The effect of coordination of Alkanes, Xe and CO_2 (η^1-OCO) on Changes in Spin State and Reactivity in Organometallic Chemistry: A Combined Experimental and Theoretical Study of the Photochemistry of $CpMn(CO)_3$

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SUPPORTING INFORMATION

(A) Sample input file for the Spin-orbit coupled calculations,

(B) Sample input file for the MESMER calculation of rate constants for spin-forbidden steps.

(C) Calculated energies **(**B3LYP**-D3BJ/def2TZVP), free energy corrections, and Cartesian coordinates for optimized species.

(A) Sample input file for the Spin-orbit coupled calculation

Input file for MOLPRO, calculation at the MECP in the absence of ligand. The resulting SOC matrix element was used for all MECPs, assuming that the incoming ligand does not make a major perturbation of the wavefunctions.

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 C                 -0.09225700    1.35038400   -1.38441500
 O                  0.10230600    2.02133200    2.30390200
```

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{casscf
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option,maxiti=5000
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save,3010.1
noexc}          !re-calculate the casscf wavefunction; save it using the MR-CI format

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noexc}

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--------------------------------
```

(B) Sample input file for the MESMER calculation of rate constants for spin-forbidden steps.

This is the input file for calculating k_{13} and k_{31} for isolated $CpMn(CO)_2$.

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```

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601.06 605.04 655.01 806.75 807.12 835.79 839.28 853.38 905.23 910.29 1002.53 1015.13 1062.20 1063.60
1120.71 1270.44 1365.06 1368.63 1435.88 1440.26 1962.05 2016.24 3178.68 3201.82 3211.27 3216.85 3223.71
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Note: The vibrational frequency analysis at the MECP was performed using the code developed by David Glowacki. (Gannon, Glowacki et al., Faraday Discussions, 2010, 147, 173-188, https://glow-wacky.com/code)

(C) Total energies, total energies with zpe, thermal and entropy corrections, and Cartesian coordinates.

xe
Geometry with 1 atoms:
Total energy: -329.345523
Gibbs free energy: -329.359408

Xe	0.00000	0.00000	0.00000

co2
Geometry with 3 atoms:
Total energy: -188.477676
Gibbs free energy: -188.483845

C	0.00000	0.00000	0.00000
O	0.00000	0.00000	1.16460
O	0.00000	0.00000	-1.16460

c2h6
Geometry with 8 atoms:
Total energy: -79.742121
Gibbs free energy: -79.687073

C	0.00000	0.00000	0.76322
H	0.00000	1.01992	1.16315
H	0.88328	-0.50996	1.16315
H	-0.88328	-0.50996	1.16315
C	0.00000	0.00000	-0.76322
H	0.00000	-1.01992	-1.16315
H	-0.88328	0.50996	-1.16315
H	0.88328	0.50996	-1.16315

c7h16
Geometry with 23 atoms:
Total energy: -276.113554
Gibbs free energy: -275.930827

C	0.00000	1.27711	-0.34124
H	-0.87793	1.27765	-1.00389
C	0.00000	0.00000	0.49536
H	-0.87801	0.00000	1.15769
H	0.87801	0.00000	1.15769
H	0.87793	1.27765	-1.00389
C	0.00000	2.55596	0.49410
H	-0.87757	2.55396	1.15539
H	0.87757	2.55396	1.15539
C	0.00000	-1.27711	-0.34124
H	0.87793	-1.27765	-1.00389
H	-0.87793	-1.27765	-1.00389
C	0.00000	3.82514	-0.35451
H	0.00000	4.72695	0.26691
H	0.88404	3.86566	-1.00189
H	-0.88404	3.86566	-1.00189
C	0.00000	-2.55596	0.49410
H	0.87757	-2.55396	1.15539
H	-0.87757	-2.55396	1.15539
C	0.00000	-3.82514	-0.35451
H	0.00000	-4.72695	0.26691
H	-0.88404	-3.86566	-1.00189
H	0.88404	-3.86566	-1.00189

c6f12
Geometry with 18 atoms:
Total energy: -1426.026532
Gibbs free energy: -1425.992554

F	0.00000	1.63147	1.55903
C	0.00000	1.49877	0.21342
C	-1.29798	0.74939	-0.21342
C	1.29798	0.74939	-0.21342
F	0.00000	2.72472	-0.34598
C	-1.29798	-0.74939	0.21342
F	-2.35968	1.36236	0.34598
F	-1.41290	0.81574	-1.55903
C	1.29798	-0.74939	0.21342
F	2.35968	1.36236	0.34598
F	1.41290	0.81574	-1.55903
C	0.00000	-1.49877	-0.21342
F	-2.35968	-1.36236	-0.34598
F	-1.41290	-0.81574	1.55903
F	2.35968	-1.36236	-0.34598
F	1.41290	-0.81574	1.55903
F	0.00000	-1.63147	-1.55903
F	0.00000	-2.72472	0.34598

c7f14
Geometry with 21 atoms:
Total energy: -1663.703468
Gibbs free energy: -1663.662705

F	1.70763	0.97503	0.00000
C	0.33540	0.99517	0.00000
C	-0.14240	0.24981	1.28916
C	-0.14240	0.24981	-1.28916
C	0.19762	-1.27532	1.28805
F	0.45164	0.78989	2.37220
F	-1.48350	0.38031	1.41671
C	0.19762	-1.27532	-1.28805
F	0.45164	0.78989	-2.37220
F	-1.48350	0.38031	-1.41671
C	-0.27567	-2.00197	0.00000
F	-0.39979	-1.84266	2.35529
F	1.53479	-1.42441	1.40712
F	-0.39979	-1.84266	-2.35529
F	1.53479	-1.42441	-1.40712
F	-1.62747	-2.04833	0.00000
F	0.20464	-3.26102	0.00000
C	-0.07788	2.50786	0.00000
F	0.42649	3.11343	1.08323
F	0.42649	3.11343	-1.08323
F	-1.40557	2.66785	0.00000

cpmnco2_s
Geometry with 15 atoms:
Total energy: -1570.633462
Gibbs free energy: -1570.565852

Mn	-0.41907	0.13852	0.00000
C	-0.13345	1.32405	1.30920
C	-0.13345	1.32405	-1.30920
O	0.14143	2.04172	2.17443
O	0.14143	2.04172	-2.17443
C	1.16662	-1.06400	-0.71020
C	1.16662	-1.06400	0.71020
C	-0.06178	-1.65323	-1.15645
H	1.96010	-0.69176	-1.34286
C	-0.06178	-1.65323	1.15645
H	1.96010	-0.69176	1.34286
C	-0.80572	-1.99911	0.00000
H	-0.36093	-1.81003	-2.18290
H	-0.36093	-1.81003	2.18290
H	-1.80685	-2.41430	0.00000

cpmnco2_t
Geometry with 15 atoms:
Total energy: -1570.639349
Gibbs free energy: -1570.571944

C	-0.01574	1.42538	1.42686
O	-0.01564	2.09214	2.36767
Mn	-0.00716	0.28460	0.00000
C	-0.01574	1.42538	-1.42686
O	-0.01564	2.09214	-2.36767
C	1.00168	-1.59700	-0.70881
C	1.00168	-1.59700	0.70881
C	-0.36099	-1.65863	-1.14746
H	1.87059	-1.56405	-1.35159
C	-0.36099	-1.65863	1.14746
H	1.87059	-1.56405	1.35159
C	-1.19186	-1.72957	0.00000
H	-0.69339	-1.67824	-2.17637
H	-0.69339	-1.67824	2.17637
H	-2.27323	-1.76419	0.00000

cpmnco2_mecp
Geometry with 15 atoms:
Total energy: -1570.629033
Gibbs free energy: -1570.564911

Mn	-0.29412	0.19766	0.00000
C	-0.09226	1.35038	1.38441
C	-0.09226	1.35038	-1.38441
O	0.10231	2.02133	2.30390
O	0.10231	2.02133	-2.30390
C	1.13371	-1.23380	-0.70840
C	1.13371	-1.23380	0.70840
C	-0.16897	-1.63966	-1.15248
H	1.96509	-0.96837	-1.34641
C	-0.16897	-1.63966	1.15248
H	1.96509	-0.96837	1.34641
C	-0.95224	-1.89840	0.00000
H	-0.48660	-1.74838	-2.17960
H	-0.48660	-1.74838	2.17960
H	-1.99740	-2.18210	0.00000

cpmnco2_xe_s
Geometry with 16 atoms:
Total energy: -1899.996897
Gibbs free energy: -1899.933807

Mn	0.41399	0.66408	0.00000
C	-0.51398	1.46485	1.29469
C	-0.51398	1.46485	-1.29469
Xe	-1.19019	-1.61503	0.00000
O	-1.04328	2.03685	2.15201
O	-1.04328	2.03685	-2.15201
C	2.19453	1.56478	-0.71005
C	2.19453	1.56478	0.71005
C	2.19453	0.20385	-1.15574
H	2.20357	2.44104	-1.34306
C	2.19453	0.20385	1.15574
H	2.20357	2.44104	1.34306
C	2.19040	-0.61638	0.00000
H	2.20485	-0.13375	-2.18214
H	2.20485	-0.13375	2.18214
H	2.15238	-1.69828	0.00000

cpmnco2_xe_t
Geometry with 16 atoms:
Total energy: -1899.988492
Gibbs free energy: -1899.932160

Mn	0.28710	1.40086	0.00000
C	-0.85787	1.35994	1.42367
C	-0.85787	1.35994	-1.42367
O	-1.52546	1.32315	2.36326
O	-1.52546	1.32315	-2.36326
C	2.10201	1.82417	-1.14734
C	2.13244	2.65517	0.00000
C	2.10201	0.46057	-0.70917
H	2.10299	2.15821	-2.17566
C	2.10201	1.82417	1.14734
H	2.10617	3.73688	0.00000
C	2.10201	0.46057	0.70917
H	2.09786	-0.40871	-1.35200
H	2.10299	2.15821	2.17566
H	2.09786	-0.40871	1.35200
Xe	-0.85605	-2.27954	0.00000

cpmnco2_xe_mecp
Geometry with 16 atoms:
Total energy: -1899.980601
Gibbs free energy: -1899.923439

Mn	0.39352	1.03197	0.00000
C	-0.69619	1.43091	1.39887
C	-0.69619	1.43091	-1.39887
O	-1.31351	1.71498	2.33236
O	-1.31351	1.71498	-2.33236
C	2.20390	1.43589	-1.14683
C	2.22188	2.27323	0.00000
C	2.20390	0.07856	-0.71180
H	2.19802	1.76930	-2.17552
C	2.20390	1.43589	1.14683
H	2.20500	3.35394	0.00000
C	2.20390	0.07856	0.71180
H	2.20260	-0.78990	-1.35533
H	2.19802	1.76930	2.17552
H	2.20260	-0.78990	1.35533
Xe	-1.06850	-1.99140	0.00000

cpmnco2_co2_s

Geometry with 18 atoms:
Total energy: -1759.129858
Gibbs free energy: -1759.057341

Mn	0.15409	0.24401	0.00000
C	-0.77560	1.04990	1.29103
C	-0.77560	1.04990	-1.29103
O	-1.30538	1.63081	2.14239
O	-1.30538	1.63081	-2.14239
C	1.93832	1.14712	-0.70970
C	1.93832	1.14712	0.70970
C	1.93832	-0.21453	-1.15567
H	1.95003	2.02328	-1.34289
C	1.93832	-0.21453	1.15567
H	1.95003	2.02328	1.34289
C	1.93385	-1.03413	0.00000
H	1.95036	-0.55170	-2.18226
H	1.95036	-0.55170	2.18226
H	1.87838	-2.11564	0.00000
O	-1.01917	-1.52265	0.00000
C	-1.89075	-2.29468	0.00000
O	-2.74539	-3.08205	0.00000

cpmnco2_co2_t
Geometry with 18 atoms:
Total energy: -1759.121129
Gibbs free energy: -1759.055150

Mn	-0.41463	0.49816	0.00000
C	-0.22634	2.71827	0.00000
C	0.39998	2.17100	1.14764
C	0.39998	2.17100	-1.14764
C	1.45612	1.30898	0.70929
C	1.45612	1.30898	-0.70929
C	-1.10156	-0.41315	1.42710
O	-1.49077	-0.94892	2.37119
C	-1.10156	-0.41315	-1.42710
O	-1.49077	-0.94892	-2.37119
H	-1.08109	3.38172	0.00000
H	0.14186	2.38334	2.17589
H	0.14186	2.38334	-2.17589
H	2.12472	0.75042	1.34909
H	2.12472	0.75042	-1.34909
C	1.04593	-2.72674	0.00000
O	2.00236	-2.05977	0.00000
O	0.09687	-3.39918	0.00000

cpmnco2_co2_mecp
Geometry with 18 atoms:
Total energy: -1759.113521
Gibbs free energy: -1759.047938

Mn	-0.10556	0.34567	0.00000
C	-1.10460	-0.52752	1.24023
C	-1.10460	-0.52752	-1.24023
O	-1.78237	-1.05722	2.01099
O	-1.78237	-1.05722	-2.01099
C	-0.41346	2.45056	-0.70300
C	-0.41346	2.45056	0.70300
C	0.84926	1.94286	-1.14808
H	-1.23657	2.74389	-1.33978
C	0.84926	1.94286	1.14808
H	-1.23657	2.74389	1.33978
C	1.63692	1.66009	0.00000
H	1.15590	1.83073	-2.17885
H	1.15590	1.83073	2.17885
H	2.64293	1.26188	0.00000
O	1.93548	-1.73658	0.00000
C	1.21711	-2.65820	0.00000
O	0.51162	-3.58085	0.00000

cpmnco2_c2h6_s
Geometry with 23 atoms:
Total energy: -1650.398219
Gibbs free energy: -1650.260952

Mn	0.13011	0.05987	-0.01857
C	-0.34526	1.62459	-0.72274
C	-0.73027	0.39777	1.50596
O	-0.56902	2.67050	-1.16874
O	-1.21883	0.62958	2.53074
H	-1.17894	-0.49813	-1.10886
C	-1.81651	-1.38231	-0.79311
C	-3.23592	-0.88773	-0.55009
H	-1.42859	-1.94564	0.05445
H	-1.74368	-2.02245	-1.67898
H	-3.92525	-1.73249	-0.44643
H	-3.29406	-0.29080	0.36410
H	-3.58870	-0.26576	-1.37877
C	2.17725	0.57294	-0.26664
C	1.99417	-0.04729	0.99679
C	1.83788	-0.37469	-1.28375
H	2.51892	1.58539	-0.43078
C	1.54316	-1.38817	0.77180
H	2.17562	0.40945	1.95949
C	1.44599	-1.57104	-0.62910
H	1.88282	-0.21191	-2.35099
H	1.32309	-2.12421	1.53195
H	1.08577	-2.46526	-1.12176

cpmnco2_c2h6_t
Geometry with 23 atoms:
Total energy: -1650.387454
Gibbs free energy: -1650.255690

Mn	0.53490	0.17473	0.00000
C	0.66828	-0.96413	1.42079
C	0.66828	-0.96413	-1.42079
O	0.73230	-1.63886	2.35388
O	0.73230	-1.63886	-2.35388
H	-1.96004	-0.73872	0.00000
C	-2.72706	-1.52413	0.00000
C	-2.09352	-2.91183	0.00000
H	-3.35287	-1.36689	-0.88530
H	-3.35287	-1.36689	0.88530
H	-2.85703	-3.69718	0.00000
H	-1.46410	-3.06220	-0.88315
H	-1.46410	-3.06220	0.88315
C	0.66828	2.14897	1.14731
C	1.48577	2.31488	0.00000
C	-0.67844	1.93170	0.70882
H	0.99606	2.20637	2.17628
C	0.66828	2.14897	-1.14731
H	2.55626	2.47169	0.00000
C	-0.67844	1.93170	-0.70882
H	-1.53755	1.79559	1.35101
H	0.99606	2.20637	-2.17628
H	-1.53755	1.79559	-1.35101

cpmnco2_c2h6_mecp
Geometry with 23 atoms:
Total energy: -1650.381050
Gibbs free energy: -1650.250810

Mn	-0.21752	-0.13638	-0.01079
C	0.49790	-1.39125	-1.10365
C	0.69768	-0.95720	1.31733
O	0.94273	-2.22499	-1.76838
O	1.26972	-1.51991	2.14914
H	1.49567	1.26364	-0.98447
C	2.18480	1.83484	-0.34023
C	3.48602	1.07055	-0.12668
H	1.67628	2.03775	0.60878
H	2.34599	2.79664	-0.84027
H	4.18468	1.64329	0.49236
H	3.30436	0.11475	0.37458
H	3.98288	0.85766	-1.07877
C	-2.47898	-0.36495	-0.54038
C	-2.38409	-0.17361	0.85077
C	-1.92239	0.78603	-1.18824
H	-2.87064	-1.24159	-1.03816
C	-1.76355	1.09773	1.08261
H	-2.69056	-0.87589	1.61380
C	-1.51540	1.70062	-0.18045
H	-1.86667	0.94561	-2.25637
H	-1.56798	1.53842	2.05048
H	-1.06756	2.67194	-0.34492

cpmnco2_c7h16_s
Geometry with 38 atoms:
Total energy: -1846.773004
Gibbs free energy: -1846.505993

Mn	0.19600	-0.98278	0.11124
C	-0.15381	-2.87562	-0.77267
C	1.24343	-2.62642	-0.71955
C	-0.75165	-1.88793	-1.61857
C	1.52220	-1.48257	-1.53439
C	0.28933	-1.03760	-2.07309
C	1.44116	-0.79053	1.37054
O	2.27961	-0.74972	2.16954
C	-1.08015	-1.29596	1.31341
O	-1.90216	-1.58988	2.07569
H	-0.67291	-3.67942	-0.26967
H	1.97056	-3.20776	-0.17030
H	-1.79895	-1.81114	-1.87354
H	2.49376	-1.04351	-1.71101
H	0.15852	-0.16637	-2.70285
C	-0.33867	1.67876	0.15443
H	-0.14655	0.71522	-0.40335
C	-1.72732	2.14700	-0.27733
H	-1.74047	2.26707	-1.37042
H	-1.88303	3.15346	0.13735
H	-0.30784	1.50969	1.23293
C	0.76852	2.64135	-0.27038
H	0.74097	2.75935	-1.36349
H	0.52817	3.63082	0.14472
C	-2.88091	1.24560	0.14893
H	-2.86231	1.12031	1.23894
H	-2.72746	0.24316	-0.26827
C	2.17600	2.24489	0.16207
H	2.20076	2.12010	1.25203
H	2.41553	1.25983	-0.25597
C	-4.24070	1.78535	-0.28608
H	-5.05202	1.12083	0.02802
H	-4.43255	2.77405	0.14743
H	-4.29545	1.88744	-1.37666
C	3.23003	3.26191	-0.26708
H	3.02866	4.24879	0.16628
H	4.23208	2.95670	0.05103
H	3.24627	3.37825	-1.35753

cpmnco2_c7h16_t
Geometry with 38 atoms:
Total energy: -1846.764760
Gibbs free energy: -1846.499153

Mn	-1.19995	-0.63404	0.45937
C	-0.97143	-1.14302	-1.80233
C	-2.23959	-0.56357	-1.55155
C	-0.88203	-2.34621	-1.05131
C	-2.96134	-1.44024	-0.67084
C	-2.12382	-2.54476	-0.37592
C	0.20763	-1.01823	1.56044
O	1.10053	-1.31687	2.22662
C	-1.89411	0.86626	1.22540
O	-2.38133	1.81201	1.67140
H	-0.18257	-0.71505	-2.40555
H	-2.61482	0.35831	-1.97403
H	-0.02927	-3.01074	-1.01803
H	-3.97445	-1.29204	-0.32348
H	-2.36658	-3.37957	0.26750
C	2.73431	0.13662	-0.58960
H	3.02903	0.30556	-1.63600
C	2.21693	1.44121	0.00983
H	3.02141	2.19066	0.00769
H	1.96047	1.27605	1.06566
H	1.91281	-0.59305	-0.62182
C	3.90589	-0.46942	0.17882
H	4.74126	0.24432	0.18808
H	3.60988	-0.60953	1.22664
C	0.99947	1.99904	-0.71982
H	0.20415	1.23562	-0.72264
C	4.37188	-1.80190	-0.40166
H	5.21453	-2.21575	0.16221
H	3.56246	-2.54154	-0.37980
H	4.69017	-1.69035	-1.44516
C	0.43985	3.28030	-0.11141
H	0.17744	3.09424	0.93846
H	1.22479	4.04894	-0.09802
C	-0.78335	3.80436	-0.85938
H	-1.18140	4.71384	-0.39782
H	-0.53706	4.03703	-1.90242
H	-1.58662	3.05874	-0.86606
H	1.24792	2.17159	-1.77777

cpmnco2_c7h16_mecp
Geometry with 38 atoms:
Total energy: -1846.756446
Gibbs free energy: -1846.496948

Mn	-1.06048	-0.59872	0.28166
C	-0.87767	-1.17274	-1.85403
C	-2.22843	-0.88740	-1.53337
C	-0.43396	-2.23453	-1.02945
C	-2.64159	-1.81747	-0.52046
C	-1.53667	-2.64861	-0.21298
C	0.20970	-0.86809	1.55408
O	1.02019	-1.12606	2.33553
C	-2.11486	0.63089	1.10467
O	-2.85608	1.36661	1.59728
H	-0.26356	-0.62137	-2.55394
H	-2.84795	-0.12941	-1.99153
H	0.55408	-2.67327	-1.03212
H	-3.62484	-1.86820	-0.07393
H	-1.51768	-3.44500	0.51797
C	2.70470	0.34267	-0.52980
H	2.95917	0.50887	-1.58709
C	2.07877	1.60920	0.04584
H	2.78914	2.44409	-0.03944
H	1.89883	1.47086	1.12054
H	1.95097	-0.45641	-0.52120
C	3.94015	-0.13918	0.22572
H	4.71051	0.64392	0.20665
H	3.67508	-0.28404	1.28127
C	0.77074	1.98869	-0.63604

H	0.05690	1.14061	-0.54267
C	4.50826	-1.43775	-0.34032
H	5.38628	-1.77425	0.22089
H	3.76087	-2.23928	-0.29914
H	4.80704	-1.31636	-1.38851
C	0.09770	3.23751	-0.08117
H	-0.13187	3.07831	0.98068
H	0.80931	4.07384	-0.11800
C	-1.17519	3.61006	-0.83645
H	-1.66100	4.48864	-0.40014
H	-0.95528	3.83488	-1.88701
H	-1.89779	2.78679	-0.81589
H	0.93115	2.10088	-1.71857

cpmnco2_c6f12_s
Geometry with 33 atoms:
Total energy: -2996.673985
Gibbs free energy: -2996.557758

Mn	2.58871	0.09147	-0.16323
C	2.44036	1.42572	-1.34000
C	2.68107	1.20032	1.23015
O	2.43449	2.27528	-2.12705
O	2.83447	1.89957	2.14120
C	4.37926	-0.56427	-1.08159
C	4.48825	-0.70234	0.32741
C	3.32237	-1.42176	-1.53229
H	4.99503	0.06781	-1.70588
C	3.49952	-1.64470	0.76176
H	5.20080	-0.19208	0.96021
C	2.79185	-2.07044	-0.39021
H	2.99658	-1.55318	-2.55417
H	3.33378	-1.97685	1.77661
H	1.93963	-2.73916	-0.39021
F	0.35488	-0.29619	-0.13316
C	-0.56603	-0.22764	0.89214
C	-1.55016	-1.41694	0.69234
C	-1.25820	1.16554	0.82666
F	0.07257	-0.36587	2.05633
C	-2.45382	-1.24984	-0.56689
F	-0.83383	-2.55423	0.57058
F	-2.33396	-1.50909	1.78689
C	-2.15862	1.32871	-0.43646
F	-0.31971	2.12650	0.82273
F	-2.02649	1.30068	1.93086
C	-3.15178	0.14261	-0.62966
F	-3.39540	-2.21244	-0.55385
F	-1.68590	-1.40159	-1.66933
F	-2.86135	2.47090	-0.32101
F	-1.36243	1.40757	-1.52498
F	-4.08673	0.19816	0.34508
F	-3.75717	0.27097	-1.82557

cpmnco2_c6f12_t
Geometry with 33 atoms:
Total energy: -2996.671415
Gibbs free energy: -2996.560914

Mn	-3.05237	0.25066	0.42460
C	-2.63042	1.95518	-0.08910
C	-2.13424	0.09011	1.99268
O	-2.38572	3.01583	-0.46948
O	-1.56354	-0.07871	2.98070
C	-3.17303	-1.31932	-1.14728
C	-4.12243	-0.30086	-1.41553
C	-3.45891	-1.86400	0.12869
H	-2.33434	-1.58258	-1.77766
C	-5.03752	-0.24486	-0.32061
H	-4.15896	0.31538	-2.30325
C	-4.62769	-1.20517	0.63995
H	-2.91116	-2.65496	0.62165
H	-5.87951	0.42853	-0.23662
H	-5.11121	-1.41928	1.58283
F	-0.21135	0.65700	-1.74433
C	1.03783	0.35674	-1.33296
C	1.48202	1.39225	-0.25584
F	0.52308	1.47091	0.69256
C	1.05441	-1.10957	-0.80709
F	0.83182	-1.94571	-1.84276
F	0.05706	-1.26212	0.09368
C	2.40049	-1.49309	-0.12400
C	2.82825	1.00699	0.42969
C	2.84098	-0.45973	0.95653
F	1.87687	0.44351	-2.38921
F	1.61908	2.59684	-0.84221
F	3.82789	1.15149	-0.46980
F	3.04620	1.84335	1.46261
F	4.08832	-0.76512	1.36619
F	1.99833	-0.54976	2.00843
F	3.36099	-1.56950	-1.07205
F	2.26395	-2.70184	0.45663

cpmnco2_c6f12_mecp
Geometry with 33 atoms:
Total energy: -2996.662207
Gibbs free energy: -2996.552050

Mn	2.90782	0.18316	-0.12263
C	2.42370	1.59713	-1.15786
C	2.87354	0.95978	1.51718
O	2.18110	2.47103	-1.87232
O	2.92977	1.41389	2.57774
C	4.59792	-0.46327	-1.28407
C	4.81163	-0.79231	0.07701
C	3.44199	-1.18294	-1.73705
H	5.19296	0.21494	-1.87954
C	3.78873	-1.71794	0.47466
H	5.60093	-0.41292	0.71088
C	2.97085	-1.96605	-0.65509
H	3.02296	-1.15164	-2.73301
H	3.68119	-2.16512	1.45280
H	2.08490	-2.58811	-0.66750
F	0.23452	-0.47390	0.01723
C	-0.74438	-0.35998	0.95641
C	-1.80664	-1.46027	0.66610
C	-1.32241	1.08404	0.89055
F	-0.20782	-0.56996	2.17029
C	-2.60386	-1.19372	-0.64640
F	-1.17858	-2.65031	0.56165
F	-2.67245	-1.51308	1.70088
C	-2.12143	1.35067	-0.42127
F	-0.30818	1.96482	0.97225
F	-2.14782	1.26192	1.94627
C	-3.18627	0.25040	-0.71570
F	-3.61649	-2.07843	-0.72822
F	-1.77552	-1.37894	-1.69947
F	-2.74396	2.54040	-0.31678
F	-1.25195	1.39854	-1.45447
F	-4.18154	0.35627	0.19330
F	-3.69526	0.45502	-1.94604

cpmnco2_c7f14_s
Geometry with 36 atoms:
Total energy: -3234.350757
Gibbs free energy: -3234.225594

Mn	2.54973	-0.47443	-0.06662
C	2.14512	-2.20176	0.13138
C	2.70117	-0.20687	1.68963
O	1.97374	-3.34286	0.22961
O	2.89618	-0.02819	2.81743
C	4.28881	-0.97114	-1.16444
C	4.55004	0.15518	-0.34006
C	3.27314	-0.60457	-2.10809
H	4.78040	-1.93157	-1.09971
C	3.69695	1.22627	-0.76185
H	5.27418	0.19770	0.46142
C	2.91868	0.74016	-1.84330
H	2.85781	-1.23726	-2.87936
H	3.66436	2.22225	-0.34427
H	2.13303	1.29063	-2.34567
F	0.33988	0.14012	-0.35368
C	-0.71498	0.90077	0.13592
C	-1.74060	0.99653	-1.04183
C	-1.31905	0.13374	1.35556
C	-2.36973	-0.38125	-1.42735
F	-1.11909	1.47893	-2.13857
F	-2.74247	1.83639	-0.70333
C	-1.96991	-1.23602	0.97203
F	-0.35657	-0.12084	2.25881
F	-2.26680	0.91321	1.92745
C	-2.97538	-1.12891	-0.20745
F	-3.34097	-0.15924	-2.33443
F	-1.41633	-1.15568	-1.98900
F	-2.61467	-1.71012	2.05540
F	-0.99044	-2.09830	0.63015
F	-4.06925	-0.45404	0.21363
F	-3.34416	-2.36647	-0.58804
C	-0.12298	2.29851	0.52916
F	0.53717	2.81127	-0.52065
F	0.73839	2.17272	1.54073
F	-1.08582	3.15243	0.88830

cpmnco2_c7f14_t
Geometry with 36 atoms:
Total energy: -3234.348979
Gibbs free energy: -3234.229806

Mn	3.15419	-0.37855	0.49090
C	2.26368	-1.78705	1.23134
C	3.03031	0.89523	1.80056
O	1.69705	-2.70813	1.63288
O	2.97216	1.74328	2.57955
C	3.11498	0.58666	-1.46793
C	2.94307	-0.81387	-1.60818
C	4.39497	0.81595	-0.88239
H	2.39232	1.34876	-1.72408
C	4.13396	-1.45263	-1.12066
H	2.08099	-1.31631	-2.02267
C	5.03019	-0.43978	-0.69810
H	4.81462	1.78170	-0.63633
H	4.32046	-2.51740	-1.10792
H	6.00269	-0.59601	-0.25045
F	0.12609	0.60164	0.44898
C	-1.06376	1.02062	-0.09385
C	-1.29672	0.19267	-1.39812
C	-2.18166	0.73517	0.96136
C	-1.53249	-1.32944	-1.13599
F	-0.21401	0.29387	-2.20039
F	-2.37148	0.68008	-2.05829
C	-2.40784	-0.78815	1.22717
F	-1.84925	1.30237	2.13734
F	-3.35087	1.26776	0.53413
C	-2.63382	-1.60330	-0.07567
F	-1.89036	-1.90680	-2.30107
F	-0.37444	-1.88271	-0.71518
F	-3.49042	-0.92175	2.01955
F	-1.33026	-1.28420	1.87003
F	-3.83306	-1.26155	-0.60054
F	-2.64485	-2.91712	0.21921
C	-0.89304	2.55185	-0.38175
F	0.12697	2.73897	-1.23571
F	-0.60149	3.19644	0.75308
F	-1.99486	3.09056	-0.91307

cpmnco2_c7f14_mecp
Geometry with 36 atoms:
Total energy: -3234.339436
Gibbs free energy: -3234.220802

Mn	3.42550	-0.39962	0.59645
C	2.38043	-1.65602	1.37872
C	2.91243	1.04443	1.56257
O	1.67503	-2.47613	1.78325
O	2.55563	2.01000	2.08647
C	3.09850	0.49302	-1.32600
C	2.86131	-0.90119	-1.40816
C	4.47423	0.68817	-0.96872
H	2.37127	1.27400	-1.49543
C	4.08819	-1.57966	-1.10179
H	1.92087	-1.37426	-1.65139
C	5.07205	-0.59081	-0.84903
H	4.96896	1.63984	-0.83544
H	4.23934	-2.64974	-1.09248
H	6.09523	-0.78189	-0.55027
F	0.14825	0.50709	0.35318
C	-1.04966	0.98843	-0.11091
C	-1.38382	0.20267	-1.41960
C	-2.12019	0.72066	0.99616
C	-1.66300	-1.31565	-1.17775
F	-0.33972	0.28200	-2.27421
F	-2.47198	0.74308	-2.01278
C	-2.39086	-0.79886	1.24019
F	-1.70432	1.24547	2.16495
F	-3.28874	1.30762	0.64431
C	-2.71654	-1.57313	-0.06617
F	-2.10321	-1.85308	-2.33344
F	-0.50558	-1.92167	-0.83083
F	-3.43605	-0.91081	2.08528
F	-1.30196	-1.35010	1.81374
F	-3.92700	-1.17270	-0.51903
F	-2.76423	-2.89270	0.19919
C	-0.83212	2.51888	-0.37103
F	0.15357	2.68690	-1.26932
F	-0.46361	3.12501	0.76090
F	-1.93588	3.11120	-0.83914