2.4813765	-3.8369059
C	-1.3907421	-2.5563180	-3.0677811
C	-0.5030393	-2.5395661	-4.2768478

H	0.4851455	-2.1097204	-4.0225480
H	-0.3368939	-3.5592905	-4.6861045
H	-0.9504210	-1.9306064	-5.0869792
N	2.4643495	-2.1066402	-0.7853188
N	3.1431290	-0.9382951	-0.6425926
N	-1.9267398	-2.6002836	-0.9866342
N	-0.8675287	-2.6070887	-1.8291408

Conf-2

C	0.2177908	0.4412594	1.4580510
C	0.4105591	1.7573735	2.1471984
H	1.4403172	1.8233977	2.5621022
H	0.2789045	2.6224239	1.4670025
C	-0.9045771	1.1134122	4.2361193
C	-0.3077481	-0.2442344	4.4174355
H	-0.7399637	-0.9529810	3.6798444
H	0.7931077	-0.2464976	4.2895384
H	-0.5380351	-0.6205158	5.4318563
C	-1.9036568	1.7698038	4.9551256
H	-2.4192897	1.3889190	5.8428846
C	-2.1231520	3.0014092	4.2776558
C	-3.1055361	4.0830904	4.6084173
H	-4.1473667	3.7008398	4.5847347
H	-2.9323492	4.4938517	5.6247681
H	-3.0181277	4.9125815	3.8813991
C	-0.9645404	-0.1092670	0.9579653
C	-2.2648300	0.6221799	0.8406535
H	-2.0840788	1.7139724	0.8349552
H	-2.7625092	0.3681549	-0.1203604
C	-4.2162202	1.1678929	2.3543294
C	-4.4802414	2.4989436	1.7295309
H	-5.3250192	2.9977077	2.2387135
H	-3.5902558	3.1578264	1.8104242
H	-4.7384253	2.4078308	0.6531347
C	-4.8584827	0.4767311	3.3857739
H	-5.7184461	0.8270380	3.9669583
C	-4.1476454	-0.7474742	3.5237361
C	-4.3750043	-1.8655555	4.4954356
H	-5.4200048	-2.2363350	4.4583670
H	-3.6953980	-2.7083305	4.2666798
H	-4.1802000	-1.5416264	5.5395727
N	1.1908005	-0.5316441	1.3944484
H	2.2030721	-0.4188447	1.5316074
N	-0.5803466	1.9627650	3.2023357

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N	-3.1405143	-0.8135166	2.6314268
C	0.6707752	-1.6881329	0.8492740
C	1.5877754	-2.8279462	0.5289756
H	2.0323792	-3.2822352	1.4386739
H	1.0405387	-3.6195389	-0.0138423
C	2.7532785	-2.2862599	-1.6640928
C	1.7197310	-2.9014169	-2.5510294
H	1.9940024	-2.7440175	-3.6106762
H	1.6362317	-3.9974568	-2.3898063
H	0.7102502	-2.4578924	-2.3884920
C	3.8907573	-1.5252670	-1.9475596
H	4.2730924	-1.2753382	-2.9432171
C	4.4368330	-1.1581325	-0.6845195
C	5.6601038	-0.3428139	-0.3918001
H	6.5790562	-0.8352081	-0.7729247
H	5.6055471	0.6579912	-0.8680645
H	5.7718923	-0.2069336	0.7006849
C	-0.6815403	-1.4670141	0.5858736
C	-1.6718501	-2.4735792	0.0846360
H	-1.1834178	-3.4544216	-0.0914397
H	-2.4597047	-2.6173947	0.8501379
C	-3.6710937	-1.7857560	-1.3368451
C	-4.7213866	-2.0315511	-0.2994174
H	-5.6742683	-1.5674463	-0.6144339
H	-4.9100715	-3.1168931	-0.1550069
H	-4.4444219	-1.6150320	0.6903235
C	-3.7706543	-1.2977726	-2.6429336
H	-4.6895663	-0.9863793	-3.1517434
C	-2.4423254	-1.3048062	-3.1587057
C	-1.9615924	-0.8983503	-4.5192278
H	-2.2992800	0.1258742	-4.7792118
H	-0.8559526	-0.9194414	-4.5525902
H	-2.3448188	-1.5786221	-5.3087568
N	2.7003167	-2.3647165	-0.2942182
N	3.6931624	-1.6628687	0.3175096
N	-2.3343803	-2.0483197	-1.1453827
N	-1.5813825	-1.7596202	-2.2333396

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C	0.2851713	0.7599336	1.5113554
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H	1.7113116	2.0902773	2.4070935

H	0.6081929	2.9131967	1.2704167
C	-0.6055376	1.8730292	4.2317165
C	-0.0929619	0.5140856	4.5882932
H	-0.6363741	-0.2765473	4.0251823
H	0.9858461	0.3986906	4.3624808
H	-0.2395077	0.3274251	5.6690244
C	-1.5584249	2.6823199	4.8550910
H	-2.0763471	2.4658762	5.7958707
C	-1.7103952	3.8224494	4.0151546
C	-2.6110010	5.0074709	4.1924032
H	-3.6785922	4.7056052	4.2202024
H	-2.3973903	5.5435665	5.1403144
H	-2.4710246	5.7153026	3.3537598
C	-0.9736525	0.1887116	1.2950814
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H	-2.9710813	0.1761057	2.0748652
H	-2.2435078	1.8076902	1.9703006
C	-2.8188048	2.0506268	-0.7123887
C	-1.8312298	3.1512502	-0.4936604
H	-2.0345253	3.9905426	-1.1848411
H	-1.8431888	3.5437200	0.5447600
H	-0.7954002	2.7984128	-0.6910492
C	-3.6579387	1.7636429	-1.7937544
H	-3.7784592	2.3647391	-2.7019318
C	-4.3142471	0.5469038	-1.4551207
C	-5.3294417	-0.2263682	-2.2425979
H	-4.9220758	-0.5622417	-3.2193796
H	-5.6466997	-1.1196938	-1.6716383
H	-6.2311091	0.3839919	-2.4586107
N	1.2292812	-0.2260370	1.3094025
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N	-3.9120783	0.1143149	-0.2462243
C	0.6188867	-1.4066899	0.9502039
C	1.4435101	-2.6336889	0.7104571
H	1.8520973	-3.0436541	1.6595499
H	0.8219835	-3.4243872	0.2526913
C	2.7293301	-2.6832710	-1.4929689
C	1.7443841	-3.5181000	-2.2471777
H	2.0831737	-3.6494890	-3.2911673
H	1.6253056	-4.5294396	-1.8043006
H	0.7409350	-3.0433019	-2.2760336

C	3.9172872	-2.0673303	-1.8956640
H	4.3711307	-2.1177598	-2.8912794
C	4.4012579	-1.3767602	-0.7489793
C	5.6379381	-0.5421366	-0.6075601
H	6.5524987	-1.1304814	-0.8280259
H	5.6284930	0.3204943	-1.3056577
H	5.7178903	-0.1549677	0.4257774
C	-0.7601272	-1.1870925	0.9384663
C	-1.8400128	-2.2203390	0.8085906
H	-2.7714578	-1.7535082	0.4211790
H	-1.5515933	-3.0312093	0.1127438
C	-2.1030652	-4.1786206	2.4358644
C	-1.8144158	-5.2690112	1.4526024
H	-1.8642405	-6.2511926	1.9582473
H	-2.5435514	-5.2856523	0.6154145
H	-0.8003712	-5.1789282	1.0065203
C	-2.4038683	-4.2372004	3.8007989
H	-2.4817037	-5.1434150	4.4117110
C	-2.5853028	-2.8857173	4.2080221
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H	-2.1133868	-2.5633387	6.3010398
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H	-3.8536464	-2.7824021	5.9644984
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C	-1.1699433	1.0436153	1.6776926
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H	-2.9496392	2.1978052	1.9837279
C	-2.9334142	1.8781008	4.6421371
C	-4.3585597	1.8240270	4.1921332
H	-4.6773176	2.7644872	3.6956300
H	-4.5359253	0.9919191	3.4784487
H	-5.0210682	1.6643444	5.0625386
C	-2.3665305	1.7484179	5.9134902
H	-2.9066881	1.5919641	6.8533797
C	-0.9618309	1.8664765	5.7229794
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H	0.1628875	0.8012818	7.2381979

H	1.1155692	1.9648331	6.2546746
C	-1.4754449	0.2553557	0.5668193
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H	-2.9259272	-0.6337204	-0.7422755
H	-3.5937801	0.5839436	0.3800282
C	-3.3312205	1.3322047	-2.5096998
C	-4.2694845	0.2296643	-2.8794790
H	-4.6889608	0.4103900	-3.8860108
H	-3.7419288	-0.7472133	-2.8968782
H	-5.1202814	0.1486416	-2.1695629
C	-2.9700467	2.5100300	-3.1680839
H	-3.3247654	2.8410801	-4.1503126
C	-2.0408005	3.1580124	-2.3061178
C	-1.2915854	4.4378351	-2.5236195
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H	-0.7621922	4.7267538	-1.5957049
H	-0.5351312	4.3325976	-3.3302268
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N	-1.8485357	2.4376587	-1.1863492
C	0.6087797	-0.3025915	1.3133388
C	1.9346265	-0.9365355	1.5998487
H	2.5517179	-1.0139564	0.6835935
H	2.5000523	-0.3225510	2.3302211
C	1.4114594	-2.7028885	3.3520890
C	1.1467794	-1.7421783	4.4677863
H	0.8987878	-2.2948301	5.3926488
H	2.0289191	-1.1034260	4.6868871
H	0.2984886	-1.0626352	4.2415461
C	1.3080690	-4.0937558	3.2813525
H	1.0193941	-4.7674987	4.0957999
C	1.6621754	-4.4371746	1.9436382
C	1.7296682	-5.7931925	1.3082384
H	2.4776067	-6.4430902	1.8086734
H	0.7527080	-6.3168223	1.3624525
H	2.0134640	-5.6941357	0.2435817
C	-0.3419476	-0.5938453	0.3287109
C	-0.1837302	-1.5466619	-0.8187322
H	0.8019265	-2.0564882	-0.7689238
H	-0.9469130	-2.3499117	-0.8024029
C	0.2694797	0.2298400	-2.5959235

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H	1.7469903	1.7675264	-2.4722477
H	0.6987135	1.6289188	-1.0210682
H	2.0066330	0.4312964	-1.3060890
C	-0.2196866	0.4118815	-3.8903949
H	0.0530050	1.2188714	-4.5786527
C	-1.1504551	-0.6414665	-4.1021365
C	-1.9866202	-0.9160098	-5.3147115
H	-1.3583099	-1.0690410	-6.2167400
H	-2.5946676	-1.8274730	-5.1598069
H	-2.6703066	-0.0693277	-5.5345547
N	1.8256716	-2.3028124	2.1044949
N	1.9664958	-3.3345929	1.2374181
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C	-3.7388254	-2.3771290	-0.7044769
N	-2.3755571	-2.2272612	-0.6006123
C	-4.5565524	-3.1820543	0.2559840
C	-2.7017666	-0.2326584	-3.5562297
C	-1.4908697	-2.7704129	0.4306572
C	-0.4867389	-1.7648918	0.9010571
C	-0.7652251	-0.4854639	1.4934097
C	0.4611299	0.1504550	1.6973757
N	1.4527557	-0.7106609	1.2828871
C	0.9003462	-1.8672238	0.7753347
C	0.7314132	1.5274250	2.2205388
N	0.5431014	1.6529802	3.6643945
C	1.4154528	1.2761848	4.6557553
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N	-0.6634352	2.0402174	4.1462142
C	2.7954887	0.7750643	4.3720364
C	-1.7222291	2.3029972	6.3635659
C	-2.0996846	0.1575415	1.7245659
N	-2.5318655	0.9625165	0.5707297
C	-3.8171646	1.1866336	0.1453453
C	-3.7104794	2.0826201	-0.9223294
C	-2.3189027	2.3506633	-1.0545334
N	-1.6181059	1.6688584	-0.1326200

C	-5.0176869	0.5806999	0.7960840
C	-1.6176294	3.2346207	-2.0412381
C	1.7930550	-2.8692708	0.1097129
N	2.6692117	-2.2023925	-0.8486537
C	2.3936431	-1.8930385	-2.1577506
C	3.4047523	-1.0128827	-2.5523336
C	4.2202526	-0.8184277	-1.4015822
N	3.7529981	-1.5358899	-0.3623357
C	1.1901959	-2.4124414	-2.8735909
C	5.4476493	0.0289809	-1.2527028
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H	0.0310320	2.2354042	1.7367467
H	2.7771021	-0.1597471	3.7731674
H	3.4026331	1.5163239	3.8098652
H	3.3242589	0.5599686	5.3188462
H	1.1114605	1.2789463	6.8646911
H	-2.0623905	1.4400560	6.9734531
H	-1.4553794	3.1166963	7.0696846
H	-2.5709496	2.6480152	5.7431871
H	-2.8841235	-0.6034413	1.9015203
H	-2.0512642	0.8138542	2.6210452
H	-5.9313961	0.8855461	0.2529286
H	-4.9798710	-0.5268389	0.7830195
H	-5.1275692	0.9043624	1.8529326
H	-4.5380541	2.4838270	-1.5182242
H	-1.9734778	4.2842284	-1.9803668
H	-0.5290381	3.2216323	-1.8437745
H	-1.7818495	2.8927518	-3.0847246
H	2.4536849	-0.5071442	1.1669179
H	2.4563038	-3.3953806	0.8276527
H	1.1916644	-3.6327656	-0.4170059
H	1.2074741	-2.0818732	-3.9285638
H	1.1527614	-3.5226637	-2.8723882
H	0.2479366	-2.0372020	-2.4103325
H	3.5299440	-0.5721405	-3.5473218
H	6.2701856	-0.3258821	-1.9082752
H	5.2474370	1.0859718	-1.5248748
H	5.8053548	-0.0039427	-0.2060390
H	-0.9771744	-3.6764869	0.0411504
H	-2.1419448	-3.1117291	1.2609455
H	-5.6272731	-3.1058821	-0.0098649
H	-4.2843161	-4.2589230	0.2419429
H	-4.4488566	-2.8325392	1.3054260
H	-5.1251725	-1.5311886	-2.2307677

H	-3.3088475	0.6907692	-3.4654262
H	-1.6386131	0.0622948	-3.6324818
H	-2.9982772	-0.7416955	-4.4970774

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C	0.4396906	0.6477648	1.1981260
C	0.7457495	2.1131270	1.1305099
H	0.2756300	2.6985665	1.9449019
H	1.8435626	2.2750136	1.2000806
C	0.3487210	2.2316716	-1.3894012
C	1.1414412	1.0203456	-1.7651010
H	1.3640361	1.0375173	-2.8485372
H	2.1062862	0.9503270	-1.2259566
H	0.5710386	0.0891461	-1.5543732
C	-0.4491738	3.0732777	-2.1700128
H	-0.5808145	3.0138294	-3.2561762
C	-1.0309203	4.0075933	-1.2653312
C	-1.9746788	5.1360647	-1.5549939
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H	-2.8876189	4.7808537	-2.0765841
H	-2.2780819	5.6221293	-0.6084858
C	-0.7683834	-0.0072421	0.9455407
C	-2.0483602	0.6946767	0.6158627
H	-1.9487037	1.7804413	0.8210943
H	-2.2481740	0.6026424	-0.4742124
C	-4.5219810	0.5663253	1.0360760
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H	-5.9507969	1.6046347	-0.1805363
H	-4.3496587	2.4084402	-0.0962609
H	-4.5535785	0.9366018	-1.0900207
C	-5.3124908	-0.0256925	2.0253306
H	-6.4019165	0.0446225	2.1180808
C	-4.4037872	-0.7346477	2.8618638
C	-4.6927035	-1.5705797	4.0728066
H	-5.3263302	-2.4486940	3.8267501
H	-3.7435170	-1.9376402	4.5070431
H	-5.2297695	-0.9892011	4.8505689
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N	-3.2312339	0.1951981	1.3215722
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C	0.9063207	-1.5539753	0.9923450

C	1.8474008	-2.6933565	0.7519977
H	2.4205424	-2.9788978	1.6579124
H	1.2962060	-3.5855080	0.4038345
C	2.7030866	-2.4011433	-1.6263988
C	1.6019890	-3.1603683	-2.2910352
H	1.7897149	-3.2217332	-3.3790820
H	1.5192789	-4.1984494	-1.9065497
H	0.6206474	-2.6535361	-2.1422958
C	3.7356396	-1.6196354	-2.1514373
H	3.9691107	-1.4796357	-3.2124202
C	4.4090251	-1.0616392	-1.0276607
C	5.5947142	-0.1451973	-1.0033462
H	6.4948943	-0.6318214	-1.4333171
H	5.4081309	0.7751987	-1.5942893
H	5.8271894	0.1459491	0.0385340
C	-0.4676074	-1.4051917	0.7992299
C	-1.4412492	-2.4587892	0.3768046
H	-0.9363195	-3.4381447	0.2336625
H	-2.2292451	-2.5848280	1.1451773
C	-3.4566240	-2.0776174	-1.1395734
C	-4.4731201	-2.6834535	-0.2281005
H	-5.4889144	-2.4891469	-0.6175267
H	-4.3447570	-3.7834837	-0.1442463
H	-4.4211050	-2.2564216	0.7933777
C	-3.5928643	-1.4712294	-2.3933916
H	-4.5288456	-1.3174691	-2.9416104
C	-2.2723319	-1.1237889	-2.7978763
C	-1.8200063	-0.4083386	-4.0348125
H	-2.0059224	0.6836960	-3.9539614
H	-0.7330941	-0.5520925	-4.1834290
H	-2.3530011	-0.7719521	-4.9357445
N	2.8301449	-2.3085202	-0.2618332
N	3.8378296	-1.4758047	0.1191034
N	-2.1119301	-2.0597090	-0.8650909
N	-1.3832490	-1.4923140	-1.8597080