Electronic Supporting Information for

Carbon Dioxide Hydrogenation Catalysed by Well-defined Mn(I) PNP Pincer Hydride Complexes

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1. GENERAL METHODS AND MATERIALS

The complexes [Mn(PNP^{NH}-*i*Pr)(CO)$_2$H] (**Mn1**) and [Mn(PNP^{NMe}-*i*Pr)(CO)$_2$H] (**Mn2**) were synthesised as previously described by some of us.[1] $NaBHEt_3$ and DBU were obtained from commercial suppliers and used as received. All manipulations were carried out using standard Schlenk and glovebox techniques. A H_2:CO_2 (1:1) gas mixture was purchased from Air Liquide and used as received. Solvents were freshly distilled over appropriate drying agents, collected over Linde type 3Å or 4Å molecular sieves under nitrogen, and degassed with nitrogen or argon. Deuterated solvents for NMR measurements were purchased from commercial suppliers and stored onto activated 4Å molecular sieves under Ar before use. The ^{1}H, ^{13}C{^{1}H}, and ^{31}P{^{1}H} NMR spectra were recorded on a Bruker AVANCE-250 spectrometer (operating at 250.13, 101.26, and 62.90 MHz, respectively), on a Bruker Avance II 300 spectrometer (operating at 300.13, 75.47, and 121.50 MHz, respectively) and a Bruker Avance II 400 spectrometer (operating at 400.13, 100.61, and 161.98 MHz, respectively) at room temperature. Peak positions are relative to tetramethylsilane and were calibrated against the residual solvent resonance (^{1}H) or the deuterated solvent multiplet (^{13}C). ^{31}P{^{1}H} NMR were referenced to 85% H_3PO_4, with the downfield shift taken as positive. Mass spectra were obtained on a Shimadzu GCMS-QP2010S with a SPB1 column (32m, internal diameter 0.25mm, 0.25 μm film thickness). IR data were obtained on a Perkin Elmer Spectrum BXII spectrophotometer and by ATR crystal using a Bruker Tensor 27 mid-range FTIR spectrophotometer.

2. SYNTHETIC PROCEDURES

2a. Synthesis of [Mn(PNP^{NH}-*i*Pr)(η^1-OC(O)H)(CO)$_2$] (Mn3). [Mn(PNP^{NH}-*i*Pr)(CO)$_2$H] (**Mn1**) (225 mg, 0.5 mmol) was dissolved in THF and the solution purged with CO_2 (1 atm) for 1 min. An off white suspension formed and after 15 min the solid was collected on a glass frit and dried under reduced pressure. Yield: 255 mg (99%). Anal. Calcd. for $C_{20}H_{36}MnN_3O_5P_2$ (515.40). C, 46.61; H, 7.04; N, 8.15. Found: C, 46.70; H, 7.10; N, 8.02. ^{1}H NMR (250 MHz, δ, DMSO-d_6, 20 °C) 8.21 (s, 1H, *H*COO), 8.19 (b, 2H, N*H*), 7.33 (t, J_{HH} = 7.8 Hz, 1H, py^4), 6.28 (d, J_{HH} = 7.8 Hz, 2H, py^{3,5}), 2.51 (m, 2H, C*H*), 2.23 (m, 2H, C*H*), 1.41-0.96 (m, 24H, CH_3). ^{13}P{^{1}H} NMR (101 MHz, δ, DMSO-d_6, 20 °C) 136.7 (s). IR (ATR, cm^{-1}): 1923 (ν_{CO}), 1842 (ν_{CO}), 1593 (ν_{CO}). The same procedure using CH_2Cl_2 gave identical results. Due to the poor solubility of this complex in all common solvents, the recording of a ^{13}C NMR spectrum was precluded.

The reversibility of the reaction was tested by placing **Mn3** (50 mg, 0.10 mmol) together with DBU (100 equivs) in an autoclave which was then charged with THF (5.0 mL) and pressurised with H_2 (70 bar), leaving it stirring at room temperature for 3 h. Analysis of the solution recovered after the desired time showed quantitative formation of **Mn1** by NMR and IR analyses.

2b. High temperature reactivity of DBU with HCOOH.

An equimolar amount of HCOOH (2.0 mmol; 300 μL) and DBU (2.0 mmol; 74 μL) in THF (5 mL) and H_2O (0.5 mL) were placed in a teflon-coated steel autoclave and heated to 120 °C for 72h. After cooling to room temperature, an aliquot of the mixture was diluted in D_2O and analysed by ^1H NMR, which revealed formation of a product with a characteristic N-formyl signal at 8.00 ppm, which matches perfectly with the signal observed for the undesired side-product (**4**) formed under catalytic conditions at high temperatures (>100 °C, see main text). The mixture was then concentrated under vacuum and the desired product **4** was extracted in CD_2Cl_2 from H_2O/CD_2Cl_2. The product was extracted in the CD_2Cl_2 phase, which was dried with Na_2SO_4 and analysed by GC-MS, ^1H NMR, $^{13}C\{^1H\}$ NMR, 2D ^1H-$^{13}C\{^1H\}$ NMR, $^{13}C\{^1H\}$ NMR-Jmod.

GC-MS (*m*/*z*): 198 [$M^{+\cdot}$], 170 [198-HCO], 153 [170-OH].

^1H NMR (400 MHz, CD_2Cl_2): 8.09 ppm (s, 1H, $\underline{H}CO$); 3.40 (t, 2H, $NC\underline{H_2}$); 3.32 (m, 2H, $NC\underline{H_2}$); 3.19 (t, 2H, $NC\underline{H_2}$); 2.90 (1H, $O\underline{H}$); (2.49 (m, 2H, $C\underline{H_2}C$-OH); 1.73-1.70 (m, 2H, $CH_2C\underline{H_2}CH_2$) 1.65-1.62 (m, 6H, $CH_2C\underline{H_2}CH_2$).

$^{13}C\{^1H\}$ NMR: 177,26 ($\underline{C}$-OH); 161.72 ($H\underline{C}(O)$-N); 49.94 ($N\underline{C}H_2$); 45.34 ($N\underline{C}H_2$); 37.38 ($\underline{C}H_2C$-OH); 34.46 ($N\underline{C}H_2$);30.25 ($CH_2\underline{C}H_2CH_2$); 28.78 ($CH_2\underline{C}H_2CH_2$); 27.63 ($CH_2\underline{C}H_2CH_2$); 23.79 ($CH_2\underline{C}H_2CH_2$).

IR (ν, cm^{-1}, $CHCl_3$): 3355 (s.br., OH); 1771 (s. sh., C=O).

3. NMR AND IR SPECTRA

Figure S1. ^{1}H NMR spectrum of **Mn3** (250 MHz, DMSO-d_6).

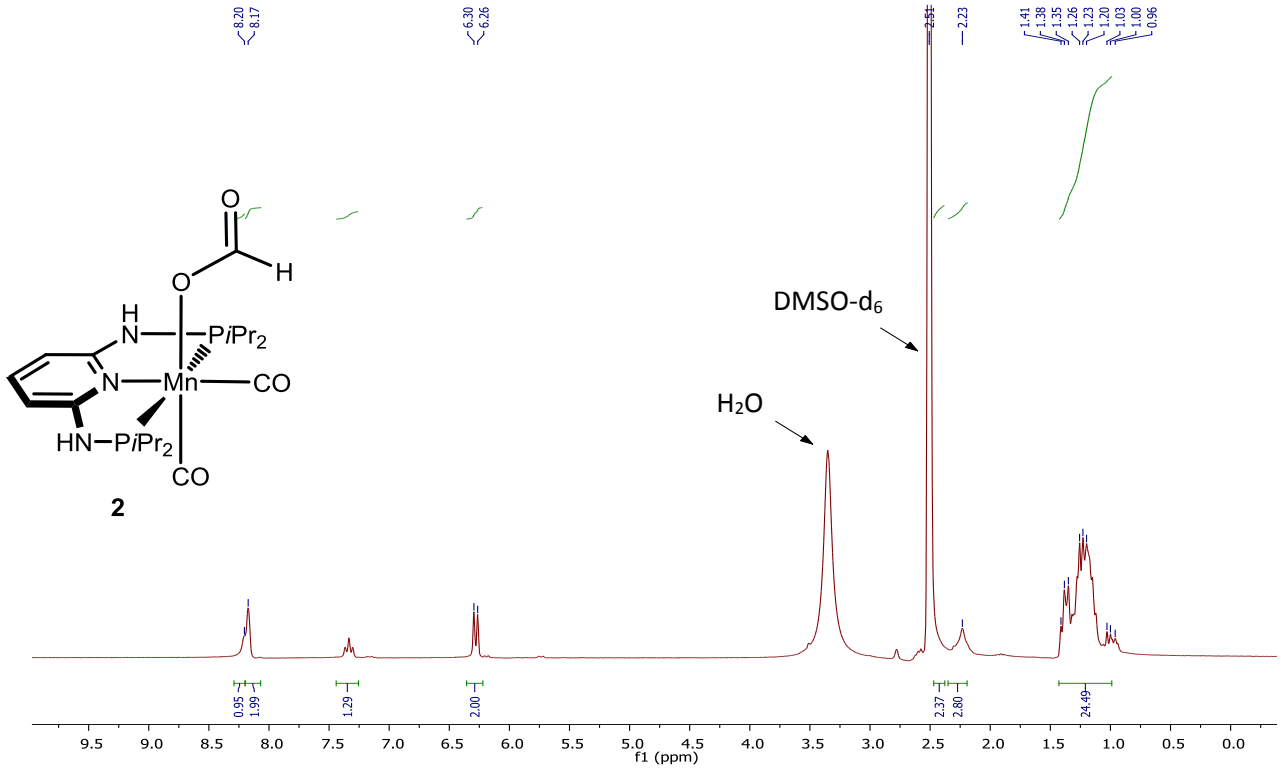


Figure S2. $^{31}P\{^{1}H\}$ NMR spectrum of **Mn3** (101 MHz, DMSO-d_6)

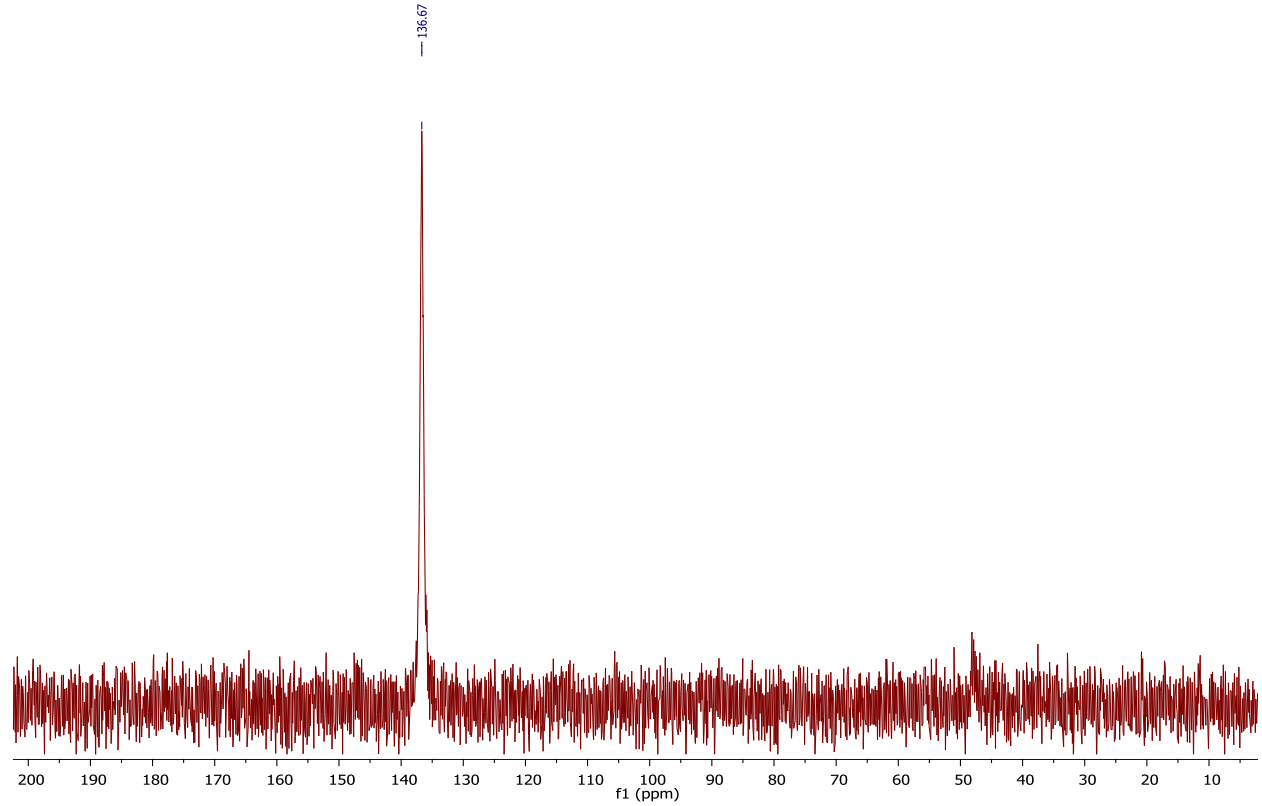


Figure S3: IR spectrum of **Mn3**

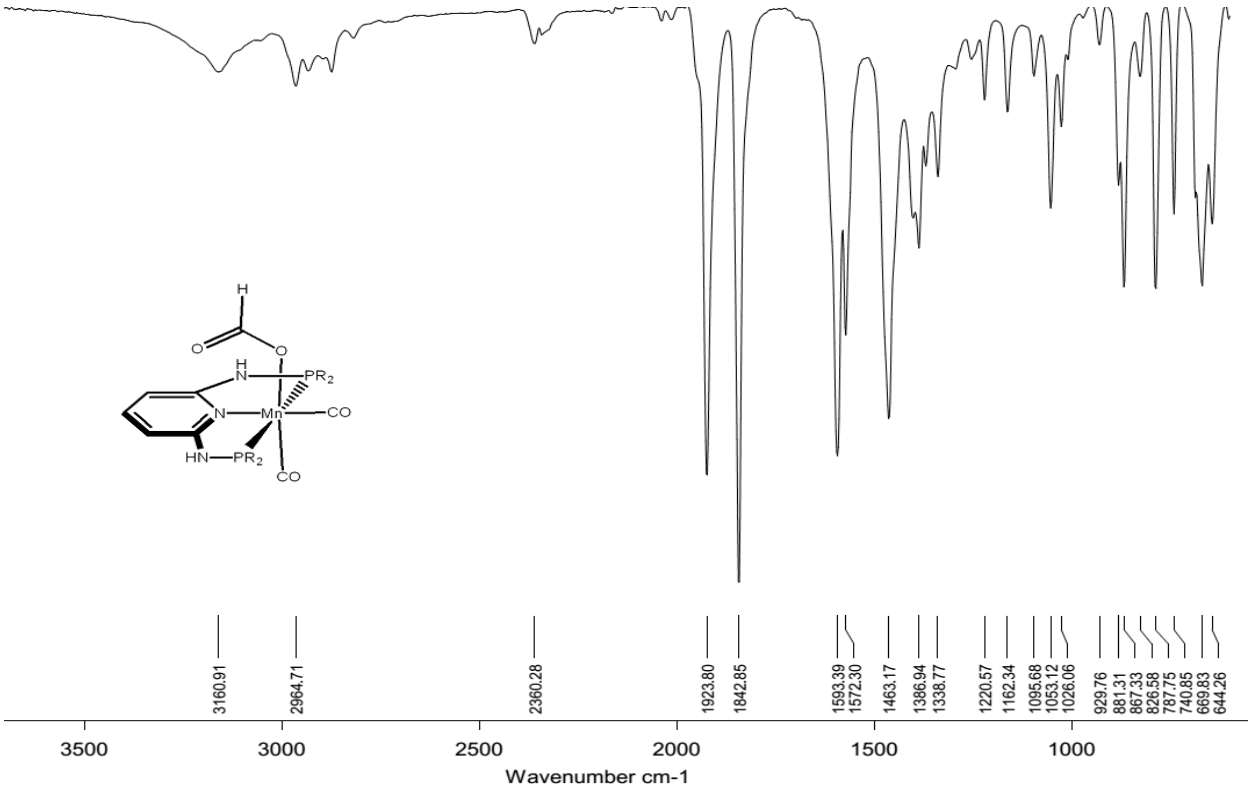


Figure S4: ^{1}H NMR spectrum of **4** (400 MHz, CD_2Cl_2):

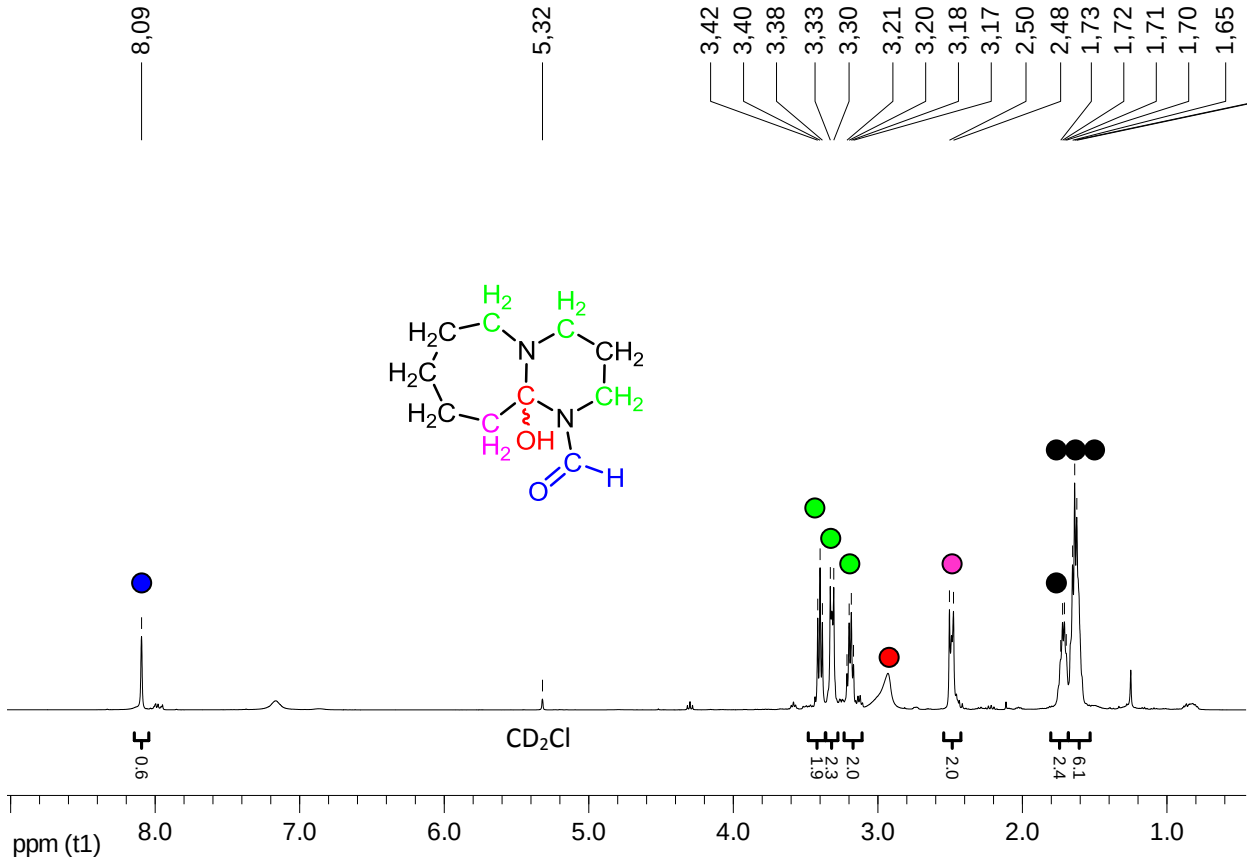


Figure S5: $^{13}C\{^{1}H\}$ NMR spectrum of **4** (100.61MHz, CD_2Cl_2).

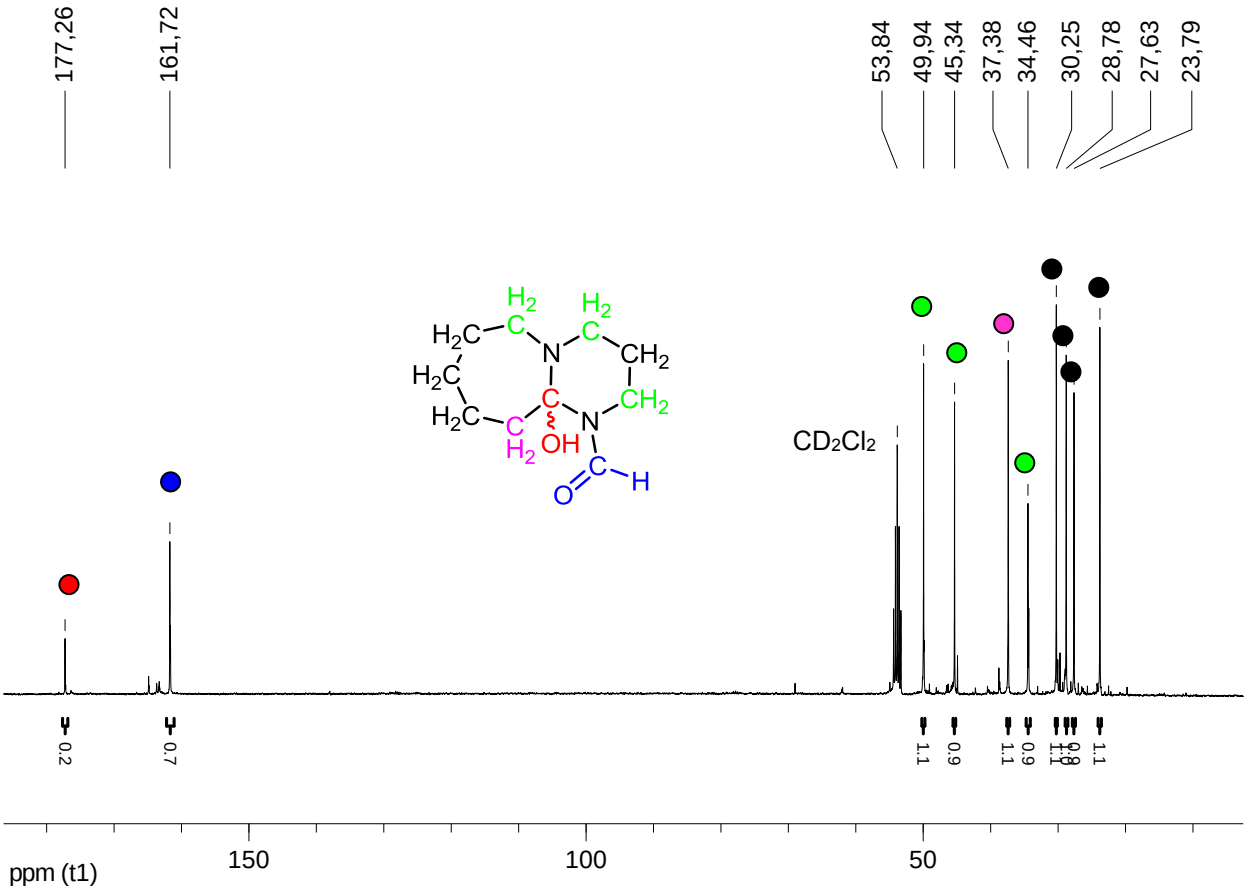


Figure S6: 2D ^{1}H-$^{13}C\{^{1}H\}$ NMR of **4** (400 and 100.61 MHz, CD_2Cl_2) highlighting the correlation of ^{1}H signal at 8.09 ppm and $^{13}C\{^{1}H\}$ signal at 161.72.

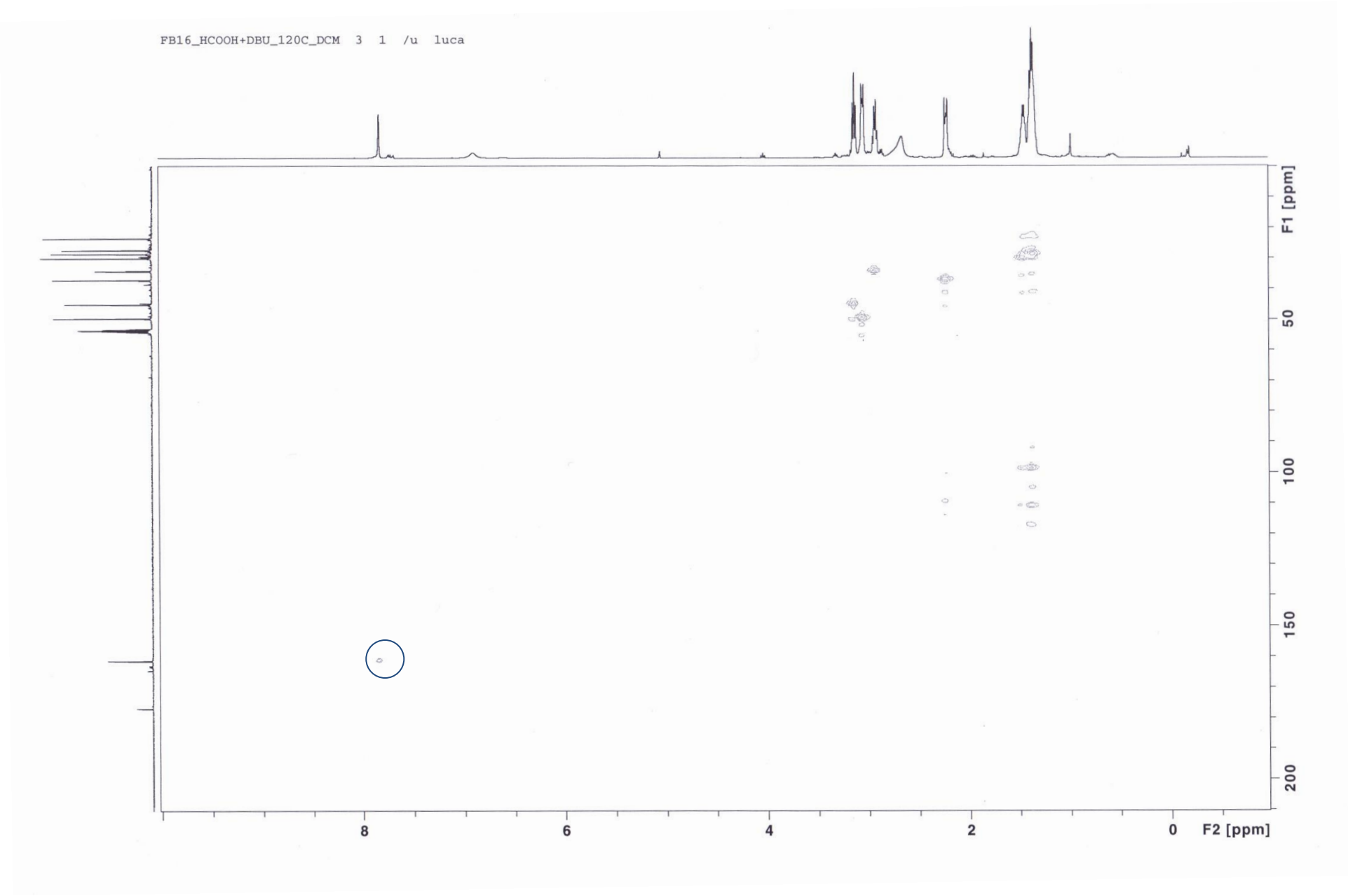


Figure S7: $^{13}C\{^{1}H\}$ NMR-Jmod spectrum optimised for the detection of quaternary carbons of **4** (100.61MHz, CD_2Cl_2).

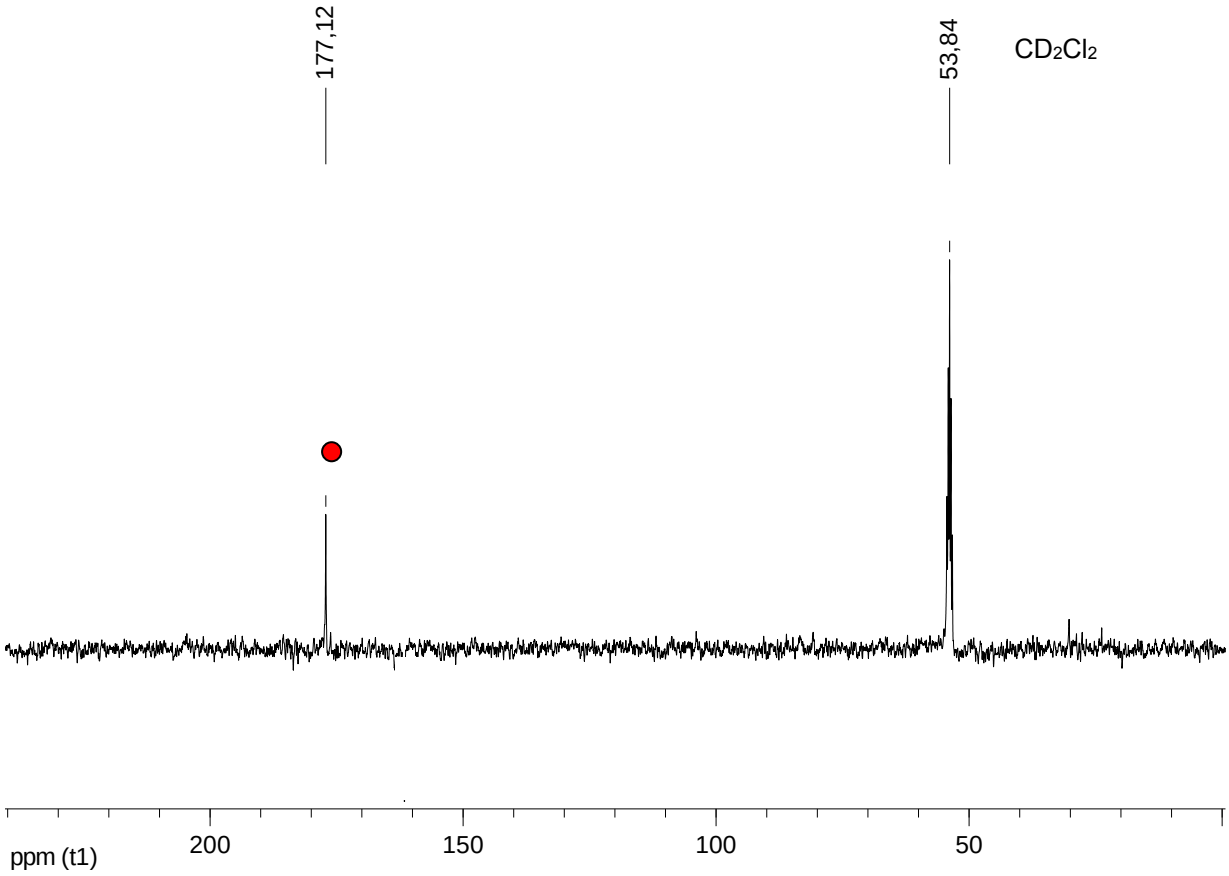
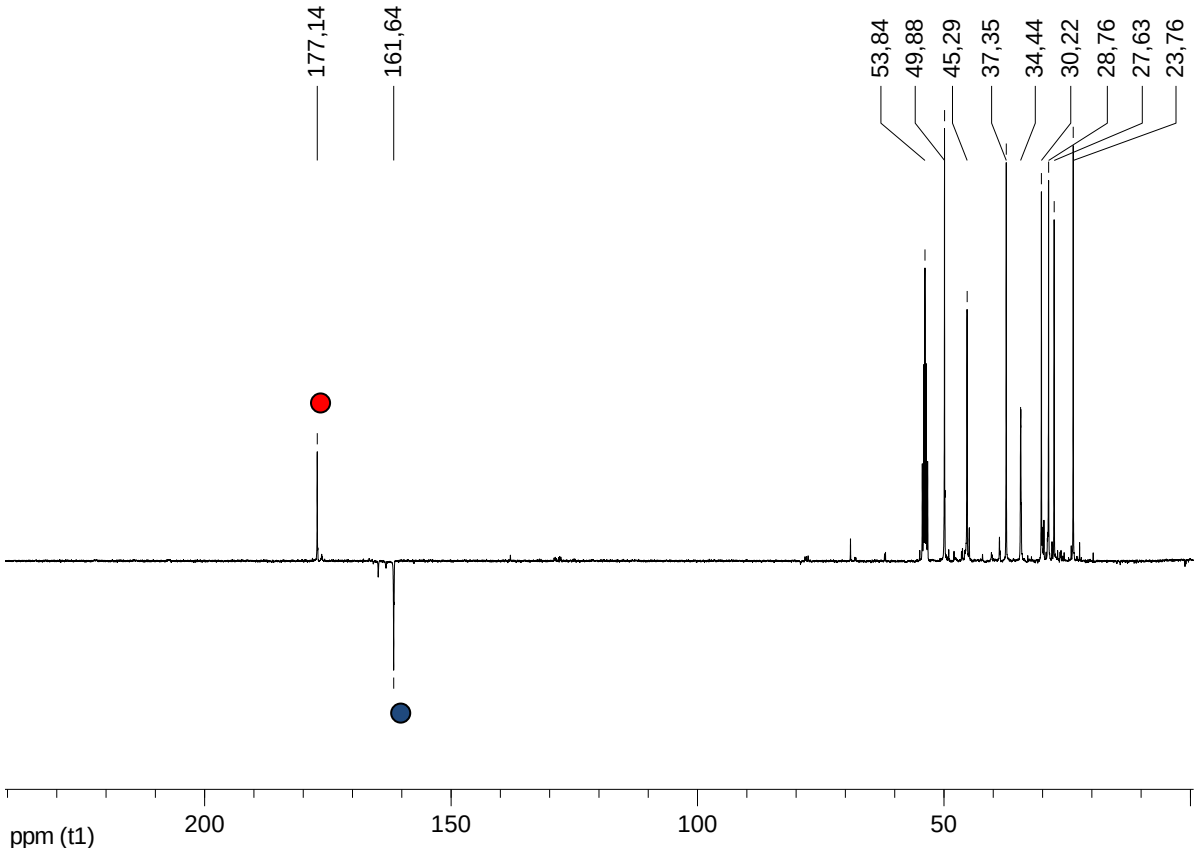


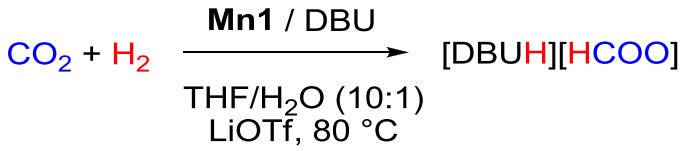
Figure S8: $^{13}C\{^{1}H\}$ NMR-Jmod spectrum of **4** (100.61MHz, CD_2Cl_2).



4. GENERAL PROCEDURES AND ADDITIONAL TABLES FOR CATALYTIC TESTS

General Procedure for Carbon Dioxide Catalytic Hydrogenation: In a typical experiment, the catalytic mixture containing solvent, catalyst, base and additive (if any) was prepared in a Schlenk tube under nitrogen and subsequently injected into a 40 mL magnetically stirred teflon-lined stainless steel autoclave built at CNR-ICCOM kept under a nitrogen atmosphere. Then, the autoclave was pressurised with a H_2/CO_2 (1:1) gas mixture at the desired pressure and placed into an oil bath pre-heated to the desired temperature and left stirring at 400 rpm for the set reaction time. After the run, the autoclave was cooled to < 10 °C using an ice bath, the pressure was gently released and the reaction mixture was transferred in a round bottom flask. The autoclave beaker was thoroughly rinsed with H_2O and the washings added to the rest of the mixture. The volume of the mixture was then gently reduced using a rotavapor at room temperature until an homogeneous mixture is obtained. DMF (300 µL) were added to the mixture as internal standard and the formate content was determined by integration of the corresponding ^{1}H NMR signal vs. DMF. All tests were repeated at least twice to check for reproducibility. Average error (TON) ca. 6%.

Table S1. Lewis acid quantity screening for CO_2 hydrogenation catalysed by **Mn1**.



entry[a]	LiOTf (mmol)	DBU/LiOTf	TON	Standard deviation	yield(%)[b,c]
1	-	-	9100	±700	16
2	0.5	20	13200	±1100	26
3	1.0	10	16799	±700	33
4	1.5	6.67	12426	±174	25
5	2.0	5	11000	±1000	22

[a] Reaction conditions: 80 bar of CO_2:H_2 (1:1), 0.2 µmol of Mn catalyst (**1**) in 5 mL THF + 0.5 mL H_2O, 1.5 mL DBU (10 mmol), at 80 °C for 24h. [b] Formate amount quantified by integration of the corresponding ^{1}H NMR signal using 300 µL DMF as internal standard. [c] Reported values are the average of two runs.

5. COMPUTATIONAL DETAILS

Computational details

All calculations were performed using the GAUSSIAN 09 software package[2] and the PBE0 functional, without symmetry constraints. That functional uses a hybrid generalized gradient approximation (GGA), including 25 % mixture of Hartree-Fock[3] exchange with DFT[4] exchange-correlation, given by Perdew, Burke and Ernzerhof functional (PBE).[5] The basis set used for the calculations consisted of the Stuttgart/Dresden ECP (SDD) basis set[6] to describe the electrons of Mn, and a standard 6-31G(d,p) basis set[7] for all other atoms. Transition state optimisations were performed with the Synchronous Transit-Guided Quasi-Newton Method (STQN) developed by Schlegel *et al*,[8] following extensive searches of the Potential Energy Surface. Frequency calculations were performed to confirm the nature of the stationary points, yielding one imaginary frequency for the transition states and none for the minima. Each transition state was further confirmed by following its vibrational mode downhill on both sides and obtaining the minima presented on the energy profiles. The electronic energies were converted to free energy at 298.15 K and 1 atm by using zero point energy and thermal energy corrections based on structural and vibration frequency data calculated at the same level. Solvent effects (THF) were considered in all calculations using the Polarizable Continuum Model (PCM) initially devised by Tomasi and coworkers[9] with radii and non-electrostatic terms of the SMD solvation model, developed by Truhler *et al*.[10] A Natural Population Analysis (NPA)[11] and the resulting Wiberg indices[12] were used to study the electronic structure and bonding of the optimised species.

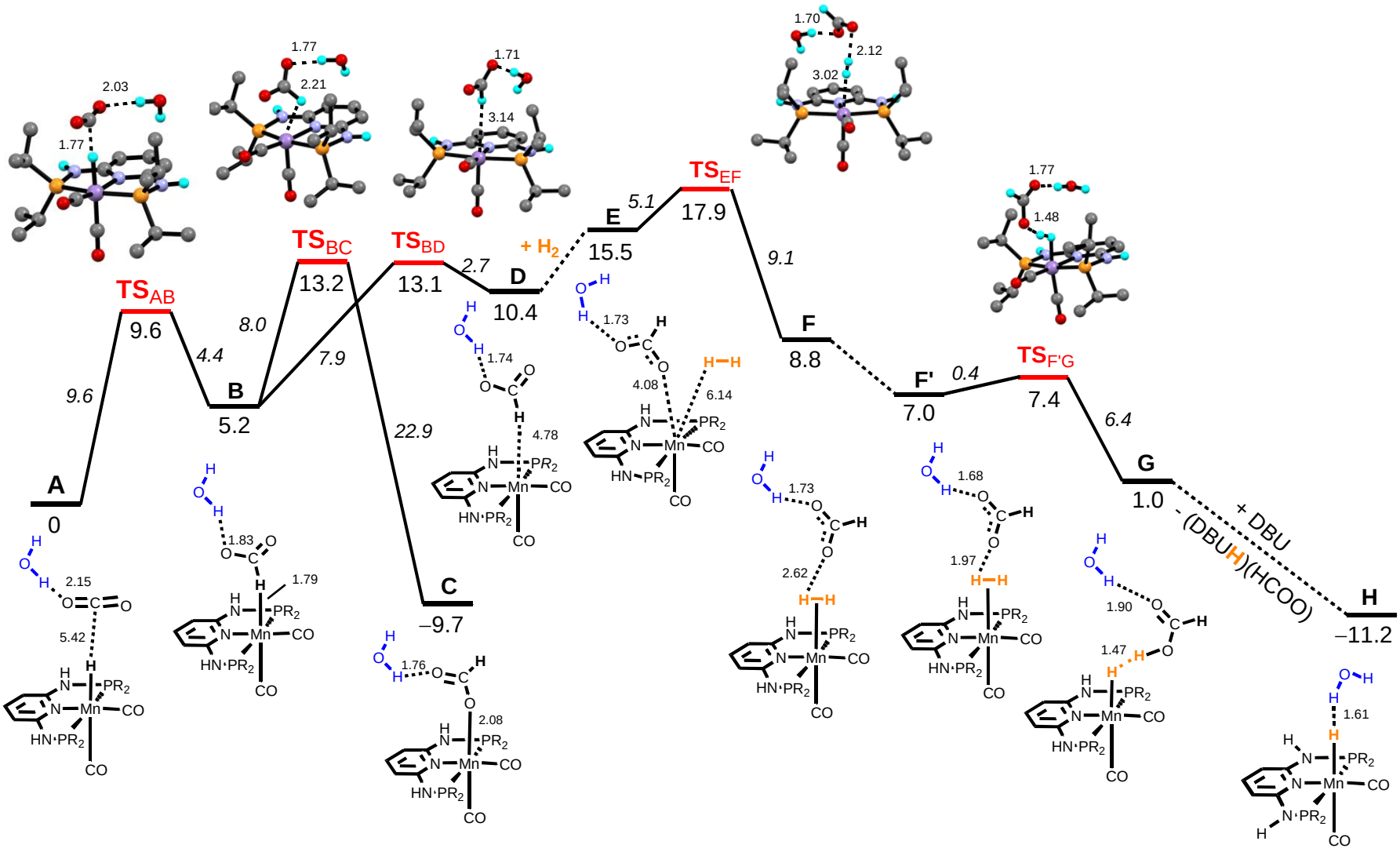


Figure S9. Free energy profile calculated for the hydrogenation of CO_2 catalysed by the hydride complex **Mn1** (denoted as **A**), in a mechanism *without ligand N–H bond participation*. The free energy values (kcal/mol) are referred to the initial reactants (**A**) and relevant distances (Å) are presented.

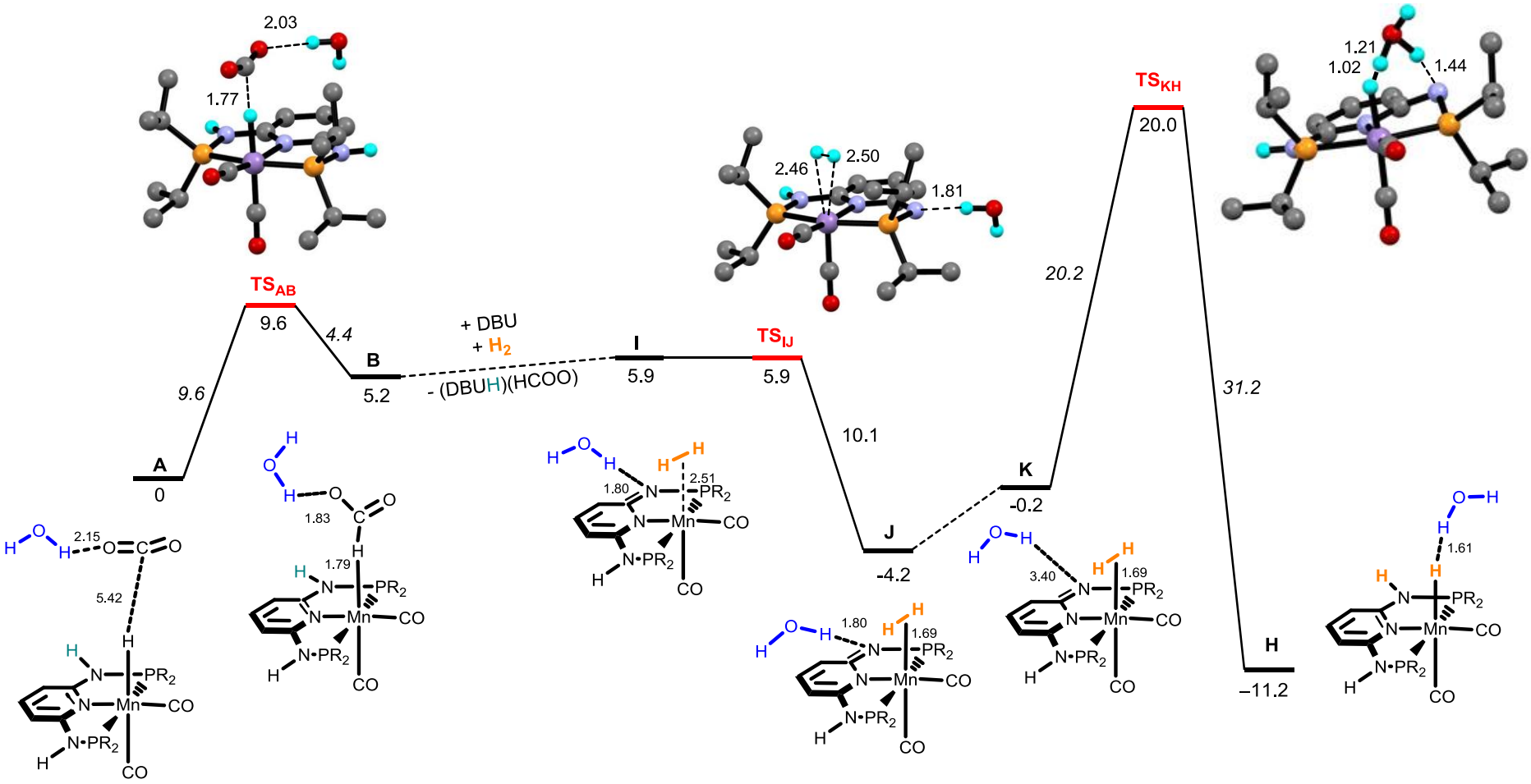


Figure S10. Free energy profile calculated for the hydrogenation of CO_2 catalysed by the hydride complex **Mn1** (denoted as **A**), in a bifunctional mechanism *with ligand N–H bond participation*. The free energy values (kcal/mol) are referred to the initial reactants (**A**) and relevant distances (Å) are presented.

6. ATOMIC COORDINATES FOR ALL THE OPTIMISED STRUCTURES (PBE0)

H_2

H	-0.679315	-0.384670	-1.964211
H	-0.259598	-0.949623	-1.721206

H_2O

O	0.466288	-0.366241	0.000000
H	0.461908	0.597045	0.000000
H	-0.470596	-0.590204	0.000000

DBU

C	-2.691722	0.097069	0.231075
C	-2.710113	-1.111276	1.165853
C	-1.307888	-1.640209	1.461808
C	-0.398398	-1.630080	0.230713
C	0.380668	-0.352274	-0.013287
N	-0.284391	0.857268	-0.038450
C	-1.600122	1.112474	0.548725
N	1.642744	-0.521609	-0.233571
C	2.485907	0.627289	-0.507899
C	1.722176	1.821028	-1.054274
C	0.517809	2.068757	-0.168997
H	-3.657301	0.612230	0.287430
H	-2.577152	-0.218095	-0.812676
H	-3.317581	-1.903241	0.710369
H	-3.205839	-0.843675	2.107251
H	-1.376386	-2.662367	1.850115
H	-0.841753	-1.047811	2.259202
H	-0.984795	-1.876777	-0.664705
H	0.370354	-2.400719	0.317565
H	-1.518638	1.249575	1.639847
H	-1.909372	2.082036	0.144784
H	3.268058	0.317475	-1.213174
H	3.013347	0.914185	0.415076
H	1.384251	1.611247	-2.076291
H	2.350952	2.716632	-1.091405
H	0.842076	2.424136	0.822431
H	-0.120690	2.850132	-0.595815

$(DBUH)^+(HCOO)^-$

C	-2.278930	1.854550	0.973215
O	3.698498	-2.292183	0.340772
C	-1.582870	2.964477	0.188296
C	4.023349	-1.160707	-0.044028
C	-0.435219	2.438175	-0.670029
H	5.112141	-0.897449	-0.022522
C	0.393562	1.368014	0.043050
O	3.276988	-0.226756	-0.475540
C	-0.122115	-0.044841	-0.082843
N	-1.412046	-0.368192	0.088333
C	-2.529547	0.584535	0.170801
N	0.792038	-0.949676	-0.341735
C	0.536063	-2.375547	-0.431013
C	-0.712562	-2.715953	0.352942
C	-1.825387	-1.769374	-0.054118
H	-3.251650	2.214487	1.325873
H	-1.710692	1.594485	1.873571
H	-1.205798	3.714036	0.894517
H	-2.309380	3.477084	-0.453213
H	0.227903	3.263347	-0.948951
H	-0.820617	2.031434	-1.612660
H	0.481326	1.605353	1.110773
H	1.413868	1.350563	-0.346017
H	-2.871343	0.830313	-0.844410
H	-3.340504	0.028257	0.646803
H	1.435640	-2.868331	-0.049268
H	0.418437	-2.657998	-1.485537
H	-0.520052	-2.615934	1.426967
H	-1.022547	-3.746665	0.161847
H	-2.132273	-1.954389	-1.092099
H	-2.703390	-1.916238	0.580165
H	1.837805	-0.643872	-0.399740

A

Mn	0.460034	0.100684	0.330669
O	-4.467317	1.409516	1.798080
P	-0.425799	-1.927185	0.462098
O	-4.043428	3.587879	-0.361276
C	-4.138531	1.361804	2.917683
H	-4.287625	2.984963	0.348345
P	0.711896	2.286909	0.048072
H	-0.566550	0.467964	1.506223
H	-3.679266	3.000042	-1.036028
N	-1.141762	0.408017	-0.982051
O	-3.826547	1.312140	4.037082
N	-1.757575	-1.781441	-0.636126
N	-0.480817	2.603672	-1.167923
C	-1.987746	-0.601544	-1.281466
C	-3.042108	-0.451089	-2.195079
C	-3.205103	0.783685	-2.802091
C	-2.358012	1.842399	-2.492053
C	-1.334635	1.614438	-1.558100
C	0.482407	-3.374465	-0.294751
C	-0.307987	-4.677742	-0.375423
C	1.862763	-3.603262	0.320650
C	-1.251397	-2.612490	1.988361
C	-0.257706	-2.701883	3.146232
C	-2.467744	-1.787348	2.396295
C	1.572070	-0.320310	-0.981766
C	2.237846	2.937947	-0.812166
O	2.322109	-0.605752	-1.831926
C	2.241541	4.442187	-1.070203
C	3.538926	2.479717	-0.155190
C	0.289736	3.571804	1.331603
C	-1.148399	3.435608	1.824791
C	1.271068	3.516048	2.501673
C	1.663132	-0.093315	1.598302
O	2.446536	-0.213614	2.456790
H	-2.388099	-2.546418	-0.839539
H	-3.695614	-1.289303	-2.409850
H	-4.004187	0.928740	-3.524011
H	-2.447765	2.811371	-2.972628
H	0.632556	-2.998109	-1.316611
H	0.234093	-5.398748	-0.998700
H	-1.298741	-4.546633	-0.823846
H	-0.437131	-5.135867	0.610924
H	2.438119	-4.288560	-0.312555
H	1.793986	-4.060501	1.312889
H	2.435948	-2.675969	0.412488
H	-1.590177	-3.623616	1.728057
H	-0.744146	-3.157894	4.016262
H	0.086079	-1.705246	3.442985
H	0.622817	-3.304896	2.908617
H	-2.929835	-2.228885	3.287042
H	-3.225501	-1.747899	1.608505
H	-2.168589	-0.763466	2.644887
H	2.155459	2.422116	-1.779524
H	3.070394	4.699850	-1.740004
H	2.381727	5.010924	-0.144850
H	1.319221	4.790356	-1.548011
H	4.387039	2.742359	-0.798248
H	3.560738	1.397481	-0.002160
H	3.703754	2.961298	0.813744
H	0.388944	4.543501	0.829978
H	-1.366317	4.248006	2.528661
H	-1.287689	2.487829	2.355738
H	-1.881473	3.492720	1.013385
H	0.992800	4.264246	3.252848
H	2.301736	3.722654	2.199967
H	1.249602	2.535232	2.990181
H	-0.648659	3.530043	-1.539754

TS_{AB}

Mn	0.232497	0.201591	0.520420
O	-3.186282	1.072330	2.166151
P	-0.566931	-1.903889	0.491918

O	-4.182504	2.950305	0.062970
C	-2.204546	0.960530	2.824162
H	-3.908520	2.336994	0.755846
P	0.623715	2.381917	0.116468
H	-0.976876	0.578506	1.602948
H	-3.831769	2.553618	-0.743435
N	-1.221228	0.470551	-0.945001
O	-1.570521	0.950894	3.820996
N	-1.855375	-1.727469	-0.642984
N	-0.511773	2.655721	-1.157724
C	-2.053763	-0.538633	-1.285464
C	-3.069718	-0.384121	-2.239053
C	-3.211550	0.853987	-2.845211
C	-2.367759	1.905845	-2.508565
C	-1.371639	1.670467	-1.548462
C	0.476371	-3.226952	-0.309558
C	-0.298698	-4.441748	-0.811305
C	1.632256	-3.630954	0.605621
C	-1.338605	-2.819783	1.930645
C	-0.596210	-2.492059	3.225768
C	-2.838003	-2.573096	2.067476
C	1.501237	-0.248126	-0.617118
C	2.234728	2.801141	-0.735604
O	2.345331	-0.561135	-1.361288
C	2.355362	4.245832	-1.212998
C	3.468481	2.372186	0.059970
C	0.286090	3.869523	1.188214
C	-1.139924	3.906738	1.726360
C	1.293793	3.995805	2.330185
C	1.269376	0.065509	1.942298
O	1.939820	0.001371	2.892532
H	-2.456640	-2.495341	-0.912043
H	-3.715614	-1.220864	-2.480630
H	-3.989995	1.005224	-3.587965
H	-2.450293	2.881875	-2.974288
H	0.894570	-2.710934	-1.182507
H	0.386305	-5.124062	-1.328209
H	-1.080016	-4.164724	-1.526194
H	-0.763492	-5.007689	0.003326
H	2.334730	-4.269835	0.058711
H	1.278127	-4.200532	1.471952
H	2.189592	-2.763328	0.975279
H	-1.189911	-3.884828	1.714608
H	-0.963937	-3.137703	4.031963
H	-0.760676	-1.453275	3.524509
H	0.483051	-2.650770	3.141489
H	-3.209013	-3.089686	2.960434
H	-3.399989	-2.952063	1.208973
H	-3.073518	-1.510675	2.177145
H	2.170328	2.155187	-1.621600
H	3.240722	4.347478	-1.851547
H	2.476208	4.942141	-0.376511
H	1.490781	4.566474	-1.804457
H	4.355069	2.433755	-0.581448
H	3.393524	1.343680	0.423192
H	3.646718	3.021621	0.921843
H	0.414093	4.723054	0.508897
H	-1.347775	4.910053	2.116692
H	-1.254519	3.212513	2.562388
H	-1.900409	3.680942	0.972754
H	1.010540	4.834801	2.976288
H	2.310650	4.184865	1.977989
H	1.309711	3.093410	2.952117
H	-0.640188	3.567538	-1.578627

B

Mn	0.539151	0.159507	0.671256
O	-2.816965	0.028337	2.007841
P	0.069718	-2.053597	0.377962
O	-4.144529	2.025305	0.560313
C	-1.722553	0.161177	2.567541
H	-3.708262	1.326988	1.081417
P	0.612375	2.425384	0.533132
H	-0.836240	0.412126	1.785104
H	-3.829010	1.862009	-0.334871
N	-0.917339	0.379281	-0.775022
O	-1.339015	0.124296	3.729975
N	-1.201156	-1.917236	-0.774260
N	-0.561682	2.662738	-0.706202
C	-1.570772	-0.699284	-1.269309
C	-2.577717	-0.584875	-2.236073
C	-2.902566	0.681808	-2.694619
C	-2.244273	1.801859	-2.203307
C	-1.244885	1.608248	-1.239952
C	1.334688	-3.072518	-0.535551
C	0.777943	-4.335300	-1.188414
C	2.529608	-3.381661	0.365841
C	-0.564635	-3.248088	1.672715
C	0.060809	-2.942332	3.034399
C	1.869919	0.033708	-0.461698
C	-2.088210	-3.310728	1.748187
C	2.134691	3.175239	-0.246972
O	2.743500	-0.047354	-1.226660
C	2.020529	4.670029	-0.535316
C	3.429892	2.848060	0.497761
C	0.055416	3.670362	1.799112
C	-1.350539	3.397719	2.327566
C	1.051544	3.799076	2.950657
C	1.627199	-0.000969	2.069658
O	2.343898	-0.088895	2.977469
H	-1.682829	-2.723146	-1.151455
H	-3.076656	-1.474820	-2.602696
H	-3.680278	0.800562	-3.443922
H	-2.475058	2.803449	-2.548636
H	1.668072	-2.401502	-1.336108
H	1.576598	-4.829843	-1.753274
H	-0.029489	-4.116152	-1.894126
H	0.406727	-5.058338	-0.454382
H	3.323911	-3.853348	-0.223257
H	2.257890	-4.077663	1.166854
H	2.947211	-2.479797	0.825878
H	-0.200809	-4.230504	1.347805
H	-0.211797	-3.735329	3.740727
H	-0.298689	-1.990316	3.436095
H	1.153711	-2.904760	2.990092
H	-2.373765	-4.000488	2.551107
H	-2.530997	-3.685882	0.820423
H	-2.531433	-2.334465	1.965273
H	2.156354	2.644503	-1.208333
H	2.870927	4.987810	-1.149491
H	2.042241	5.263649	0.384417
H	1.109369	4.923781	-1.087626
H	4.285983	3.106511	-0.135455
H	3.515132	1.787529	0.749341
H	3.525261	3.421938	1.423621
H	0.035729	4.617331	1.242434
H	-1.710584	4.294764	2.845342
H	-1.341830	2.583916	3.057405
H	-2.075709	3.153430	1.544871
H	0.656949	4.502554	3.692479
H	2.025106	4.176654	2.629170
H	1.204138	2.839792	3.457338
H	-0.833719	3.586959	-1.017887

TS_{BC}

Mn	0.527618	0.165171	0.713290
O	-2.959361	-0.040775	2.345630
P	0.061462	-2.062131	0.407294
O	-4.077191	1.831092	0.672709
C	-1.750152	0.270192	2.353569
H	-3.744132	1.123736	1.268053
P	0.605893	2.443877	0.555031
H	-1.412436	0.898012	1.471563
H	-3.785741	1.554905	-0.201698
N	-0.911353	0.380332	-0.769837
O	-0.863848	0.010395	3.196658
N	-1.201045	-1.916375	-0.755535
N	-0.559571	2.665891	-0.696734
C	-1.554518	-0.701319	-1.271340
C	-2.538751	-0.590108	-2.261107
C	-2.853953	0.676174	-2.729855
C	-2.207623	1.798316	-2.228948
C	-1.228994	1.609171	-1.244810
C	1.338783	-3.061422	-0.513153
C	0.782697	-4.292166	-1.225175
C	2.512296	-3.416979	0.398987
C	-0.588899	-3.278705	1.671501
C	0.075343	-3.050312	3.030135

C	1.845840	0.039910	-0.412630
C	-2.111009	-3.278079	1.789435
C	2.138671	3.168003	-0.230277
O	2.715505	-0.044364	-1.183326
C	2.038167	4.658676	-0.543532
C	3.428524	2.841620	0.523794
C	0.053342	3.719768	1.795516
C	-1.357400	3.486002	2.332968
C	1.051675	3.860193	2.944104
C	1.626769	-0.002235	2.115918
O	2.366737	-0.100682	3.000137
H	-1.674210	-2.723518	-1.141469
H	-3.031111	-1.480588	-2.635218
H	-3.616376	0.792006	-3.495124
H	-2.437606	2.798748	-2.577651
H	1.697154	-2.367403	-1.282138
H	1.592824	-4.784662	-1.775251
H	0.008014	-4.032976	-1.953585
H	0.369156	-5.030569	-0.530083
H	3.321098	-3.854555	-0.196581
H	2.222900	-4.156515	1.153013
H	2.917043	-2.541690	0.918146
H	-0.274751	-4.259993	1.294912
H	-0.200132	-3.869069	3.705413
H	-0.262104	-2.104142	3.463060
H	1.167946	-3.031878	2.966446
H	-2.401816	-4.005431	2.556882
H	-2.598849	-3.576020	0.856266
H	-2.501695	-2.299516	2.086470
H	2.159017	2.622329	-1.183032
H	2.892176	4.957381	-1.162171
H	2.064816	5.268002	0.365670
H	1.130073	4.911423	-1.101284
H	4.288347	3.083241	-0.110946
H	3.504336	1.784521	0.791739
H	3.525964	3.428629	1.441059
H	0.047412	4.653812	1.216977
H	-1.707042	4.409899	2.808860
H	-1.356994	2.703539	3.096666
H	-2.084555	3.207385	1.563218
H	0.664745	4.582828	3.671428
H	2.029320	4.220699	2.615768
H	1.193001	2.909494	3.469839
H	-0.823246	3.588005	-1.021936

C

Mn	0.721693	0.177320	0.579505
O	-2.744340	0.557306	2.975393
P	0.153069	-2.006515	0.335535
O	-5.119595	0.768017	1.651257
C	-1.972161	0.479095	2.003931
H	-4.321981	0.745301	2.224053
P	0.805981	2.444552	0.458947
H	-2.408089	0.545957	0.986584
H	-5.327495	-0.163535	1.532517
N	-0.773291	0.437691	-0.853922
O	-0.714153	0.327090	2.078122
N	-1.089263	-1.852778	-0.849526
N	-0.369724	2.712521	-0.772950
C	-1.433382	-0.629183	-1.358233
C	-2.426437	-0.496520	-2.336087
C	-2.725082	0.778934	-2.792803
C	-2.054286	1.885239	-2.292934
C	-1.073595	1.671962	-1.316472
C	1.359731	-3.155783	-0.490949
C	0.736173	-4.407609	-1.102326
C	2.502003	-3.503481	0.463762
C	-0.586588	-3.065853	1.690991
C	0.036410	-2.700378	3.039444
C	1.954297	0.033833	-0.656475
C	-2.111327	-3.022927	1.753067
C	2.319967	3.248770	-0.266087
O	2.773880	-0.069995	-1.480616
C	2.091071	4.648452	-0.831149
C	3.473113	3.230630	0.736664
C	0.326839	3.592327	1.857466
C	-1.162686	3.924824	1.892570
C	0.801541	3.010059	3.190165
C	1.950019	-0.039441	1.842941
O	2.773086	-0.186008	2.650238
H	-1.595008	-2.649260	-1.215071
H	-2.936670	-1.376221	-2.712270
H	-3.493073	0.912149	-3.549792
H	-2.270758	2.891665	-2.633313
H	1.766929	-2.545858	-1.307216
H	1.514394	-4.989504	-1.609601
H	-0.026779	-4.167905	-1.849752
H	0.285239	-5.060055	-0.346788
H	3.276830	-4.060856	-0.074450
H	2.157585	-4.135827	1.289452
H	2.971083	-2.610643	0.890382
H	-0.293312	-4.094025	1.442718
H	-0.329251	-3.389981	3.809596
H	-0.234961	-1.679820	3.324387
H	1.128485	-2.771517	3.025211
H	-2.451308	-3.702432	2.543663
H	-2.577651	-3.347999	0.818524
H	-2.490020	-2.026265	1.996237
H	2.578134	2.583937	-1.100073
H	3.018951	5.009977	-1.289284
H	1.811088	5.369548	-0.055697
H	1.320859	4.661993	-1.608727
H	4.391737	3.574302	0.248393
H	3.662501	2.227722	1.132781
H	3.281399	3.900961	1.581602
H	0.875710	4.524287	1.671367
H	-1.353914	4.617105	2.721016
H	-1.780922	3.038334	2.059204
H	-1.503853	4.410403	0.973680
H	0.607056	3.727809	3.995895
H	1.875216	2.797749	3.191290
H	0.270940	2.079947	3.413197
H	-0.620852	3.639103	-1.092487

TS_{BD}

Mn	0.648771	0.137748	0.587035
O	-3.748555	0.849083	2.881564
P	0.190201	-2.083786	0.307495
O	-4.249982	2.316450	0.676843
C	-2.637296	0.299009	2.688863
H	-4.126133	1.767529	1.492292
P	0.683780	2.425170	0.484568
H	-2.320823	0.209922	1.608192
H	-3.974931	1.734252	-0.037717
N	-0.842050	0.353768	-0.805297
O	-1.832863	-0.154304	3.529027
N	-1.036133	-1.955377	-0.891354
N	-0.549420	2.649795	-0.696206
C	-1.467418	-0.733539	-1.326465
C	-2.502177	-0.622930	-2.259911
C	-2.884758	0.647595	-2.664255
C	-2.250640	1.772567	-2.158206
C	-1.219669	1.587149	-1.229639
C	1.480797	-3.130831	-0.528111
C	0.926323	-4.392101	-1.186326
C	2.620811	-3.450872	0.438406
C	-0.499258	-3.208573	1.631473
C	0.084499	-2.828904	2.993620
C	1.960375	0.034826	-0.553931
C	-2.024183	-3.224270	1.677038
C	2.156792	3.219393	-0.334205
O	2.813624	-0.040237	-1.340974
C	1.987807	4.717044	-0.579768
C	3.481801	2.913106	0.366136
C	0.137939	3.589629	1.823170
C	-1.203228	3.163299	2.408483
C	1.190341	3.731377	2.921585
C	1.780168	-0.027530	1.959964
O	2.527188	-0.119252	2.841178
H	-1.518192	-2.762467	-1.266121
H	-2.978857	-1.517263	-2.644914
H	-3.688322	0.762712	-3.386300
H	-2.529398	2.775294	-2.461251
H	1.869157	-2.479886	-1.320419
H	1.743899	-4.922702	-1.687578
H	0.172919	-4.165570	-1.947036
H	0.487534	-5.084375	-0.460076
H	3.424996	-3.962045	-0.102095

H	2.290887	-4.116757	1.242932
H	3.046757	-2.550218	0.892561
H	-0.148573	-4.212560	1.360769
H	-0.208581	-3.584684	3.732205
H	-0.315879	-1.860583	3.315741
H	1.178204	-2.786889	2.985851
H	-2.344866	-3.928304	2.453756
H	-2.472732	-3.548190	0.733596
H	-2.422016	-2.240976	1.942063
H	2.161876	2.710353	-1.307685
H	2.816699	5.079005	-1.198655
H	2.005445	5.284616	0.356278
H	1.059502	4.954835	-1.109881
H	4.309526	3.226960	-0.279395
H	3.614106	1.848300	0.575990
H	3.581080	3.456470	1.309649
H	0.016780	4.557725	1.317820
H	-1.543683	3.931703	3.113022
H	-1.106873	2.226680	2.964609
H	-1.988916	3.037106	1.656915
H	0.787812	4.362480	3.721732
H	2.112400	4.198745	2.568138
H	1.442147	2.761961	3.366057
H	-0.868337	3.571523	-0.969140

D

Mn	0.792427	0.090759	0.553150
O	-4.011748	1.524307	2.552996
P	0.318668	-2.126594	0.319229
O	-4.370575	3.134226	0.392242
C	-3.422476	0.465349	2.230993
H	-4.314272	2.571893	1.199190
P	0.752619	2.371889	0.502926
H	-3.903370	-0.128517	1.399234
H	-4.144719	2.519941	-0.313189
N	-0.790556	0.296830	-0.737797
O	-2.378631	-0.022544	2.719176
N	-0.964700	-2.013105	-0.818818
N	-0.529193	2.596468	-0.622944
C	-1.435595	-0.795002	-1.222424
C	-2.522896	-0.694178	-2.095599
C	-2.940415	0.572867	-2.474717
C	-2.293163	1.703742	-1.998297
C	-1.212046	1.526889	-1.126279
C	1.553252	-3.197166	-0.563902
C	0.972989	-4.499951	-1.108460
C	2.778016	-3.448426	0.314313
C	-0.317082	-3.190164	1.717042
C	0.365946	-2.783479	3.023878
C	2.019222	0.022569	-0.681096
C	-1.836390	-3.143810	1.856625
C	2.150283	3.265046	-0.339223
O	2.815440	-0.022135	-1.527702
C	1.854251	4.730595	-0.648392
C	3.483565	3.108612	0.390041
C	0.248171	3.393897	1.970616
C	-1.217672	3.165362	2.327873
C	1.147380	3.090446	3.170277
C	2.046324	-0.073994	1.810979
O	2.890602	-0.176141	2.599709
H	-1.471293	-2.823928	-1.150869
H	-3.011948	-1.592690	-2.454288
H	-3.782258	0.681306	-3.152833
H	-2.592675	2.704378	-2.289172
H	1.857595	-2.577779	-1.417051
H	1.747964	-5.027309	-1.676279
H	0.132697	-4.329964	-1.788824
H	0.641724	-5.172400	-0.310158
H	3.540302	-3.981534	-0.264397
H	2.530238	-4.069575	1.181845
H	3.227109	-2.518077	0.676320
H	-0.011528	-4.214235	1.467464
H	0.070223	-3.476337	3.820078
H	0.061479	-1.775980	3.325725
H	1.457795	-2.807058	2.955506
H	-2.131497	-3.808432	2.677774
H	-2.347974	-3.492724	0.954251
H	-2.176904	-2.128704	2.100362
H	2.213821	2.720541	-1.291104
H	2.662581	5.138408	-1.265881
H	1.801524	5.336690	0.261702
H	0.922181	4.863879	-1.206829
H	4.293008	3.463255	-0.257389
H	3.700939	2.068832	0.652652
H	3.515036	3.706469	1.306103
H	0.391054	4.440410	1.671529
H	-1.474110	3.800042	3.184845
H	-1.416072	2.127447	2.616736
H	-1.907827	3.415196	1.517628
H	0.899039	3.774834	3.989230
H	2.213096	3.206517	2.955891
H	0.981013	2.070385	3.532663
H	-0.894788	3.513356	-0.848678

E

Mn	0.812067	0.267486	-0.264985
O	-1.886169	1.872698	1.953086
H	-0.586824	0.545966	6.443497
P	-0.334924	-1.697915	-0.430575
H	-0.543303	0.686958	5.705929
O	-4.165390	0.999796	0.770650
C	-1.573184	1.487884	3.111262
H	-3.390098	1.359792	1.259500
P	1.510991	2.440911	-0.410880
H	-3.929373	1.142479	-0.151409
H	-2.407954	1.492998	3.862624
N	-0.751676	0.975825	-1.398055
O	-0.459773	1.105463	3.524951
N	-1.704320	-1.132691	-1.308029
N	0.283550	3.046626	-1.454703
C	-1.782183	0.160986	-1.736027
C	-2.880596	0.614806	-2.476124
C	-2.886943	1.940228	-2.889057
C	-1.835639	2.785754	-2.570103
C	-0.780107	2.267155	-1.812465
C	0.346834	-3.003499	-1.571189
C	-0.619915	-4.158044	-1.820723
C	1.730843	-3.511320	-1.164566
C	-1.141667	-2.585627	0.983975
C	1.831751	-0.161772	-1.609054
C	-0.135764	-3.403813	1.791259
C	-1.882807	-1.597187	1.878078
C	3.065381	2.785694	-1.371588
O	2.492293	-0.423088	-2.530542
C	3.156840	4.209693	-1.913846
C	4.300271	2.412553	-0.552595
C	1.598507	3.632081	1.026441
C	0.271198	4.336113	1.295664
C	2.100819	2.905804	2.276360
C	2.043629	-0.308923	0.893393
O	2.855733	-0.703263	1.620290
H	-2.486193	-1.735164	-1.534364
H	-3.686321	-0.068068	-2.720669
H	-3.724244	2.318118	-3.469132
H	-1.818742	3.824682	-2.879220
H	0.455360	-2.435614	-2.505706
H	-0.220589	-4.802982	-2.611776
H	-1.607293	-3.816229	-2.148226
H	-0.747860	-4.776360	-0.926692
H	2.157416	-4.089884	-1.991408
H	1.683476	-4.172184	-0.295303
H	2.429160	-2.702392	-0.934391
H	-1.867560	-3.266220	0.517661
H	-0.633827	-3.809188	2.679075
H	0.699130	-2.785127	2.138876
H	0.270689	-4.248048	1.229508
H	-2.456379	-2.156739	2.627182
H	-2.583649	-0.958458	1.331306
H	-1.180420	-0.950676	2.413158
H	2.997759	2.102450	-2.226405
H	4.074671	4.310785	-2.504158
H	3.200722	4.957577	-1.115184
H	2.318861	4.456479	-2.572937
H	5.194006	2.493170	-1.180908
H	4.252412	1.386795	-0.172795
H	4.436523	3.086808	0.299465
H	2.341868	4.382906	0.730420
H	0.395863	5.001798	2.158337

H	-0.521354	3.616613	1.532088
H	-0.049821	4.954065	0.451113
H	2.318258	3.645408	3.056569
H	3.022799	2.343750	2.095777
H	1.335658	2.220918	2.662337
H	0.240324	4.019609	-1.730752

TS_{EF}

Mn	0.909155	0.272082	-0.170428
O	-2.991162	2.010190	1.741396
H	0.561952	0.350324	2.828822
P	-0.281811	-1.669666	-0.307568
H	-0.007648	0.795147	3.043735
O	-4.734208	0.468875	0.402694
C	-2.734345	1.728536	2.940932
H	-4.158254	1.052128	0.958757
P	1.612705	2.443887	-0.271265
H	-4.411326	0.646612	-0.486370
H	-3.560883	1.206816	3.501994
N	-0.681711	1.018631	-1.240337
O	-1.695737	1.960468	3.591003
N	-1.585315	-1.112972	-1.285660
N	0.315526	3.107609	-1.185830
C	-1.680093	0.198045	-1.652327
C	-2.759282	0.659586	-2.415492
C	-2.790397	2.004945	-2.755595
C	-1.775969	2.859725	-2.353287
C	-0.727113	2.327436	-1.596741
C	0.415197	-3.046264	-1.351918
C	-0.541680	-4.220661	-1.541407
C	1.796543	-3.517281	-0.897544
C	-1.181139	-2.473321	1.106126
C	1.822014	-0.139653	-1.596692
C	-0.212879	-3.134807	2.085294
C	-2.101970	-1.484757	1.815750
C	3.077276	2.818599	-1.359646
O	2.397323	-0.395956	-2.574067
C	3.253680	4.298156	-1.692731
C	4.376770	2.210066	-0.834741
C	1.764839	3.583602	1.194472
C	0.412507	4.016421	1.756434
C	2.638624	2.953454	2.280358
C	2.216551	-0.341387	0.879944
O	3.081394	-0.752619	1.533416
H	-2.368432	-1.708090	-1.526709
H	-3.529611	-0.033414	-2.735480
H	-3.616165	2.390882	-3.346720
H	-1.775375	3.913077	-2.609490
H	0.532690	-2.540512	-2.320051
H	-0.132867	-4.901310	-2.296870
H	-1.531647	-3.907340	-1.889375
H	-0.666288	-4.794076	-0.617367
H	2.195000	-4.221262	-1.636653
H	1.758709	-4.039281	0.062557
H	2.512432	-2.695953	-0.808523
H	-1.800497	-3.251123	0.638828
H	-0.782606	-3.579190	2.908935
H	0.478775	-2.405388	2.520908
H	0.375468	-3.932946	1.625387
H	-2.652801	-2.019253	2.599389
H	-2.840543	-1.023413	1.152923
H	-1.535701	-0.687745	2.304214
H	2.802180	2.293788	-2.283798
H	4.005516	4.400375	-2.483354
H	3.609764	4.871389	-0.830916
H	2.333358	4.763270	-2.060337
H	5.147414	2.276766	-1.610734
H	4.269224	1.154903	-0.565342
H	4.748279	2.751342	0.040764
H	2.276397	4.474027	0.807279
H	0.588621	4.729845	2.570769
H	-0.175044	3.189205	2.174803
H	-0.199445	4.524662	1.005190
H	2.830298	3.694593	3.064335
H	3.608273	2.610911	1.908580
H	2.133259	2.102851	2.746684
H	0.265030	4.090615	-1.422513

F

Mn	0.793542	0.197702	0.098675
O	-2.367205	2.017118	2.139738
H	-0.098130	0.998957	1.318982
P	-0.310470	-1.767013	-0.144283
H	-0.387925	0.238780	1.303468
O	-4.374223	0.854714	0.730301
C	-2.108451	1.448074	3.237091
H	-3.699468	1.317396	1.282063
P	1.484812	2.356725	-0.031741
H	-4.069268	1.010120	-0.169129
H	-3.006814	1.076905	3.804540
N	-0.698708	0.884450	-1.166562
O	-0.999751	1.246515	3.765232
N	-1.617844	-1.233741	-1.126891
N	0.311528	2.961534	-1.134865
C	-1.690409	0.057668	-1.567369
C	-2.747737	0.497890	-2.373318
C	-2.750168	1.826667	-2.776131
C	-1.735216	2.686244	-2.384465
C	-0.719581	2.175199	-1.568776
C	0.465520	-3.086329	-1.205717
C	-0.458368	-4.266094	-1.497394
C	1.831462	-3.559449	-0.706065
C	-1.203987	-2.648088	1.223433
C	1.862172	-0.212185	-1.259694
C	-0.238522	-3.376522	2.156686
O	2.555446	-0.467508	-2.152270
C	-2.108288	-1.700939	2.006014
C	3.084968	2.731535	-0.899534
C	3.198197	4.171437	-1.394773
C	4.277232	2.338077	-0.028967
C	1.475751	3.527183	1.423309
C	0.136595	4.241639	1.590712
C	1.858839	2.785298	2.705645
C	1.993030	-0.369789	1.286116
O	2.771403	-0.750508	2.055907
H	-2.371907	-1.852272	-1.399319
H	-3.525864	-0.195900	-2.670927
H	-3.556342	2.196300	-3.403630
H	-1.715903	3.728556	-2.681889
H	0.620259	-2.531734	-2.141842
H	0.003349	-4.910183	-2.254365
H	-1.431986	-3.952156	-1.888265
H	-0.625694	-4.877207	-0.604814
H	2.332115	-4.118018	-1.504548
H	1.739640	-4.230714	0.152135
H	2.489929	-2.734827	-0.419076
H	-1.832428	-3.388656	0.709695
H	-0.805128	-3.835729	2.974194
H	0.481713	-2.683888	2.606141
H	0.317429	-4.172453	1.655625
H	-2.753507	-2.294440	2.664884
H	-2.758102	-1.090990	1.369606
H	-1.525143	-1.031299	2.646861
H	3.061368	2.074625	-1.777483
H	4.140509	4.289824	-1.941630
H	3.205959	4.895217	-0.572978
H	2.389395	4.438103	-2.082198
H	5.203856	2.459420	-0.600584
H	4.224755	1.295069	0.299620
H	4.353948	2.973513	0.859965
H	2.251425	4.269758	1.198770
H	0.194665	4.890814	2.473008
H	-0.684407	3.531234	1.752160
H	-0.105942	4.877777	0.733664
H	2.048484	3.518342	3.498990
H	2.767645	2.185406	2.593137
H	1.035278	2.141393	3.038293
H	0.277673	3.937652	-1.400575

F'

Mn	0.679715	0.210695	-0.010124
O	-2.356066	1.150553	3.844645
H	-0.211344	0.550798	1.508478
P	-0.372824	-1.771788	-0.275942
H	-0.701475	0.676992	0.876117
O	-3.152858	1.709177	1.352622
C	-1.215656	0.758542	4.184872

H	-2.819786	1.486099	2.259901
P	1.302558	2.383427	-0.093897
H	-2.866737	2.617571	1.223567
H	-1.087615	0.568785	5.284290
N	-0.707700	0.831673	-1.424841
O	-0.200399	0.549822	3.478724
N	-1.522038	-1.330604	-1.482027
N	0.166634	2.963869	-1.253354
C	-1.591624	-0.047395	-1.950399
C	-2.528339	0.329835	-2.919048
C	-2.539490	1.653270	-3.333734
C	-1.646385	2.570996	-2.800411
C	-0.737410	2.119598	-1.837133
C	0.543071	-3.152875	-1.126361
C	-0.333125	-4.330872	-1.543349
C	1.770719	-3.622593	-0.347723
C	-1.387641	-2.573865	1.059456
C	1.837679	-0.208006	-1.283144
C	-0.552054	-2.743604	2.330546
O	2.585472	-0.481583	-2.127223
C	-2.663719	-1.791465	1.355667
C	2.919331	2.807371	-0.919193
C	3.118343	4.295749	-1.195068
C	4.135876	2.207136	-0.215995
C	1.122896	3.564041	1.329650
C	-0.336290	3.779396	1.719881
C	1.928881	3.076912	2.536105
C	1.839534	-0.308523	1.241564
O	2.633263	-0.659292	2.009180
H	-2.205124	-1.983139	-1.845716
H	-3.219697	-0.404231	-3.317127
H	-3.257201	1.975410	-4.083095
H	-1.638724	3.611417	-3.105234
H	0.890936	-2.649351	-2.038271
H	0.242980	-4.996465	-2.196177
H	-1.222317	-4.020227	-2.101464
H	-0.657001	-4.922089	-0.680865
H	2.375220	-4.279354	-0.983335
H	1.490501	-4.196528	0.540847
H	2.407860	-2.792204	-0.029487
H	-1.665096	-3.563157	0.673518
H	-1.126714	-3.322412	3.063122
H	-0.323949	-1.769092	2.777136
H	0.386911	-3.277912	2.158440
H	-3.223313	-2.309303	2.143524
H	-3.315334	-1.714031	0.480581
H	-2.448990	-0.780373	1.713579
H	2.800256	2.296481	-1.884615
H	4.002011	4.431160	-1.829065
H	3.289677	4.860857	-0.273253
H	2.270844	4.745996	-1.722483
H	5.009600	2.286157	-0.872365
H	4.000753	1.149897	0.030173
H	4.374332	2.742919	0.707720
H	1.534894	4.518220	0.976487
H	-0.382014	4.526775	2.520613
H	-0.782751	2.857891	2.104954
H	-0.938345	4.150312	0.884619
H	1.917082	3.852108	3.311174
H	2.976348	2.868982	2.299808
H	1.474178	2.174109	2.958716
H	0.140798	3.931538	-1.549166

$TS_{F'G}$

Mn	0.707737	0.201894	0.006588
O	-2.272061	1.189311	3.585876
H	-0.268981	0.528545	1.781735
P	-0.362786	-1.768770	-0.239596
H	-0.573626	0.678331	0.971749
O	-3.448329	1.920567	1.209424
C	-1.165388	0.768828	3.959643
H	-2.995540	1.611671	2.021925
P	1.312811	2.372959	-0.076666
H	-3.057054	2.784886	1.053248
H	-1.007063	0.659799	5.058073
N	-0.702898	0.826982	-1.394287
O	-0.161713	0.436530	3.255592
N	-1.535888	-1.325931	-1.423319
N	0.190674	2.951024	-1.251408
C	-1.604043	-0.045648	-1.898579
C	-2.555053	0.332835	-2.853505
C	-2.562522	1.653511	-3.276819
C	-1.652243	2.566284	-2.764338
C	-0.730862	2.111623	-1.813862
C	0.535878	-3.145579	-1.120799
C	-0.339929	-4.332567	-1.512031
C	1.798591	-3.603808	-0.392974
C	-1.377749	-2.595825	1.081557
C	1.847983	-0.209041	-1.278009
C	-0.526531	-2.869927	2.323167
O	2.586574	-0.473743	-2.136495
C	-2.620108	-1.788078	1.444727
C	2.936955	2.806725	-0.884362
C	3.138951	4.295376	-1.155730
C	4.146140	2.204145	-0.170689
C	1.108961	3.570521	1.332434
C	-0.358232	3.803619	1.681212
C	1.892234	3.098066	2.558691
C	1.878211	-0.319351	1.241083
O	2.682977	-0.676619	1.997360
H	-2.225969	-1.977780	-1.774552
H	-3.259515	-0.398042	-3.234231
H	-3.290662	1.977401	-4.015364
H	-1.641129	3.605145	-3.074534
H	0.844593	-2.633201	-2.042136
H	0.218541	-4.987579	-2.190562
H	-1.253787	-4.029886	-2.033778
H	-0.623491	-4.933146	-0.641699
H	2.391785	-4.241483	-1.058245
H	1.561787	-4.194850	0.497135
H	2.431469	-2.765961	-0.086519
H	-1.700993	-3.551908	0.649960
H	-1.110459	-3.461754	3.037716
H	-0.245122	-1.932118	2.813538
H	0.384807	-3.432947	2.101673
H	-3.192223	-2.335692	2.203118
H	-3.277045	-1.628913	0.584958
H	-2.364773	-0.812898	1.870112
H	2.828386	2.296989	-1.851618
H	4.025543	4.432270	-1.785468
H	3.306879	4.858342	-0.231881
H	2.294124	4.748143	-1.685465
H	5.030224	2.297053	-0.811371
H	4.011569	1.142826	0.057194
H	4.367506	2.727152	0.764742
H	1.532743	4.519530	0.979542
H	-0.419888	4.530006	2.500074
H	-0.844945	2.884987	2.021874
H	-0.922705	4.208206	0.835565
H	1.859836	3.875813	3.330594
H	2.945455	2.898631	2.340745
H	1.445210	2.189766	2.976537
H	0.163175	3.918953	-1.545674

G

Mn	0.750484	0.183913	-0.025354
O	-2.342127	1.326789	3.612571
H	-0.320632	0.485326	2.561770
P	-0.334805	-1.760902	-0.255846
H	-0.358785	0.580928	1.098306
O	-3.565603	2.006113	1.110229
C	-1.356238	0.868343	4.155183
H	-3.120723	1.716881	1.921533
P	1.326651	2.345234	-0.095086
H	-3.139109	2.844851	0.909480
H	-1.272427	0.784605	5.249455
N	-0.695024	0.822868	-1.400901
O	-0.271549	0.414339	3.567247
N	-1.537055	-1.321802	-1.414564
N	0.204876	2.939905	-1.265206
C	-1.608215	-0.042748	-1.891247
C	-2.573669	0.339026	-2.831794
C	-2.583707	1.659992	-3.254368
C	-1.662242	2.568240	-2.753454
C	-0.727964	2.106968	-1.817465
C	0.534100	-3.145393	-1.162580
C	-0.347914	-4.331228	-1.542643
C	1.814552	-3.607264	-0.468552

C	-1.345400	-2.613312	1.057441
C	1.893499	-0.226498	-1.311471
C	-0.483808	-2.947103	2.275688
O	2.656273	-0.500177	-2.151844
C	-2.569927	-1.799447	1.462026
C	2.948736	2.798902	-0.903548
C	3.150358	4.287079	-1.175946
C	4.159464	2.195775	-0.192782
C	1.127457	3.563855	1.302287
C	-0.339058	3.806240	1.644683
C	1.913245	3.112321	2.533610
C	1.871096	-0.317428	1.241376
O	2.620893	-0.653260	2.069384
H	-2.229465	-1.975083	-1.757694
H	-3.286283	-0.389610	-3.201894
H	-3.321733	1.987312	-3.981667
H	-1.651623	3.607844	-3.061635
H	0.823854	-2.625629	-2.086229
H	0.193398	-4.981426	-2.239865
H	-1.275170	-4.026391	-2.039385
H	-0.610001	-4.939594	-0.670710
H	2.403096	-4.226438	-1.155437
H	1.600063	-4.218288	0.414062
H	2.442690	-2.767613	-0.156880
H	-1.693440	-3.550387	0.604210
H	-1.068095	-3.543686	2.985757
H	-0.164122	-2.037622	2.793436
H	0.410534	-3.522667	2.021666
H	-3.127996	-2.340748	2.235143
H	-3.246897	-1.624990	0.621028
H	-2.291924	-0.825887	1.876977
H	2.840064	2.287565	-1.870049
H	4.034079	4.426352	-1.809652
H	3.322165	4.851114	-0.253207
H	2.302772	4.739833	-1.701640
H	5.043301	2.281779	-0.835177
H	4.018221	1.136035	0.039398
H	4.386247	2.721480	0.740266
H	1.552728	4.509126	0.941955
H	-0.407587	4.502520	2.488775
H	-0.843020	2.880334	1.938552
H	-0.888938	4.242987	0.805665
H	1.872670	3.892983	3.302022
H	2.967784	2.919793	2.316994
H	1.486407	2.201456	2.965100
H	0.177525	3.909816	-1.551908

H

Mn	0.019403	-1.387729	-0.733367
P	-2.164815	-0.927553	-0.691789
P	2.241393	-1.237219	-0.615263
N	0.165077	0.691231	-0.874358
N	-2.136386	0.780906	-0.945871
N	2.456718	0.469767	-0.764033
C	-0.945325	1.452781	-0.979048
C	-0.888247	2.846291	-1.109388
C	0.362153	3.447488	-1.124507
C	1.514479	2.683173	-1.011953
C	1.372965	1.295020	-0.886065
C	-3.235077	-1.495783	-2.108072
C	-4.528441	-0.708694	-2.300265
C	-3.504233	-2.996872	-2.012809
C	-3.282712	-1.167475	0.794904
C	-2.921440	-2.455450	1.535354
C	-3.271962	0.025688	1.746866
C	3.272721	-1.866605	-2.035755
C	4.682710	-1.288326	-2.123459
C	3.292589	-3.394354	-2.059958
C	3.251172	-1.707913	0.890960
C	3.331688	-0.587490	1.924164
C	2.702377	-2.988785	1.519210
C	0.027546	-1.639255	-2.482288
O	0.032619	-1.851455	-3.632082
C	-0.116666	-3.109519	-0.396933
O	-0.213437	-4.250175	-0.167002
O	0.076338	0.537774	2.780148
H	-0.038241	-0.108832	3.486053
H	0.034329	-1.181447	0.867197
H	-2.975705	1.344918	-0.978369
H	3.365839	0.912744	-0.747583
H	-1.804099	3.421009	-1.191116
H	0.439450	4.526935	-1.223061
H	2.503229	3.128391	-1.017267
H	-2.592566	-1.315992	-2.979730
H	-5.053245	-1.080637	-3.188086
H	-4.344150	0.358618	-2.458596
H	-5.212978	-0.817769	-1.451981
H	-4.000239	-3.344222	-2.926276
H	-4.166735	-3.232300	-1.172359
H	-2.582910	-3.576116	-1.893532
H	-4.297656	-1.278077	0.392328
H	-3.662265	-2.650105	2.319819
H	-1.940596	-2.368518	2.014225
H	-2.896290	-3.329690	0.878282
H	-3.930552	-0.185239	2.598206
H	-3.634605	0.941177	1.270200
H	-2.270266	0.224042	2.144180
H	2.705090	-1.518585	-2.908936
H	5.172871	-1.656783	-3.032327
H	5.308536	-1.587627	-1.275658
H	4.681685	-0.194972	-2.179479
H	3.775823	-3.745253	-2.978953
H	2.284376	-3.820472	-2.030728
H	3.861081	-3.801816	-1.216543
H	4.265073	-1.912867	0.525112
H	3.895833	-0.941268	2.795632
H	2.341341	-0.276318	2.274671
H	3.844095	0.298047	1.536526
H	3.364916	-3.314678	2.329727
H	2.624574	-3.811969	0.802958
H	1.707520	-2.821524	1.944669
H	0.066510	-0.015569	1.973792

I

Mn	0.082814	-1.476876	-0.282261
P	-2.166855	-1.110948	-0.254637
P	2.358540	-1.149553	-0.282750
N	0.145739	0.574635	-0.321692
N	-2.176525	0.598706	-0.342111
N	2.516459	0.526225	-0.356261
C	-0.995783	1.308451	-0.347952
C	-1.006001	2.699778	-0.383594
C	0.230285	3.353017	-0.400231
C	1.406237	2.640040	-0.388110
C	1.373504	1.216740	-0.353156
C	-3.159782	-1.604603	-1.748755
C	-4.487879	-0.865416	-1.885901
C	-3.349744	-3.118261	-1.826387
C	-3.265808	-1.530934	1.201401
C	-2.916422	-2.913723	1.753078
C	-3.207675	-0.472414	2.299232
C	3.300602	-1.739568	-1.778652
C	4.741437	-1.234943	-1.840160
C	3.240153	-3.252999	-1.973225
C	3.416676	-1.689034	1.169639
C	3.419918	-0.657661	2.294025
C	3.009739	-3.066813	1.688964
C	0.083202	-1.706150	-2.003455
O	0.084250	-1.833836	-3.162018
H	-3.030133	1.141863	-0.341295
H	-1.946440	3.239315	-0.398988
H	0.258872	4.440051	-0.425014
H	2.377620	3.121967	-0.400783
H	-2.510550	-1.295107	-2.577746
H	-4.968021	-1.156333	-2.827152
H	-4.357930	0.220813	-1.911063
H	-5.183793	-1.112346	-1.077058
H	-3.795067	-3.381796	-2.792205
H	-4.027757	-3.479367	-1.045725
H	-2.403643	-3.662418	-1.738615
H	-4.290063	-1.563165	0.808591
H	-3.646120	-3.198212	2.519850
H	-1.925626	-2.914581	2.219480
H	-2.925350	-3.690433	0.983493
H	-3.850168	-0.779963	3.132365
H	-3.552857	0.505966	1.954209
H	-2.193741	-0.350838	2.696631
H	2.738471	-1.263580	-2.593752

H	5.145779	-1.404207	-2.845422
H	5.387515	-1.778176	-1.141476
H	4.825238	-0.166770	-1.618330
H	3.682270	-3.520189	-2.940268
H	2.215977	-3.637929	-1.959233
H	3.811206	-3.777735	-1.199649
H	4.438374	-1.754783	0.774683
H	4.080052	-0.996958	3.101273
H	2.422011	-0.519496	2.726685
H	3.772143	0.317621	1.949179
H	3.730731	-3.409392	2.440963
H	2.970364	-3.823642	0.900474
H	2.025366	-3.032433	2.168082
C	0.072918	-3.235954	-0.047640
O	0.067790	-4.393065	0.071364
H	0.479285	-1.199853	2.176764
H	-0.274085	-1.181432	2.186640
H	3.999910	1.539536	-0.500407
H	4.629304	2.413379	-1.581418
O	4.757898	2.154136	-0.663145

TS_{IJ}

Mn	0.080804	-1.476198	-0.283619
P	-2.168150	-1.110103	-0.257036
P	2.355952	-1.149753	-0.277240
N	0.143368	0.575775	-0.321107
N	-2.178488	0.599208	-0.351050
N	2.514090	0.526176	-0.348176
C	-0.997888	1.309358	-0.354580
C	-1.007871	2.700567	-0.395472
C	0.228609	3.353481	-0.409742
C	1.404444	2.640379	-0.390424
C	1.371355	1.217212	-0.350655
C	-3.163966	-1.608677	-1.747407
C	-4.493926	-0.872413	-1.882404
C	-3.351351	-3.122759	-1.822571
C	-3.261212	-1.525710	1.204398
C	-2.911468	-2.908143	1.756803
C	-3.194288	-0.465360	2.299870
C	3.300333	-1.736898	-1.773392
C	4.742086	-1.234286	-1.830101
C	3.238938	-3.249433	-1.974705
C	3.413667	-1.690893	1.174807
C	3.411407	-0.663642	2.303077
C	3.013079	-3.073095	1.687495
C	0.083278	-1.691250	-2.006757
O	0.083907	-1.811656	-3.165975
H	-3.032271	1.142077	-0.352702
H	-1.948181	3.240114	-0.417095
H	0.257508	4.440395	-0.438923
H	2.375899	3.122188	-0.401908
H	-2.517223	-1.299168	-2.578405
H	-4.976133	-1.166540	-2.821599
H	-4.366419	0.214030	-1.910523
H	-5.186962	-1.118986	-1.071007
H	-3.800331	-3.388068	-2.786204
H	-4.025274	-3.484515	-1.038698
H	-2.403804	-3.664858	-1.738623
H	-4.287592	-1.556046	0.817041
H	-3.637309	-3.189648	2.528315
H	-1.918027	-2.909460	2.217441
H	-2.926105	-3.686479	0.988944
H	-3.833376	-0.769132	3.136992
H	-3.537947	0.513461	1.954588
H	-2.177873	-0.346388	2.691976
H	2.740613	-1.256930	-2.587829
H	5.148029	-1.400297	-2.835271
H	5.385931	-1.781566	-1.132512
H	4.827379	-0.167119	-1.604052
H	3.684773	-3.512627	-2.941149
H	2.214568	-3.633892	-1.966871
H	3.806438	-3.778286	-1.201338
H	4.436096	-1.750252	0.780781
H	4.072575	-1.002891	3.109492
H	2.412664	-0.531116	2.735107
H	3.760006	0.314185	1.961652
H	3.733556	-3.414072	2.440705
H	2.981536	-3.826983	0.895829
H	2.026770	-3.047967	2.163417
C	0.068989	-3.238030	-0.071328
O	0.062520	-4.396795	0.030724
H	0.493953	-1.274709	2.137643
H	-0.250077	-1.156378	2.177436
H	3.997490	1.539431	-0.494961
H	4.626945	2.407751	-1.580239
O	4.755288	2.153531	-0.660514

J

Mn	0.080824	-1.464037	-0.255262
P	-2.139279	-1.096474	-0.227016
P	2.336313	-1.136383	-0.259840
N	0.145179	0.605720	-0.317072
N	-2.168234	0.614019	-0.299683
N	2.506947	0.533152	-0.374304
C	-0.993619	1.333249	-0.345817
C	-1.005089	2.724728	-0.418444
C	0.231536	3.373732	-0.470098
C	1.407705	2.658197	-0.454896
C	1.369839	1.237570	-0.380336
C	-3.164374	-1.578984	-1.703814
C	-4.519067	-0.880294	-1.779768
C	-3.308915	-3.093449	-1.839562
C	-3.180314	-1.528243	1.262398
C	-2.872445	-2.947593	1.740588
C	-2.987450	-0.524581	2.396170
C	3.313215	-1.768033	-1.717459
C	4.776294	-1.328265	-1.709572
C	3.193161	-3.271879	-1.956268
C	3.335334	-1.618129	1.246523
C	3.112031	-0.635748	2.392419
C	3.051110	-3.048920	1.697660
C	0.087903	-1.573377	-2.021402
O	0.090077	-1.644864	-3.179800
H	-3.028704	1.146016	-0.297142
H	-1.945387	3.264395	-0.436111
H	0.262084	4.459513	-0.526331
H	2.379927	3.136869	-0.497588
H	-2.547049	-1.216222	-2.536445
H	-5.013244	-1.150201	-2.720097
H	-4.427411	0.210136	-1.765605
H	-5.185889	-1.182090	-0.965347
H	-3.755584	-3.332108	-2.811201
H	-3.968186	-3.505314	-1.068384
H	-2.346364	-3.611708	-1.782094
H	-4.226601	-1.485158	0.934818
H	-3.561195	-3.219402	2.548554
H	-1.853203	-3.014905	2.136183
H	-2.976172	-3.696610	0.950859
H	-3.592375	-0.829994	3.257618
H	-3.290798	0.487038	2.113621
H	-1.943372	-0.484034	2.729409
H	2.808570	-1.250562	-2.545248
H	5.224258	-1.527943	-2.690555
H	5.359128	-1.890533	-0.971571
H	4.894159	-0.260844	-1.498424
H	3.643801	-3.526626	-2.922725
H	2.154881	-3.616384	-1.975726
H	3.725921	-3.845523	-1.190741
H	4.386355	-1.544330	0.939340
H	3.744977	-0.912301	3.244051
H	2.073101	-0.648442	2.745792
H	3.357051	0.388823	2.101126
H	3.721563	-3.318734	2.522294
H	3.195605	-3.783389	0.900872
H	2.023482	-3.148812	2.064602
C	0.065268	-3.231090	-0.119279
O	0.056215	-4.391547	-0.050256
H	0.539696	-1.305502	1.363098
H	-0.281629	-1.307926	1.394402
H	3.996608	1.525151	-0.581150
H	4.625899	2.311007	-1.725845
O	4.756766	2.122524	-0.790750

K

Mn	-0.011117	-1.439842	-0.643831
P	-2.203368	-0.947296	-0.657506
P	2.258116	-1.239908	-0.652523
N	0.175415	0.608265	-0.851743

N	-2.132542	0.749638	-0.889070
N	2.535671	0.404655	-0.833616
C	-0.917174	1.396081	-0.939370
C	-0.849541	2.783944	-1.066063
C	0.421528	3.361492	-1.089363
C	1.556973	2.582079	-0.998390
C	1.444165	1.162284	-0.900011
C	-3.257050	-1.493609	-2.091367
C	-4.587750	-0.755483	-2.212651
C	-3.456194	-3.007689	-2.123131
C	-3.267933	-1.185738	0.857418
C	-3.059306	-2.580591	1.450285
C	-3.008741	-0.111911	1.910698
C	3.205785	-1.999267	-2.065881
C	4.640139	-1.485814	-2.169780
C	3.153643	-3.524486	-2.098467
C	3.221030	-1.739183	0.874392
C	3.156727	-0.651931	1.943242
C	2.752987	-3.078415	1.440742
C	-0.003143	-1.681862	-2.396080
O	0.002699	-1.836525	-3.546601
C	-0.123328	-3.189579	-0.382243
O	-0.196017	-4.341788	-0.242987
O	0.867576	2.322271	2.259848
H	1.695570	1.899230	2.510293
H	-0.368029	-1.115267	0.977904
H	-2.959433	1.332111	-0.915678
H	1.001033	2.537672	1.326704
H	-1.756636	3.373984	-1.129890
H	0.515980	4.441614	-1.175125
H	2.551503	3.013487	-1.024049
H	-2.631904	-1.210403	-2.948664
H	-5.078345	-1.047498	-3.148208
H	-4.464210	0.331658	-2.239043
H	-5.273611	-1.006003	-1.396772
H	-3.921595	-3.295954	-3.072281
H	-4.120429	-3.342599	-1.319663
H	-2.511605	-3.553909	-2.037095
H	-4.308693	-1.098509	0.521542
H	-3.782221	-2.747524	2.256896
H	-2.056468	-2.677810	1.880707
H	-3.189541	-3.382531	0.718252
H	-3.635008	-0.307576	2.788607
H	-3.241275	0.893230	1.548948
H	-1.965376	-0.116987	2.247844
H	2.652729	-1.619047	-2.935474
H	5.079012	-1.806778	-3.122004
H	5.275860	-1.884052	-1.371184
H	4.678991	-0.393704	-2.128276
H	3.563991	-3.890025	-3.047068
H	2.133333	-3.910960	-2.009494
H	3.755104	-3.963802	-1.295342
H	4.264833	-1.836196	0.549239
H	3.760964	-0.945820	2.809820
H	2.129910	-0.502381	2.300762
H	3.530797	0.304232	1.567526
H	3.415770	-3.391835	2.256313
H	2.742750	-3.877680	0.695083
H	1.741126	-2.995385	1.853541
H	0.452307	-1.181253	0.958656

TS_{KH}

Mn	-0.078330	-1.422939	-0.461229
P	-2.246607	-0.916581	-0.701170
P	2.187812	-1.170516	-0.336424
N	0.134817	0.614490	-0.849245
N	-2.116610	0.673569	-1.364678
N	2.343193	0.511456	-0.023743
C	-0.918512	1.340233	-1.280068
C	-0.807975	2.696428	-1.607338
C	0.433598	3.300653	-1.455763
C	1.515912	2.577955	-0.976069
C	1.345843	1.221519	-0.653561
C	-3.242905	-1.747739	-2.040159
C	-4.625539	-1.146884	-2.280915
C	-3.320404	-3.264213	-1.875411
C	-3.408999	-0.717885	0.744236
C	-3.413195	-1.988664	1.594299
C	-3.048690	0.498878	1.591882
C	3.119589	-1.400833	-1.943156
C	4.465141	-0.682589	-1.988436
C	3.261440	-2.872393	-2.326744
C	3.333787	-1.997828	0.892007
C	3.479751	-1.294182	2.237249
C	2.933265	-3.457380	1.109529
C	-0.007838	-1.888925	-2.158030
O	0.011206	-2.221595	-3.276062
C	-0.255772	-3.100698	0.049840
O	-0.390784	-4.205242	0.397191
O	0.921140	0.589490	2.049919
H	1.308490	0.252765	2.869694
H	-0.267099	-1.100504	1.181024
H	-2.929975	1.237831	-1.576827
H	1.710536	0.619494	1.265211
H	-1.676992	3.243215	-1.956961
H	0.552429	4.351665	-1.707034
H	2.489417	3.031332	-0.828896
H	-2.621679	-1.537035	-2.920964
H	-5.045462	-1.558969	-3.205892
H	-4.602427	-0.058066	-2.395778
H	-5.322034	-1.392081	-1.472483
H	-3.756670	-3.707673	-2.777779
H	-3.957327	-3.550555	-1.032260
H	-2.335221	-3.715830	-1.728022
H	-4.411868	-0.563995	0.326809
H	-4.157667	-1.897771	2.393671
H	-2.435872	-2.144281	2.064204
H	-3.656314	-2.885526	1.017146
H	-3.733922	0.565727	2.444999
H	-3.125874	1.433611	1.029063
H	-2.031444	0.424263	1.991056
H	2.452340	-0.920187	-2.671606
H	4.859152	-0.698658	-3.011708
H	5.210332	-1.170523	-1.349839
H	4.378869	0.359928	-1.670978
H	3.604459	-2.958780	-3.364414
H	2.317676	-3.420501	-2.242845
H	4.004187	-3.374386	-1.697004
H	4.316281	-1.975877	0.404258
H	4.287336	-1.770124	2.805604
H	2.571789	-1.398732	2.842078
H	3.728743	-0.234170	2.134267
H	3.717169	-3.975895	1.674312
H	2.779830	-4.004251	0.175300
H	2.006380	-3.524720	1.688034
H	0.285194	-0.315227	1.538907

$B{\cdot}Li(THF)_2$

Mn	-0.714131	0.315148	0.650247
O	-4.267223	-0.057037	2.046607
P	-0.739611	-1.953134	0.331121
Li	-4.860659	-0.093163	4.021313
C	-3.152392	0.152380	2.566485
P	-1.065635	2.570005	0.507159
H	-2.311198	0.473952	1.865156
N	-2.086497	0.273613	-0.884051
O	-2.865586	0.105616	3.782320
N	-1.842287	-2.028155	-0.984581
N	-2.237072	2.582026	-0.749373
C	-2.443153	-0.898936	-1.466301
C	-3.360113	-0.962039	-2.519788
C	-3.912339	0.224551	-2.977635
C	-3.559075	1.435886	-2.402810
C	-2.638054	1.421727	-1.350876
C	0.784963	-2.752220	-0.371577
C	0.531231	-4.100168	-1.042351
C	1.888787	-2.848970	0.680815
C	-1.377108	-3.191787	1.576125
C	-0.924263	-2.811444	2.986639
C	0.703829	0.455209	-0.357444
C	-2.891689	-3.368189	1.502336
C	0.306699	3.612351	-0.193385
O	1.641252	0.547967	-1.038262
C	-0.148177	4.965867	-0.732610
C	1.448751	3.760113	0.810844
C	-1.796737	3.631000	1.860936
C	-3.323042	3.655880	1.837800
C	-1.260101	3.205983	3.228684

C	0.315832	0.331606	2.107073
O	1.012021	0.344249	3.033138
H	-2.118886	-2.902974	-1.411792
H	-3.616076	-1.920860	-2.956144
H	-4.625860	0.205183	-3.796729
H	-3.971898	2.377797	-2.745876
H	1.102780	-2.043950	-1.146351
H	1.463271	-4.452394	-1.498468
H	-0.215004	-4.038689	-1.840624
H	0.211495	-4.865632	-0.327572
H	2.815716	-3.189590	0.206988
H	1.634962	-3.572669	1.462563
H	2.095083	-1.886598	1.159949
H	-0.906217	-4.145154	1.307095
H	-1.181687	-3.621478	3.678849
H	-1.424654	-1.901852	3.332784
H	0.156329	-2.654601	3.054263
H	-3.205565	-4.071444	2.282337
H	-3.214011	-3.778684	0.541198
H	-3.424200	-2.425283	1.663306
H	0.662851	3.015088	-1.042071
H	0.699948	5.459524	-1.220291
H	-0.498304	5.634517	0.060528
H	-0.940725	4.872805	-1.481809
H	2.292469	4.268656	0.331868
H	1.809795	2.793601	1.176943
H	1.149891	4.363846	1.674524
H	-1.438687	4.646781	1.654652
H	-3.679887	4.253829	2.684518
H	-3.757716	2.656076	1.930952
H	-3.716588	4.110495	0.924352
H	-1.580970	3.935147	3.981873
H	-0.167093	3.167215	3.255911
H	-1.646296	2.225835	3.525316
H	-2.640679	3.438309	-1.108024
C	-5.516029	2.416338	5.554655
C	-7.121593	1.836010	3.921814
C	-6.480075	3.578570	5.383349
C	-7.726627	2.875870	4.849070
H	-6.928430	2.247864	2.923350
H	-4.465052	2.692720	5.428630
H	-6.095325	4.288488	4.642756
H	-5.638964	1.931278	6.531719
H	-6.649358	4.114843	6.320336
H	-8.413978	3.545088	4.325679
H	-8.270940	2.389051	5.665936
H	-7.729287	0.931639	3.818407
O	-5.864659	1.473727	4.523396
C	-4.813801	-2.828923	5.157282
C	-5.580985	-3.638094	6.190920
C	-6.575210	-1.506239	6.008031
C	-6.200620	-2.541143	7.053387
H	-3.802524	-2.584255	5.504597
H	-6.365571	-4.230970	5.708175
H	-7.547221	-1.731808	5.550587
H	-6.592190	-0.479431	6.382883
H	-7.065309	-2.877013	7.631085
H	-5.457312	-2.131931	7.746780
H	-4.929636	-4.315842	6.748121
H	-4.741694	-3.319808	4.182418
O	-5.552800	-1.600622	4.997486

C·Li(THF)$_2$

Mn	-1.215715	-0.229328	0.219493
O	-4.348463	-0.120771	3.104724
P	-1.850683	-2.365994	-0.252807
Li	-3.679273	0.386144	4.756298
C	-3.714298	-0.194240	2.025045
P	-1.076914	2.039587	0.357982
H	-4.310807	-0.281796	1.099695
N	-2.886732	0.225490	-0.942208
O	-2.459589	-0.172353	1.920220
N	-3.238508	-2.044397	-1.220234
N	-2.439595	2.469539	-0.603437
C	-3.629168	-0.761377	-1.495235
C	-4.750379	-0.495714	-2.290038
C	-5.091602	0.830562	-2.512329
C	-4.338665	1.857017	-1.961592
C	-3.230561	1.511961	-1.178905
C	-0.775714	-3.370278	-1.389608
C	-1.486821	-4.533574	-2.076044
C	0.483302	-3.831160	-0.655686
C	-2.409424	-3.623940	1.020002
C	-1.676727	-3.389700	2.341577
C	-0.141863	-0.226248	-1.166131
C	-3.921648	-3.671305	1.223132
C	0.317723	2.904842	-0.516206
O	0.577620	-0.218642	-2.082897
C	0.047191	4.369554	-0.850296
C	1.624779	2.735959	0.257548
C	-1.270946	3.016875	1.941971
C	-2.721786	3.358179	2.271705
C	-0.595039	2.281400	3.100558
C	0.158551	-0.623264	1.273628
O	1.079159	-0.883091	1.933831
H	-3.799454	-2.781403	-1.627808
H	-5.322306	-1.314678	-2.711783
H	-5.957320	1.067325	-3.124712
H	-4.583347	2.900869	-2.123557
H	-0.482104	-2.649226	-2.162209
H	-0.795237	-5.016784	-2.775549
H	-2.355387	-4.205875	-2.656006
H	-1.815361	-5.299058	-1.364874
H	1.168546	-4.310675	-1.363253
H	0.249526	-4.566220	0.122404
H	1.018760	-2.998237	-0.188373
H	-2.095050	-4.596171	0.621276
H	-1.947056	-4.176377	3.055863
H	-1.951422	-2.420967	2.767089
H	-0.588833	-3.410990	2.223344
H	-4.155965	-4.445293	1.963235
H	-4.461105	-3.921593	0.304956
H	-4.319864	-2.725539	1.601650
H	0.400928	2.351947	-1.460120
H	0.900167	4.777073	-1.404848
H	-0.079064	4.985132	0.046921
H	-0.837786	4.495209	-1.481767
H	2.459227	3.116894	-0.341378
H	1.836351	1.687617	0.492521
H	1.611853	3.300491	1.196365
H	-0.732769	3.957636	1.770926
H	-2.749268	3.934666	3.204248
H	-3.332565	2.461718	2.414915
H	-3.194398	3.968376	1.496758
H	-0.617401	2.914715	3.995475
H	0.453548	2.048092	2.891261
H	-1.114990	1.344200	3.318143
H	-2.700793	3.432032	-0.775042
C	-4.822149	2.779012	6.120383
C	-6.291394	0.932965	5.983535
C	-6.251755	3.291738	6.106340
C	-7.018235	2.088201	6.649812
H	-6.689193	0.731325	4.981437
H	-4.186267	3.231519	5.352902
H	-6.567278	3.513620	5.080745
H	-4.351091	2.922512	7.100681
H	-6.371730	4.195098	6.709378
H	-8.082491	2.101858	6.402369
H	-6.915482	2.028828	7.738867
H	-6.308280	0.006383	6.564713
O	-4.919505	1.364476	5.858147
C	-1.147652	-1.055091	5.413714
C	-0.121064	-1.024780	6.533422
C	-1.512000	0.875776	6.727999
C	-0.055149	0.465639	6.858093
H	-0.686535	-0.878901	4.435347
H	-0.481489	-1.588832	7.400502
H	-2.066912	0.698376	7.657757
H	-1.649400	1.919325	6.429654
H	0.344766	0.678617	7.852437
H	0.557513	0.991589	6.117390
H	0.838256	-1.445113	6.221364
H	-1.723248	-1.984344	5.372960
O	-2.055868	0.029302	5.695812

Fe1

Fe	-0.064746	-0.390279	0.229969
P	-2.243362	-0.144484	0.235065
P	2.115266	-0.132566	0.190115
N	-0.073032	1.672497	0.133233
N	-2.378647	1.590492	0.167759
N	2.234179	1.598705	0.071199
C	-1.238141	2.359633	0.120657
C	-1.284067	3.761180	0.061703
C	-0.079911	4.453789	0.009204
C	1.127655	3.764537	0.012421
C	1.087766	2.363266	0.073271
C	-3.251298	-0.631749	-1.282988
C	-4.739936	-0.257810	-1.238388
C	-3.047383	-2.100127	-1.688905
C	-3.334424	-0.548603	1.715552
C	-3.343615	-2.062248	1.989323
C	-2.879243	0.224966	2.961877
C	3.076884	-0.715029	-1.322363
C	4.327121	0.085253	-1.719635
C	3.364338	-2.225119	-1.267206
C	3.115548	-0.465247	1.753648
C	2.940862	-1.905541	2.262631
C	4.593704	-0.049070	1.742297
H	-2.237964	4.276639	0.055353
H	-0.082417	5.539005	-0.036696
H	2.078916	4.282934	-0.032395
H	-2.756801	-0.013730	-2.043027
H	-5.195185	-0.413561	-2.223295
H	-4.904240	0.793021	-0.973522
H	-5.294826	-0.875913	-0.524761
H	-3.489799	-2.275024	-2.676636
H	-3.529846	-2.792634	-0.991707
H	-1.985915	-2.351335	-1.744432
H	-4.354901	-0.230822	1.462026
H	-3.964831	-2.278510	2.865987
H	-2.332812	-2.426030	2.197437
H	-3.745014	-2.640218	1.152501
H	-3.528667	-0.024599	3.809213
H	-2.921467	1.307151	2.809451
H	-1.849043	-0.034792	3.221125
H	2.314022	-0.551964	-2.092929
H	4.686354	-0.262781	-2.695375
H	5.149635	-0.037880	-1.009955
H	4.113997	1.153962	-1.821158
H	3.697446	-2.573925	-2.251291
H	2.477134	-2.803590	-0.995244
H	4.160258	-2.461699	-0.553393
H	2.576439	0.190059	2.449881
H	3.377330	-1.997033	3.264165
H	3.444075	-2.634137	1.620116
H	1.884966	-2.175520	2.329199
H	4.998757	-0.095446	2.760202
H	4.743951	0.975480	1.385157
H	5.201220	-0.716719	1.123648
H	-0.028090	-0.281546	1.787452
H	3.113046	2.096064	0.046320
C	-0.054135	-2.128575	0.286706
O	-0.039733	-3.295332	0.319059
H	-3.262211	2.080883	0.173432
H	-0.088619	-0.410766	-1.335004

Fe2

Fe	-0.067646	-0.257403	0.260613
P	-2.240786	-0.057737	0.234210
P	2.109709	0.002555	0.203611
N	-0.097522	1.779183	0.094801
N	-2.430289	1.685972	0.169513
N	2.242649	1.749350	0.070333
C	-1.278494	2.447030	0.048939
C	-1.335255	3.844145	-0.105560
C	-0.141054	4.545781	-0.183722
C	1.074108	3.879131	-0.117794
C	1.061830	2.478024	0.013580
C	-3.206732	-0.659503	-1.285436
C	-4.742533	-0.663757	-1.202601
C	-2.696266	-2.030181	-1.766046
C	-3.315118	-0.527932	1.708238
C	-3.232688	-2.043876	1.962050
C	-2.913484	0.256014	2.965922
C	2.978037	-0.675297	-1.333155
C	4.285340	-0.033073	-1.822102
C	3.108970	-2.207552	-1.242373
C	3.152931	-0.410046	1.741486
C	2.612137	-1.683469	2.419395
C	4.685277	-0.507523	1.622303
H	-2.281495	4.360888	-0.172338
H	-0.156966	5.625568	-0.301720
H	2.002190	4.427393	-0.180911
H	-2.895996	0.082052	-2.033264
H	-5.158207	-0.962325	-2.172157
H	-5.168351	0.313099	-0.960151
H	-5.107078	-1.385190	-0.463702
H	-3.163682	-2.278066	-2.726343
H	-2.948621	-2.831954	-1.064293
H	-1.613652	-2.020174	-1.900100
H	-4.355422	-0.284024	1.458187
H	-3.866393	-2.310168	2.815742
H	-2.208756	-2.347151	2.196262
H	-3.571093	-2.634479	1.105703
H	-3.535418	-0.058500	3.812353
H	-3.039825	1.334948	2.838506
H	-1.864448	0.071617	3.213164
H	2.202053	-0.461190	-2.077111
H	4.581248	-0.506702	-2.766065
H	5.115928	-0.166481	-1.123372
H	4.168796	1.034543	-2.022756
H	3.410175	-2.605770	-2.218074
H	2.167492	-2.688060	-0.967802
H	3.872244	-2.513160	-0.519678
H	2.905390	0.436654	2.395601
H	3.140358	-1.844826	3.366710
H	2.768944	-2.572897	1.800621
H	1.545453	-1.593934	2.626404
H	5.109893	-0.680897	2.618286
H	5.160220	0.392939	1.227406
H	4.990020	-1.349900	0.994962
H	-0.058906	-0.091523	1.813140
C	-0.047558	-1.990573	0.386314
O	-0.035549	-3.155479	0.468980
H	-0.069403	-0.321517	-1.301427
C	3.493440	2.501482	0.135889
H	3.511209	3.166937	1.008375
H	4.329543	1.814814	0.215137
H	3.647024	3.109120	-0.764411
C	-3.714040	2.376366	0.238467
H	-3.996432	2.823188	-0.724079
H	-4.491158	1.672174	0.528261
H	-3.690557	3.169346	0.994685

Fe3

Fe	-0.062645	-0.394703	-0.203248
P	-2.287661	-0.161419	0.082269
P	2.170766	-0.138412	0.039383
N	-0.070750	1.652285	-0.055853
N	-2.384912	1.561627	-0.009955
N	2.245577	1.584554	-0.068569
C	-1.241111	2.333313	0.005157
C	-1.286677	3.730013	0.072958
C	-0.082772	4.425256	0.085819
C	1.127725	3.7417950	0.042891
C	1.093902	2.344860	-0.024423
C	-3.471218	-0.685436	-1.274296
C	-4.891907	-0.114586	-1.129487
C	-3.502613	-2.209366	-1.486690
C	-3.084699	-0.609072	1.719604
C	-2.821507	-2.079654	2.093793
C	-2.623973	0.329249	2.846151
C	3.303556	-0.706774	-1.344671
C	4.608868	0.086359	-1.524927
C	3.563718	-2.222613	-1.280376
C	2.893208	-0.503795	1.731537
C	2.711560	-1.966258	2.173993
C	4.338586	-0.027123	1.950895
C	-0.088716	-0.318115	-2.034503
O	-0.105028	-0.270095	-3.182925
H	-3.262728	2.054918	0.086712
H	-2.239280	4.244835	0.115731

H	-0.087394	5.509399	0.137242
H	2.076053	4.265909	0.063007
H	-3.007435	-0.228499	-2.158268
H	-5.472365	-0.359963	-2.024428
H	-4.903847	0.975757	-1.034833
H	-5.422300	-0.543313	-0.273711
H	-4.043597	-2.433629	-2.411055
H	-4.025744	-2.721763	-0.674301
H	-2.503490	-2.644094	-1.579169
H	-4.163397	-0.472756	1.570857
H	-3.384326	-2.326641	2.999318
H	-1.761929	-2.245698	2.308441
H	-3.125987	-2.784591	1.316925
H	-3.117573	0.040151	3.779326
H	-2.871664	1.375145	2.648464
H	-1.543254	0.257259	3.003571
H	2.679093	-0.510043	-2.225432
H	5.098001	-0.246277	-2.446273
H	5.314499	-0.074228	-0.706875
H	4.431619	1.160516	-1.631721
H	4.024484	-2.550060	-2.217279
H	2.647384	-2.805310	-1.145446
H	4.254075	-2.478475	-0.471886
H	2.229306	0.113685	2.351626
H	3.013130	-2.059783	3.222185
H	3.332857	-2.654509	1.595395
H	1.672868	-2.295474	2.101499
H	4.572893	-0.075512	3.019266
H	4.501292	1.008455	1.635574
H	5.061020	-0.663276	1.432565
H	-0.045207	-0.417139	1.314891
H	3.120479	2.087080	0.004430
C	-0.050791	-2.165382	-0.053040
O	-0.040669	-3.308358	0.091880

Fe4

Fe	-1.377199	1.026754	-0.964264
P	-2.508493	2.053130	-2.607366
P	-0.101878	0.631287	0.854472
N	0.071393	2.378373	-1.409402
N	-1.315191	3.216897	-3.105420
N	1.308575	1.555551	0.411422
C	-0.087321	3.229975	-2.458332
C	0.942389	4.094195	-2.860216
C	2.124434	4.092094	-2.134099
C	2.279134	3.263137	-1.031773
C	1.223314	2.405325	-0.687270
C	-2.891957	1.044008	-4.160176
C	-3.715931	1.747997	-5.253307
C	-3.523223	-0.323003	-3.826130
C	-4.024519	3.091097	-2.243156
C	-5.201601	2.233887	-1.744173
C	-3.718232	4.231398	-1.260633
C	0.450726	-1.161058	1.071711
C	1.788611	-1.466200	1.767094
C	-0.687893	-1.992269	1.699002
C	-0.678560	1.358845	2.500249
C	-2.172416	1.085421	2.764716
C	0.142967	1.018791	3.758108
H	0.826987	4.739545	-3.717942
H	2.935911	4.750597	-2.427570
H	3.195440	3.281124	-0.462162
H	-1.882310	0.857484	-4.550964
H	-3.819933	1.072785	-6.108696
H	-3.249189	2.661995	-5.624362
H	-4.727345	1.989252	-4.911509
H	-3.573507	-0.922672	-4.740351
H	-4.544639	-0.224733	-3.448371
H	-2.945608	-0.892367	-3.095970
H	-4.315808	3.528990	-3.205347
H	-6.073140	2.878407	-1.593034
H	-4.976191	1.758467	-0.786153
H	-5.492777	1.455743	-2.453455
H	-4.611682	4.852810	-1.142066
H	-2.906006	4.877133	-1.604190
H	-3.446134	3.841826	-0.275667
H	0.556629	-1.480133	0.028361
H	1.932357	-2.551997	1.770203
H	1.812115	-1.137114	2.809136
H	2.640665	-1.034849	1.238571
H	-0.443708	-3.054730	1.603663
H	-1.654831	-1.837762	1.214428
H	-0.803128	-1.780644	2.765516
H	-0.572191	2.432151	2.291549
H	-2.475385	1.632332	3.663296
H	-2.373249	0.026275	2.946532
H	-2.805058	1.423704	1.943332
H	-0.269467	1.577097	4.604954
H	1.196533	1.291781	3.682904
H	0.077685	-0.042147	4.013348
H	-1.997611	2.107433	-0.102784
C	-2.753962	0.042261	-0.427614
O	-3.666965	-0.555136	-0.055098
C	-1.570048	4.249229	-4.119205
H	-0.995800	4.067676	-5.034451
H	-2.626736	4.261132	-4.375432
H	-1.314478	5.239377	-3.729717
C	2.499270	1.688267	1.2646180
H	2.429955	1.000613	2.0993320
H	3.406491	1.441212	0.7042320
H	2.590476	2.706447	1.6591760
C	-0.562979	-0.221915	-2.025541
O	-0.035056	-0.998666	-2.689583

Mn1

P	2.172376	-0.275839	0.122846
P	-2.260946	-0.127079	0.164750
N	0.020485	1.587669	-0.137677
N	2.331401	1.430609	-0.190182
N	-2.287544	1.612432	0.028524
C	1.207833	2.231851	-0.218428
C	1.300401	3.628215	-0.321281
C	0.120546	4.363858	-0.322769
C	-1.107436	3.722510	-0.212693
C	-1.115866	2.321826	-0.112173
C	3.105213	-0.505933	1.750641
C	4.613442	-0.207869	1.725334
C	3.242316	-1.058753	-1.219861
C	4.492538	-0.294079	-1.683887
C	-4.419930	0.420374	2.020607
C	-3.323292	-1.861412	2.159714
C	-3.558378	-0.665012	-1.100546
C	-3.381737	-2.159907	-1.430299
C	-0.045104	-0.796159	-1.807219
O	-0.026945	-1.017554	-2.957310
H	-3.139990	2.154805	0.045222
H	2.270088	4.108083	-0.392505
H	0.159209	5.446406	-0.402651
H	-2.039016	4.277157	-0.197468
H	5.026388	-0.316388	2.734921
H	4.818486	0.822242	1.409283
H	5.170854	-0.881053	1.071727
H	4.907582	-0.785734	-2.571649
H	5.284177	-0.264871	-0.931300
H	4.251008	0.733732	-1.9721300
H	-4.782375	0.290871	3.046955
H	-5.220157	0.080181	1.354112
H	-4.276565	1.494704	1.866758
H	-3.630378	-1.965551	3.206666
H	-2.408066	-2.442500	2.022292
H	-4.112940	-2.309945	1.547278
H	-4.192270	-2.491989	-2.089356
H	-3.394320	-2.796526	-0.542206
H	-2.434638	-2.331709	-1.948908
H	3.221823	1.908886	-0.199136
C	-3.500189	0.171701	-2.388691
H	-3.699396	1.231571	-2.209184
H	-2.522020	0.089566	-2.870882
H	-4.251122	-0.194666	-3.098314
C	3.543264	-2.529659	-0.880128
H	2.637526	-3.076210	-0.599827
H	3.974284	-3.032068	-1.753169
H	4.262867	-2.625045	-0.060440
C	2.429171	0.300985	2.871117
H	1.360759	0.086288	2.928528
H	2.893857	0.057828	3.833426
H	2.550691	1.377643	2.705237
C	-0.095420	-2.251292	0.427955

O	-0.101429	-3.360884	0.796893
H	-2.360678	0.022829	2.507667
C	-3.120791	-0.374595	1.824836
H	-4.545543	-0.525018	-0.640648
H	2.543884	-1.059485	-2.063797
H	2.962035	-0.531221	-0.027485
H	-0.128151	-0.313563	1.554085

Mn2

P	2.204187	-0.228669	0.089069
P	-2.186563	-0.275100	0.127806
N	-0.020156	1.562044	-0.046137
N	2.317856	1.529952	0.112103
N	-2.360046	1.471119	-0.055155
C	1.142767	2.260610	0.009138
C	1.160161	3.668106	-0.022931
C	-0.052738	4.340774	-0.051863
C	-1.250339	3.640205	-0.047859
C	-1.201006	2.233517	-0.052071
C	3.124588	-0.699779	1.666441
C	2.553986	0.021768	2.895681
C	3.388850	-0.721037	-1.317024
C	4.902725	-0.579085	-1.081158
C	-4.417062	-0.419927	2.045852
C	-2.449783	-1.948929	2.434477
C	-3.509559	-0.924255	-1.048608
C	-3.494003	-2.463927	-1.065562
C	0.050141	-0.531452	-1.965351
O	0.116811	-0.549750	-3.133887
H	2.090680	4.216247	-0.031120
H	-0.065067	5.426932	-0.068990
H	-2.192557	4.167695	-0.037653
H	3.125084	-0.262594	3.787338
H	1.506809	-0.250939	3.050887
H	2.603197	1.109929	2.7973170
H	5.438531	-0.855049	-1.996870
H	5.256209	-1.250373	-0.291379
H	5.210015	0.437208	-0.826457
H	-4.669487	-0.538464	3.106199
H	-4.984209	-1.179984	1.497877
H	-4.780851	0.563018	1.738220
H	-2.735315	-2.008083	3.491562
H	-1.368560	-2.071832	2.364732
H	-2.925138	-2.792248	1.923723
H	-4.247492	-2.831296	-1.771611
H	-3.721966	-2.897158	-0.088175
H	-2.520903	-2.848283	-1.384201
C	-3.348603	-0.367886	-2.4716610
H	-3.342260	0.725135	-2.495433
H	-2.421933	-0.714344	-2.932955
H	-4.182622	-0.712580	-3.094273
C	3.078988	-2.138732	-1.836252
H	2.025927	-2.264327	-2.086078
H	3.664915	-2.328939	-2.742917
H	3.349068	-2.909496	-1.107629
C	3.107191	-2.224782	1.874069
H	3.589933	-2.766392	1.056107
H	3.644533	-2.476287	2.795767
H	2.084888	-2.600924	1.967874
C	0.031589	-2.311822	0.006403
O	0.042369	-3.469577	0.170059
H	-2.384704	0.187727	2.431556
C	-2.900931	-0.594453	1.859538
H	-4.486306	-0.607740	-0.662625
H	3.090915	-0.013611	-2.102510
H	4.169584	-0.389519	1.539123
Mn	0.012403	-0.539964	-0.164555
H	0.027220	-0.498848	1.432363
C	-3.638645	2.174283	-0.116449
H	-3.667204	2.855196	-0.974960
H	-4.446824	1.457121	-0.240806
H	-3.834281	2.757142	0.793522
C	3.557750	2.265045	0.350403
H	3.433916	2.988653	1.164384
H	4.341625	1.572051	0.646279
H	3.896785	2.804249	-0.543763

Fe(PNP^{H}-iPr)(H)(CO)(OCHO)

P	2.325812	-0.229271	-0.099373
P	-2.116680	-0.262215	-0.164818
N	0.092947	1.534100	-0.386425
N	2.407462	1.490682	-0.290225
N	-2.214549	1.423894	-0.558979
C	1.250139	2.229990	-0.443554
C	1.284844	3.615237	-0.650120
C	0.073123	4.281330	-0.804860
C	-1.124335	3.580624	-0.769342
C	-1.075131	2.194086	-0.558120
C	3.391930	-0.501372	1.417108
C	4.730785	0.250788	1.414940
C	3.592198	-1.994294	1.728454
C	3.302299	-0.898111	-1.560832
C	3.015531	-2.397992	-1.761561
C	2.981060	-0.120271	-2.846763
C	-3.293034	-0.494321	1.284145
C	-4.515336	0.435542	1.326868
C	-3.680892	-1.970502	1.472281
C	-2.872083	-1.013006	-1.720964
C	-2.671002	-2.533235	-1.832696
C	-4.325472	-0.615725	-2.019989
H	2.232339	4.141186	-0.682668
H	0.065136	5.356117	-0.961485
H	-2.078792	4.078474	-0.896058
H	2.738052	-0.084564	2.191348
H	5.246804	0.088343	2.368177
H	4.600712	1.332143	1.306403
H	5.403251	-0.098934	0.622928
H	4.022087	-2.102840	2.730307
H	4.285984	-2.469299	1.026298
H	2.650471	-2.549341	1.713649
H	4.368105	-0.769569	-1.327505
H	3.632060	-2.784572	-2.581045
H	1.965248	-2.554414	-2.024230
H	3.231362	-2.997078	-0.873983
H	3.528549	-0.557646	-3.689382
H	3.258679	0.934616	-2.775526
H	1.911258	-0.173089	-3.072370
H	-2.645958	-0.193785	2.111814
H	-5.070062	0.253836	2.254677
H	-5.209572	0.274708	0.496966
H	-4.212558	1.486411	1.344082
H	-4.151637	-2.098673	2.453442
H	-2.812699	-2.636105	1.438320
H	-4.400939	-2.309532	0.720591
H	-2.228276	-0.544688	-2.475908
H	-2.961234	-2.866309	-2.836106
H	-3.284457	-3.087212	-1.116874
H	-1.627321	-2.814035	-1.678335
H	-4.595024	-0.937606	-3.032826
H	-4.479360	0.467087	-1.974371
H	-5.030352	-1.091598	-1.331511
H	-3.089987	1.927057	-0.537099
H	3.278012	1.998292	-0.361387
O	0.364570	-0.007903	2.060325
C	-0.266104	0.882034	2.741498
O	-1.254640	1.547493	2.415248
H	0.170099	1.030055	3.757080
C	0.111834	-2.208577	0.338418
O	0.121550	-3.361106	0.487496
Fe	0.105997	-0.477200	0.057969
H	0.082139	-0.769908	-1.436376

Fe(PNP^{Me}-iPr)(H)(CO)(OCHO)

Fe	**-0.006874**	**-0.467660**	**0.118446**
P	**-2.210393**	**-0.270927**	**0.197924**
P	**2.215235**	**-0.187877**	**0.143634**
N	**-0.041874**	**1.573026**	**0.082817**
N	**-2.377999**	**1.471292**	**0.235813**
N	**2.302602**	**1.553367**	**-0.045780**
C	**-1.226375**	**2.237750**	**0.123117**
C	**-1.288876**	**3.639850**	**0.054730**
C	**-0.097776**	**4.345099**	**-0.040043**
C	**1.119221**	**3.681482**	**-0.067230**
C	**1.116635**	**2.274929**	**-0.012370**
C	**-3.216772**	**-0.816056**	**-1.308050**
C	**-4.747554**	**-0.845435**	**-1.165956**
C	**-2.692433**	**-2.160806**	**-1.849865**

C	-3.201688	-0.807331	1.701011
C	-3.163294	-2.336957	1.870080
C	-2.718374	-0.103400	2.977711
C	3.103711	-0.949703	-1.327500
C	4.378752	-0.296750	-1.879636
C	3.311835	-2.458720	-1.089787
C	3.166040	-0.505628	1.750688
C	2.702448	-1.816275	2.414191
C	4.704014	-0.450335	1.715412
H	-2.235289	4.159777	0.057826
H	-0.118700	5.429621	-0.096121
H	2.040947	4.238051	-0.139709
H	-2.947694	-0.045318	-2.041002
H	-5.191262	-1.120028	-2.129614
H	-5.177085	0.117840	-0.879666
H	-5.076135	-1.594496	-0.438097
H	-3.220916	-2.405297	-2.778449
H	-2.867653	-2.984715	-1.150167
H	-1.625037	-2.100647	-2.067809
H	-4.244181	-0.516538	1.518401
H	-3.774275	-2.624062	2.733172
H	-2.145493	-2.693205	2.049140
H	-3.556678	-2.867483	0.998851
H	-3.336280	-0.418036	3.826616
H	-2.782701	0.985463	2.899298
H	-1.677655	-0.360115	3.192637
H	2.315366	-0.846229	-2.082686
H	4.702571	-0.863198	-2.760337
H	5.211354	-0.302972	-1.168280
H	4.202606	0.728162	-2.212532
H	3.601673	-2.927572	-2.036373
H	2.402786	-2.959514	-0.748164
H	4.109859	-2.662820	-0.367971
H	2.800958	0.321545	2.374446
H	3.167813	-1.905737	3.402692
H	2.996090	-2.695758	1.833673
H	1.619728	-1.835305	2.543653
H	5.091081	-0.596968	2.730644
H	5.097544	0.503018	1.358008
H	5.124347	-1.245631	1.093587
H	-0.000904	-0.379224	1.635835
C	0.020091	-2.208455	0.323813
O	0.037472	-3.352070	0.530918
C	3.549738	2.318311	-0.095755
H	3.668952	2.949781	0.794069
H	4.393026	1.638842	-0.150263
H	3.582296	2.956964	-0.985531
C	-3.659951	2.161584	0.358463
H	-3.938700	2.676911	-0.569411
H	-4.439349	1.440518	0.595047
H	-3.632482	2.896404	1.170974
O	0.118353	-0.521569	-1.937601
C	-0.052722	0.418675	-2.812792
O	0.512539	0.508727	-3.896862
H	-0.800926	1.200885	-2.525457

[Fe(PNP^{H}-iPr)(CO)$_2$(OCHO)]$^+$

P	2.397751	-0.189728	0.057870
P	-2.220677	-0.201437	-0.072111
N	0.086351	1.532498	-0.435101
N	2.408270	1.505160	-0.234553
N	-2.237339	1.441638	-0.587179
C	1.249172	2.229451	-0.452266
C	1.285377	3.607850	-0.676975
C	0.079836	4.271560	-0.879031
C	-1.120923	3.574858	-0.851679
C	-1.083428	2.197666	-0.614300
C	3.281708	-0.391794	1.694641
C	4.570131	0.442625	1.786923
C	3.540430	-1.869804	2.034385
C	3.547412	-0.941860	-1.227582
C	3.209896	-2.427200	-1.464968
C	3.577232	-0.157223	-2.549208
C	-3.232580	-0.354824	1.500810
C	-4.347247	0.697685	1.624877
C	-3.740556	-1.788658	1.731144
C	-3.113141	-1.032784	-1.504384
C	-2.971188	-2.565331	-1.532094
C	-4.578208	-0.597949	-1.682957
H	2.231751	4.135665	-0.686588
H	0.077925	5.342471	-1.055076
H	-2.070459	4.076761	-0.994272
H	2.546037	-0.002198	2.402781
H	5.005445	0.314373	2.783172
H	4.385321	1.513244	1.659350
H	5.330042	0.127475	1.063567
H	3.916646	-1.936720	3.059795
H	4.298217	-2.316529	1.383338
H	2.633398	-2.478401	1.983633
H	4.546562	-0.889482	-0.777437
H	3.982258	-2.877946	-2.095843
H	2.256853	-2.541237	-1.989119
H	3.163029	-3.008654	-0.540931
H	4.273052	-0.646337	-3.238309
H	3.913504	0.873680	-2.416586
H	2.598955	-0.132740	-3.037066
H	-2.495956	-0.126279	2.270569
H	-4.844363	0.564513	2.591185
H	-5.114274	0.605090	0.850629
H	-3.936225	1.709991	1.615020
H	-4.140645	-1.855780	2.747635
H	-2.946850	-2.537733	1.648548
H	-4.547019	-2.063176	1.046765
H	-2.551135	-0.631075	-2.356489
H	-3.349388	-2.941059	-2.488022
H	-3.545313	-3.050662	-0.740516
H	-1.931702	-2.894512	-1.446228
H	-4.952288	-0.985038	-2.636366
H	-4.692940	0.489674	-1.713277
H	-5.225303	-0.991862	-0.895418
H	-3.102201	1.965772	-0.612369
H	3.268756	2.036552	-0.242985
O	0.259811	-0.033036	1.949615
C	-0.261969	0.960389	2.614776
O	-1.126238	1.744172	2.242058
H	0.164789	1.033509	3.635248
C	0.089307	-0.834455	-1.759446
C	0.055853	-2.183956	0.559173
O	0.029440	-3.256644	0.957837
O	0.079401	-1.037752	-2.889310
Fe	0.085940	-0.450783	0.001556

[Fe(PNP^{Me}-iPr)(CO)$_2$(OCHO)]$^+$

P	2.368499	-0.311551	0.050362
P	-2.221093	-0.241623	-0.077472
N	0.106406	1.484169	-0.291808
N	2.466153	1.397998	-0.212970
N	-2.255264	1.465586	-0.374178
C	1.295154	2.150121	-0.303600
C	1.346304	3.544838	-0.417817
C	0.151387	4.241226	-0.535880
C	-1.062416	3.574206	-0.529415
C	-1.063156	2.178316	-0.387481
C	3.156778	-0.672639	1.719904
C	4.536808	-0.042327	1.972616
C	3.199842	-2.185295	2.009439
C	3.490963	-1.112310	-1.233760
C	3.080405	-2.581577	-1.471030
C	3.558446	-0.361493	-2.575307
C	-3.126939	-0.709342	1.508984
C	-4.294531	0.190181	1.942117
C	-3.521095	-2.198391	1.517087
C	-3.109057	-0.974424	-1.581104
C	-2.788628	-2.468215	-1.796924
C	-4.631710	-0.753404	-1.680557
H	2.286570	4.074192	-0.408790
H	0.168326	5.322436	-0.629979
H	-1.984198	4.127503	-0.615448
H	2.429086	-0.227374	2.401978
H	4.885157	-0.363181	2.959965
H	4.508197	1.048042	1.984131
H	5.293565	-0.368254	1.250606
H	3.475419	-2.329551	3.058690
H	3.954968	-2.698237	1.406030
H	2.236879	-2.677481	1.861347
H	4.492189	-1.109859	-0.784419

H	3.843630	-3.071328	-2.083695
H	2.136457	-2.644737	-2.020983
H	2.978398	-3.160444	-0.551290
H	4.215538	-0.915474	-3.253521
H	3.962399	0.647179	-2.483324
H	2.581107	-0.292784	-3.058130
H	-2.336624	-0.573693	2.245782
H	-4.655625	-0.168063	2.912039
H	-5.142646	0.156878	1.251741
H	-3.972221	1.223076	2.079495
H	-3.824155	-2.463863	2.534911
H	-2.696814	-2.863247	1.246395
H	-4.369075	-2.412968	0.862058
H	-2.637242	-0.413480	-2.397806
H	-3.135321	-2.759991	-2.793106
H	-3.299282	-3.107463	-1.074472
H	-1.721262	-2.692674	-1.750755
H	-4.999590	-1.258158	-2.579860
H	-4.906351	0.297610	-1.775301
H	-5.171160	-1.178271	-0.830444
O	0.201784	-0.284259	1.943371
C	-0.292711	0.656045	2.701423
O	-1.146215	1.486639	2.415565
H	0.145242	0.626332	3.7199740
C	0.077310	-0.699842	-1.830039
C	0.013593	-2.294512	0.327617
O	-0.028424	-3.406529	0.600411
O	0.062642	-0.758626	-2.977088
Fe	0.068047	-0.516473	-0.042694
C	3.746694	2.111651	-0.330969
H	4.564948	1.395345	-0.334578
H	3.785101	2.678752	-1.266177
H	3.899839	2.799036	0.507385
C	-3.501648	2.244997	-0.432545
H	-3.587075	2.768414	-1.390552
H	-4.352536	1.581306	-0.329589
H	-3.542271	2.971436	0.384451

[Mn(PNP^{H}-iPr)(CO)$_2$(OCHO)]

Mn	0.092532	-0.534837	0.016453
P	2.375265	-0.182865	0.051868
P	-2.196340	-0.227701	-0.063050
N	0.077958	1.518133	-0.492320
N	2.396062	1.515261	-0.298194
N	-2.241285	1.410600	-0.638276
C	1.231762	2.220739	-0.541838
C	1.263631	3.593387	-0.823542
C	0.054071	4.242060	-1.047186
C	-1.141310	3.539415	-0.988663
C	-1.091381	2.168251	-0.695705
C	3.304982	-0.269123	1.680560
C	4.585436	0.576827	1.740878
C	3.574971	-1.721597	2.108339
C	3.575458	-0.913494	-1.208338
C	3.334289	-2.427444	-1.365459
C	3.501837	-0.211239	-2.574036
C	-3.263477	-0.252057	1.488433
C	-4.395085	0.785997	1.536584
C	-3.752185	-1.669224	1.830167
C	-3.131844	-1.084089	-1.459349
C	-3.045138	-2.619569	-1.402860
C	-4.575674	-0.615330	-1.695100
H	2.208553	4.123962	-0.856999
H	0.045105	5.305804	-1.266386
H	-2.095714	4.027627	-1.149155
H	2.562193	0.147200	2.367337
H	5.022870	0.508384	2.743444
H	4.392947	1.637583	1.551459
H	5.349723	0.231421	1.034671
H	3.936181	-1.734985	3.142663
H	4.347025	-2.193805	1.491171
H	2.672671	-2.337670	2.067602
H	4.584428	-0.765864	-0.800989
H	4.111965	-2.860177	-2.005067
H	2.368262	-2.620810	-1.838351
H	3.353696	-2.962400	-0.412928
H	4.210967	-0.682395	-3.264289
H	3.752662	0.850744	-2.510954
H	2.505169	-0.296863	-3.015506
H	-2.537768	0.051184	2.244055
H	-4.899099	0.719620	2.507744
H	-5.157273	0.634190	0.765645
H	-3.996404	1.800706	1.456300
H	-4.146494	-1.676511	2.852499
H	-2.945588	-2.408001	1.787314
H	-4.558395	-2.003223	1.169747
H	-2.535478	-0.758774	-2.320426
H	-3.398652	-3.039129	-2.351509
H	-3.666767	-3.038926	-0.607895
H	-2.021238	-2.967981	-1.249813
H	-4.949681	-1.036058	-2.635913
H	-4.652970	0.473393	-1.777527
H	-5.250577	-0.947822	-0.901098
H	-3.104113	1.936445	-0.656301
H	3.251683	2.051173	-0.339696
O	0.268179	0.084102	2.014737
C	-0.240390	1.089630	2.638914
O	-1.135797	1.855246	2.271305
H	0.214868	1.237875	3.646133
C	0.097829	-1.040484	-1.688573
C	0.091008	-2.233283	0.617557
O	0.089084	-3.322155	1.025348
O	0.094306	-1.359781	-2.813107

[Mn(PNP^{Me}-iPr)(CO)$_2$(OCHO)]

Mn	0.073244	-0.590368	-0.056259
P	2.346577	-0.311539	0.045679
P	-2.195175	-0.258464	-0.079861
N	0.106937	1.483381	-0.336627
N	2.462949	1.408644	-0.254719
N	-2.252496	1.461561	-0.403513
C	1.288862	2.152631	-0.368393
C	1.341614	3.548173	-0.520933
C	0.145563	4.238484	-0.654798
C	-1.065803	3.568824	-0.626258
C	-1.059713	2.172506	-0.444925
C	3.171472	-0.577363	1.723830
C	4.569827	0.017812	1.949605
C	3.158784	-2.066208	2.118264
C	3.531767	-1.079271	-1.207396
C	3.229283	-2.583922	-1.363581
C	3.493124	-0.399270	-2.587173
C	-3.132885	-0.643613	1.514947
C	-4.315169	0.243634	1.926163
C	-3.496530	-2.138134	1.587520
C	-3.145091	-0.987348	-1.553385
C	-2.880745	-2.497708	-1.726401
C	-4.657306	-0.720908	-1.672552
H	2.281414	4.079130	-0.525449
H	0.159492	5.317623	-0.778524
H	-1.989104	4.117970	-0.723885
H	2.454999	-0.069993	2.375086
H	4.913849	-0.257354	2.953622
H	4.579330	1.107999	1.896836
H	5.314684	-0.370238	1.244644
H	3.386884	-2.153830	3.186386
H	3.922128	-2.637356	1.579131
H	2.187533	-2.534186	1.950665
H	4.544677	-0.977800	-0.796076
H	3.988984	-3.043348	-2.006085
H	2.255849	-2.736416	-1.836617
H	3.227072	-3.123322	-0.414699
H	4.177671	-0.924062	-3.263719
H	3.800943	0.647389	-2.556673
H	2.495302	-0.446611	-3.028815
H	-2.343217	-0.462730	2.243820
H	-4.679628	-0.094791	2.903536
H	-5.160783	0.187331	1.232596
H	-4.005313	1.283376	2.040371
H	-3.784517	-2.379101	2.617031
H	-2.658469	-2.789130	1.324670
H	-4.346522	-2.391735	0.946899
H	-2.644141	-0.476967	-2.385692
H	-3.209643	-2.803499	-2.725892
H	-3.439035	-3.095353	-1.001973
H	-1.825724	-2.754857	-1.634014

H	-5.042370	-1.240828	-2.557665
H	-4.899150	0.335657	-1.797580
H	-5.213072	-1.101791	-0.810585
O	0.197663	-0.195841	2.009958
C	-0.276325	0.755530	2.739770
O	-1.158617	1.574085	2.468469
H	0.195386	0.788721	3.750458
C	0.081240	-0.887724	-1.807867
C	0.027742	-2.342238	0.345726
O	-0.009861	-3.471918	0.624827
O	0.062746	-1.061097	-2.964050
C	3.732984	2.120463	-0.396579
H	3.900291	2.826211	0.426497
H	4.553816	1.406401	-0.399809
H	3.765905	2.677204	-1.340275
C	-3.488430	2.243809	-0.459462
H	-3.590949	2.753871	-1.425399
H	-4.342426	1.588797	-0.331344
H	-3.517049	2.990998	0.341372

7. X-RAY CRYSTAL STRUCTURE DETERMINATION

X-ray diffraction data were collected at T = 100 K in a dry stream of nitrogen on a Bruker Kappa APEX II diffractometer system using graphite-monochromatized Mo-$K\alpha$ radiation (λ = 0.71073 Å) and fine sliced φ- and ω-scans. Data were reduced to intensity values with SAINT and an absorption correction was applied with the multi-scan approach implemented in SADABS.[13] The structure was solved by charge flipping using SUPERFLIP[14] and refined against F with JANA2006.[15] Non-hydrogen atoms were refined anisotropically. The H atoms connected to C atoms were placed in calculated positions and thereafter refined as riding on the parent atoms. The hydride H was located from difference Fourier maps and freely refined. Molecular graphics were generated with the program MERCURY.[16] Crystal data and experimental details are given in Table S2.

Table S2. Details for the crystal structure determination.

formula	$C_{21}H_{38}MnN_3O_2P_2$
fw	481.4
cryst.size, mm	0.60 x 0.40 x 0.17
color, shape	yellow, irregular
crystal system	orthorhombic
space group	*Pbca* (no. 61)
a, Å	11.717(3)
b, Å	14.835(4)
c, Å	28.548(7)
V, Å^3	4962(2)
T, K	100
Z,Z'	8,1
ρ_{calc}, g cm^{-3}	1.2889
μ, mm^{-1} (MoKα)	0.682
F(000)	2048
absorption corrections,	multi-scan, 0.66–
θ range, deg	3.89–30.14
no. of rflns measd	33947
R_{int}	0.0448
no. of rflns unique	7196
no. of rflns $I>3\sigma(I)$	5714
no. of params /	266 / 0
R ($I > 3\sigma(I)$) [a]	0.0389
R (all data)	0.0517
wR ($I > 3\sigma(I)$)	0.0465
wR (all data)	0.0476
GooF	2.19
Diff.Four.peaks	-0.44 / 0.69
CCDC no.	1520528

[a] $R = \Sigma||F_o|-|F_c|| \,/\, \Sigma|F_o|$, $wR = \Sigma w(|F_o| - |F_c|) \,/\, \Sigma w|F_o|$, GooF = $\{\Sigma[w(F_o^2 - F_c^2)^2] \,/\, (n-p)\}^{½}$

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