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Supporting Information

69451 Weinheim, Germany

Preparation of a Dihydrogen Complex of Cobalt**

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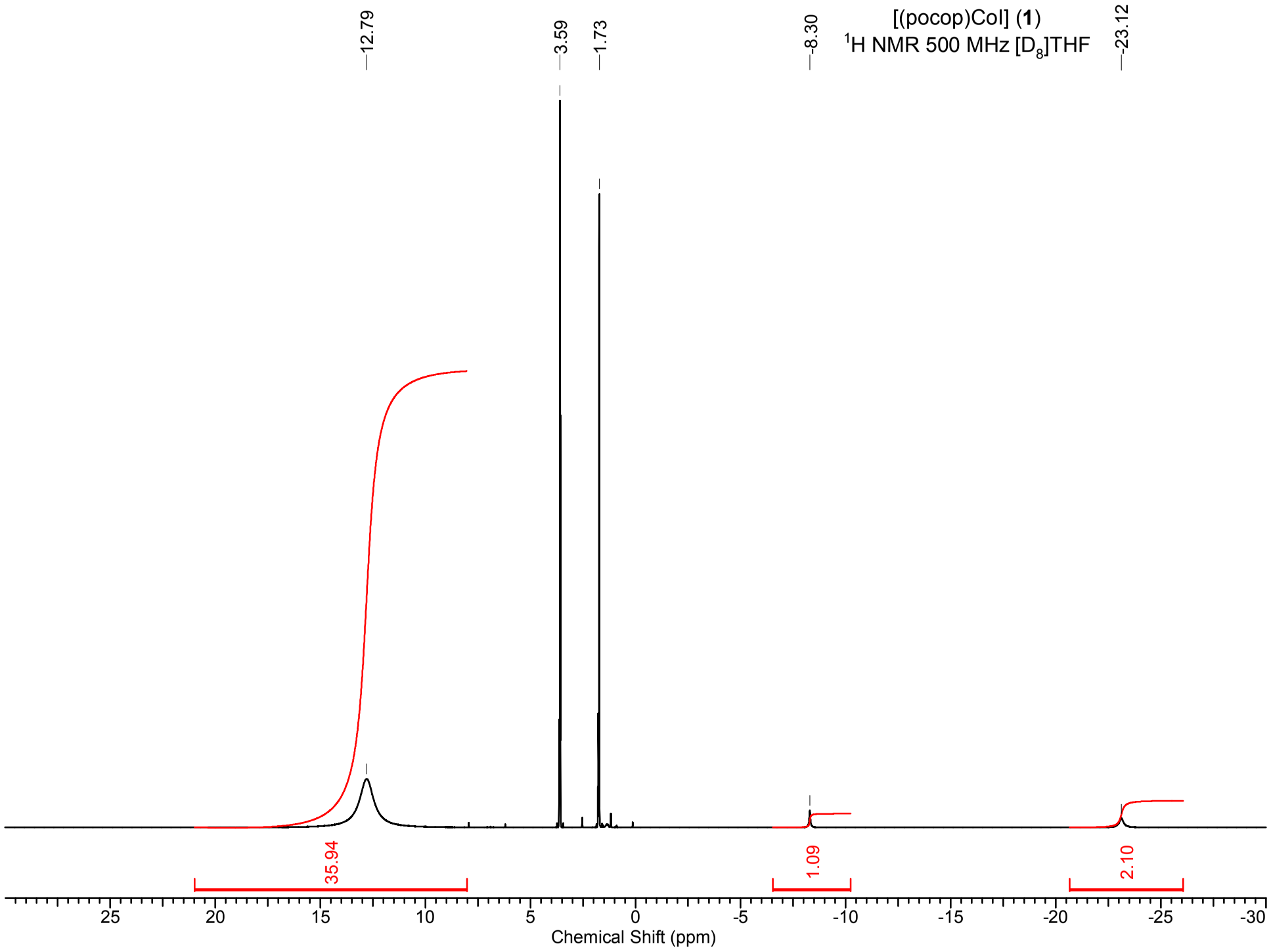
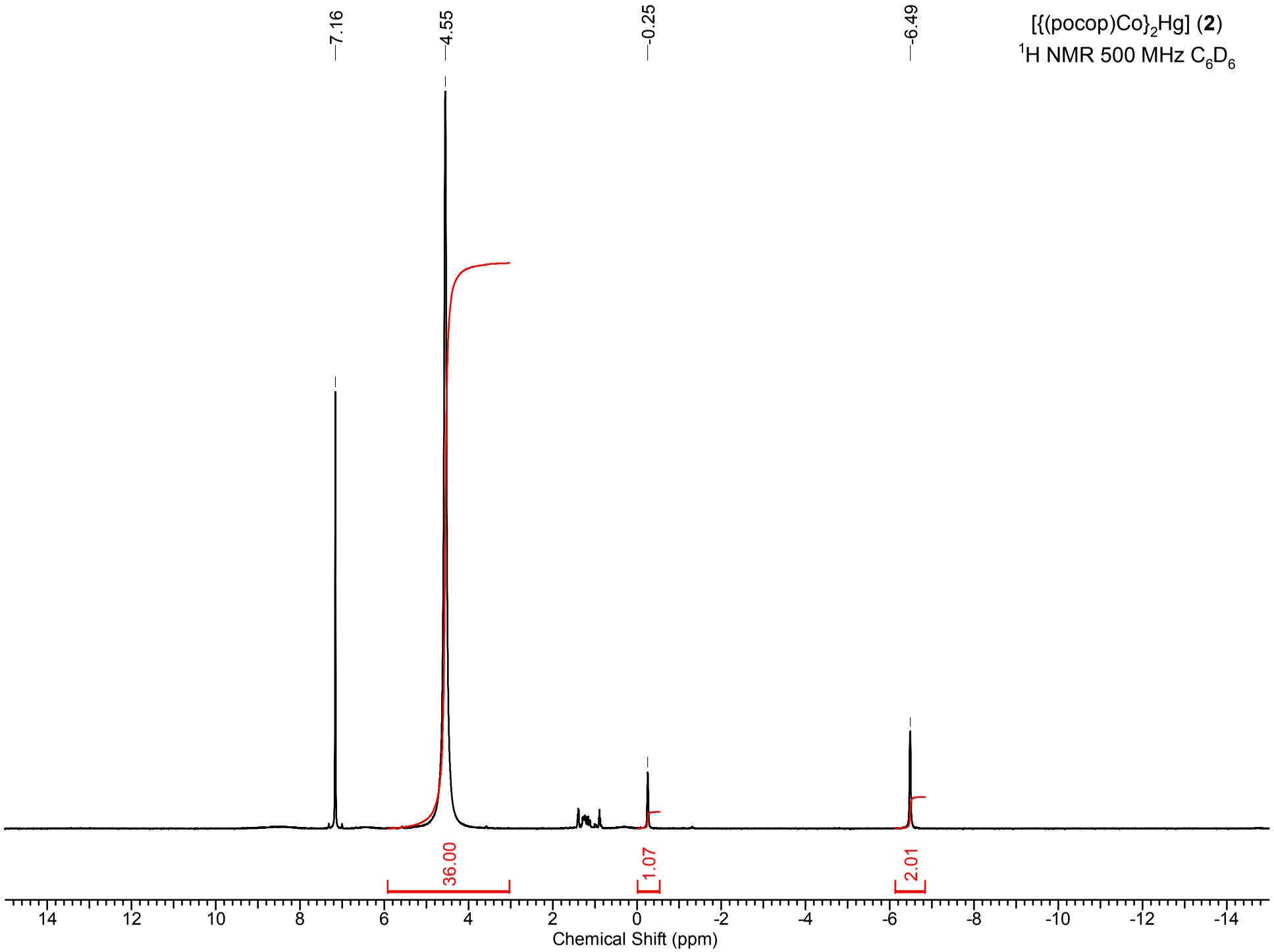
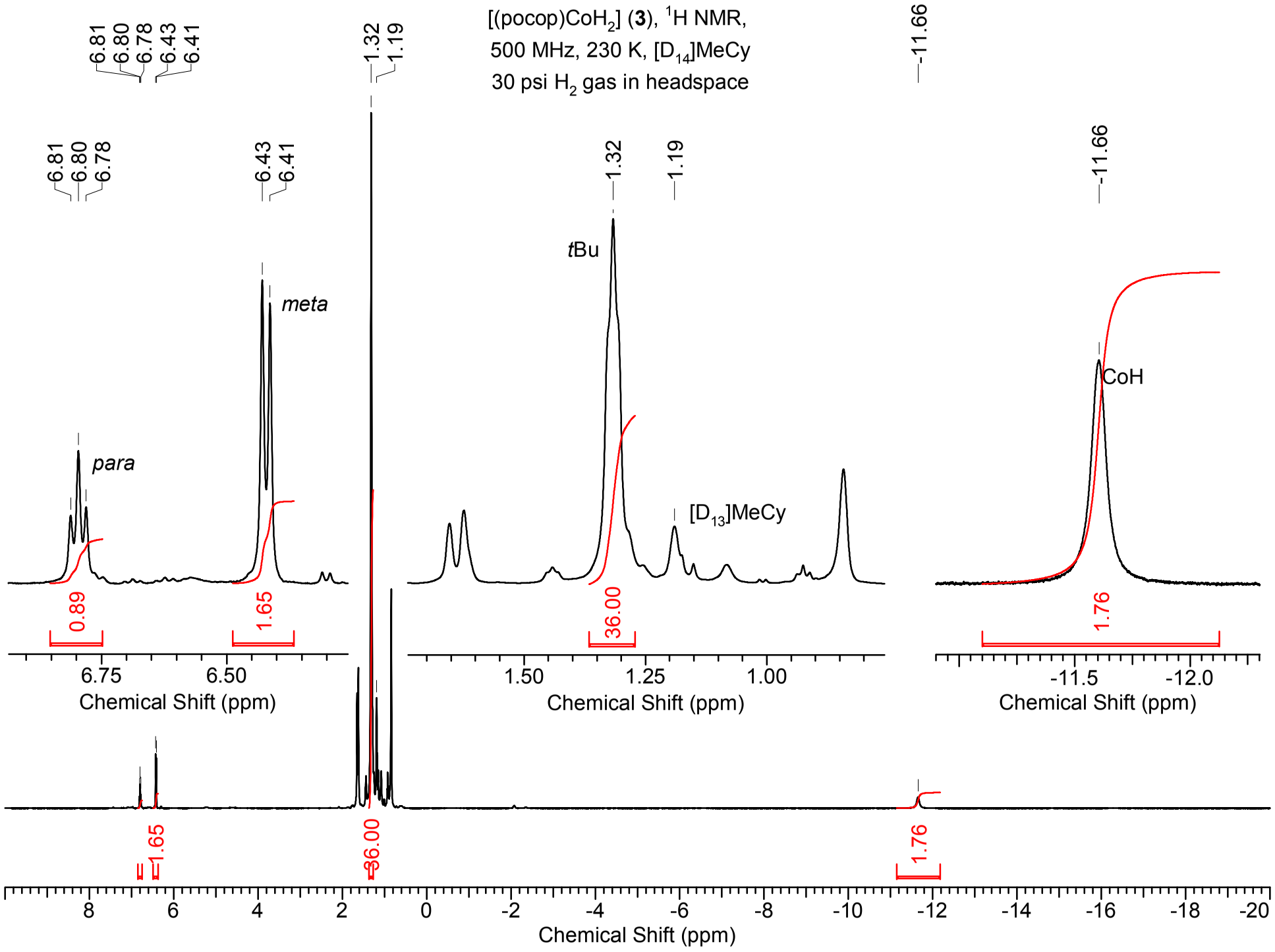
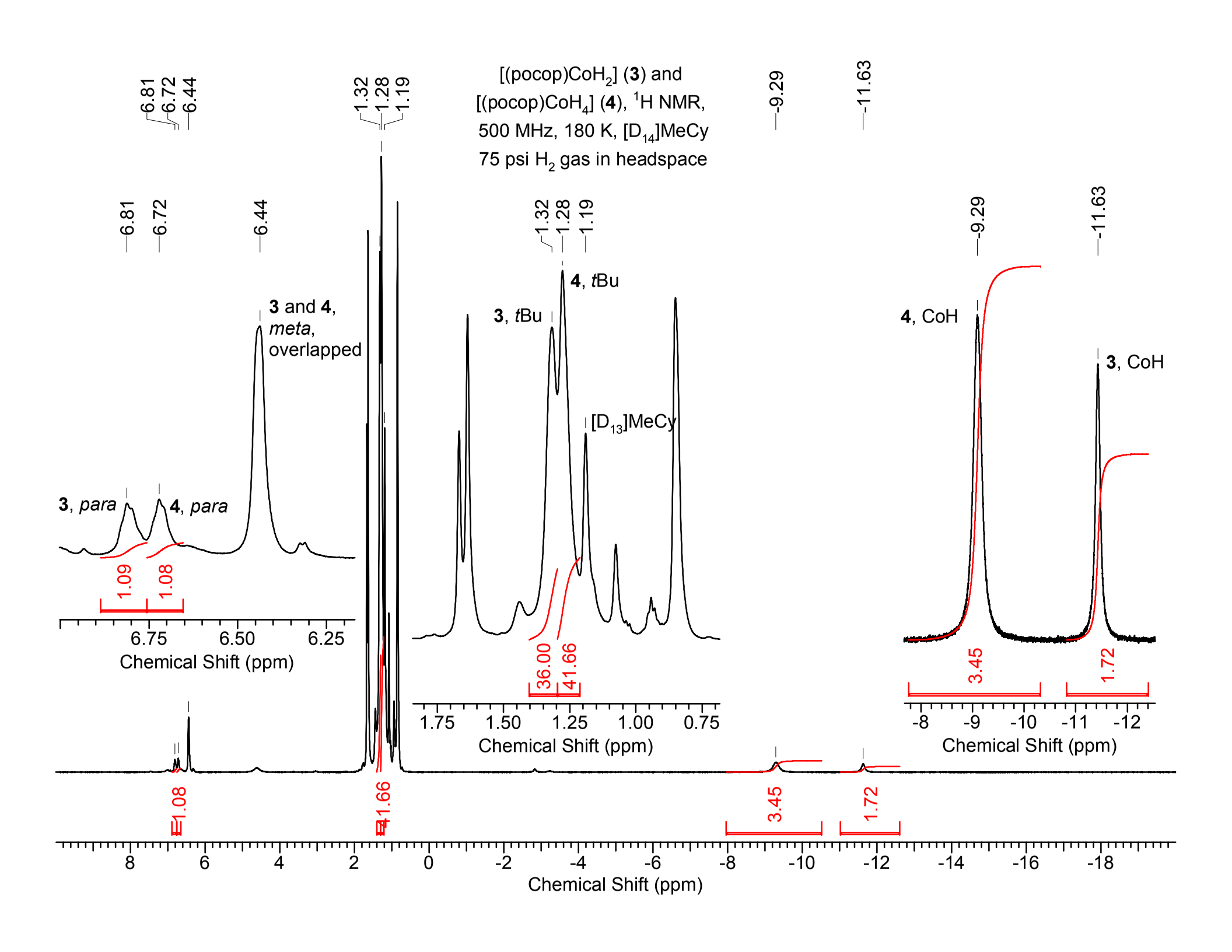
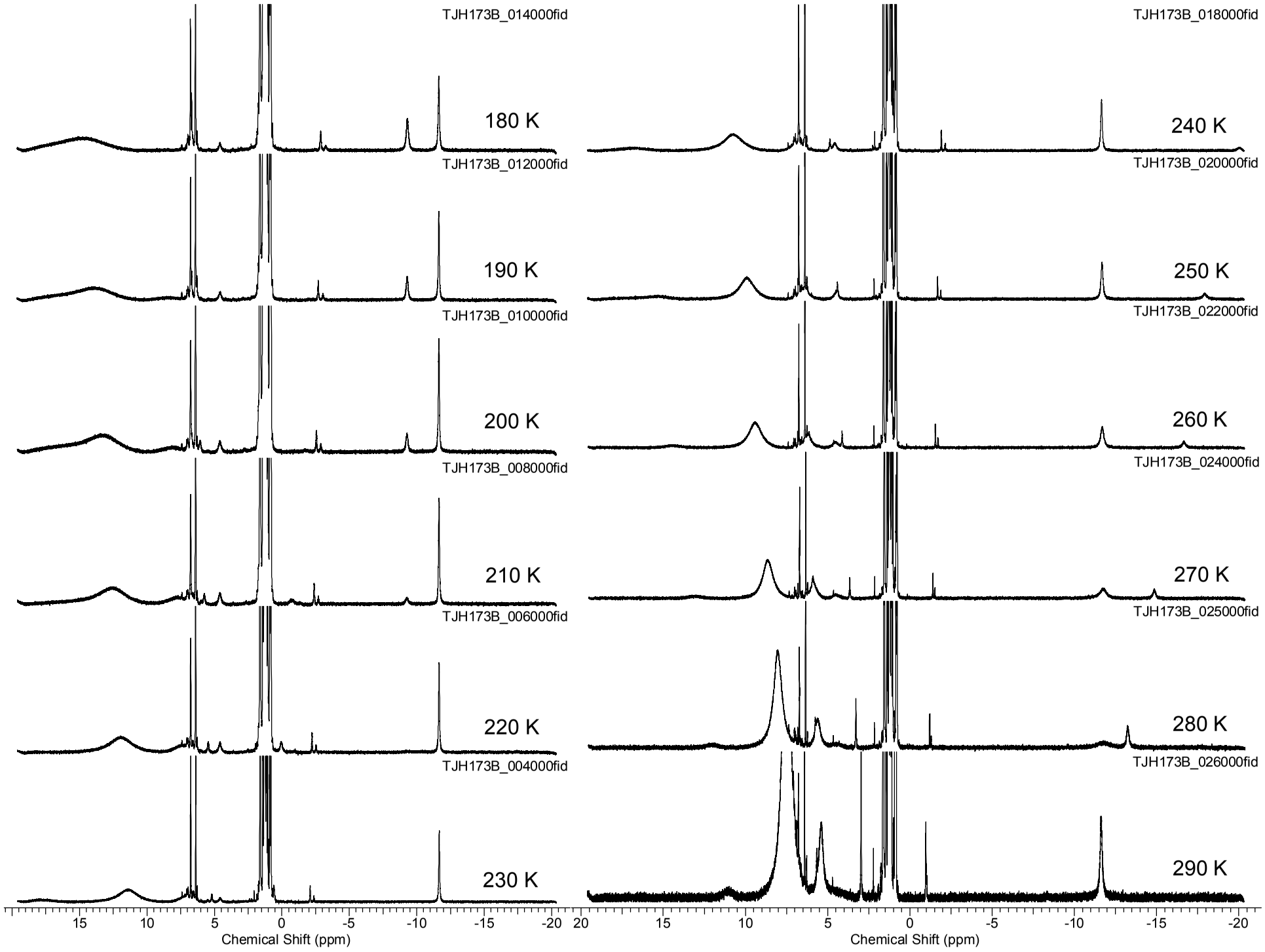
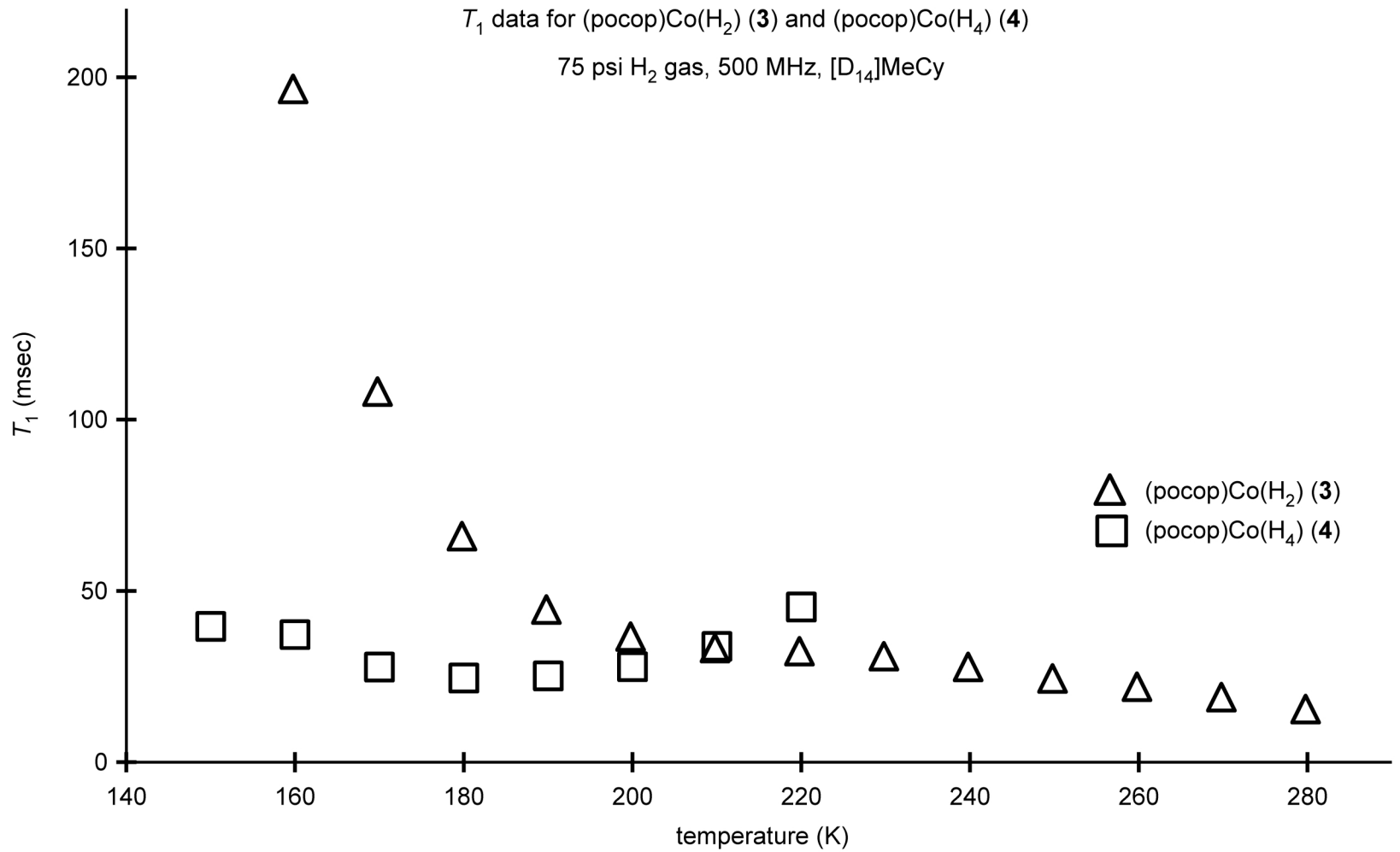

12.79
3.59
1.73
8.30
-23.12
[(pocop)CoI] (1)
^{1}H NMR 500 MHz [D_8]THF
35.94
1.09
2.10
25
20
15
10
5
0
-5
-10
-15
-20
-25
-30
Chemical Shift (ppm)


7.16
4.55
-0.25
-6.49
[{(pocop)Co}2Hg] (2)
1H NMR 500 MHz C6D6
36.00
1.07
2.01
14
12
10
8
6
4
2
0
-2
-4
-6
-8
-10
-12
-14
Chemical Shift (ppm)


[(pocop)CoH2] (3), 1H NMR,
500 MHz, 230 K, [D14]MeCy
30 psi H2 gas in headspace
6.81
6.80
6.78
6.43
6.41
1.32
1.19
-11.66
para
meta
tBu
[D13]MeCy
CoH
0.89
1.65
36.00
1.76
Chemical Shift (ppm)


[(pocop)CoH2] (3) and
[(pocop)CoH4] (4), 1H NMR,
500 MHz, 180 K, [D14]MeCy
75 psi H2 gas in headspace
6.81
6.72
6.44
1.32
1.28
1.19
-9.29
-11.63
3 and 4, meta, overlapped
3, para
4, para
1.09
1.08
6.75
6.50
6.25
Chemical Shift (ppm)
3, tBu
4, tBu
[D13]MeCy
36.00
41.66
1.75
1.50
1.25
1.00
0.75
Chemical Shift (ppm)
4, CoH
3, CoH
3.45
1.72
-8
-9
-10
-11
-12
Chemical Shift (ppm)
1.08
41.66
3.45
1.72
8
6
4
2
0
-2
-4
-6
-8
-10
-12
-14
-16
-18
Chemical Shift (ppm)


TJH173B_014000fid
180 K
TJH173B_012000fid
190 K
TJH173B_010000fid
200 K
TJH173B_008000fid
210 K
TJH173B_006000fid
220 K
TJH173B_004000fid
230 K
15 10 5 0 -5 -10 -15 -20
Chemical Shift (ppm)
TJH173B_018000fid
240 K
TJH173B_020000fid
250 K
TJH173B_022000fid
260 K
TJH173B_024000fid
270 K
TJH173B_025000fid
280 K
TJH173B_026000fid
290 K
20 15 10 5 0 -5 -10 -15 -20
Chemical Shift (ppm)


T_1 data for (pocop)Co(H_2) (**3**) and (pocop)Co(H_4) (**4**)
75 psi H_2 gas, 500 MHz, [D_{14}]MeCy
T_1 (msec)
200
150
100
50
0
140
160
180
200
220
240
260
280
temperature (K)
(pocop)Co(H_2) (**3**)
(pocop)Co(H_4) (**4**)

Computational details: The DFT calculations were carried out using the mPW1PW91 and PBE1PBE (also known as PBE0) functionals implemented in Gaussian 03.[#] Additionally, geometry optimizations and frequency calculations for cis-$CoH_2(H_2)$(POCOP), trans-$CoH_2(H_2)$(POCOP), and the transition states for H_2 loss from these complexes were carried out using the mPW1K functional. The basis sets included SDD (with ECP) for Hg, 6-311+G(2d) for Co, 6-311+G(d) for P, 6-31++G(p) for H-Co, and 6-31+G(d,p) for all other atoms. The nature of all stationary points was verified by frequency calculations. The (POCOP)Co fragment can have C_2 or C_s symmetry, therefore, the hydride and dihydrogen complexes resulting from H_2 addition to (POCOP)Co can also adopt C_2 or C_s symmetrical structures. Possible isomers were explored in every case. A D_2 symmetrical structure was found to be a minimum for the triplet $[(POCOP)Co]_2Hg$.

References:

#1 Gaussian 03, Revision E.01, Frisch, M. J.; Trucks, G. W.; Schlegel, H. B.; Scuseria, G. E.; Robb, M. A.; Cheeseman, J. R.; Montgomery, Jr., J. A.; Vreven, T.; Kudin, K. N.; Burant, J. C.; Millam, J. M.; Iyengar, S. S.; Tomasi, J.; Barone, V.; Mennucci, B.; Cossi, M.; Scalmani, G.; Rega, N.; Petersson, G. A.; Nakatsuji, H.; Hada, M.; Ehara, M.; Toyota, K.; Fukuda, R.; Hasegawa, J.; Ishida, M.; Nakajima, T.; Honda, Y.; Kitao, O.; Nakai, H.; Klene, M.; Li, X.; Knox, J. E.; Hratchian, H. P.; Cross, J. B.; Bakken, V.; Adamo, C.; Jaramillo, J.; Gomperts, R.; Stratmann, R. E.; Yazyev, O.; Austin, A. J.; Cammi, R.; Pomelli, C.; Ochterski, J. W.; Ayala, P. Y.; Morokuma, K.; Voth, G. A.; Salvador, P.; Dannenberg, J. J.; Zakrzewski, V. G.; Dapprich, S.; Daniels, A. D.; Strain, M. C.; Farkas, O.; Malick, D. K.; Rabuck, A. D.; Raghavachari, K.; Foresman, J. B.; Ortiz, J. V.; Cui, Q.; Baboul, A. G.; Clifford, S.; Cioslowski, J.; Stefanov, B. B.; Liu, G.; Liashenko, A.; Piskorz, P.; Komaromi, I.; Martin, R. L.; Fox, D. J.; Keith, T.; Al-Laham, M. A.; Peng, C. Y.; Nanayakkara, A.; Challacombe, M.; Gill, P. M. W.; Johnson, B.; Chen, W.; Wong, M. W.; Gonzalez, C.; and Pople, J. A.; Gaussian, Inc., Wallingford CT, 2004.

#2 Frish, A.; Frish, M. J.; Trucks, G. W. Gaussian 03 User's Reference, Gaussian, Inc., Pittsburgh PA, 2003.

Reaction enthalpies (kcal mol^{-1}), POCOP = (POCOP = κ^3-C_6H_3-1,3-[OP(*t*Bu)$_2$]$_2$)

1) singlet Co(POCOP) → triplet Co(POCOP) ΔH = -18.1 (mPW1PW91); -17.9 (PBE0)

2) triplet Co(POCOP) + H_2 → Co(H_2)(POCOP) ΔH = -3.3 (mPW1PW91); -5.1 (PBE0)

3) Co(H_2)(POCOP) → Co(H)$_2$(POCOP) ΔH = +2.4 (mPW1PW91); +2.5 (PBE0)

4) Co(H_2)(POCOP) + H_2 → cis-CoH_2(H_2)(POCOP) ΔH = -3.7 (mPW1PW91); -4.9 (PBE0)

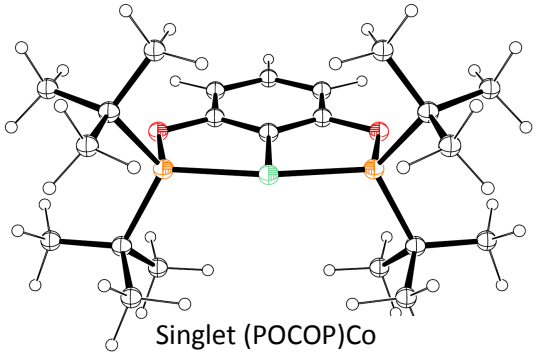
5) cis-CoH_2(H_2)(POCOP) → trans-CoH_2(H_2)(POCOP) ΔH = +1.6 (mPW1PW91); +1.6 (PBE0)

6) cis-CoH_2(H_2)(POCOP) → Co(H_2)$_2$(POCOP) ΔH = +4.8 (mPW1PW91); +4.7 (PBE0)

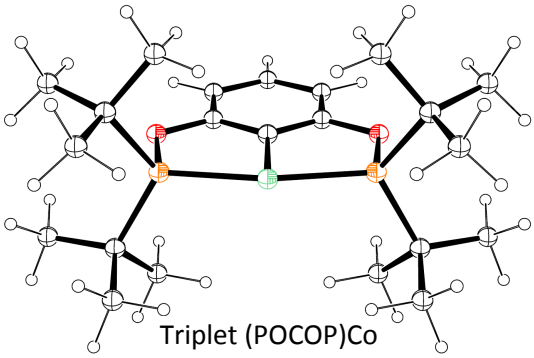
Barrier height for H_2 loss from cis-CoH_2(H_2)(POCOP): $\Delta H^{‡}$ = 12.7 (mPW1K)

Barrier height for H_2 loss from trans-CoH_2(H_2)(POCOP): $\Delta H^{‡}$ = 17.8 (mPW1K)

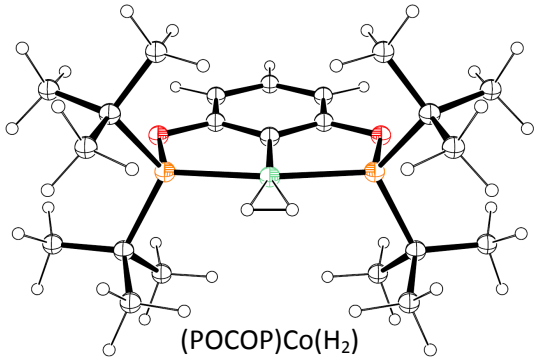
Representative structures of the complexes calculated in this work:



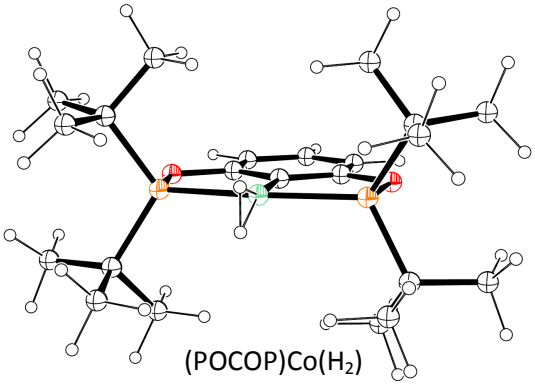
Singlet (POCOP)Co



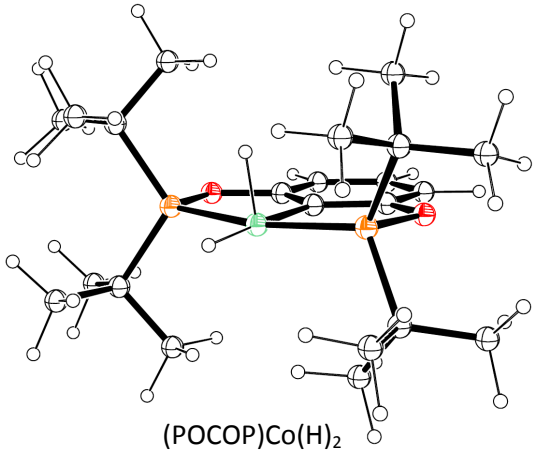
Triplet (POCOP)Co



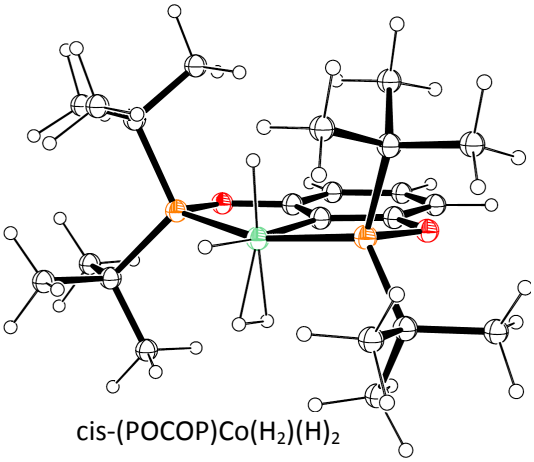
(POCOP)Co(H_2)



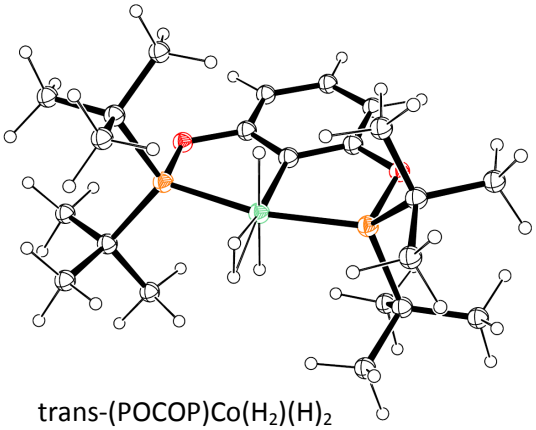
(POCOP)Co(H_2)



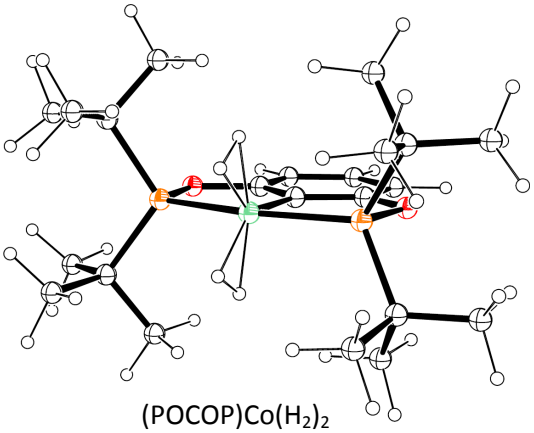
(POCOP)Co($H)_2$



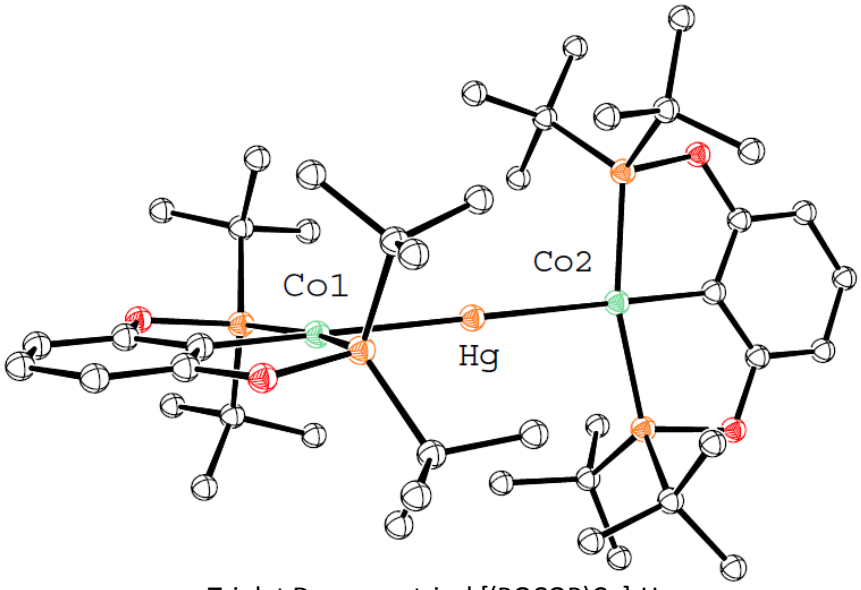
cis-(POCOP)Co(H_2)($H)_2$



trans-(POCOP)Co(H_2)($H)_2$



(POCOP)Co($H_2)_2$



Triplet D_2 symmetrical $[(POCOP)Co]_2Hg$

Optimized geometries and energies (mPW1PW91)

C_2 symmetrical singlet (POCOP)Co: E = -3077.72430728
Sum of electronic and thermal Enthalpies -3077.115163
0 1

P	-1.61292000	1.44571400	0.28337300
P	1.61292000	-1.44571400	0.28337300
O	-1.78868700	1.57332400	-1.37825400
C	-0.88624800	0.78297200	-2.06992800
C	0.00000000	0.00000000	-4.14812300
C	0.90979100	-0.80511100	-3.46158700
C	0.88624800	-0.78297200	-2.06992800
C	0.00000000	0.00000000	-1.32179800
O	1.78868700	-1.57332400	-1.37825400
C	-1.21623200	3.22856500	0.73967800
C	-0.78865800	3.25646100	2.21394100
C	-2.32963700	4.24692700	0.48934500
C	0.00000000	3.59185600	-0.12795400
C	-3.37702200	0.96352400	0.73109900
C	-3.58941800	1.10675100	2.24157500
C	-4.45567100	1.72764800	-0.04384200
C	-3.46961700	-0.52423100	0.35024400
C	1.21623200	-3.22856500	0.73967800
C	0.00000000	-3.59185600	-0.12795400
C	2.32963700	-4.24692700	0.48934500
C	0.78865800	-3.25646100	2.21394100
C	3.37702200	-0.96352400	0.73109900
C	4.45567100	-1.72764800	-0.04384200
C	3.58941800	-1.10675100	2.24157500
C	3.46961700	0.52423100	0.35024400
H	-0.26423500	3.64724900	-1.18605800
H	0.80386300	2.85714200	-0.01883100
H	0.38199300	4.57060000	0.18411100
H	-2.70600800	4.18984000	-0.53491200
H	-3.16782900	4.12262500	1.17918400
H	-1.93222600	5.25741100	0.64211700
H	-0.44479400	4.26472000	2.47155300
H	-1.60345300	3.00383100	2.89644700
H	0.04065500	2.56569800	2.39868800
H	-4.53213700	2.77253200	0.25714100
H	-4.26763500	1.69138200	-1.11884600
H	-5.42857900	1.25924900	0.14596300
H	-3.63860500	2.15262000	2.55488000
H	-4.53936200	0.63679000	2.52011000
H	-2.79870400	0.61069200	2.81496200
H	-3.29682200	-0.67614300	-0.71856600
H	-2.73629400	-1.12523400	0.89605000
H	-4.47290600	-0.89639200	0.58876800
H	-0.04065500	-2.56569800	2.39868800
H	1.60345300	-3.00383100	2.89644700
H	0.44479400	-4.26472000	2.47155300
H	-0.38199300	-4.57060000	0.18411100
H	-0.80386300	-2.85714200	-0.01883100
H	0.26423500	-3.64724900	-1.18605800
H	1.93222600	-5.25741100	0.64211700
H	2.70600800	-4.18984000	-0.53491200
H	3.16782900	-4.12262500	1.17918400
H	2.73629400	1.12523400	0.89605000
H	4.47290600	0.89639200	0.58876800
H	3.29682200	0.67614300	-0.71856600
H	2.79870400	-0.61069200	2.81496200
H	3.63860500	-2.15262000	2.55488000
H	4.53936200	-0.63679000	2.52011000
H	5.42857900	-1.25924900	0.14596300
H	4.53213700	-2.77253200	0.25714100
H	4.26763500	-1.69138200	-1.11884600
H	1.62004200	-1.43327000	-3.98758900
H	0.00000000	0.00000000	-5.23327000
C	-0.90979100	0.80511100	-3.46158700
H	-1.62004200	1.43327000	-3.98758900
Co	0.00000000	0.00000000	0.55120300

C_s symmetrical singlet (POCOP)Co: E = -3077.72417605
Sum of electronic and thermal Enthalpies -3077.115045
0 1

P	0.27911100	0.04315700	2.16637400
P	0.27911100	0.04315700	-2.16637400
O	-1.37549500	-0.10884000	2.38242000
C	-2.06261700	-0.18387200	1.18256200
C	-3.44627200	-0.33356200	1.21480800
C	-4.12887700	-0.40693300	0.00000000
C	-3.44627200	-0.33356200	-1.21480800
C	-2.06261700	-0.18387200	-1.18256200
C	-1.31871100	-0.10206800	0.00000000
O	-1.37549500	-0.10884000	-2.38242000
C	0.56330700	1.61572400	3.16207900
C	2.06134100	1.80433500	3.42195700
C	-0.22549000	1.68450900	4.47449000
C	0.06639300	2.74285600	2.24087500
C	0.90225900	-1.49287300	3.06016900
C	2.39868700	-1.64366300	2.75188200
C	0.66339000	-1.52978300	4.56993200
C	0.14973200	-2.66210500	2.40455500
C	0.90225900	-1.49287300	-3.06016900
C	0.14973200	-2.66210500	-2.40455500
C	0.66339000	-1.52978300	-4.56993200
C	2.39868700	-1.64366300	-2.75188200
C	0.56330700	1.61572400	-3.16207900
C	-0.22549000	1.68450900	-4.47449000
C	2.06134100	1.80433500	-3.42195700
C	0.06639300	2.74285600	-2.24087500
H	-0.99590500	2.63198600	2.00764500
H	0.61457600	2.76133000	1.29451300
H	0.20499000	3.70740500	2.74325200
H	-1.28614200	1.48598900	4.30740700

H	0.14164600	0.98522300	5.22570900
H	-0.13106300	2.69402200	4.89151500
H	2.23620800	2.80898500	3.82305000
H	2.44643600	1.08927300	4.15343700
H	2.65153600	1.71176200	2.50385200
H	1.28123100	-0.80405700	5.10409500
H	-0.38549700	-1.34800700	4.81668000
H	0.92734200	-2.52331700	4.95125400
H	3.00413600	-0.84371000	3.18465400
H	2.76037300	-2.59089700	3.16827500
H	2.57939500	-1.66566000	1.67215800
H	-0.91672400	-2.63552400	2.63781400
H	0.25832700	-2.64716200	1.31565500
H	0.56138900	-3.60650900	2.77862900
H	2.57939500	-1.66566000	-1.67215800
H	3.00413600	-0.84371000	-3.18465400
H	2.76037300	-2.59089700	-3.16827500
H	0.56138900	-3.60650900	-2.77862900
H	0.25832700	-2.64716200	-1.31565500
H	-0.91672400	-2.63552400	-2.63781400
H	0.92734200	-2.52331700	-4.95125400
H	-0.38549700	-1.34800700	-4.81668000
H	1.28123100	-0.80405700	-5.10409500
H	0.61457600	2.76133000	-1.29451300
H	0.20499000	3.70740500	-2.74325200
H	-0.99590500	2.63198600	-2.00764500
H	2.65153600	1.71176200	-2.50385200
H	2.44643600	1.08927300	-4.15343700
H	2.23620800	2.80898500	-3.82305000
H	-0.13106300	2.69402200	-4.89151500
H	0.14164600	0.98522300	-5.22570900
H	-1.28614200	1.48598900	-4.30740700
H	-3.96904800	-0.39119600	2.16300200
H	-5.20769200	-0.52400100	0.00000000
H	-3.96904800	-0.39119600	-2.16300200
Co	0.54491300	0.08763300	0.00000000

C_2 symmetrical triplet (POCOP)Co: E = -3077.75264194

Sum of electronic and thermal Enthalpies -3077.143966

0 3

P	0.00000000	2.21036400	0.32837500
P	0.00000000	-2.21036400	0.32837500
O	-0.00816400	2.37904800	-1.35267900
C	-0.00243900	1.18475400	-2.06210800
C	0.00000000	0.00000000	-4.13567100
C	0.00170500	-1.22103700	-3.45565400
C	0.00243900	-1.18475400	-2.06210800
C	0.00000000	0.00000000	-1.33588400
O	0.00816400	-2.37904800	-1.35267900
C	1.56191400	3.18024200	0.72025400
C	1.84424000	3.09744100	2.22565800
C	1.53865800	4.63818300	0.25742000
C	2.67762500	2.43223600	-0.02904800
C	-1.58403300	3.15027800	0.71866000
C	-1.61533900	3.54165400	2.19919600
C	-1.82355000	4.37510300	-0.16921500
C	-2.69759300	2.12270500	0.45105100
C	-1.56191400	-3.18024200	0.72025400
C	-2.67762500	-2.43223600	-0.02904800
C	-1.53865800	-4.63818300	0.25742000
C	-1.84424000	-3.09744100	2.22565800
C	1.58403300	-3.15027800	0.71866000
C	1.82355000	-4.37510300	-0.16921500
C	1.61533900	-3.54165400	2.19919600
C	2.69759300	-2.12270500	0.45105100
H	2.54125200	2.48219200	-1.11108500
H	2.72376500	1.37678800	0.25803400
H	3.64273300	2.88848200	0.21846200
H	1.24911900	4.72013200	-0.79283500
H	0.85940400	5.24823900	0.85789600
H	2.54129900	5.06889100	0.36471500
H	2.82678100	3.53712300	2.43171000
H	1.10948900	3.64170800	2.82236800
H	1.86007700	2.06004500	2.57337200
H	-1.11256700	5.17847200	0.02709900
H	-1.76156000	4.11404700	-1.22710600
H	-2.82791200	4.76779300	0.02887200
H	-0.92689900	4.36062000	2.42167300
H	-2.62337300	3.88242100	2.46128100
H	-1.37108900	2.69612900	2.85057900
H	-2.68889600	1.77345500	-0.58513400
H	-2.60363600	1.25236800	1.10989600
H	-3.67297400	2.58391300	0.64434700
H	-1.86007700	-2.06004500	2.57337200
H	-1.10948900	-3.64170800	2.82236800
H	-2.82678100	-3.53712300	2.43171000
H	-3.64273300	-2.88848200	0.21846200
H	-2.72376500	-1.37678800	0.25803400
H	-2.54125200	-2.48219200	-1.11108500
H	-2.54129900	-5.06889100	0.36471500
H	-1.24911900	-4.72013200	-0.79283500
H	-0.85940400	-5.24823900	0.85789600
H	2.60363600	-1.25236800	1.10989600
H	3.67297400	-2.58391300	0.64434700
H	2.68889600	-1.77345500	-0.58513400
H	1.37108900	-2.69612900	2.85057900
H	0.92689900	-4.36062000	2.42167300
H	2.62337300	-3.88242100	2.46128100
H	2.82791200	-4.76779300	0.02887200
H	1.11256700	-5.17847200	0.02709900
H	1.76156000	-4.11404700	-1.22710600
H	0.00329300	-2.16359300	-3.99224700
H	0.00000000	0.00000000	-5.22124100
C	-0.00170500	1.22103700	-3.45565400
H	-0.00329300	2.16359300	-3.99224700
Co	0.00000000	0.00000000	0.62384600

C_s symmetrical triplet (POCOP)Co: E = -3077.75247058

Sum of electronic and thermal Enthalpies -3077.143805

0 3

P	0.32926500	0.01014900	2.21212200
P	0.32926500	0.01014900	-2.21212200
O	-1.35181500	0.00003600	2.37913900
C	-2.06083900	-0.01292700	1.18464000
C	-3.45404600	-0.04309700	1.22098400
C	-4.13399400	-0.05722400	0.00000000
C	-3.45404600	-0.04309700	-1.22098400
C	-2.06083900	-0.01292700	-1.18464000
C	-1.33463900	0.00452000	0.00000000
O	-1.35181500	0.00003600	-2.37913900
C	0.70076000	1.57567800	3.18969400
C	2.17964500	1.61344800	3.58742500
C	-0.19219600	1.77500000	4.41824400
C	0.42252800	2.71098300	2.18970700
C	0.73683900	-1.56880000	3.14913400
C	2.24650700	-1.82853900	3.07183800
C	0.26231800	-1.58657900	4.60333600
C	0.00974700	-2.67685200	2.36898600
C	0.73683900	-1.56880000	-3.14913400
C	0.00974700	-2.67685200	-2.36898600
C	0.26231800	-1.58657900	-4.60333600
C	2.24650700	-1.82853900	-3.07183800
C	0.70076000	1.57567800	-3.18969400
C	-0.19219600	1.77500000	-4.41824400
C	2.17964500	1.61344800	-3.58742500
C	0.42252800	2.71098300	-2.18970700
H	-0.61305200	2.69905300	1.83900500
H	1.08162300	2.64594100	1.31762500
H	0.60369700	3.67663700	2.67548700
H	-1.24909200	1.71737900	4.15235000
H	0.00401200	1.04085700	5.20045300
H	0.00140900	2.76792400	4.84109600
H	2.43030600	2.61701200	3.94933300
H	2.40562200	0.91147600	4.39402800
H	2.83738200	1.39229900	2.74052000
H	0.84974700	-0.91497000	5.23405500
H	-0.79192900	-1.31161200	4.68385700
H	0.37884100	-2.59798400	5.01048200
H	2.82789200	-1.10162300	3.64231900
H	2.46237300	-2.82045000	3.48506000
H	2.60341000	-1.80976700	2.03758300
H	-1.07430500	-2.55106600	2.40066900
H	0.31740600	-2.70126800	1.31855100
H	0.25746100	-3.64828000	2.81152600
H	2.60341000	-1.80976700	-2.03758300
H	2.82789200	-1.10162300	-3.64231900
H	2.46237300	-2.82045000	-3.48506000
H	0.25746100	-3.64828000	-2.81152600
H	0.31740600	-2.70126800	-1.31855100
H	-1.07430500	-2.55106600	-2.40066900
H	0.37884100	-2.59798400	-5.01048200
H	-0.79192900	-1.31161200	-4.68385700
H	0.84974700	-0.91497000	-5.23405500
H	1.08162300	2.64594100	-1.31762500
H	0.60369700	3.67663700	-2.67548700
H	-0.61305200	2.69905300	-1.83900500
H	2.83738200	1.39229900	-2.74052000
H	2.40562200	0.91147600	-4.39402800
H	2.43030600	2.61701200	-3.94933300
H	0.00140900	2.76792400	-4.84109600
H	0.00401200	1.04085700	-5.20045300
H	-1.24909200	1.71737900	-4.15235000
H	-3.99032500	-0.05619600	2.16362600
H	-5.21930300	-0.08092400	0.00000000
H	-3.99032500	-0.05619600	-2.16362600
Co	0.62526200	0.02524400	0.00000000

C_2 symmetrical (POCOP)Co(H_2) : E = -3078.93870168

Sum of electronic and thermal Enthalpies -3078.311954

0 1

P	0.79080400	1.98116000	0.25638400
P	-0.79080400	-1.98116000	0.25638400
O	0.82676700	2.22882600	-1.40458700
C	0.41139300	1.10680900	-2.09267000
C	0.00000000	0.00000000	-4.17325300
C	-0.42333200	-1.13781500	-3.48574100
C	-0.41139300	-1.10680900	-2.09267000
C	0.00000000	0.00000000	-1.33789900
O	-0.82676700	-2.22882600	-1.40458700
C	2.60921000	2.23301500	0.67200500
C	2.84379800	1.86529600	2.14363500
C	3.14607000	3.63634400	0.38315500
C	3.35886500	1.21844700	-0.20758300
C	-0.28025200	3.44682300	0.75654200
C	-0.14757600	3.71909400	2.25838300
C	0.00000000	4.72460100	-0.04289800
C	-1.71751500	2.98859800	0.45462200
C	-2.60921000	-2.23301500	0.67200500
C	-3.35886500	-1.21844700	-0.20758300
C	-3.14607000	-3.63634400	0.38315500
C	-2.84379800	-1.86529600	2.14363500
C	0.28025200	-3.44682300	0.75654200
C	0.00000000	-4.72460100	-0.04289800
C	0.14757600	-3.71909400	2.25838300
C	1.71751500	-2.98859800	0.45462200
H	3.27999700	1.46844300	-1.26769300
H	2.97046700	0.20528400	-0.06823100
H	4.41932900	1.22320700	0.06855400
H	2.92126600	3.95211400	-0.63840300
H	2.75121500	4.38228500	1.07699400
H	4.23625100	3.63155700	0.49829900
H	3.91491200	1.93951800	2.36301400
H	2.32051600	2.52912800	2.83554000
H	2.52997800	0.83810900	2.34920800
H	0.97183500	5.16166800	0.18735600

H	-0.04849900	4.53871800	-1.11745300
H	-0.76411000	5.46954500	0.20769500
H	0.82663400	4.14086400	2.51735000
H	-0.90905400	4.44757200	2.55846900
H	-0.30520300	2.81584400	2.85608300
H	-1.85497300	2.76884300	-0.60762100
H	-1.97704700	2.08832100	1.01967200
H	-2.41625100	3.78751900	0.72917400
H	-2.52997800	-0.83810900	2.34920800
H	-2.32051600	-2.52912800	2.83554000
H	-3.91491200	-1.93951800	2.36301400
H	-4.41932900	-1.22320700	0.06855400
H	-2.97046700	-0.20528400	-0.06823100
H	-3.27999700	-1.46844300	-1.26769300
H	-4.23625100	-3.63155700	0.49829900
H	-2.92126600	-3.95211400	-0.63840300
H	-2.75121500	-4.38228500	1.07699400
H	1.97704700	-2.08832100	1.01967200
H	2.41625100	-3.78751900	0.72917400
H	1.85497300	-2.76884300	-0.60762100
H	0.30520300	-2.81584400	2.85608300
H	-0.82663400	-4.14086400	2.51735000
H	0.90905400	-4.44757200	2.55846900
H	0.76411000	-5.46954500	0.20769500
H	-0.97183500	-5.16166800	0.18735600
H	0.04849900	-4.53871800	-1.11745300
H	-0.75452300	-2.02636000	-4.01167300
H	0.11102400	0.41590000	2.10022300
H	-0.11102400	-0.41590000	2.10022300
H	0.00000000	0.00000000	-5.25859200
C	0.42333200	1.13781500	-3.48574100
H	0.75452300	2.02636000	-4.01167300
Co	0.00000000	0.00000000	0.58225500

C_s symmetrical (POCOP)Co(H_2) : E = -3078.93587363

Sum of electronic and thermal Enthalpies -3078.309134

0 1

P	0.25740500	0.02341200	2.13274600
P	0.25740500	0.02341200	-2.13274600
O	-1.40125000	0.00066700	2.37758100
C	-2.08938700	-0.02457900	1.18015700
C	-3.48072800	-0.07304600	1.21365800
C	-4.16745100	-0.09625000	0.00000000
C	-3.48072800	-0.07304600	-1.21365800
C	-2.08938700	-0.02457900	-1.18015700
C	-1.33480000	0.00146900	0.00000000
O	-1.40125000	0.00066700	-2.37758100
C	0.68259100	1.56025200	3.13698300
C	2.18419500	1.60925800	3.43514300
C	-0.12510600	1.69937500	4.43218300
C	0.31639000	2.73076900	2.20848000
C	0.74524200	-1.56997500	3.00848700
C	2.23242000	-1.85295500	2.75545200
C	0.44906800	-1.59306900	4.50970200
C	-0.08288200	-2.66652300	2.31885400
C	0.74524200	-1.56997500	-3.00848700
C	-0.08288200	-2.66652300	-2.31885400
C	0.44906800	-1.59306900	-4.50970200
C	2.23242000	-1.85295500	-2.75545200
C	0.68259100	1.56025200	-3.13698300
C	-0.12510600	1.69937500	-4.43218300
C	2.18419500	1.60925800	-3.43514300
C	0.31639000	2.73076900	-2.20848000
H	-0.74700900	2.72589600	1.95477300
H	0.88291800	2.69233700	1.27379600
H	0.54099700	3.67727800	2.71419000
H	-1.19576400	1.60342400	4.24264300
H	0.15769600	0.96563700	5.18715800
H	0.05723300	2.69385000	4.85604700
H	2.43549200	2.59006000	3.85432800
H	2.48530000	0.85568500	4.16707500
H	2.78727900	1.47598800	2.53139000
H	1.11314500	-0.93362400	5.07360900
H	-0.58614400	-1.31482000	4.72111100
H	0.60523500	-2.61013200	4.88799300
H	2.88846700	-1.09793300	3.19481000
H	2.49389200	-2.81739400	3.20561300
H	2.44762400	-1.91393000	1.68490500
H	-1.15075000	-2.54819800	2.51392400
H	0.06662400	-2.65394800	1.23553100
H	0.23126300	-3.64471100	2.70035900
H	2.44762400	-1.91393000	-1.68490500
H	2.88846700	-1.09793300	-3.19481000
H	2.49389200	-2.81739400	-3.20561300
H	0.23126300	-3.64471100	-2.70035900
H	0.06662400	-2.65394800	-1.23553100
H	-1.15075000	-2.54819800	-2.51392400
H	0.60523500	-2.61013200	-4.88799300
H	-0.58614400	-1.31482000	-4.72111100
H	1.11314500	-0.93362400	-5.07360900
H	0.88291800	2.69233700	-1.27379600
H	0.54099700	3.67727800	-2.71419000
H	-0.74700900	2.72589600	-1.95477300
H	2.78727900	1.47598800	-2.53139000
H	2.48530000	0.85568500	-4.16707500
H	2.43549200	2.59006000	-3.85432800
H	0.05723300	2.69385000	-4.85604700
H	0.15769600	0.96563700	-5.18715800
H	-1.19576400	1.60342400	-4.24264300
H	-4.00529500	-0.09141600	2.16223600
H	-5.25200900	-0.13330900	0.00000000
H	-4.00529500	-0.09141600	-2.16223600
H	2.09614300	0.20231400	-0.43126000
H	2.09614300	0.20231400	0.43126000
Co	0.58418700	0.09045000	0.00000000

C_s symmetrical (POCOP)Co(H_2) : E = -3078.93555631

Sum of electronic and thermal Enthalpies -3078.309363

0 1

P	0.02031800	-0.27226400	2.15163800
P	0.02031800	-0.27226400	-2.15163800
O	-0.04929500	1.39294500	2.37948500
C	-0.08447900	2.07998100	1.18428600
C	-0.15357700	3.47103100	1.21621800
C	-0.18681800	4.15347500	0.00000000
C	-0.15357700	3.47103100	-1.21621800
C	-0.08447900	2.07998100	-1.18428600
C	-0.04714600	1.33323000	0.00000000
O	-0.04929500	1.39294500	-2.37948500
C	1.58977000	-0.63369400	3.12984100
C	1.70250300	-2.13516200	3.41252500
C	1.71948700	0.17024200	4.42783400
C	2.72695200	-0.21313700	2.18306500
C	-1.54133500	-0.78696200	3.06747100
C	-1.76888300	-2.29285300	2.87759900
C	-1.55949100	-0.43372200	4.55638600
C	-2.67772000	-0.02992700	2.35986200
C	-1.54133500	-0.78696200	-3.06747100
C	-2.67772000	-0.02992700	-2.35986200
C	-1.55949100	-0.43372200	-4.55638600
C	-1.76888300	-2.29285300	-2.87759900
C	1.58977000	-0.63369400	-3.12984100
C	1.71948700	0.17024200	-4.42783400
C	1.70250300	-2.13516200	-3.41252500
C	2.72695200	-0.21313700	-2.18306500
H	2.67044600	0.84972400	1.93291500
H	2.69810100	-0.77968200	1.24838200
H	3.69065200	-0.39607100	2.67275000
H	1.57299300	1.23715200	4.24891300
H	1.01450600	-0.14975100	5.19521600
H	2.72946400	0.02930100	4.83049300
H	2.70698000	-2.35621800	3.79070200
H	0.98916900	-2.46643500	4.17149200
H	1.55163200	-2.73379300	2.50861400
H	-0.87977700	-1.06142700	5.13749900
H	-1.30336300	0.61461200	4.72697900
H	-2.56920700	-0.59982300	4.94990800
H	-0.99356900	-2.90111500	3.34833800
H	-2.72572200	-2.56898700	3.33507200
H	-1.81568800	-2.55752900	1.81783900
H	-2.59313900	1.04957600	2.50185600
H	-2.68315500	-0.23210200	1.28494800
H	-3.63716100	-0.35720800	2.77636800
H	-1.81568800	-2.55752900	-1.81783900
H	-0.99356900	-2.90111500	-3.34833800
H	-2.72572200	-2.56898700	-3.33507200
H	-3.63716100	-0.35720800	-2.77636800
H	-2.68315500	-0.23210200	-1.28494800
H	-2.59313900	1.04957600	-2.50185600
H	-2.56920700	-0.59982300	-4.94990800
H	-1.30336300	0.61461200	-4.72697900
H	-0.87977700	-1.06142700	-5.13749900
H	2.69810100	-0.77968200	-1.24838200
H	3.69065200	-0.39607100	-2.67275000
H	2.67044600	0.84972400	-1.93291500
H	1.55163200	-2.73379300	-2.50861400
H	0.98916900	-2.46643500	-4.17149200
H	2.70698000	-2.35621800	-3.79070200
H	2.72946400	0.02930100	-4.83049300
H	1.01450600	-0.14975100	-5.19521600
H	1.57299300	1.23715200	-4.24891300
H	-0.17960000	3.99907800	2.16261600
H	-0.23989400	5.23755300	0.00000000
H	-0.17960000	3.99907800	-2.16261600
H	0.57240400	-2.04833100	0.00000000
H	-0.31130000	-2.08542800	0.00000000
Co	0.06059000	-0.58264400	0.00000000

C_s symmetrical (POCOP)Co(H)$_2$: E = -3078.93092772

Sum of electronic and thermal Enthalpies -3078.305500

0 1

C	-0.72433800	-1.55906100	3.06930900
P	-0.26796300	0.00882800	2.13701300
C	-0.72433800	-1.55906100	-3.06930900
H	4.03453500	0.03261900	2.16321800
C	-0.73726000	1.57713000	3.05280200
C	3.50064200	0.01842300	1.21984400
C	2.10792800	-0.00288600	1.18929300
C	4.18025100	0.02629900	0.00000000
C	1.37454700	-0.02420100	0.00000000
P	-0.26796300	0.00882800	-2.13701300
C	2.10792800	-0.00288600	-1.18929300
H	-0.88901500	1.27620600	0.00000000
C	-0.73726000	1.57713000	-3.05280200
C	0.08850700	-1.79611400	-4.34604400
H	-0.13825300	-2.79926200	-4.72562100
H	-0.15196700	-1.08481200	-5.13658100
H	1.16104000	-1.74188300	-4.14961300
C	-2.22782100	-1.57696700	-3.36482700
H	-2.81616100	-1.35222300	-2.47034800
H	-2.50256500	-0.86907500	-4.15063300
H	-2.51192600	-2.57651300	-3.71289000
C	-2.21730100	1.88725700	-2.79040200
H	-2.42960300	1.93815800	-1.72005600
H	-2.46006100	2.85706000	-3.23915300
H	-2.88475000	1.14365100	-3.23099200
C	0.12431600	2.69576900	-2.44444800
H	1.18636500	2.53989800	-2.64476500
H	-0.17385900	3.65024300	-2.89213900
H	-0.01220300	2.76932700	-1.36316400
C	-0.46283900	1.51313400	-4.55811100
H	0.56986400	1.22486400	-4.76898400
H	-1.13411100	0.82216500	-5.07292300
H	-0.62695800	2.50691100	-4.99012700
C	-0.40424300	-2.68141700	-2.06668600

H	-1.00790000	-2.57955600	-1.15833900
H	-0.64266600	-3.65207100	-2.51671500
H	0.65310900	-2.69204200	-1.78729700
C	0.08850700	-1.79611400	4.34604400
H	-0.15196700	-1.08481200	5.13658100
H	-0.13825300	-2.79926200	4.72562100
H	1.16104000	-1.74188300	4.14961300
C	-0.40424300	-2.68141700	2.06668600
H	0.65310900	-2.69204200	1.78729700
H	-0.64266600	-3.65207100	2.51671500
H	-1.00790000	-2.57955600	1.15833900
C	-2.22782100	-1.57696700	3.36482700
H	-2.81616100	-1.35222300	2.47034800
H	-2.51192600	-2.57651300	3.71289000
H	-2.50256500	-0.86907500	4.15063300
C	0.12431600	2.69576900	2.44444800
H	1.18636500	2.53989800	2.64476500
H	-0.01220300	2.76932700	1.36316400
H	-0.17385900	3.65024300	2.89213900
C	-2.21730100	1.88725700	2.79040200
H	-2.46006100	2.85706000	3.23915300
H	-2.42960300	1.93815800	1.72005600
H	-2.88475000	1.14365100	3.23099200
C	-0.46283900	1.51313400	4.55811100
H	-0.62695800	2.50691100	4.99012700
H	-1.13411100	0.82216500	5.07292300
H	0.56986400	1.22486400	4.76898400
O	1.40324100	0.00260400	-2.37735200
O	1.40324100	0.00260400	2.37735200
Co	-0.55010700	-0.09611700	0.00000000
H	-2.06031400	-0.22179200	0.00000000
H	4.03453500	0.03261900	-2.16321800
C	3.50064200	0.01842300	-1.21984400
H	5.26550200	0.04353400	0.00000000

C_s cis-(POCOP)Co(H)$_2$(H$_2$) : E = -3080.11837689

Sum of electronic and thermal Enthalpies -3079.473140

0 1

C	0.67386600	1.61418000	3.07465300
P	0.26467500	0.01689600	2.15158800
C	0.67386600	1.61418000	-3.07465300
H	-4.02797200	-0.04329300	2.16255700
C	0.76595100	-1.50529500	3.16679800
C	-3.49974400	-0.07468500	1.21628500
C	-2.10708500	-0.09476500	1.18299400
C	-4.18466200	-0.07739700	0.00000000
C	-1.37601100	-0.15023600	0.00000000
P	0.26467500	0.01689600	-2.15158800
C	-2.10708500	-0.09476500	-1.18299400
H	0.58146100	-1.71986900	0.00000000
C	0.76595100	-1.50529500	-3.16679800
C	-0.14607400	1.78882400	-4.36139100
H	0.03198700	2.79725100	-4.75097800
H	0.12786500	1.08582500	-5.14554000
H	-1.21529400	1.68760700	-4.16474400
C	2.17763600	1.67156600	-3.36617400
H	2.76700200	1.48725600	-2.46281500
H	2.48236700	0.95686200	-4.13434600
H	2.43308700	2.67195700	-3.73282800
C	2.24112500	-1.83622700	-2.89892200
H	2.44154900	-2.00016200	-1.83845600
H	2.50230600	-2.75480400	-3.43652800
H	2.91479000	-1.04923000	-3.24438000
C	-0.11594600	-2.66543300	-2.67433300
H	-1.16690600	-2.49672400	-2.91659600
H	0.20817500	-3.58588900	-3.17241800
H	-0.04239100	-2.82883500	-1.59784200
C	0.54238800	-1.37395500	-4.67732300
H	-0.48303100	-1.08083300	-4.91315100
H	1.23070900	-0.66498000	-5.14132200
H	0.72358500	-2.34999400	-5.14223700
C	0.31219800	2.78172700	-2.14250700
H	0.95971900	2.81349100	-1.26557000
H	0.43895500	3.71887200	-2.69614600
H	-0.72563800	2.72991200	-1.80243700
C	-0.14607400	1.78882400	4.36139100
H	0.12786500	1.08582500	5.14554000
H	0.03198700	2.79725100	4.75097800
H	-1.21529400	1.68760700	4.16474400
C	0.31219800	2.78172700	2.14250700
H	-0.72563800	2.72991200	1.80243700
H	0.43895500	3.71887200	2.69614600
H	0.95971900	2.81349100	1.26557000
C	2.17763600	1.67156600	3.36617400
H	2.76700200	1.48725600	2.46281500
H	2.43308700	2.67195700	3.73282800
H	2.48236700	0.95686200	4.13434600
C	-0.11594600	-2.66543300	2.67433300
H	-1.16690600	-2.49672400	2.91659600
H	-0.04239100	-2.82883500	1.59784200
H	0.20817500	-3.58588900	3.17241800
C	2.24112500	-1.83622700	2.89892200
H	2.50230600	-2.75480400	3.43652800
H	2.44154900	-2.00016200	1.83845600
H	2.91479000	-1.04923000	3.24438000
C	0.54238800	-1.37395500	4.67732300
H	0.72358500	-2.34999400	5.14223700
H	1.23070900	-0.66498000	5.14132200
H	-0.48303100	-1.08083300	4.91315100
O	-1.39838300	-0.02457600	-2.37114200
O	-1.39838300	-0.02457600	2.37114200
Co	0.56651600	-0.10850900	0.00000000
H	1.38507600	-1.46175100	0.00000000
H	-4.02797200	-0.04329300	-2.16255700
C	-3.49974400	-0.07468500	-1.21628500
H	-5.26963300	-0.06189500	0.00000000
H	0.44365400	1.31543900	0.00000000

H	2.02792000	0.25013400	0.00000000

C_s cis-(POCOP)Co$(H)_2(H_2)$: E = -3080.12026680

Sum of electronic and thermal Enthalpies -3079.475389

0 1

C	-0.80582000	-1.42253100	3.35217600
P	-0.26871400	-0.06566600	2.14810400
C	-0.80582000	-1.42253100	-3.35217600
H	4.02725300	-0.06711700	2.16299700
C	-0.63642300	1.64850600	2.85667700
C	3.49789300	-0.09731200	1.21731900
C	2.10614800	-0.15421600	1.18486300
C	4.18115400	-0.07525600	0.00000000
C	1.37890000	-0.19651000	0.00000000
P	-0.26871400	-0.06566600	-2.14810400
C	2.10614800	-0.15421600	-1.18486300
H	-0.70158400	1.13863800	0.00000000
C	-0.63642300	1.64850600	-2.85667700
C	0.02384600	-1.44118000	-4.64474400
H	-0.25984500	-2.32555600	-5.22656200
H	-0.14411600	-0.57014500	-5.27497100
H	1.09146200	-1.50738200	-4.42648300
C	-2.30070000	-1.28070400	-3.66179900
H	-2.89739800	-1.20814700	-2.74726500
H	-2.51565800	-0.41002100	-4.28504500
H	-2.63905300	-2.16647000	-4.21099600
C	-2.06973300	2.04904200	-2.48103600
H	-2.22699400	1.99866700	-1.40209000
H	-2.24681700	3.07901200	-2.81036400
H	-2.82022500	1.41619900	-2.96049000
C	0.35277900	2.61425400	-2.18477200
H	1.38205000	2.40738800	-2.48532300
H	0.10514500	3.63652700	-2.49127700
H	0.29922000	2.56409200	-1.09633900
C	-0.44507100	1.77843800	-4.37166300
H	0.55540300	1.47065900	-4.68422400
H	-1.18608300	1.21326400	-4.94010300
H	-0.56612500	2.83274400	-4.64562500
C	-0.57997700	-2.76975800	-2.64703000
H	-1.27893000	-2.92056200	-1.82340800
H	-0.74595500	-3.57512200	-3.37062600
H	0.44083600	-2.86977500	-2.26716800
C	0.02384600	-1.44118000	4.64474400
H	-0.14411600	-0.57014500	5.27497100
H	-0.25984500	-2.32555600	5.22656200
H	1.09146200	-1.50738200	4.42648300
C	-0.57997700	-2.76975800	2.64703000
H	0.44083600	-2.86977500	2.26716800
H	-0.74595500	-3.57512200	3.37062600
H	-1.27893000	-2.92056200	1.82340800
C	-2.30070000	-1.28070400	3.66179900
H	-2.89739800	-1.20814700	2.74726500
H	-2.63905300	-2.16647000	4.21099600
H	-2.51565800	-0.41002100	4.28504500
C	0.35277900	2.61425400	2.18477200
H	1.38205000	2.40738800	2.48532300
H	0.29922000	2.56409200	1.09633900
H	0.10514500	3.63652700	2.49127700
C	-2.06973300	2.04904200	2.48103600
H	-2.24681700	3.07901200	2.81036400
H	-2.22699400	1.99866700	1.40209000
H	-2.82022500	1.41619900	2.96049000
C	-0.44507100	1.77843800	4.37166300
H	-0.56612500	2.83274400	4.64562500
H	-1.18608300	1.21326400	4.94010300
H	0.55540300	1.47065900	4.68422400
O	1.39417300	-0.16616300	-2.37334000
O	1.39417300	-0.16616300	2.37334000
Co	-0.56266500	-0.29825500	0.00000000
H	-2.06557100	-0.22863100	0.00000000
H	4.02725300	-0.06711700	-2.16299700
C	3.49789300	-0.09731200	-1.21731900
H	5.26536800	-0.03119100	0.00000000
H	-0.27020900	-1.87476700	0.00000000
H	-1.10533900	-1.78294700	0.00000000

C_2 trans-(POCOP)Co$(H)_2(H_2)$: E = -3080.11778080

Sum of electronic and thermal Enthalpies -3079.472781

0 1

P	0.71666000	2.04659800	0.26113200
P	-0.71666000	-2.04659800	0.26113200
O	0.59079400	2.29883100	-1.38259500
C	0.29217700	1.14400800	-2.08451000
C	0.00000000	0.00000000	-4.16478000
C	-0.29973800	-1.17546400	-3.47616900
C	-0.29217700	-1.14400800	-2.08451000
C	0.00000000	0.00000000	-1.34632800
O	-0.59079400	-2.29883100	-1.38259500
C	2.57015900	2.31928200	0.54272400
C	2.93454300	1.81363100	1.94546900
C	3.06225200	3.76001700	0.37179700
C	3.28786000	1.45147300	-0.50438000
C	-0.29154400	3.52472800	0.87101400
C	-0.04586200	3.74090900	2.36860000
C	0.00000000	4.80993300	0.08125900
C	-1.77490500	3.18745700	0.65377300
C	-2.57015900	-2.31928200	0.54272400
C	-3.28786000	-1.45147300	-0.50438000
C	-3.06225200	-3.76001700	0.37179700
C	-2.93454300	-1.81363100	1.94546900
C	0.29154400	-3.52472800	0.87101400
C	0.00000000	-4.80993300	0.08125900
C	0.04586200	-3.74090900	2.36860000
C	1.77490500	-3.18745700	0.65377300
H	3.14002800	1.84106100	-1.51387200
H	2.94266800	0.41561900	-0.48009700
H	4.36203400	1.46138900	-0.28801100
H	2.78770900	4.17409800	-0.60118000

H	2.69926600	4.42617200	1.15721800
H	4.15678000	3.76024000	0.43114100
H	4.01677900	1.90971000	2.08764200
H	2.44869000	2.38527500	2.74078400
H	2.67128200	0.76022000	2.06310400
H	0.99149000	5.21595700	0.27010100
H	-0.10959200	4.64585100	-0.99264700
H	-0.72755700	5.57247600	0.38118100
H	0.96548100	4.09625900	2.57894500
H	-0.74319000	4.49963800	2.74047600
H	-0.21889400	2.82789500	2.94734600
H	-1.98316900	2.93840200	-0.39006900
H	-2.10001300	2.34786900	1.26823100
H	-2.37278700	4.06692500	0.91857500
H	-2.67128200	-0.76022000	2.06310400
H	-2.44869000	-2.38527500	2.74078400
H	-4.01677900	-1.90971000	2.08764200
H	-4.36203400	-1.46138900	-0.28801100
H	-2.94266800	-0.41561900	-0.48009700
H	-3.14002800	-1.84106100	-1.51387200
H	-4.15678000	-3.76024000	0.43114100
H	-2.78770900	-4.17409800	-0.60118000
H	-2.69926600	-4.42617200	1.15721800
H	2.10001300	-2.34786900	1.26823100
H	2.37278700	-4.06692500	0.91857500
H	1.98316900	-2.93840200	-0.39006900
H	0.21889400	-2.82789500	2.94734600
H	-0.96548100	-4.09625900	2.57894500
H	0.74319000	-4.49963800	2.74047600
H	0.72755700	-5.57247600	0.38118100
H	-0.99149000	-5.21595700	0.27010100
H	0.10959200	-4.64585100	-0.99264700
H	-0.53687600	-2.09506300	-3.99902800
H	1.41422400	-0.48614200	0.55766200
H	0.40389100	-0.15255500	2.08449000
H	-0.40389100	0.15255500	2.08449000
H	-1.41422400	0.48614200	0.55766200
H	0.00000000	0.00000000	-5.24960300
C	0.29973800	1.17546400	-3.47616900
H	0.53687600	2.09506300	-3.99902800
Co	0.00000000	0.00000000	0.57203300

C_s (POCOP)Co(H_2)$_2$: E = -3080.11220174

Sum of electronic and thermal Enthalpies -3079.467749

0 1

P	-0.26859000	0.03372300	2.16614800
P	-0.26859000	0.03372300	-2.16614800
O	1.38395500	-0.10294800	2.37543000
C	2.07182700	-0.16865100	1.17614700
C	3.45864300	-0.29114100	1.21178700
C	4.14618800	-0.35176600	0.00000000
C	3.45864300	-0.29114100	-1.21178700
C	2.07182700	-0.16865100	-1.17614700
C	1.32292000	-0.10335600	0.00000000
O	1.38395500	-0.10294800	-2.37543000
C	-0.84179500	-1.50027600	3.11749000
C	-2.35328300	-1.69569100	2.93967000
C	-0.50573800	-1.48809700	4.61236600
C	-0.09669000	-2.68648400	2.48107100
C	-0.54893500	1.62157000	3.15960500
C	-2.04386800	1.83203500	3.41977300
C	0.23853000	1.65809900	4.47748000
C	-0.01622300	2.77260100	2.28801000
C	-0.54893500	1.62157000	-3.15960500
C	-0.01622300	2.77260100	-2.28801000
C	0.23853000	1.65809900	-4.47748000
C	-2.04386800	1.83203500	-3.41977300
C	-0.84179500	-1.50027600	-3.11749000
C	-0.50573800	-1.48809700	-4.61236600
C	-2.35328300	-1.69569100	-2.93967000
C	-0.09669000	-2.68648400	-2.48107100
H	0.97921600	-2.61962800	2.65482200
H	-0.25898200	-2.75155000	1.40308500
H	-0.46131000	-3.61438700	2.93568700
H	0.54429900	-1.24863000	4.79375700
H	-1.13266300	-0.79155800	5.17295700
H	-0.69347200	-2.48806300	5.02028900
H	-2.65102800	-2.62552600	3.43733600
H	-2.93427700	-0.88520500	3.38548200
H	-2.63704700	-1.77493000	1.88882500
H	-0.16013900	0.98407600	5.23319800
H	1.29152900	1.41819300	4.31714900
H	0.18288000	2.67324300	4.88647100
H	-2.43857100	1.12167400	4.15076600
H	-2.20264700	2.83776900	3.82482500
H	-2.63454600	1.74799000	2.50223500
H	1.01922000	2.60405100	1.98113200
H	-0.61541300	2.92536200	1.39018100
H	-0.04960100	3.69840200	2.87315300
H	-2.63454600	1.74799000	-2.50223500
H	-2.43857100	1.12167400	-4.15076600
H	-2.20264700	2.83776900	-3.82482500
H	-0.04960100	3.69840200	-2.87315300
H	-0.61541300	2.92536200	-1.39018100
H	1.01922000	2.60405100	-1.98113200
H	0.18288000	2.67324300	-4.88647100
H	1.29152900	1.41819300	-4.31714900
H	-0.16013900	0.98407600	-5.23319800
H	-0.25898200	-2.75155000	-1.40308500
H	-0.46131000	-3.61438700	-2.93568700
H	0.97921600	-2.61962800	-2.65482200
H	-2.63704700	-1.77493000	-1.88882500
H	-2.93427700	-0.88520500	-3.38548200
H	-2.65102800	-2.62552600	-3.43733600
H	-0.69347200	-2.48806300	-5.02028900
H	-1.13266300	-0.79155800	-5.17295700
H	0.54429900	-1.24863000	-4.79375700

H	3.97911300	-0.33606000	2.16187000
H	5.22706700	-0.44600200	0.00000000
H	3.97911300	-0.33606000	-2.16187000
Co	-0.63111500	0.04332300	0.00000000
H	-0.96930800	1.53938400	0.00000000
H	-1.77864600	1.08596600	0.00000000
H	-1.09820800	-1.44642900	0.00000000
H	-1.84374600	-0.93442700	0.00000000

C_2 (POCOP)Co(H_2)$_2$: E = -3080.11225418

Sum of electronic and thermal Enthalpies -3079.467928

0 1

P	0.00000000	2.16612500	0.27109000
P	0.00000000	-2.16612500	0.27109000
O	0.00496400	2.37543900	-1.38723100
C	0.00580500	1.17621900	-2.07840900
C	0.00000000	0.00000000	-4.16077900
C	-0.00769200	-1.21181600	-3.47062900
C	-0.00580500	-1.17621900	-2.07840900
C	0.00000000	0.00000000	-1.32690200
O	-0.00496400	-2.37543900	-1.38723100
C	1.58495100	3.09922300	0.72097000
C	1.89811300	2.91946700	2.21255300
C	1.56414500	4.59441000	0.38625200
C	2.70022500	2.44754600	-0.11490300
C	-1.55049500	3.17587000	0.67468300
C	-1.64204800	3.43829300	2.18115100
C	-1.63429000	4.49465000	-0.10815900
C	-2.74932000	2.31714300	0.23408100
C	-1.58495100	-3.09922300	0.72097000
C	-2.70022500	-2.44754600	-0.11490300
C	-1.56414500	-4.59441000	0.38625200
C	-1.89811300	-2.91946700	2.21255300
C	1.55049500	-3.17587000	0.67468300
C	1.63429000	-4.49465000	-0.10815900
C	1.64204800	-3.43829300	2.18115100
C	2.74932000	-2.31714300	0.23408100
H	2.55202700	2.62475400	-1.18215700
H	2.76027600	1.36822900	0.04031000
H	3.66036300	2.88783700	0.17660500
H	1.24701600	4.77936700	-0.64238000
H	0.92433200	5.16233300	1.06483500
H	2.58046200	4.98983300	0.49690300
H	2.84974900	3.41485700	2.43582200
H	1.13743000	3.36709400	2.85612300
H	1.99767800	1.86846800	2.48928200
H	-0.92235000	5.24251600	0.23562500
H	-1.47988500	4.33211900	-1.17668700
H	-2.63692700	4.91563900	0.02728200
H	-0.89364500	4.15920200	2.51989100
H	-2.62701700	3.85707600	2.41620100
H	-1.52596800	2.51940300	2.76423800
H	-2.66088900	1.99889100	-0.80792500
H	-2.87217100	1.42827900	0.85309800
H	-3.66170300	2.91642100	0.32814700
H	-1.99767800	-1.86846800	2.48928200
H	-1.13743000	-3.36709400	2.85612300
H	-2.84974900	-3.41485700	2.43582200
H	-3.66036300	-2.88783700	0.17660500
H	-2.76027600	-1.36822900	0.04031000
H	-2.55202700	-2.62475400	-1.18215700
H	-2.58046200	-4.98983300	0.49690300
H	-1.24701600	-4.77936700	-0.64238000
H	-0.92433200	-5.16233300	1.06483500
H	2.87217100	-1.42827900	0.85309800
H	3.66170300	-2.91642100	0.32814700
H	2.66088900	-1.99889100	-0.80792500
H	1.52596800	-2.51940300	2.76423800
H	0.89364500	-4.15920200	2.51989100
H	2.62701700	-3.85707600	2.41620100
H	2.63692700	-4.91563900	0.02728200
H	0.92235000	-5.24251600	0.23562500
H	1.47988500	-4.33211900	-1.17668700
H	-0.01372400	-2.16186100	-3.99306100
H	1.49346300	0.01903400	1.03337300
H	1.01048800	-0.01481500	1.81206900
H	-1.01048800	0.01481500	1.81206900
H	-1.49346300	-0.01903400	1.03337300
H	0.00000000	0.00000000	-5.24575900
C	0.00769200	1.21181600	-3.47062900
H	0.01372400	2.16186100	-3.99306100
Co	0.00000000	0.00000000	0.63291100

Optimized geometries and energies (PBE0)

C_2 symmetrical singlet (POCOP)Co: E = -3076.12767697
Sum of electronic and thermal Enthalpies -3075.519560
0 1

P	-1.61180900	1.44090100	0.28397300
P	1.61180900	-1.44090100	0.28397300
O	-1.79104900	1.57077400	-1.37798200
C	-0.88773600	0.78215600	-2.06835000
C	0.00000000	0.00000000	-4.14719700
C	0.91088800	-0.80413000	-3.46046600
C	0.88773600	-0.78215600	-2.06835000
C	0.00000000	0.00000000	-1.31957000
O	1.79104900	-1.57077400	-1.37798200
C	-1.21661500	3.22252900	0.73901100
C	-0.79087600	3.25207300	2.21277400
C	-2.33016300	4.23855500	0.48538000
C	0.00000000	3.58326700	-0.12774500
C	-3.37380600	0.95737100	0.73148400
C	-3.58618300	1.10246200	2.24083100
C	-4.45229200	1.71858900	-0.04484700
C	-3.46248800	-0.53013200	0.35179500
C	1.21661500	-3.22252900	0.73901100
C	0.00000000	-3.58326700	-0.12774500
C	2.33016300	-4.23855500	0.48538000
C	0.79087600	-3.25207300	2.21277400
C	3.37380600	-0.95737100	0.73148400
C	4.45229200	-1.71858900	-0.04484700
C	3.58618300	-1.10246200	2.24083100
C	3.46248800	0.53013200	0.35179500
H	-0.26313800	3.63434600	-1.18789600
H	0.80515000	2.84816500	-0.01452100
H	0.38098300	4.56468400	0.18195900
H	-2.70608500	4.17798500	-0.54042800
H	-3.16977500	4.11466700	1.17582700
H	-1.93315300	5.25099300	0.63607100
H	-0.44654900	4.26197500	2.46929200
H	-1.60743400	3.00007500	2.89565100
H	0.03929100	2.56040400	2.39891500
H	-4.53056700	2.76507600	0.25509000
H	-4.26268300	1.68099200	-1.12101300
H	-5.42564800	1.24801700	0.14517500
H	-3.63781800	2.15021300	2.55250400
H	-4.53617400	0.62989300	2.52027100
H	-2.79301400	0.60869300	2.81554500
H	-3.28759600	-0.68226200	-0.71824200
H	-2.72704600	-1.12985400	0.89923800
H	-4.46661000	-0.90448100	0.58971200
H	-0.03929100	-2.56040400	2.39891500
H	1.60743400	-3.00007500	2.89565100
H	0.44654900	-4.26197500	2.46929200
H	-0.38098300	-4.56468400	0.18195900
H	-0.80515000	-2.84816500	-0.01452100
H	0.26313800	-3.63434600	-1.18789600
H	1.93315300	-5.25099300	0.63607100
H	2.70608500	-4.17798500	-0.54042800
H	3.16977500	-4.11466700	1.17582700
H	2.72704600	1.12985400	0.89923800
H	4.46661000	0.90448100	0.58971200
H	3.28759600	0.68226200	-0.71824200
H	2.79301400	-0.60869300	2.81554500
H	3.63781800	-2.15021300	2.55250400
H	4.53617400	-0.62989300	2.52027100
H	5.42564800	-1.24801700	0.14517500
H	4.53056700	-2.76507600	0.25509000
H	4.26268300	-1.68099200	-1.12101300
H	1.62309200	-1.43236700	-3.98660200
H	0.00000000	0.00000000	-5.23369700
C	-0.91088800	0.80413000	-3.46046600
H	-1.62309200	1.43236700	-3.98660200
Co	0.00000000	0.00000000	0.55227200

C_s symmetrical singlet (POCOP)Co: E = -3076.12760405
Sum of electronic and thermal Enthalpies -3075.519384
0 1

P	0.27895400	0.04801300	2.16213800
P	0.27895400	0.04801300	-2.16213800
O	-1.37435000	-0.12035600	2.38251900
C	-2.06059400	-0.19487800	1.18321700
C	-3.44338600	-0.35640600	1.21506000
C	-4.12563900	-0.43422000	0.00000000
C	-3.44338600	-0.35640600	-1.21506000
C	-2.06059400	-0.19487800	-1.18321700
C	-1.31736200	-0.10348900	0.00000000
O	-1.37435000	-0.12035600	-2.38251900
C	0.55112800	1.61629600	3.16557700
C	2.04589000	1.81366100	3.43142100
C	-0.24398200	1.67189600	4.47328100
C	0.05100100	2.74280200	2.24644200
C	0.91485500	-1.48690800	3.04350200
C	2.41471500	-1.61499100	2.74799800
C	0.65925400	-1.54528100	4.54966100
C	0.18394700	-2.65608200	2.36540900
C	0.91485500	-1.48690800	-3.04350200
C	0.18394700	-2.65608200	-2.36540900
C	0.65925400	-1.54528100	-4.54966100
C	2.41471500	-1.61499100	-2.74799800
C	0.55112800	1.61629600	-3.16557700
C	-0.24398200	1.67189600	-4.47328100
C	2.04589000	1.81366100	-3.43142100
C	0.05100100	2.74280200	-2.24644200
H	-1.00737500	2.61791700	1.99556600
H	0.61452000	2.77663300	1.30791900
H	0.16785600	3.70639900	2.75918200
H	-1.30357900	1.46601400	4.29935000
H	0.12489100	0.97023300	5.22350600
H	-0.15946500	2.68111300	4.89687800
H	2.21237100	2.82025100	3.83513000
H	2.43409700	1.09916000	4.16399400
H	2.63978800	1.72694500	2.51334700

H	1.26429800	-0.82044300	5.10246600
H	-0.39546000	-1.37545800	4.78658700
H	0.92833900	-2.54278400	4.92103300
H	3.00651500	-0.81322700	3.19898500
H	2.78385100	-2.56581900	3.15298900
H	2.60469100	-1.61767000	1.66809100
H	-0.88899600	-2.63707600	2.57566300
H	0.31662200	-2.63270700	1.27773900
H	0.59401700	-3.60133100	2.74297100
H	2.60469100	-1.61767000	-1.66809100
H	3.00651500	-0.81322700	-3.19898500
H	2.78385100	-2.56581900	-3.15298900
H	0.59401700	-3.60133100	-2.74297100
H	0.31662200	-2.63270700	-1.27773900
H	-0.88899600	-2.63707600	-2.57566300
H	0.92833900	-2.54278400	-4.92103300
H	-0.39546000	-1.37545800	-4.78658700
H	1.26429800	-0.82044300	-5.10246600
H	0.61452000	2.77663300	-1.30791900
H	0.16785600	3.70639900	-2.75918200
H	-1.00737500	2.61791700	-1.99556600
H	2.63978800	1.72694500	-2.51334700
H	2.43409700	1.09916000	-4.16399400
H	2.21237100	2.82025100	-3.83513000
H	-0.15946500	2.68111300	-4.89687800
H	0.12489100	0.97023300	-5.22350600
H	-1.30357900	1.46601400	-4.29935000
H	-3.96587800	-0.42004900	2.16464600
H	-5.20485500	-0.55994800	0.00000000
H	-3.96587800	-0.42004900	-2.16464600
Co	0.54324800	0.10051900	0.00000000

C_2 symmetrical triplet (POCOP)Co: E = -3076.15579883
Sum of electronic and thermal Enthalpies -3075.548160
0 3

P	0.00316700	2.20571400	0.32917900
P	-0.00316700	-2.20571400	0.32917900
O	-0.00332200	2.37900500	-1.35250000
C	0.00000000	1.18544300	-2.06062600
C	0.00000000	0.00000000	-4.13477500
C	-0.00089600	-1.22125500	-3.45464700
C	0.00000000	-1.18544300	-2.06062600
C	0.00000000	0.00000000	-1.33386600
O	0.00332200	-2.37900500	-1.35250000
C	1.56337600	3.17470200	0.72118600
C	1.84372000	3.09538000	2.22614500
C	1.53992800	4.63028800	0.25392500
C	2.67753100	2.42302600	-0.02511800
C	-1.58057900	3.14350900	0.71774000
C	-1.61266800	3.53562900	2.19707400
C	-1.82089500	4.36624300	-0.17124200
C	-2.69052400	2.11325600	0.44957900
C	-1.56337600	-3.17470200	0.72118600
C	-2.67753100	-2.42302600	-0.02511800
C	-1.53992800	-4.63028800	0.25392500
C	-1.84372000	-3.09538000	2.22614500
C	1.58057900	-3.14350900	0.71774000
C	1.82089500	-4.36624300	-0.17124200
C	1.61266800	-3.53562900	2.19707400
C	2.69052400	-2.11325600	0.44957900
H	2.54076800	2.46905600	-1.10882500
H	2.72202100	1.36700300	0.26636100
H	3.64431700	2.87961200	0.22131300
H	1.24900700	4.70844100	-0.79779400
H	0.85981200	5.24265200	0.85371400
H	2.54394200	5.06174700	0.35939400
H	2.82797300	3.53482800	2.43196400
H	1.10796000	3.64266700	2.82140400
H	1.85776100	2.05732000	2.57642900
H	-1.10977000	5.17157500	0.02440600
H	-1.75812300	4.10309600	-1.23008400
H	-2.82709200	4.75821000	0.02657100
H	-0.92498600	4.35734900	2.41886300
H	-2.62284700	3.87475800	2.45884500
H	-1.36611300	2.68993000	2.84976900
H	-2.67983800	1.76358200	-0.58809400
H	-2.59399900	1.24180400	1.10929800
H	-3.66850700	2.57236600	0.64271200
H	-1.85776100	-2.05732000	2.57642900
H	-1.10796000	-3.64266700	2.82140400
H	-2.82797300	-3.53482800	2.43196400
H	-3.64431700	-2.87961200	0.22131300
H	-2.72202100	-1.36700300	0.26636100
H	-2.54076800	-2.46905600	-1.10882500
H	-2.54394200	-5.06174700	0.35939400
H	-1.24900700	-4.70844100	-0.79779400
H	-0.85981200	-5.24265200	0.85371400
H	2.59399900	-1.24180400	1.10929800
H	3.66850700	-2.57236600	0.64271200
H	2.67983800	-1.76358200	-0.58809400
H	1.36611300	-2.68993000	2.84976900
H	0.92498600	-4.35734900	2.41886300
H	2.62284700	-3.87475800	2.45884500
H	2.82709200	-4.75821000	0.02657100
H	1.10977000	-5.17157500	0.02440600
H	1.75812300	-4.10309600	-1.23008400
H	-0.00132100	-2.16521000	-3.99160100
H	0.00000000	0.00000000	-5.22170800
C	0.00089600	1.22125500	-3.45464700
H	0.00132100	2.16521000	-3.99160100
Co	0.00000000	0.00000000	0.62447100

C_s symmetrical triplet (POCOP)Co: E = -3076.15564537
Sum of electronic and thermal Enthalpies -3075.547982
0 3

P	0.33089700	0.01046100	2.20740300
P	0.33089700	0.01046100	-2.20740300
O	-1.35079900	-0.00575900	2.37898000
C	-2.05844800	-0.02078000	1.18532100
C	-3.45207300	-0.05420100	1.22119100

C	-4.13209900	-0.06966900	0.00000000
C	-3.45207300	-0.05420100	-1.22119100
C	-2.05844800	-0.02078000	-1.18532100
C	-1.33171900	-0.00207600	0.00000000
O	-1.35079900	-0.00575900	-2.37898000
C	0.69471900	1.57735200	3.18253400
C	2.17490300	1.62691500	3.56975000
C	-0.19318100	1.76941000	4.41475900
C	0.40004900	2.70800100	2.18301100
C	0.74222800	-1.56457300	3.14536500
C	2.25102200	-1.82349600	3.06294200
C	0.27378800	-1.57919300	4.60064700
C	0.01284100	-2.67361200	2.37013000
C	0.74222800	-1.56457300	-3.14536500
C	0.01284100	-2.67361200	-2.37013000
C	0.27378800	-1.57919300	-4.60064700
C	2.25102200	-1.82349600	-3.06294200
C	0.69471900	1.57735200	-3.18253400
C	-0.19318100	1.76941000	-4.41475900
C	2.17490300	1.62691500	-3.56975000
C	0.40004900	2.70800100	-2.18301100
H	-0.63759700	2.68271300	1.83412500
H	1.05890100	2.65088200	1.30822900
H	0.57104500	3.67692000	2.66915300
H	-1.25179500	1.69412400	4.15413600
H	0.01886800	1.04191700	5.20100600
H	-0.01230400	2.76879000	4.83164800
H	2.42022500	2.63358000	3.93083700
H	2.41254800	0.92489700	4.37482400
H	2.82856900	1.41134000	2.71637400
H	0.86743300	-0.90813300	5.22861400
H	-0.78057400	-1.30011500	4.68578200
H	0.38883200	-2.59201900	5.00828300
H	2.83580600	-1.08904700	3.62312300
H	2.46939000	-2.81202600	3.48649100
H	2.60264400	-1.81594700	2.02523700
H	-1.07274600	-2.55058400	2.41062400
H	0.31252000	-2.69662100	1.31559300
H	0.26768100	-3.64557000	2.81086500
H	2.60264400	-1.81594700	-2.02523700
H	2.83580600	-1.08904700	-3.62312300
H	2.46939000	-2.81202600	-3.48649100
H	0.26768100	-3.64557000	-2.81086500
H	0.31252000	-2.69662100	-1.31559300
H	-1.07274600	-2.55058400	-2.41062400
H	0.38883200	-2.59201900	-5.00828300
H	-0.78057400	-1.30011500	-4.68578200
H	0.86743300	-0.90813300	-5.22861400
H	1.05890100	2.65088200	-1.30822900
H	0.57104500	3.67692000	-2.66915300
H	-0.63759700	2.68271300	-1.83412500
H	2.82856900	1.41134000	-2.71637400
H	2.41254800	0.92489700	-4.37482400
H	2.42022500	2.63358000	-3.93083700
H	-0.01230400	2.76879000	-4.83164800
H	0.01886800	1.04191700	-5.20100600
H	-1.25179500	1.69412400	-4.15413600
H	-3.98876000	-0.06807000	2.16520100
H	-5.21872600	-0.09544100	0.00000000
H	-3.98876000	-0.06807000	-2.16520100
Co	0.62651700	0.02593700	0.00000000

D_2 triplet $[(POCOP)Co]_2Hg$: E = -6305.84027449

Sum of electronic and thermal Enthalpies -6304.618546

0 3

Hg	0.00000000	0.00000000	0.00000000
Co	0.00000000	-0.00000000	2.76433900
Co	-0.00000000	-0.00000000	-2.76433900
P	-1.46138700	1.59343300	3.08984400
P	1.46138700	-1.59343300	3.08984400
C	0.00000000	-0.00000000	4.72077400
P	-1.46138700	-1.59343300	-3.08984400
P	1.46138700	1.59343300	-3.08984400
C	-0.00000000	-0.00000000	-4.72077400
O	-1.44147800	1.88297300	4.76537900
C	-3.28741400	1.15858200	2.93274400
C	-1.07528800	3.35372200	2.54661100
O	1.44147800	-1.88297300	4.76537900
C	3.28741400	-1.15858200	2.93274400
C	1.07528800	-3.35372200	2.54661100
C	-0.71796700	0.94694700	5.45598800
C	0.71796700	-0.94694700	5.45598800
O	-1.44147800	-1.88297300	-4.76537900
C	-3.28741400	-1.15858200	-2.93274400
C	-1.07528800	-3.35372200	-2.54661100
O	1.44147800	1.88297300	-4.76537900
C	3.28741400	1.15858200	-2.93274400
C	1.07528800	3.35372200	-2.54661100
C	-0.71796700	-0.94694700	-5.45598800
C	0.71796700	0.94694700	-5.45598800
C	-3.60101500	0.76826800	1.49008400
C	-4.22976000	2.26684500	3.40515700
C	-3.48688900	-0.07951600	3.82220700
C	-1.53204000	3.57308300	1.10356700
C	-1.66304500	4.43891400	3.45527600
C	0.45752400	3.43860800	2.62495500
C	3.48688900	0.07951600	3.82220700
C	4.22976000	-2.26684500	3.40515700
C	3.60101500	-0.76826800	1.49008400
C	1.66304500	-4.43891400	3.45527600
C	1.53204000	-3.57308300	1.10356700
C	-0.45752400	-3.43860800	2.62495500
C	-0.73410500	0.97237100	6.85074400
C	0.73410500	-0.97237100	6.85074400
C	-3.60101500	-0.76826800	-1.49008400
C	-4.22976000	-2.26684500	-3.40515700
C	-3.48688900	0.07951600	-3.82220700
C	-1.53204000	-3.57308300	-1.10356700
C	-1.66304500	-4.43891400	-3.45527600

C	0.45752400	-3.43860800	-2.62495500
C	3.48688900	-0.07951600	-3.82220700
C	4.22976000	2.26684500	-3.40515700
C	3.60101500	0.76826800	-1.49008400
C	1.66304500	4.43891400	-3.45527600
C	1.53204000	3.57308300	-1.10356700
C	-0.45752400	3.43860800	-2.62495500
C	-0.73410500	-0.97237100	-6.85074400
C	0.73410500	0.97237100	-6.85074400
H	-4.64195200	0.42631900	1.42455300
H	-3.48119700	1.59917500	0.78948700
H	-2.95345100	-0.04924900	1.16192900
H	-3.97057700	2.61783300	4.40814600
H	-4.23705800	3.12098800	2.72167700
H	-5.25311900	1.87110400	3.44074700
H	-3.32073300	0.14519300	4.87919200
H	-2.81359000	-0.89562100	3.53832100
H	-4.51938700	-0.43296500	3.70634800
H	-2.62156800	3.64179400	1.02573500
H	-1.11689600	4.51782900	0.73159200
H	-1.18695400	2.77452100	0.43809300
H	-2.75204300	4.49079800	3.40167900
H	-1.37761200	4.28404300	4.49819600
H	-1.27056300	5.41202800	3.13256200
H	0.81127100	3.29469800	3.65152100
H	0.93513300	2.68358600	1.99037400
H	0.78573900	4.43094900	2.29004400
H	4.51938700	0.43296500	3.70634800
H	2.81359000	0.89562100	3.53832100
H	3.32073300	-0.14519300	4.87919200
H	5.25311900	-1.87110400	3.44074700
H	3.97057700	-2.61783300	4.40814600
H	4.23705800	-3.12098800	2.72167700
H	2.95345100	0.04924900	1.16192900
H	3.48119700	-1.59917500	0.78948700
H	4.64195200	-0.42631900	1.42455300
H	1.27056300	-5.41202800	3.13256200
H	2.75204300	-4.49079800	3.40167900
H	1.37761200	-4.28404300	4.49819600
H	1.18695400	-2.77452100	0.43809300
H	2.62156800	-3.64179400	1.02573500
H	1.11689600	-4.51782900	0.73159200
H	-0.93513300	-2.68358600	1.99037400
H	-0.78573900	-4.43094900	2.29004400
H	-0.81127100	-3.29469800	3.65152100
C	0.00000000	-0.00000000	7.53096500
H	-1.30590800	1.72630400	7.38255700
H	1.30590800	-1.72630400	7.38255700
H	-4.64195200	-0.42631900	-1.42455300
H	-3.48119700	-1.59917500	-0.78948700
H	-2.95345100	0.04924900	-1.16192900
H	-3.97057700	-2.61783300	-4.40814600
H	-4.23705800	-3.12098800	-2.72167700
H	-5.25311900	-1.87110400	-3.44074700
H	-3.32073300	-0.14519300	-4.87919200
H	-2.81359000	0.89562100	-3.53832100
H	-4.51938700	0.43296500	-3.70634800
H	-2.62156800	-3.64179400	-1.02573500
H	-1.11689600	-4.51782900	-0.73159200
H	-1.18695400	-2.77452100	-0.43809300
H	-2.75204300	-4.49079800	-3.40167900
H	-1.37761200	-4.28404300	-4.49819600
H	-1.27056300	-5.41202800	-3.13256200
H	0.81127100	-3.29469800	-3.65152100
H	0.93513300	-2.68358600	-1.99037400
H	0.78573900	-4.43094900	-2.29004400
H	4.51938700	-0.43296500	-3.70634800
H	2.81359000	-0.89562100	-3.53832100
H	3.32073300	0.14519300	-4.87919200
H	5.25311900	1.87110400	-3.44074700
H	3.97057700	2.61783300	-4.40814600
H	4.23705800	3.12098800	-2.72167700
H	2.95345100	-0.04924900	-1.16192900
H	3.48119700	1.59917500	-0.78948700
H	4.64195200	0.42631900	-1.42455300
H	1.27056300	5.41202800	-3.13256200
H	2.75204300	4.49079800	-3.40167900
H	1.37761200	4.28404300	-4.49819600
H	1.18695400	2.77452100	-0.43809300
H	2.62156800	3.64179400	-1.02573500
H	1.11689600	4.51782900	-0.73159200
H	-0.93513300	2.68358600	-1.99037400
H	-0.78573900	4.43094900	-2.29004400
H	-0.81127100	3.29469800	-3.65152100
C	-0.00000000	-0.00000000	-7.53096500
H	-1.30590800	-1.72630400	-7.38255700
H	1.30590800	1.72630400	-7.38255700
H	0.00000000	-0.00000000	8.61792400
H	-0.00000000	-0.00000000	-8.61792400

C_s symmetrical (POCOP)Co(H_2): E = -3077.33480733

Sum of electronic and thermal Enthalpies -3076.709767

0 1

C	0.63598300	1.58795600	3.12287200
P	0.27225100	0.01993200	2.14667500
C	0.63598300	1.58795600	-3.12287200
H	-3.99986700	-0.17681400	2.16430700
C	0.78558800	-1.54095600	3.06067400
C	-3.47134900	-0.15060800	1.21658400
C	-2.07981500	-0.08186300	1.18507500
C	-4.15378400	-0.18351600	0.00000000
C	-1.33285800	-0.04430700	0.00000000
P	0.27225100	0.01993200	-2.14667500
C	-2.07981500	-0.08186300	-1.18507500
H	2.07694200	-0.32994300	0.00000000
C	0.78558800	-1.54095600	-3.06067400
C	-0.16792500	1.72020300	-4.41958000
H	-0.02486700	2.73167900	-4.82146200
H	0.15054300	1.01428900	-5.18872200

H	-1.23638000	1.57538400	-4.23951300
C	2.13686000	1.69740000	-3.40500800
H	2.73550500	1.54294800	-2.49993000
H	2.46663200	0.98368900	-4.16635900
H	2.36032200	2.70348000	-3.78155700
C	2.29026300	-1.76978200	-2.86992200
H	2.55427900	-1.81585300	-1.80847000
H	2.56530100	-2.72873200	-3.32696500
H	2.90041700	-0.99457900	-3.34168300
C	0.02685200	-2.67445800	-2.35196800
H	-1.05407600	-2.58724300	-2.49325600
H	0.35236600	-3.63601000	-2.76861200
H	0.23015700	-2.67881100	-1.27562300
C	0.43251400	-1.55816600	-4.54873700
H	-0.61677400	-1.29951800	-4.71926000
H	1.06237000	-0.87840400	-5.13018200
H	0.59708400	-2.56950000	-4.94257100
C	0.21743500	2.72311200	-2.17399700
H	0.78486100	2.69105400	-1.23809200
H	0.40178100	3.68866600	-2.66262300
H	-0.84691100	2.66708200	-1.92325000
C	-0.16792500	1.72020300	4.41958000
H	0.15054300	1.01428900	5.18872200
H	-0.02486700	2.73167900	4.82146200
H	-1.23638000	1.57538400	4.23951300
C	0.21743500	2.72311200	2.17399700
H	-0.84691100	2.66708200	1.92325000
H	0.40178100	3.68866600	2.66262300
H	0.78486100	2.69105400	1.23809200
C	2.13686000	1.69740000	3.40500800
H	2.73550500	1.54294800	2.49993000
H	2.36032200	2.70348000	3.78155700
H	2.46663200	0.98368900	4.16635900
C	0.02685200	-2.67445800	2.35196800
H	-1.05407600	-2.58724300	2.49325600
H	0.23015700	-2.67881100	1.27562300
H	0.35236600	-3.63601000	2.76861200
C	2.29026300	-1.76978200	2.86992200
H	2.56530100	-2.72873200	3.32696500
H	2.55427900	-1.81585300	1.80847000
H	2.90041700	-0.99457900	3.34168300
C	0.43251400	-1.55816600	4.54873700
H	0.59708400	-2.56950000	4.94257100
H	1.06237000	-0.87840400	5.13018200
H	-0.61677400	-1.29951800	4.71926000
O	-1.39351500	-0.04789700	-2.37956700
O	-1.39351500	-0.04789700	2.37956700
Co	0.58215200	0.06076400	0.00000000
H	2.05039600	0.56135100	0.00000000
H	-3.99986700	-0.17681400	-2.16430700
C	-3.47134900	-0.15060800	-1.21658400
H	-5.23925200	-0.23638400	0.00000000

C_2 symmetrical (POCOP)Co(H_2): E = -3077.33554130
Sum of electronic and thermal Enthalpies -3076.710035

0 1

P	0.00000000	2.12659200	0.25715000
P	0.00000000	-2.12659200	0.25715000
O	-0.09233700	2.37527700	-1.39946900
C	-0.04549200	1.17988100	-2.08816200
C	0.00000000	0.00000000	-4.16791600
C	0.04617200	-1.21313900	-3.48072700
C	0.04549200	-1.17988100	-2.08816200
C	0.00000000	0.00000000	-1.33293600
O	0.09233700	-2.37527700	-1.39946900
C	1.60671400	3.02672700	0.63961700
C	1.98470200	2.79083700	2.10713200
C	1.58640600	4.52462400	0.33124800
C	2.65836100	2.34511200	-0.25095900
C	-1.52262100	3.09893800	0.78706200
C	-1.47065000	3.40368300	2.28615800
C	-1.74668400	4.38593300	-0.01344600
C	-2.69220600	2.14118800	0.50611900
C	-1.60671400	-3.02672700	0.63961700
C	-2.65836100	-2.34511200	-0.25095900
C	-1.58640600	-4.52462400	0.33124800
C	-1.98470200	-2.79083700	2.10713200
C	1.52262100	-3.09893800	0.78706200
C	1.74668400	-4.38593300	-0.01344600
C	1.47065000	-3.40368300	2.28615800
C	2.69220600	-2.14118800	0.50611900
H	2.47083500	2.53294100	-1.31188300
H	2.67222000	1.26052000	-0.09691100
H	3.64925600	2.74464200	-0.00069800
H	1.24029200	4.72316700	-0.68755200
H	0.95842000	5.08227300	1.03229000
H	2.60569300	4.92214800	0.42135100
H	2.96469600	3.24505900	2.30070300
H	1.27275200	3.23850700	2.80635400
H	2.06083800	1.72189600	2.33126100
H	-1.01037600	5.15909800	0.21417400
H	-1.72192400	4.19241900	-1.08890500
H	-2.73597200	4.78935400	0.23801100
H	-0.71875100	4.16121000	2.52756300
H	-2.44422400	3.79420900	2.60778800
H	-1.26444600	2.50676100	2.88142000
H	-2.74546500	1.87522600	-0.55458900
H	-2.59700500	1.21294600	1.08018200
H	-3.63547400	2.62971500	0.78312300
H	-2.06083800	-1.72189600	2.33126100
H	-1.27275200	-3.23850700	2.80635400
H	-2.96469600	-3.24505900	2.30070300
H	-3.64925600	-2.74464200	-0.00069800
H	-2.67222000	-1.26052000	-0.09691100
H	-2.47083500	-2.53294100	-1.31188300
H	-2.60569300	-4.92214800	0.42135100
H	-1.24029200	-4.72316700	-0.68755200
H	-0.95842000	-5.08227300	1.03229000
H	2.59700500	-1.21294600	1.08018200

H	3.63547400	-2.62971500	0.78312300
H	2.74546500	-1.87522600	-0.55458900
H	1.26444600	-2.50676100	2.88142000
H	0.71875100	-4.16121000	2.52756300
H	2.44422400	-3.79420900	2.60778800
H	2.73597200	-4.78935400	0.23801100
H	1.01037600	-5.15909800	0.21417400
H	1.72192400	-4.19241900	-1.08890500
H	0.08168700	-2.16255300	-4.00574000
H	-0.07147200	0.42937600	2.09928200
H	0.07147200	-0.42937600	2.09928200
H	0.00000000	0.00000000	-5.25446200
C	-0.04617200	1.21313900	-3.48072700
H	-0.08168700	2.16255300	-4.00574000
Co	0.00000000	0.00000000	0.58865400

C_s symmetrical (POCOP)Co(H)$_2$: E = -3077.33034384
Sum of electronic and thermal Enthalpies -3076.705990
0 1

C	0.73357300	-1.55419100	-3.06153800
P	0.26781400	0.01069300	-2.13226100
C	0.73357300	-1.55419100	3.06153800
H	-4.03495400	0.01434600	-2.16485800
C	0.72863500	1.57940100	-3.04804500
C	-3.50062000	0.00218800	-1.22012500
C	-2.10738300	-0.01341700	-1.19002900
C	-4.18032000	0.00733000	0.00000000
C	-1.37350600	-0.03170100	0.00000000
P	0.26781400	0.01069300	2.13226100
C	-2.10738300	-0.01341700	1.19002900
H	0.88230100	1.28173700	0.00000000
C	0.72863500	1.57940100	3.04804500
C	-0.07906100	-1.79966000	4.33576100
H	0.15558000	-2.80299100	4.71398100
H	0.15451000	-1.08695700	5.12903900
H	-1.15300600	-1.75353900	4.13690700
C	2.23601600	-1.56194400	3.35823700
H	2.82414800	-1.32988400	2.46368500
H	2.50505800	-0.85349700	4.14750700
H	2.52700900	-2.56185200	3.70391500
C	2.20591400	1.89748800	2.78490600
H	2.41746800	1.94834200	1.71289800
H	2.44333800	2.87028500	3.23335700
H	2.87851600	1.15691700	3.22628900
C	-0.13985100	2.69192100	2.44042300
H	-1.20223900	2.52838000	2.64094500
H	0.15261300	3.64926200	2.88905500
H	-0.00392400	2.76647800	1.35757000
C	0.45482500	1.51138700	4.55241200
H	-0.57750300	1.21594800	4.76282900
H	1.13114900	0.82256300	5.06647200
H	0.61309100	2.50677800	4.98636900
C	0.42207300	-2.67453500	2.05507300
H	1.02907900	-2.56647500	1.14778600
H	0.66422600	-3.64656700	2.50354700
H	-0.63578400	-2.68911500	1.77179900
C	-0.07906100	-1.79966000	-4.33576100
H	0.15451000	-1.08695700	-5.12903900
H	0.15558000	-2.80299100	-4.71398100
H	-1.15300600	-1.75353900	-4.13690700
C	0.42207300	-2.67453500	-2.05507300
H	-0.63578400	-2.68911500	-1.77179900
H	0.66422600	-3.64656700	-2.50354700
H	1.02907900	-2.56647500	-1.14778600
C	2.23601600	-1.56194400	-3.35823700
H	2.82414800	-1.32988400	-2.46368500
H	2.52700900	-2.56185200	-3.70391500
H	2.50505800	-0.85349700	-4.14750700
C	-0.13985100	2.69192100	-2.44042300
H	-1.20223900	2.52838000	-2.64094500
H	-0.00392400	2.76647800	-1.35757000
H	0.15261300	3.64926200	-2.88905500
C	2.20591400	1.89748800	-2.78490600
H	2.44333800	2.87028500	-3.23335700
H	2.41746800	1.94834200	-1.71289800
H	2.87851600	1.15691700	-3.22628900
C	0.45482500	1.51138700	-4.55241200
H	0.61309100	2.50677800	-4.98636900
H	1.13114900	0.82256300	-5.06647200
H	-0.57750300	1.21594800	-4.76282900
O	-1.40367200	-0.00479100	2.37750000
O	-1.40367200	-0.00479100	-2.37750000
Co	0.54975600	-0.09310900	0.00000000
H	2.06234000	-0.20651100	0.00000000
H	-4.03495400	0.01434600	2.16485800
C	-3.50062000	0.00218800	1.22012500
H	-5.26698100	0.02032600	0.00000000

C_s cis-(POCOP)Co(H)$_2$(H)$_2$: E = -3078.51552674
Sum of electronic and thermal Enthalpies -3077.871679
0 1

C	-0.82630000	-1.41155600	3.34513200
P	-0.26992400	-0.06284000	2.14285300
C	-0.82630000	-1.41155600	-3.34513200
H	4.02557100	-0.11320300	2.16469300
C	-0.61278400	1.65468400	2.85109800
C	3.49563400	-0.13755200	1.21755600
C	2.10296200	-0.17990900	1.18545900
C	4.17924200	-0.12229700	0.00000000
C	1.37495000	-0.21379000	0.00000000
P	-0.26992400	-0.06284000	-2.14285300
C	2.10296200	-0.17990900	-1.18545900
H	-0.68504700	1.14847700	0.00000000
C	-0.61278400	1.65468400	-2.85109800
C	0.00048800	-1.44205000	-4.63825500
H	-0.29122300	-2.32822200	-5.21595600
H	-0.16256400	-0.57193800	-5.27340400
H	1.06933800	-1.51546200	-4.42093900
C	-2.31914500	-1.25076800	-3.65094300
H	-2.91278700	-1.17027600	-2.73329400

H	-2.52514100	-0.37652200	-4.27480100
H	-2.67019900	-2.13376500	-4.19947000
C	-2.03903200	2.07706200	-2.47567100
H	-2.19495500	2.03858800	-1.39450000
H	-2.20268500	3.10778000	-2.81432100
H	-2.80021100	1.44941400	-2.94843300
C	0.39065000	2.60580300	-2.18105700
H	1.41758300	2.38634700	-2.48614600
H	0.15403600	3.63275300	-2.48570600
H	0.34060200	2.55469400	-1.09096200
C	-0.42032500	1.77974200	-4.36564000
H	0.57547000	1.45282000	-4.67874100
H	-1.17307700	1.22704800	-4.93379500
H	-0.52248800	2.83738900	-4.63994700
C	-0.61642700	-2.75975300	-2.63854600
H	-1.31731400	-2.90067700	-1.81293000
H	-0.79347600	-3.56472600	-3.36205700
H	0.40480000	-2.87171300	-2.25866300
C	0.00048800	-1.44205000	4.63825500
H	-0.16256400	-0.57193800	5.27340400
H	-0.29122300	-2.32822200	5.21595600
H	1.06933800	-1.51546200	4.42093900
C	-0.61642700	-2.75975300	2.63854600
H	0.40480000	-2.87171300	2.25866300
H	-0.79347600	-3.56472600	3.36205700
H	-1.31731400	-2.90067700	1.81293000
C	-2.31914500	-1.25076800	3.65094300
H	-2.91278700	-1.17027600	2.73329400
H	-2.67019900	-2.13376500	4.19947000
H	-2.52514100	-0.37652200	4.27480100
C	0.39065000	2.60580300	2.18105700
H	1.41758300	2.38634700	2.48614600
H	0.34060200	2.55469400	1.09096200
H	0.15403600	3.63275300	2.48570600
C	-2.03903200	2.07706200	2.47567100
H	-2.20268500	3.10778000	2.81432100
H	-2.19495500	2.03858800	1.39450000
H	-2.80021100	1.44941400	2.94843300
C	-0.42032500	1.77974200	4.36564000
H	-0.52248800	2.83738900	4.63994700
H	-1.17307700	1.22704800	4.93379500
H	0.57547000	1.45282000	4.67874100
O	1.39157000	-0.18602900	-2.37319400
O	1.39157000	-0.18602900	2.37319400
Co	-0.56624600	-0.29148300	0.00000000
H	-2.06811900	-0.19084800	0.00000000
H	4.02557100	-0.11320300	-2.16469300
C	3.49563400	-0.13755200	-1.21755600
H	5.26522400	-0.08934600	0.00000000
H	-0.29349300	-1.86640000	0.00000000
H	-1.13368100	-1.76272900	0.00000000

C_2 trans-(POCOP)Co(H)$_2$(H)$_2$: E = -3078.51280898

Sum of electronic and thermal Enthalpies -3077.869097

0 1

P	0.72088400	2.03955000	0.25944100
P	-0.72088400	-2.03955000	0.25944100
O	0.59949600	2.29657300	-1.38470500
C	0.29746600	1.14351800	-2.08655600
C	0.00000000	0.00000000	-4.16720900
C	-0.30567200	-1.17436400	-3.47868000
C	-0.29746600	-1.14351800	-2.08655600
C	0.00000000	0.00000000	-1.34882000
O	-0.59949600	-2.29657300	-1.38470500
C	2.57315200	2.31004900	0.54581300
C	2.92763300	1.81284400	1.95265000
C	3.06451400	3.74829100	0.36412400
C	3.29244200	1.43350200	-0.49150500
C	-0.28110500	3.51973800	0.87099400
C	-0.01885300	3.74575400	2.36354800
C	0.00000000	4.79869600	0.06913800
C	-1.76614400	3.18082100	0.67430300
C	-2.57315200	-2.31004900	0.54581300
C	-3.29244200	-1.43350200	-0.49150500
C	-3.06451400	-3.74829100	0.36412400
C	-2.92763300	-1.81284400	1.95265000
C	0.28110500	-3.51973800	0.87099400
C	0.00000000	-4.79869600	0.06913800
C	0.01885300	-3.74575400	2.36354800
C	1.76614400	-3.18082100	0.67430300
H	3.14320800	1.81136000	-1.50685600
H	2.94954800	0.39568800	-0.45524000
H	4.36782700	1.44933300	-0.27488800
H	2.78464300	4.15472500	-0.61217700
H	2.70358000	4.42095600	1.14688000
H	4.16056500	3.74877100	0.41930300
H	4.01229900	1.89326800	2.09712100
H	2.44751000	2.39956400	2.74213200
H	2.64708100	0.76322800	2.07897900
H	0.99486900	5.20705400	0.24229900
H	-0.12304500	4.62639200	-1.00341900
H	-0.72540400	5.56313600	0.37402200
H	0.99305900	4.11150900	2.56070000
H	-0.71951600	4.50119700	2.73992800
H	-0.17757000	2.83272700	2.94907500
H	-1.98716100	2.91993800	-0.36564700
H	-2.08491800	2.34694000	1.30243700
H	-2.36042100	4.06504800	0.93697000
H	-2.64708100	-0.76322800	2.07897900
H	-2.44751000	-2.39956400	2.74213200
H	-4.01229900	-1.89326800	2.09712100
H	-4.36782700	-1.44933300	-0.27488800
H	-2.94954800	-0.39568800	-0.45524000
H	-3.14320800	-1.81136000	-1.50685600
H	-4.16056500	-3.74877100	0.41930300
H	-2.78464300	-4.15472500	-0.61217700
H	-2.70358000	-4.42095600	1.14688000
H	2.08491800	-2.34694000	1.30243700
H	2.36042100	-4.06504800	0.93697000

H	1.98716100	-2.91993800	-0.36564700
H	0.17757000	-2.83272700	2.94907500
H	-0.99305900	-4.11150900	2.56070000
H	0.71951600	-4.50119700	2.73992800
H	0.72540400	-5.56313600	0.37402200
H	-0.99486900	-5.20705400	0.24229900
H	0.12304500	-4.62639200	-1.00341900
H	-0.54752400	-2.09394300	-4.00234700
H	1.41094000	-0.49634500	0.54266800
H	0.40634200	-0.15575700	2.07849600
H	-0.40634200	0.15575700	2.07849600
H	-1.41094000	0.49634500	0.54266800
H	0.00000000	0.00000000	-5.25339100
C	0.30567200	1.17436400	-3.47868000
H	0.54752400	2.09394300	-4.00234700
Co	0.00000000	0.00000000	0.56795600

C_s (POCOP)Co(H_2)$_2$: E = -3078.50751840

Sum of electronic and thermal Enthalpies -3077.864156

0 1

P	-0.26880000	0.03256400	2.16051900
P	-0.26880000	0.03256400	-2.16051900
O	1.38470700	-0.09696600	2.37521800
C	2.07230100	-0.16055600	1.17682800
C	3.46001700	-0.27802700	1.21208600
C	4.14785400	-0.33618800	0.00000000
C	3.46001700	-0.27802700	-1.21208600
C	2.07230100	-0.16055600	-1.17682800
C	1.32301500	-0.09835100	0.00000000
O	1.38470700	-0.09696600	-2.37521800
C	-0.83578500	-1.50193600	3.11149300
C	-2.34473500	-1.70633400	2.92956000
C	-0.50453900	-1.48466200	4.60654000
C	-0.08119600	-2.68332800	2.47930800
C	-0.55675800	1.61837500	3.15201600
C	-2.05210000	1.82088800	3.41092800
C	0.23009900	1.65939500	4.46925400
C	-0.02885000	2.77016800	2.27983500
C	-0.55675800	1.61837500	-3.15201600
C	-0.02885000	2.77016800	-2.27983500
C	0.23009900	1.65939500	-4.46925400
C	-2.05210000	1.82088800	-3.41092800
C	-0.83578500	-1.50193600	-3.11149300
C	-0.50453900	-1.48466200	-4.60654000
C	-2.34473500	-1.70633400	-2.92956000
C	-0.08119600	-2.68332800	-2.47930800
H	0.99494700	-2.60955600	2.65823500
H	-0.23809100	-2.74971000	1.39907900
H	-0.44310800	-3.61411000	2.93350100
H	0.54477200	-1.23761200	4.79078600
H	-1.13874800	-0.79023200	5.16433100
H	-0.68739800	-2.48652600	5.01571200
H	-2.63879900	-2.63674000	3.43139600
H	-2.93233400	-0.89588600	3.37031300
H	-2.62497500	-1.79211300	1.87685000
H	-0.16626900	0.98412000	5.22696200
H	1.28542900	1.42318600	4.30863900
H	0.17026100	2.67631800	4.87685200
H	-2.44368900	1.10826900	4.14359500
H	-2.21654600	2.82767000	3.81487400
H	-2.64226000	1.73200400	2.49173500
H	1.00739900	2.60308800	1.96934700
H	-0.63161700	2.92273700	1.38264600
H	-0.06225000	3.69647200	2.86671200
H	-2.64226000	1.73200400	-2.49173500
H	-2.44368900	1.10826900	-4.14359500
H	-2.21654600	2.82767000	-3.81487400
H	-0.06225000	3.69647200	-2.86671200
H	-0.63161700	2.92273700	-1.38264600
H	1.00739900	2.60308800	-1.96934700
H	0.17026100	2.67631800	-4.87685200
H	1.28542900	1.42318600	-4.30863900
H	-0.16626900	0.98412000	-5.22696200
H	-0.23809100	-2.74971000	-1.39907900
H	-0.44310800	-3.61411000	-2.93350100
H	0.99494700	-2.60955600	-2.65823500
H	-2.62497500	-1.79211300	-1.87685000
H	-2.93233400	-0.89588600	-3.37031300
H	-2.63879900	-2.63674000	-3.43139600
H	-0.68739800	-2.48652600	-5.01571200
H	-1.13874800	-0.79023200	-5.16433100
H	0.54477200	-1.23761200	-4.79078600
H	3.98100900	-0.32090800	2.16356500
H	5.23042300	-0.42657600	0.00000000
H	3.98100900	-0.32090800	-2.16356500
Co	-0.63023700	0.03953000	0.00000000
H	-0.96631500	1.53320800	0.00000000
H	-1.78211300	1.07283300	0.00000000
H	-1.08239100	-1.45270400	0.00000000
H	-1.83665100	-0.94101100	0.00000000

Optimized geometries and energies (mPW1K)

C_s cis-(POCOP)Co(H)$_2$(H_2): E = -3080.02758091
Sum of electronic and thermal Enthalpies -3079.369950
0 1

C	-0.79886700	-1.40581700	3.35721000
P	-0.26836300	-0.06594600	2.15838100
C	-0.79886700	-1.40581700	-3.35721000
H	3.99847200	-0.07380400	2.15305200
C	-0.62470600	1.63668900	2.85516000
C	3.47186000	-0.10319300	1.21146500
C	2.08690400	-0.15946800	1.17826600
C	4.15183400	-0.08107300	0.00000000
C	1.36226000	-0.20004800	0.00000000
P	-0.26836300	-0.06594600	-2.15838100
C	2.08690400	-0.15946800	-1.17826600
H	-0.70804900	1.13310600	0.00000000
C	-0.62470600	1.63668900	-2.85516000
C	0.03237000	-1.42835100	-4.64010000
H	-0.24877100	-2.30909300	-5.21911500
H	-0.13051400	-0.56199500	-5.26965700
H	1.09410100	-1.49558700	-4.41751400
C	-2.28555000	-1.26308200	-3.67243400
H	-2.88332200	-1.18917900	-2.76441100
H	-2.49567400	-0.39651500	-4.29443700
H	-2.62079000	-2.14502100	-4.21963000
C	-2.05158000	2.03843300	-2.48371300
H	-2.21122100	1.98142300	-1.41036500
H	-2.22320000	3.06614400	-2.80621800
H	-2.79893800	1.41358600	-2.96763200
C	0.36037900	2.59372600	-2.17976200
H	1.38500200	2.38833600	-2.47989600
H	0.11506900	3.61296400	-2.48040500
H	0.30592400	2.53768400	-1.09676100
C	-0.42871000	1.77352200	-4.36199700
H	0.56699700	1.46387000	-4.67126700
H	-1.16688800	1.21759800	-4.93395100
H	-0.54316600	2.82518100	-4.62857800
C	-0.58188300	-2.74795400	-2.65406000
H	-1.28510100	-2.89601500	-1.83993800
H	-0.74272700	-3.54980700	-3.37507400
H	0.43145500	-2.84932300	-2.26791100
C	0.03237000	-1.42835100	4.64010000
H	-0.13051400	-0.56199500	5.26965700
H	-0.24877100	-2.30909300	5.21911500
H	1.09410100	-1.49558700	4.41751400
C	-0.58188300	-2.74795400	2.65406000
H	0.43145500	-2.84932300	2.26791100
H	-0.74272700	-3.54980700	3.37507400
H	-1.28510100	-2.89601500	1.83993800
C	-2.28555000	-1.26308200	3.67243400
H	-2.88332200	-1.18917900	2.76441100
H	-2.62079000	-2.14502100	4.21963000
H	-2.49567400	-0.39651500	4.29443700
C	0.36037900	2.59372600	2.17976200
H	1.38500200	2.38833600	2.47989600
H	0.30592400	2.53768400	1.09676100
H	0.11506900	3.61296400	2.48040500
C	-2.05158000	2.03843300	2.48371300
H	-2.22320000	3.06614400	2.80621800
H	-2.21122100	1.98142300	1.41036500
H	-2.79893800	1.41358600	2.96763200
C	-0.42871000	1.77352200	4.36199700
H	-0.54316600	2.82518100	4.62857800
H	-1.16688800	1.21759800	4.93395100
H	0.56699700	1.46387000	4.67126700
O	1.37985700	-0.17202600	-2.36029300
O	1.37985700	-0.17202600	2.36029300
Co	-0.57276200	-0.29672000	0.00000000
H	-2.07469800	-0.26983000	0.00000000
H	3.99847200	-0.07380400	-2.15305200
C	3.47186000	-0.10319300	-1.21146500
H	5.23114400	-0.03752700	0.00000000
H	-0.26859900	-1.88402700	0.00000000
H	-1.08262500	-1.80770200	0.00000000

C_2 trans-(POCOP)Co(H)$_2$(H_2): E = -3080.02589460
Sum of electronic and thermal Enthalpies -3079.368357
0 1

P	0.72049800	2.05713200	0.26000700
P	-0.72049800	-2.05713200	0.26000700
O	0.59297400	2.28423000	-1.36985400
C	0.29362900	1.13595400	-2.06818100
C	0.00000000	0.00000000	-4.13852100
C	-0.30186700	-1.16889600	-3.45300400
C	-0.29362900	-1.13595400	-2.06818100
C	0.00000000	0.00000000	-1.33267100
O	-0.59297400	-2.28423000	-1.36985400
C	2.55701500	2.32854000	0.54166500
C	2.91369100	1.84108500	1.94513600
C	3.04827100	3.75970900	0.35401500
C	3.27607000	1.45130600	-0.48663300
C	-0.27707500	3.52774700	0.85482300
C	-0.02197200	3.76568400	2.34063600
C	0.00000000	4.79799600	0.04957000
C	-1.75555900	3.18602100	0.65863300
C	-2.55701500	-2.32854000	0.54166500
C	-3.27607000	-1.45130600	-0.48663300
C	-3.04827100	-3.75970900	0.35401500
C	-2.91369100	-1.84108500	1.94513600
C	0.27707500	-3.52774700	0.85482300
C	0.00000000	-4.79799600	0.04957000
C	0.02197200	-3.76568400	2.34063600
C	1.75555900	-3.18602100	0.65863300
H	3.12716700	1.82223500	-1.49780300

H	2.93760600	0.41904200	-0.44603300
H	4.34525600	1.47046200	-0.27149000
H	2.76992900	4.15960400	-0.61837400
H	2.68979400	4.43247800	1.12903600
H	4.13788200	3.75957500	0.40861500
H	3.99050800	1.93509400	2.09104000
H	2.42757000	2.42039300	2.72789000
H	2.64865100	0.79413400	2.07290700
H	0.98710800	5.20884600	0.22241300
H	-0.11802600	4.61952900	-1.01613300
H	-0.72476700	5.55745400	0.34525500
H	0.98264300	4.13284500	2.53756200
H	-0.72138900	4.51806200	2.70654600
H	-0.18011400	2.86236200	2.92970500
H	-1.97260300	2.91640100	-0.37326600
H	-2.07185900	2.36178300	1.28958100
H	-2.34916600	4.06595000	0.91031900
H	-2.64865100	-0.79413400	2.07290700
H	-2.42757000	-2.42039300	2.72789000
H	-3.99050800	-1.93509400	2.09104000
H	-4.34525600	-1.47046200	-0.27149000
H	-2.93760600	-0.41904200	-0.44603300
H	-3.12716700	-1.82223500	-1.49780300
H	-4.13788200	-3.75957500	0.40861500
H	-2.76992900	-4.15960400	-0.61837400
H	-2.68979400	-4.43247800	1.12903600
H	2.07185900	-2.36178300	1.28958100
H	2.34916600	-4.06595000	0.91031900
H	1.97260300	-2.91640100	-0.37326600
H	0.18011400	-2.86236200	2.92970500
H	-0.98264300	-4.13284500	2.53756200
H	0.72138900	-4.51806200	2.70654600
H	0.72476700	-5.55745400	0.34525500
H	-0.98710800	-5.20884600	0.22241300
H	0.11802600	-4.61952900	-1.01613300
H	-0.53988400	-2.08384500	-3.97351400
H	1.40788700	-0.48851200	0.57475700
H	0.39246400	-0.14009000	2.11441000
H	-0.39246400	0.14009000	2.11441000
H	-1.40788700	0.48851200	0.57475700
H	0.00000000	0.00000000	-5.21843700
C	0.30186700	1.16889600	-3.45300400
H	0.53988400	2.08384500	-3.97351400
Co	0.00000000	0.00000000	0.57763900

C_s TS cis-(POCOP)Co(H)$_2$(H_2): E = -3080.00317856

Sum of electronic and thermal Enthalpies -3079.349763

0 1

C	-0.83671200	-1.37596900	3.37532800
P	-0.26956700	-0.07249000	2.16007200
C	-0.83671200	-1.37596900	-3.37532800
H	4.00509500	-0.10452700	2.15346800
C	-0.61299400	1.64650800	2.81935000
C	3.47367900	-0.11434000	1.21424900
C	2.08780200	-0.14336500	1.18261300
C	4.15010900	-0.10069300	0.00000000
C	1.36302700	-0.15607000	0.00000000
P	-0.26956700	-0.07249000	-2.16007200
C	2.08780200	-0.14336500	-1.18261300
H	-0.86216200	1.03892600	0.00000000
C	-0.61299400	1.64650800	-2.81935000
C	-0.00059200	-1.43841100	-4.65134800
H	-0.29836800	-2.32157200	-5.21859200
H	-0.14093300	-0.57677500	-5.29423500
H	1.05845200	-1.52601300	-4.42275700
C	-2.31510400	-1.16717900	-3.69530100
H	-2.91235200	-1.07547800	-2.78870500
H	-2.48755600	-0.29153300	-4.31557700
H	-2.68154400	-2.03334100	-4.24747000
C	-2.04551600	2.04975500	-2.47147300
H	-2.23745500	1.95438900	-1.40578700
H	-2.19713500	3.09128300	-2.75772800
H	-2.78619100	1.45363200	-2.99803800
C	0.35873700	2.58859500	-2.10614600
H	1.39079600	2.38044500	-2.37721900
H	0.12935500	3.61290200	-2.40206400
H	0.27236400	2.52043400	-1.02652000
C	-0.37883700	1.80020700	-4.31932300
H	0.61960700	1.47812700	-4.60705200
H	-1.10910300	1.26051700	-4.91618600
H	-0.47168100	2.85636400	-4.57657800
C	-0.69628700	-2.71662400	-2.65560200
H	-1.30140400	-2.74739000	-1.75157200
H	-1.04080600	-3.51092400	-3.31908100
H	0.33776900	-2.92889300	-2.39406800
C	-0.00059200	-1.43841100	4.65134800
H	-0.14093300	-0.57677500	5.29423500
H	-0.29836800	-2.32157200	5.21859200
H	1.05845200	-1.52601300	4.42275700
C	-0.69628700	-2.71662400	2.65560200
H	0.33776900	-2.92889300	2.39406800
H	-1.04080600	-3.51092400	3.31908100
H	-1.30140400	-2.74739000	1.75157200
C	-2.31510400	-1.16717900	3.69530100
H	-2.91235200	-1.07547800	2.78870500
H	-2.68154400	-2.03334100	4.24747000
H	-2.48755600	-0.29153300	4.31557700
C	0.35873700	2.58859500	2.10614600
H	1.39079600	2.38044500	2.37721900
H	0.27236400	2.52043400	1.02652000
H	0.12935500	3.61290200	2.40206400
C	-2.04551600	2.04975500	2.47147300
H	-2.19713500	3.09128300	2.75772800
H	-2.23745500	1.95438900	1.40578700
H	-2.78619100	1.45363200	2.99803800
C	-0.37883700	1.80020700	4.31932300
H	-0.47168100	2.85636400	4.57657800

H	-1.10910300	1.26051700	4.91618600
H	0.61960700	1.47812700	4.60705200
O	1.38426200	-0.17121000	-2.36612300
O	1.38426200	-0.17121000	2.36612300
Co	-0.55856400	-0.33373800	0.00000000
H	-2.06160800	-0.54355500	0.00000000
H	4.00509500	-0.10452700	-2.15346800
C	3.47367900	-0.11434000	-1.21424900
H	5.23025400	-0.07881100	0.00000000
H	0.71527400	-2.46872700	0.00000000
H	0.21154900	-3.01571500	0.00000000

C_1 TS trans-(POCOP)Co(H)$_2$(H_2): E = -3079.99180886

Sum of electronic and thermal Enthalpies -3079.339982

0 1

P	2.20057700	-0.24025300	0.03469900
P	-2.17136500	-0.26212100	0.02490900
O	2.38336700	1.36228600	-0.33052200
C	1.19381500	2.03835400	-0.46847100
C	0.00511900	4.05575400	-0.90012100
C	-1.19888500	3.37144600	-0.79960500
C	-1.16192300	2.01399900	-0.52826400
C	0.01866300	1.31234200	-0.33476400
O	-2.34153700	1.31276600	-0.45732400
C	3.13244800	-1.09301500	-1.34490000
C	2.62374100	-2.53346100	-1.39696600
C	4.65224400	-1.08901400	-1.23463600
C	2.74423600	-0.37895300	-2.64102900
C	3.11362300	-0.28531800	1.66164000
C	3.21217000	-1.72758000	2.14706100
C	4.48866100	0.37922500	1.61701000
C	2.24441400	0.51432600	2.63590900
C	-3.00591400	-0.19206500	1.69611900
C	-2.22273300	0.86453600	2.48074000
C	-4.47010500	0.22902300	1.64164200
C	-2.86389800	-1.52919400	2.42066300
C	-3.24666400	-1.11403800	-1.25000000
C	-4.45473000	-0.26981100	-1.65252600
C	-3.70219000	-2.48016300	-0.74379300
C	-2.38100000	-1.31590600	-2.49513000
H	3.13658400	0.63440000	-2.66895700
H	1.66558700	-0.32979200	-2.76908400
H	3.16260200	-0.93343400	-3.48201400
H	5.05247500	-0.08098000	-1.15783200
H	5.00959700	-1.67427600	-0.39111500
H	5.06555700	-1.53927800	-2.13840300
H	3.11393900	-3.05854800	-2.21768100
H	2.83370300	-3.08376300	-0.48129200
H	1.55040500	-2.56363300	-1.57478400
H	5.23495600	-0.22057800	1.10871200
H	4.44019000	1.35560000	1.13980700
H	4.83455600	0.52740200	2.64069800
H	3.86850600	-2.33227800	1.52317600
H	3.62294100	-1.73892700	3.15727200
H	2.22982800	-2.19719200	2.18240300
H	2.15761400	1.55555100	2.33070900
H	1.24680000	0.09099100	2.71594700
H	2.71297200	0.49171000	3.62067700
H	-1.82143300	-1.83730500	2.46982600
H	-3.44153600	-2.32514300	1.95805800
H	-3.22995100	-1.41252900	3.44146900
H	-2.60379300	0.89370300	3.50232400
H	-1.16253000	0.62222800	2.51977400
H	-2.33686500	1.85627900	2.04969700
H	-4.82017200	0.41370100	2.65827700
H	-4.60457500	1.14722400	1.07365200
H	-5.10775600	-0.54364900	1.21869200
H	-1.53674600	-1.97306800	-2.30236100
H	-2.99468900	-1.76446800	-3.27779000
H	-1.98881500	-0.37342600	-2.87163500
H	-2.87215400	-3.08306400	-0.37824400
H	-4.44251700	-2.39860600	0.04802500
H	-4.16481700	-3.02514800	-1.56730100
H	-4.97484800	-0.77805000	-2.46582400
H	-5.16486700	-0.13361100	-0.84414800
H	-4.14981500	0.71102100	-2.00652800
H	-2.14600000	3.87179400	-0.93120900
H	0.03561900	-0.42557500	-1.43137000
H	-0.32949300	-3.68166000	-0.16690800
H	-0.27969500	-3.16044100	0.36183500
H	0.02489300	-1.12911800	1.47805200
H	-0.00046600	5.11528900	-1.10856700
C	1.21624100	3.39635200	-0.73891900
H	2.15828600	3.91606700	-0.82303400
Co	0.02293000	-0.52856500	0.02354500