

SUPPORTING INFORMATION

C-H versus C-O Addition: A DFT Study of the Catalytic Cleavage of the β -O-4 Ether Linkage in Lignin by Iridium and Cobalt Pincer Complexes

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Table S1: Comparison between the M06 and M06-2X-D3 levels of theories calculated relative energies, activation energies and energies of formation for the IrPCP catalyzed cleavage of 2-Phenoxy-*I*-phenylethanol (Pathway A).

	M06-2x-d3 RE	M06-2x-d3 Ea/Ef	M06 RE	M06 Ea/Ef	Diff in RE	Diff in Ea/Ef
TS1	12.51	12.5	11.35	11.35	1.15	1.15
INT1	-6.67	-6.7	-1.38	-1.38	5.28	5.32
TS2	0.97	7.64	9.77	11.15	8.79	3.52
INT3	-30.10	-23.43	-26.48	-23.98	3.62	0.55
TS4	0.88	30.98	-1.53	24.95	2.41	6.04

Table S2: Comparison between the M06 and M06-2X-D3 levels of theories calculated relative energies, activation energies and energies of formation for the IrPCP catalyzed cleavage of 2-Phenoxy-*I*-phenylethanol along Pathway B.

	M06-2x-d3 RE	M06-2x-d3 Ea/Ef	M06 RE	M06 Ea/Ef	Diff in RE	Diff in Ea/Ef
INT1	-9.94	-9.9	-6.86	-6.9	3.07	3
TS1	29.95	39.89	27.22	34.08	2.73	5.81
INT2	-22.35	-12.41	-17.45	-10.59	4.90	1.82
TS2	4.41	26.76	5.14	22.58	0.73	4.18
INT3	-30.86	-8.51	-26.60	-9.15	4.26	0.64
INT4	-30.10	0.76	-25.64	0.96	4.46	0.20
TS4	0.88	31.74	1.24	26.88	0.35	4.87

Table S3: Comparison between the M06 and M06-2X-D3 levels of theories calculated relative energies, activation energies and energies of formation for the IrPCP catalyzed cleavage of 2-Phenoxy-*I*-phenylethanol along Pathway C.

	M06-2x-d3 RE	M06-2x-d3 Ea/Ef	M06 RE	M06 Ea/Ef	Diff in RE	Diff in Ea/Ef
INT1	-4.03	-4	-4.78	-4.8	0.75	0.8
TS1	27.29	31.32	21.98	26.76	5.31	4.57
INT2	-30.43	-26.40	-26.24	-21.47	4.18	4.93
INT3	-27.86	2.57	-29.42	-3.18	1.57	5.75
TS3	-11.92	15.94	-10.28	19.15	1.64	3.21
INT4	-16.51	11.35	-16.12	13.31	0.39	1.96
TS4	-6.14	10.37	-11.58	4.53	5.45	5.84

Cartesian coordinates (in Å) and Energies (in hartree) of the optimized structures.

Reaction between (PCP)Ir and 1 along pathway A

Reactants

Substrate (2-phenoxy-1-phenylethanol) 1

EE = -692.021667

EE + ZPE = -691.775624

G° = -691.818104

H	-0.85501	-1.15090	1.85746
C	-0.11655	-0.43987	1.47046
H	0.32056	0.08737	2.32809
C	0.96159	-1.19641	0.72063
H	1.34452	-1.95751	1.41770
C	2.13422	-0.36120	0.25336
C	4.37413	1.04170	-0.65514
C	2.25408	1.00508	0.48552
C	3.14853	-1.01330	-0.44856
C	4.25963	-0.32139	-0.89858
C	3.36916	1.70063	0.03413
H	1.46480	1.54418	0.99868
H	3.04766	-2.07742	-0.64504
H	5.04150	-0.84580	-1.43955
H	3.44639	2.76772	0.21932
H	5.24404	1.58801	-1.00652
O	-0.74416	0.53292	0.65171
C	-2.02439	0.34165	0.22277
C	-4.64347	0.15837	-0.70472
C	-2.59260	-0.90827	-0.00480
C	-2.76231	1.49643	-0.02336
C	-4.06138	1.40182	-0.48978
C	-3.90251	-0.98693	-0.46155
H	-2.00579	-1.80970	0.13498
H	-2.29165	2.45679	0.16076
H	-4.62826	2.30852	-0.67826
H	-4.33989	-1.96483	-0.63940
H	-5.66425	0.08523	-1.06503
O	0.40689	-1.93727	-0.35170
H	0.18481	-1.30665	-1.04550

Iridium pincer catalyst

EE = -1570.196996

EE + ZPE = -1569.695015

G° = -1569.753818

Ir	-0.00001	0.59837	-0.00001
P	-2.28429	0.34129	-0.08738
P	2.28427	0.34128	0.08737
C	-2.40591	-1.37804	-0.74659
H	-2.44609	-1.26907	-1.84012
H	-3.31888	-1.90588	-0.44103
C	2.40588	-1.37805	0.74659
H	3.31886	-1.90590	0.44103
H	2.44606	-1.26909	1.84011
C	-0.00001	-1.38024	-0.00002
C	-0.00002	-4.20842	-0.00001
C	-1.15925	-2.11553	-0.34369
C	1.15923	-2.11554	0.34367
C	1.14911	-3.50528	0.32807
C	-1.14914	-3.50527	-0.32809
H	2.05908	-4.04319	0.58905
H	-2.05912	-4.04318	-0.58906
H	-0.00003	-5.29400	-0.00001

C	-3.24186	1.38821	-1.29451
H	-2.53421	1.41312	-2.13775
C	-3.20293	0.34018	1.53556
H	-3.06015	1.36370	1.91330
C	3.20292	0.34016	-1.53555
H	3.06005	1.36364	-1.91336
C	3.24185	1.38819	1.29450
H	2.53419	1.41314	2.13773
C	4.56699	0.84452	1.81066
H	4.48717	-0.18752	2.16598
H	4.91039	1.45411	2.65529
H	5.35247	0.87700	1.05104
C	3.38179	2.80470	0.75653
H	4.07518	2.84341	-0.09245
H	3.77601	3.47461	1.52894
H	2.41885	3.20810	0.42230
C	4.69225	0.03603	-1.47175
H	4.89360	-0.90309	-0.94188
H	5.26538	0.82885	-0.98459
H	5.09178	-0.07731	-2.48677
C	2.49514	-0.61788	-2.48721
H	2.60345	-1.65783	-2.15470
H	2.93289	-0.54246	-3.48928
H	1.42382	-0.40204	-2.55051
C	-2.49504	-0.61772	2.48727
H	-2.60324	-1.65770	2.15484
H	-2.93279	-0.54228	3.48934
H	-1.42373	-0.40177	2.55056
C	-4.69222	0.03588	1.47179
H	-4.89347	-0.90330	0.94198
H	-5.26544	0.82860	0.98458
H	-5.09173	-0.07743	2.48682
C	-3.38174	2.80475	-0.75656
H	-3.77595	3.47465	-1.52898
H	-2.41878	3.20812	-0.42236
H	-4.07510	2.84350	0.09243
C	-4.56702	0.84458	-1.81063
H	-4.48724	-0.18747	-2.16594
H	-4.91042	1.45416	-2.65526
H	-5.35249	0.87708	-1.05099

TSA1

EE = -2262.227177

EE + ZPE = -2261.481814

G° = -2261.553828

Imaginary Freq = -756.97

Ir	-0.05760	0.42616	-0.44279
P	-2.02063	0.68997	0.79879
P	2.21311	0.84912	-0.74750
C	-2.59348	2.32551	0.16879
H	-3.35952	2.80669	0.78850
H	-3.03848	2.12715	-0.81739
C	2.31789	2.69426	-0.80175
H	2.50327	2.96506	-1.85074
H	3.17588	3.07390	-0.23018
C	1.01726	3.30522	-0.36623
C	-1.40138	4.52968	0.23774
C	0.95181	4.68282	-0.17050
C	-0.12607	2.49352	-0.22869
C	-1.34682	3.15364	0.04839
C	-0.25008	5.29707	0.13953
H	1.85584	5.28099	-0.27125

H	-0.29233	6.37099	0.29609
H	-2.35411	5.00507	0.46275
C	3.32152	0.36736	-2.18748
H	2.67469	0.61184	-3.04505
C	3.59844	-1.12912	-2.22712
H	2.67454	-1.68829	-2.38315
H	4.07846	-1.48253	-1.30622
H	4.27470	-1.36384	-3.05757
C	4.61392	1.16191	-2.35563
H	5.37160	0.87521	-1.62278
H	4.47150	2.24362	-2.28544
H	5.03334	0.95453	-3.34759
C	3.09181	0.34141	0.82910
H	2.80138	-0.71265	0.94501
C	4.60993	0.43063	0.85976
H	4.96249	0.14968	1.86056
H	4.96418	1.45128	0.66846
H	5.09617	-0.24015	0.14667
C	2.51481	1.11824	2.00764
H	1.42320	1.14283	1.98272
H	2.87521	2.15471	2.01551
H	2.82994	0.64793	2.94756
C	-3.51881	-0.41124	0.80359
H	-3.53867	-0.75657	-0.23462
C	-3.31038	-1.63247	1.68816
H	-4.08326	-2.38110	1.47675
H	-3.38252	-1.37865	2.75184
H	-2.33681	-2.10629	1.51076
C	-4.85812	0.26035	1.07206
H	-5.66132	-0.47312	0.92434
H	-5.04886	1.08933	0.38347
H	-4.94562	0.64093	2.09455
C	-1.57886	1.11509	2.56800
H	-0.89907	1.96387	2.40143
C	-0.78453	0.02052	3.26685
H	-1.42781	-0.80826	3.58421
H	-0.30246	0.42218	4.16730
H	-0.00508	-0.38610	2.61585
C	-2.72730	1.60092	3.43990
H	-3.42685	0.79272	3.68046
H	-3.29253	2.41881	2.98197
H	-2.33055	1.97467	4.39161
C	-0.25044	-1.64653	-1.52994
C	0.40913	-3.00245	-1.20480
H	1.47232	-2.89643	-1.42265
H	0.00348	-3.77171	-1.87178
O	0.20335	-3.42844	0.12977
C	1.21427	-3.26155	1.03221
C	3.15186	-2.87598	3.00179
C	0.83947	-2.94379	2.33304
C	2.56262	-3.42720	0.72607
C	3.52084	-3.22793	1.71195
C	1.80229	-2.74836	3.30835
H	-0.21859	-2.83466	2.55101
H	2.87466	-3.71618	-0.27210
H	4.57062	-3.35308	1.46112
H	1.49276	-2.47881	4.31435
H	3.90695	-2.71541	3.76443
O	0.39986	-1.29706	-2.73846
H	0.32421	-0.33707	-2.82356
C	-1.73967	-1.78546	-1.76220
C	-4.47309	-2.08836	-2.34637

C	-2.46914	-2.85738	-1.25038
C	-2.40842	-0.87163	-2.58473
C	-3.75538	-1.01585	-2.86776
C	-3.82140	-3.00692	-1.54084
H	-1.98584	-3.58421	-0.60476
H	-1.86527	-0.02899	-3.00204
H	-4.24851	-0.29183	-3.50985
H	-4.36358	-3.85468	-1.13120
H	-5.52735	-2.20737	-2.57654
H	0.19895	-1.20821	-0.21872

A2

EE = -2262.245889

EE + ZPE = -2261.499340

G° = -2261.574125

Ir	-0.22800	0.35472	-0.07020
P	-1.88868	-0.91677	0.97373
P	1.01294	2.29420	-0.35951
C	-3.45171	-0.07157	0.45500
H	-4.26670	-0.19352	1.17971
H	-3.77225	-0.57125	-0.47205
C	-0.23318	3.49652	-1.01979
H	-0.18418	3.40163	-2.11569
H	0.00419	4.54277	-0.78650
C	-1.60414	3.09258	-0.54026
C	-4.16583	2.32640	0.23206
C	-2.62974	4.03161	-0.48699
C	-1.83488	1.74671	-0.18313
C	-3.14868	1.37700	0.17525
C	-3.90376	3.65013	-0.08938
H	-2.43584	5.06773	-0.75790
H	-4.69926	4.38823	-0.03833
H	-5.17159	2.03019	0.52374
C	2.51249	2.43514	-1.45631
H	2.24672	1.73366	-2.25838
C	3.74737	1.89466	-0.74268
H	3.54128	0.97661	-0.17952
H	4.16331	2.62567	-0.04033
H	4.53403	1.66312	-1.47064
C	2.77404	3.79427	-2.09185
H	3.00617	4.56913	-1.35531
H	1.92614	4.14348	-2.68851
H	3.63522	3.72020	-2.76707
C	1.51131	2.99510	1.30201
H	2.23910	2.25975	1.67566
C	2.16549	4.36958	1.26067
H	2.37100	4.70881	2.28295
H	1.50590	5.11777	0.80427
H	3.11428	4.37896	0.71975
C	0.32792	3.01703	2.26233
H	-0.13408	2.03111	2.36434
H	-0.45050	3.71287	1.92607
H	0.66346	3.34542	3.25311
C	-2.20409	-2.72982	0.74139
H	-2.10263	-2.81512	-0.34481
C	-1.08993	-3.56094	1.36119
H	-1.14669	-4.59194	0.99155
H	-1.17199	-3.60017	2.45400
H	-0.10075	-3.16659	1.09888
C	-3.58658	-3.25833	1.09611
H	-3.68048	-4.28494	0.71955
H	-4.38753	-2.67264	0.63304

H	-3.76655	-3.28864	2.17476
C	-1.83228	-0.51716	2.80109
H	-2.00825	0.57052	2.78051
C	-0.46081	-0.76241	3.41933
H	-0.24385	-1.83399	3.49553
H	-0.43067	-0.35065	4.43554
H	0.34023	-0.30513	2.83053
C	-2.92361	-1.15510	3.64928
H	-2.74751	-2.22809	3.78244
H	-3.92702	-1.02374	3.23259
H	-2.92300	-0.70408	4.64877
C	0.54722	-0.81467	-1.65914
C	1.96673	-1.35897	-1.56259
H	2.64181	-0.50061	-1.48820
H	2.21252	-1.90115	-2.49146
O	2.13239	-2.21972	-0.45404
C	3.29978	-2.17171	0.23115
C	5.61682	-2.15585	1.77835
C	3.23568	-2.46512	1.59170
C	4.52623	-1.87161	-0.35550
C	5.67541	-1.86259	0.42494
C	4.38944	-2.46139	2.35532
H	2.26369	-2.68118	2.02563
H	4.58762	-1.65883	-1.41816
H	6.62925	-1.63027	-0.03965
H	4.32878	-2.68785	3.41569
H	6.51953	-2.14845	2.38039
O	0.67222	0.10464	-2.74578
H	-0.15552	0.59586	-2.79732
C	-0.47548	-1.86553	-2.03622
C	-2.39139	-3.77053	-2.83571
C	-0.21341	-3.23361	-1.94886
C	-1.71951	-1.47665	-2.55051
C	-2.66566	-2.41084	-2.93746
C	-1.15939	-4.17263	-2.34483
H	0.73419	-3.57657	-1.54843
H	-1.96609	-0.41994	-2.63036
H	-3.62154	-2.07524	-3.33008
H	-0.92367	-5.23040	-2.26699
H	-3.12836	-4.50483	-3.14603
H	0.98177	-0.47017	0.61813

TSA2

EE = -2262.229921

EE + ZPE = -2261.484362

G° = -2261.556354

Imaginary frequency = -431.34

Ir	0.10121	0.14091	-0.23530
H	0.62903	0.51869	-1.65849
P	2.10877	0.99300	0.71407
P	-1.98772	0.13587	-1.28042
C	-0.31706	2.13849	-0.24134
C	-0.80207	4.91680	-0.34854
C	-1.19576	2.69173	-1.19270
C	0.34469	3.02850	0.62406
C	0.09411	4.39583	0.57296
C	-1.43692	4.06010	-1.23560
H	0.61791	5.06060	1.25749
H	-2.12974	4.45827	-1.97480
H	-0.99476	5.98471	-0.38367
C	1.37937	2.46739	1.55285
H	0.91578	2.06100	2.46184

H	2.12580	3.21406	1.84865
C	-1.87614	1.75735	-2.15368
H	-2.85019	2.13446	-2.48898
H	-1.25605	1.59464	-3.04763
C	3.07873	0.12003	2.05430
H	2.28471	-0.45620	2.54183
C	4.10941	-0.84728	1.48756
H	4.52298	-1.46340	2.29457
H	4.95106	-0.32290	1.02096
H	3.68511	-1.52296	0.73740
C	3.67181	1.01785	3.13457
H	4.14199	0.39042	3.90168
H	2.90701	1.62069	3.63260
H	4.44159	1.69575	2.75645
C	3.37989	1.64705	-0.49483
H	3.80336	0.73041	-0.93371
C	2.75643	2.47138	-1.61679
H	1.96620	1.93553	-2.14733
H	3.53449	2.73836	-2.34138
H	2.32223	3.40346	-1.23598
C	4.50682	2.44916	0.14540
H	5.12009	1.86134	0.83131
H	4.12140	3.32045	0.68889
H	5.17191	2.83188	-0.63748
C	-2.41830	-1.16267	-2.54752
H	-3.06824	-1.86071	-1.99648
C	-3.16284	-0.63018	-3.76629
H	-4.06208	-0.06155	-3.51928
H	-3.46266	-1.46560	-4.40964
H	-2.51056	0.01560	-4.36533
C	-1.16364	-1.90742	-2.98304
H	-0.46228	-1.22739	-3.48381
H	-1.42374	-2.69630	-3.69865
H	-0.63734	-2.35527	-2.13618
C	-3.51064	0.30459	-0.22158
H	-3.49797	-0.61446	0.36937
C	-4.82926	0.34162	-0.98086
H	-5.65016	0.40523	-0.25606
H	-5.00126	-0.55655	-1.58123
H	-4.90883	1.21900	-1.63498
C	-3.41909	1.48427	0.73886
H	-4.25481	1.43027	1.44675
H	-3.48443	2.44362	0.21255
H	-2.48879	1.48433	1.31509
C	-0.53636	-1.18225	1.97782
C	0.34879	-2.19932	1.59918
H	1.38464	-2.14150	1.92405
O	-0.06140	-0.18778	2.86814
H	-0.16061	-0.52531	3.76589
C	-1.95717	-1.52815	2.10937
C	-4.66997	-2.24986	2.39749
C	-2.51992	-2.57566	1.35741
C	-2.79733	-0.85241	3.00052
C	-4.13186	-1.20902	3.13912
C	-3.84775	-2.93308	1.50612
H	-1.91246	-3.08758	0.61413
H	-2.40323	-0.01633	3.56993
H	-4.75879	-0.65982	3.83655
H	-4.25158	-3.74590	0.90842
H	-5.71326	-2.52707	2.50934
H	-0.02700	-3.20883	1.47080
O	0.66699	-2.04150	-0.23809

C	1.78471	-2.55569	-0.75774
C	4.15512	-3.63291	-1.81975
C	2.25052	-3.81359	-0.34776
C	2.51790	-1.86357	-1.72947
C	3.68208	-2.40165	-2.25447
C	3.42569	-4.33286	-0.86768
H	1.67872	-4.38289	0.37873
H	2.15121	-0.89407	-2.05693
H	4.23062	-1.84518	-3.01021
H	3.77210	-5.30498	-0.52746
H	5.07326	-4.04611	-2.22433

A3

EE = -1877.575979

EE + ZPE = -1876.971541

G° = -1877.036843

Ir	0.29062	-0.14033	-0.01821
H	1.03702	0.03149	1.36728
P	1.92290	-1.79988	-0.28051
P	-1.30168	1.13204	1.13895
C	-0.80870	-1.69986	0.70550
C	-2.36410	-3.86803	1.65105
C	-2.06087	-1.49268	1.32679
C	-0.37954	-3.03752	0.55278
C	-1.14882	-4.09691	1.02465
C	-2.81428	-2.56487	1.79424
H	-0.78936	-5.11652	0.89575
H	-3.77562	-2.37247	2.26797
H	-2.95595	-4.69885	2.02288
C	0.90631	-3.33484	-0.17916
H	0.69414	-3.62417	-1.21975
H	1.45553	-4.17494	0.26582
C	-2.63815	-0.10266	1.41852
H	-3.37031	0.04281	0.61100
H	-3.17385	0.06761	2.36147
C	2.86368	-1.93111	-1.87712
H	2.04751	-1.84763	-2.60781
C	3.76006	-0.71001	-2.04284
H	4.22895	-0.71578	-3.03330
H	4.56780	-0.69528	-1.30159
H	3.19148	0.22036	-1.93610
C	3.58114	-3.24065	-2.18268
H	3.83241	-3.26973	-3.24953
H	2.96402	-4.12047	-1.97113
H	4.51731	-3.34505	-1.63089
C	3.13092	-1.88269	1.14048
H	3.47464	-0.84317	1.24120
C	2.40720	-2.28746	2.41971
H	1.49450	-1.71440	2.59144
H	3.07054	-2.14113	3.27904
H	2.13245	-3.34876	2.39663
C	4.34030	-2.78506	0.94277
H	5.00996	-2.43383	0.15505
H	4.04533	-3.81621	0.71284
H	4.92022	-2.81764	1.87253
C	-0.75686	1.64767	2.85114
H	0.17396	2.20674	2.67436
C	-1.74710	2.54153	3.58700
H	-1.88136	3.51535	3.11337
H	-1.38550	2.72175	4.60599
H	-2.73163	2.06582	3.67715
C	-0.44536	0.43620	3.71996
H	-1.35115	-0.14362	3.93420

H	-0.03583	0.76978	4.67991
H	0.27934	-0.23655	3.25971
C	-2.06978	2.62314	0.34236
H	-2.14908	2.28684	-0.69605
C	-1.08958	3.79016	0.33411
H	-1.47712	4.59139	-0.30537
H	-0.11196	3.49515	-0.06161
H	-0.93381	4.21722	1.33093
C	-3.46934	3.02409	0.78971
H	-3.87241	3.75359	0.07569
H	-3.48663	3.49454	1.77598
H	-4.16291	2.17680	0.80426
O	1.25723	1.53163	-1.09212
C	2.15895	2.39669	-0.67014
C	4.09141	4.29418	0.13992
C	2.54537	3.45595	-1.51312
C	2.77253	2.32025	0.59143
C	3.72021	3.25568	0.98159
C	3.49073	4.38211	-1.11157
H	2.07821	3.52645	-2.49310
H	2.48011	1.51404	1.25930
H	4.17494	3.16870	1.96555
H	3.76442	5.18823	-1.78767
H	4.83295	5.02278	0.45098
C	-0.20321	-0.63936	-2.25328
H	-0.48263	-1.68478	-2.32332
H	0.72145	-0.34700	-2.74032
C	-1.19696	0.31696	-2.22033
O	-0.92618	1.59929	-2.47702
H	0.00727	1.77451	-2.16197
C	-2.63603	0.00347	-2.10930
C	-5.37537	-0.53043	-1.91630
C	-3.09151	-1.27256	-1.76332
C	-3.57839	0.99789	-2.38381
C	-4.93583	0.73178	-2.28880
C	-4.44675	-1.53179	-1.65877
H	-2.38652	-2.06334	-1.52654
H	-3.23229	1.98244	-2.67991
H	-5.65346	1.51671	-2.50743
H	-4.77706	-2.52265	-1.36198
H	-6.43797	-0.73687	-1.83306

TSA3

EE = -1877.530067

EE + ZPE = -1876.927780

G° = -1876.994013

Imaginary Freq = -1323.27

Ir	0.10824	0.03422	-0.13064
H	1.04841	1.09271	0.86656
P	1.85487	-1.58878	-0.10857
P	-1.45441	0.90600	1.40812
C	-0.98826	-1.66069	0.10453
C	-2.50427	-4.01252	0.40766
C	-2.24675	-1.63132	0.73201
C	-0.49337	-2.90331	-0.33431
C	-1.25511	-4.05769	-0.19336
C	-2.98529	-2.80100	0.87972
H	-0.85101	-5.00763	-0.53874
H	-3.95835	-2.75477	1.36505
H	-3.09008	-4.91885	0.52539
C	0.90133	-2.96655	-0.89043
H	0.91239	-2.76652	-1.97037
H	1.36147	-3.95106	-0.73964

C	-2.81577	-0.32179	1.19804
H	-3.46258	0.08613	0.40758
H	-3.43711	-0.43299	2.09511
C	3.32586	-1.29950	-1.22386
H	2.90823	-0.59665	-1.96021
C	4.45330	-0.57700	-0.49779
H	5.17138	-0.18237	-1.22491
H	5.00302	-1.24562	0.17205
H	4.09277	0.27097	0.09167
C	3.84290	-2.51431	-1.98453
H	4.64352	-2.19933	-2.66469
H	3.06967	-2.99127	-2.59329
H	4.26434	-3.27353	-1.31939
C	2.50611	-2.36347	1.47085
H	2.90942	-1.50596	2.03130
C	1.36218	-2.98434	2.26912
H	0.46219	-2.36891	2.28718
H	1.68321	-3.15895	3.30270
H	1.07977	-3.95481	1.84516
C	3.59688	-3.41501	1.30340
H	4.52242	-3.02713	0.87520
H	3.25325	-4.24712	0.67696
H	3.84305	-3.83999	2.28417
C	-1.08576	1.00826	3.23828
H	-0.32724	1.80435	3.29591
C	-2.26993	1.38794	4.11653
H	-2.63976	2.39654	3.92068
H	-1.97545	1.34816	5.17194
H	-3.10682	0.68993	3.99352
C	-0.44976	-0.28112	3.72530
H	-1.13680	-1.13156	3.62289
H	-0.18674	-0.19632	4.78594
H	0.45853	-0.50664	3.16101
C	-2.16302	2.57742	0.97250
H	-2.03626	2.59655	-0.11633
C	-1.30139	3.70148	1.53636
H	-1.61624	4.65643	1.10054
H	-0.24330	3.55896	1.29341
H	-1.40202	3.79533	2.62394
C	-3.64242	2.78963	1.26703
H	-3.94509	3.76809	0.87336
H	-3.87131	2.78687	2.33692
H	-4.27713	2.04238	0.78184
O	1.22084	2.09418	0.02082
C	2.52214	2.37789	-0.19143
C	5.18920	3.08999	-0.61694
C	3.01842	2.50637	-1.48937
C	3.37431	2.60396	0.89076
C	4.69755	2.95730	0.67515
C	4.34133	2.86653	-1.69465
H	2.34607	2.34204	-2.32798
H	2.97261	2.50922	1.89718
H	5.34986	3.13588	1.52515
H	4.71336	2.97664	-2.70932
H	6.22349	3.37305	-0.78328
C	0.06169	-0.06580	-2.29956
H	-0.21243	-1.02780	-2.72522
H	0.95543	0.37491	-2.74275
C	-0.97879	0.84098	-1.93822
O	-0.71160	2.20250	-2.01627
H	0.04437	2.40315	-1.43669
C	-2.41647	0.54455	-2.14249

C	-5.16301	0.03613	-2.47078
C	-2.89739	-0.76234	-2.28602
C	-3.34235	1.59086	-2.20987
C	-4.69745	1.33871	-2.36909
C	-4.25062	-1.01133	-2.43737
H	-2.21485	-1.60526	-2.24926
H	-2.98268	2.61190	-2.14812
H	-5.39333	2.17166	-2.41849
H	-4.59388	-2.03824	-2.52537
H	-6.22376	-0.16247	-2.58949

A4i

EE = -1877.575979

EE + ZPE = -1876.971541

G° = -1877.036843

Ir	-0.06417	0.08556	0.30363
P	-2.28412	-0.51691	-0.01172
P	1.93616	1.27745	0.47437
C	-2.71561	0.57996	-1.43403
H	-3.79108	0.78026	-1.51824
H	-2.42417	0.01704	-2.33480
C	1.29039	3.00954	0.35615
H	1.03276	3.32579	1.37460
H	2.05229	3.70647	-0.01721
C	-1.90371	1.84337	-1.31557
C	-0.37306	4.15482	-1.14662
C	-2.32240	3.01182	-1.94459
C	-0.69952	1.80906	-0.58261
C	0.04597	3.00176	-0.49278
C	-1.55642	4.16497	-1.87204
H	-3.25452	3.01445	-2.50662
H	-1.88281	5.07119	-2.37308
H	0.22659	5.06059	-1.07571
C	-3.41638	0.01533	1.35853
H	-3.22415	1.10086	1.35860
C	-2.98475	-0.54697	2.70736
H	-1.91084	-0.42829	2.87886
H	-3.21575	-1.61436	2.78539
H	-3.52263	-0.03660	3.51438
C	-4.90097	-0.21598	1.12027
H	-5.23807	0.12684	0.13683
H	-5.48517	0.32414	1.87423
H	-5.15504	-1.27702	1.21774
C	-2.64446	-2.24268	-0.58318
H	-1.84113	-2.38566	-1.32438
C	-2.41379	-3.24550	0.54040
H	-2.38095	-4.26149	0.13168
H	-3.23384	-3.21521	1.26787
H	-1.46869	-3.05594	1.06175
C	-3.97950	-2.45842	-1.28193
H	-4.15720	-1.74108	-2.08961
H	-4.81898	-2.39577	-0.58325
H	-4.00105	-3.46129	-1.72415
C	3.21495	1.26502	-0.88163
H	3.82736	2.15637	-0.66627
C	4.11351	0.03725	-0.87235
H	3.53053	-0.88770	-0.94642
H	4.73980	-0.01691	0.02240
H	4.78403	0.07118	-1.73892
C	2.55301	1.44082	-2.24162
H	1.91573	2.32866	-2.29707
H	1.93523	0.56859	-2.48363

H	3.32252	1.52640	-3.01728
C	2.93151	1.14299	2.04103
H	3.90769	1.60978	1.83490
C	3.12122	-0.33018	2.39627
H	3.72181	-0.41509	3.30920
H	3.62186	-0.90223	1.61058
H	2.15266	-0.81532	2.56273
C	2.26749	1.86825	3.20279
H	2.81463	1.65749	4.12838
H	1.23863	1.51525	3.34676
H	2.24573	2.95399	3.07467
O	0.61587	-1.86024	1.02383
C	1.24383	-2.42586	0.03527
C	2.69157	-3.54277	-2.13280
C	2.17580	-3.46738	0.23426
C	1.05123	-1.99572	-1.29954
C	1.77243	-2.53010	-2.35906
C	2.87575	-4.00455	-0.82829
H	2.33560	-3.81403	1.25174
H	0.26712	-1.24563	-1.51714
H	1.60266	-2.15974	-3.36723
H	3.59231	-4.80061	-0.64094
H	3.24913	-3.97645	-2.95619
H	-0.50533	0.84369	1.58293

A4ii

EE = -1954.933148

EE + ZPE = -1954.290278

G° = -1954.355885

Ir	0.18628	-0.25711	-0.03278
P	-1.48314	1.40786	0.17033
P	2.41846	-0.88290	0.01483
C	1.12881	1.37543	-1.00400
C	2.46884	3.69490	-2.00036
C	2.49405	1.36342	-1.37931
C	0.44804	2.58080	-1.29126
C	1.10586	3.71671	-1.75165
C	3.15117	2.50085	-1.83901
H	0.53537	4.62700	-1.92760
H	4.21025	2.44127	-2.08403
H	2.98458	4.58681	-2.34272
C	-1.03901	2.59529	-1.15442
H	-1.48660	2.18198	-2.06929
H	-1.45798	3.59735	-1.01279
C	3.22734	0.05798	-1.32694
H	3.04830	-0.50384	-2.25336
H	4.31111	0.16564	-1.20999
C	-3.33934	1.17648	-0.03851
H	-3.40430	0.24458	-0.61558
C	-4.06834	0.96004	1.28207
H	-5.08277	0.59686	1.07896
H	-4.16474	1.89780	1.84255
H	-3.57234	0.22447	1.91833
C	-4.03969	2.26459	-0.84576
H	-5.10007	2.00333	-0.94381
H	-3.63955	2.37323	-1.85660
H	-3.99359	3.24409	-0.35729
C	-1.30076	2.36238	1.77240
H	-1.90046	1.78187	2.48691
C	0.13823	2.38443	2.27148
H	0.53497	1.37100	2.39440
H	0.18686	2.90737	3.23485

H	0.79785	2.90731	1.56834
C	-1.84938	3.78141	1.70825
H	-2.88352	3.83242	1.35628
H	-1.23348	4.40712	1.05108
H	-1.81853	4.23722	2.70495
C	3.19738	-0.21734	1.58030
H	2.62178	0.70836	1.71731
C	2.91062	-1.12478	2.76781
H	1.83748	-1.31172	2.88331
H	3.26720	-0.65941	3.69361
H	3.41530	-2.09440	2.67793
C	4.66704	0.17296	1.49919
H	5.32474	-0.67362	1.28099
H	4.98228	0.58951	2.46338
H	4.84065	0.94593	0.74461
C	2.96887	-2.64422	-0.22174
H	2.45359	-3.21024	0.56581
C	4.46709	-2.88145	-0.09236
H	4.69985	-3.92276	-0.34552
H	4.83941	-2.70117	0.91947
H	5.03573	-2.24734	-0.78326
C	2.47135	-3.14223	-1.57600
H	3.09006	-2.74328	-2.38811
H	1.43470	-2.85181	-1.77620
H	2.53898	-4.23454	-1.62516
C	-1.32994	-1.61484	0.86082
C	-0.09047	-2.26959	0.71094
O	-1.74449	-1.24721	2.14860
H	-0.96582	-0.91289	2.60370
C	-2.47703	-2.00638	0.00519
C	-4.64179	-2.77637	-1.59767
C	-3.71856	-2.28811	0.57303
C	-2.33175	-2.13402	-1.37925
C	-3.40239	-2.51396	-2.17041
C	-4.79108	-2.66614	-0.22395
H	-3.83927	-2.20401	1.64752
H	-1.37300	-1.88412	-1.83048
H	-3.27221	-2.59514	-3.24564
H	-5.75172	-2.87781	0.23712
H	-5.48297	-3.06586	-2.22003
H	0.45854	-2.51578	1.62045
H	0.00458	-3.01157	-0.07979

TSA4

EE = -1877.530067

EE + ZPE = -1876.927780

G° = -1876.994013

Imaginary Freq = -1275.25

Ir	-0.15770	0.07506	0.05213
P	-2.06619	-1.22797	-0.12452
P	1.32127	1.86002	0.24812
C	-3.15824	-0.06226	-1.04851
H	-4.22754	-0.27148	-0.91558
H	-2.93036	-0.20804	-2.11406
C	0.16670	3.19091	0.82388
H	0.11853	3.11430	1.91576
H	0.53626	4.19626	0.57947
C	-2.79260	1.33288	-0.61662
C	-2.11383	3.93649	0.08163
C	-3.71403	2.36585	-0.76160
C	-1.50195	1.58198	-0.09459
C	-1.18944	2.91370	0.25034

C	-3.37973	3.66612	-0.41858
H	-4.70260	2.14727	-1.16084
H	-4.10232	4.46730	-0.54132
H	-1.84235	4.95510	0.35214
C	-2.98694	-1.50736	1.46625
H	-3.24009	-0.46810	1.73189
C	-2.07780	-2.06074	2.55500
H	-1.19300	-1.43206	2.68822
H	-1.73477	-3.07462	2.32223
H	-2.61858	-2.10452	3.50766
C	-4.27448	-2.31007	1.35427
H	-4.93471	-1.95290	0.55708
H	-4.83325	-2.24640	2.29534
H	-4.06768	-3.37109	1.17565
C	-1.99553	-2.77373	-1.15445
H	-1.31335	-2.44511	-1.95577
C	-1.31508	-3.91197	-0.40484
H	-1.09983	-4.73619	-1.09427
H	-1.96704	-4.31163	0.38133
H	-0.37506	-3.58833	0.05258
C	-3.30391	-3.22130	-1.79129
H	-3.80663	-2.41907	-2.34030
H	-4.00392	-3.61240	-1.04742
H	-3.10454	-4.03053	-2.50381
C	2.02540	2.63112	-1.30157
H	2.32303	3.64686	-0.99428
C	3.24875	1.90132	-1.83363
H	3.01789	0.85347	-2.05723
H	4.09193	1.91814	-1.13706
H	3.58279	2.37342	-2.76497
C	0.95559	2.72961	-2.37990
H	0.07294	3.28965	-2.05643
H	0.61839	1.72787	-2.67495
H	1.36640	3.22408	-3.26804
C	2.75843	1.95444	1.44150
H	3.36496	2.80924	1.10302
C	3.59733	0.68418	1.39904
H	4.51602	0.82101	1.98095
H	3.87891	0.37033	0.39069
H	3.04482	-0.14787	1.84996
C	2.30803	2.20473	2.87481
H	3.16040	2.08715	3.55365
H	1.54621	1.47493	3.17923
H	1.90297	3.20815	3.02861
O	1.01959	-1.81729	0.59084
C	2.24049	-2.05932	0.09202
C	4.77107	-2.66713	-0.94584
C	3.19087	-2.72279	0.87474
C	2.56902	-1.72720	-1.22488
C	3.82321	-2.02776	-1.73452
C	4.44218	-3.01659	0.35924
H	2.92301	-2.98894	1.89368
H	1.81212	-1.22602	-1.82743
H	4.06178	-1.75954	-2.76072
H	5.17185	-3.52495	0.98358
H	5.75334	-2.89802	-1.34544
H	0.63204	-0.73903	1.27124

Products

5 (Phenol)

EE = -307.325357

EE + ZPE = -307.221283

G° = -307.250277

O	0.05019	2.29241	0.00000
C	0.00000	0.93801	0.00000
C	0.02043	-1.84628	0.00000
C	-1.19782	0.23148	0.00000
C	1.21015	0.25131	0.00000
C	1.21323	-1.13252	0.00000
C	-1.18172	-1.15615	0.00000
H	-2.14317	0.77088	0.00000
H	2.13138	0.82478	0.00000
H	2.16129	-1.66192	0.00000
H	-2.12201	-1.69920	0.00000
H	0.02977	-2.93104	0.00000
H	-0.84433	2.64219	0.00000

6 (Enolate)

EE = -384.681142

EE + ZPE = -384.543763

G° = -384.575940

H	3.52334	1.01279	-0.40997
C	2.44227	1.06798	-0.44998
H	1.97923	1.93840	-0.89507
C	1.70304	0.05288	-0.00757
C	0.22795	0.03927	-0.00662
C	-2.56731	-0.00780	-0.01332
C	-0.50378	1.20384	0.23124
C	-0.46484	-1.15120	-0.23673
C	-1.85126	-1.17308	-0.24276
C	-1.88797	1.18068	0.22278
H	0.02656	2.12679	0.44619
H	0.08906	-2.06153	-0.45043
H	-2.37431	-2.10460	-0.43581
H	-2.44265	2.09396	0.41484
H	-3.65260	-0.02478	-0.01463
O	2.31755	-1.08718	0.41922
H	1.72243	-1.55902	1.00887

7 (Acetophenone)

EE = -384.706917

EE + ZPE = -384.569956

G° = -384.602631

C	-0.20468	-0.05449	-0.00022
C	2.57456	0.10935	0.00018
C	0.42842	1.18754	-0.00015
C	0.57116	-1.21343	-0.00006
C	1.95173	-1.13328	0.00013
C	1.81270	1.26892	0.00004
H	-0.15720	2.10183	-0.00025
H	0.05722	-2.16950	-0.00012
H	2.54858	-2.04001	0.00024
H	2.29880	2.23941	0.00008
H	3.65847	0.17335	0.00034
C	-1.69109	-0.20480	-0.00047
O	-2.20269	-1.30000	0.00020
C	-2.53415	1.04381	0.00011
H	-2.32510	1.65876	0.88184
H	-3.58523	0.75535	0.00051
H	-2.32584	1.65901	-0.88161

**Reaction between (PCP)Ir and 1 along path B
B2**

EE = -2262.257365

EE + ZPE = -2261.507327

G° = -2261.582851

Ir	-0.65902	0.42028	-0.33152
P	0.93382	2.01580	0.14302
P	-2.64873	-0.73939	-0.49549
C	-1.86796	2.02261	-0.33917
C	-3.57409	4.27141	0.07286
C	-3.28064	1.91128	-0.36332
C	-1.36247	3.34571	-0.21980
C	-2.19829	4.43210	0.00751
C	-4.10444	3.00930	-0.14116
H	-1.76012	5.42274	0.12121
H	-5.18450	2.86854	-0.14527
H	-4.22324	5.12090	0.26229
C	0.11035	3.56496	-0.40095
H	0.47540	4.46839	0.09956
H	0.33848	3.66796	-1.47084
C	-3.90263	0.59242	-0.71726
H	-4.83047	0.39486	-0.16460
H	-4.16828	0.59769	-1.78396
C	1.16674	2.21223	1.99390
H	0.21198	1.81253	2.36637
C	2.28641	1.31007	2.49513
H	2.25045	1.22743	3.58808
H	3.27359	1.70766	2.23067
H	2.22306	0.29835	2.07744
C	1.30517	3.63303	2.51975
H	1.41951	3.61253	3.61080
H	0.41829	4.23468	2.29788
H	2.17949	4.15049	2.11042
C	2.62621	2.07721	-0.63323
H	3.12545	1.16677	-0.27164
C	2.48234	1.96735	-2.14654
H	1.78039	1.17781	-2.43802
H	3.45641	1.75806	-2.60505
H	2.11437	2.90531	-2.57897
C	3.47667	3.28638	-0.27188
H	3.72667	3.32880	0.79205
H	2.97156	4.22307	-0.53892
H	4.42269	3.25853	-0.82824
C	-3.00467	-1.88406	-1.93375
H	-2.58513	-1.28953	-2.76047
C	-2.19813	-3.16722	-1.82367
H	-1.13229	-2.95686	-1.69847
H	-2.31744	-3.77790	-2.72637
H	-2.51849	-3.77694	-0.96919
C	-4.46167	-2.18457	-2.26505
H	-4.90526	-2.89401	-1.56160
H	-4.52223	-2.64012	-3.26112
H	-5.09080	-1.28997	-2.27891
C	-3.15485	-1.61854	1.07585
H	-2.35111	-2.35183	1.24062
C	-4.48895	-2.34955	1.06231
H	-4.73004	-2.69618	2.07491
H	-4.48196	-3.22888	0.41323
H	-5.31111	-1.69759	0.74239
C	-3.11431	-0.60797	2.21775
H	-3.22645	-1.12294	3.17984
H	-3.93329	0.11732	2.13304

H	-2.17652	-0.04100	2.22197
O	0.89376	-1.47357	-0.14033
C	1.51303	-1.88783	-1.35067
H	1.60221	-0.97859	-1.95285
H	0.87680	-2.59130	-1.90254
C	2.88750	-2.51776	-1.14734
C	0.54336	-2.42573	0.79172
C	-0.25790	-4.18926	2.78873
C	0.42961	-3.78137	0.51007
C	0.26281	-1.95062	2.06869
C	-0.13412	-2.83107	3.05947
C	0.02440	-4.65388	1.51501
H	0.63661	-4.16979	-0.48114
H	0.32422	-0.88031	2.24340
H	-0.35711	-2.44905	4.05108
H	-0.06803	-5.71145	1.28761
H	-0.57152	-4.87800	3.56614
C	3.91765	-1.53908	-0.64901
C	5.82189	0.27343	0.27935
C	4.16834	-1.41724	0.71405
C	4.62975	-0.74599	-1.54472
C	5.57907	0.15331	-1.08275
C	5.11364	-0.51324	1.17736
H	3.61910	-2.04162	1.41696
H	4.42964	-0.84030	-2.60904
H	6.13000	0.76778	-1.78938
H	5.29990	-0.42537	2.24369
H	6.56538	0.97778	0.64007
H	2.80459	-3.32805	-0.40461
O	3.19478	-3.04082	-2.42166
H	4.09023	-3.38779	-2.39595

TSB1

EE = -2262.200786

EE + ZPE = -2261.454192

G° = -2261.528539

Imaginary Freq = -568.78

Ir	-0.27880	0.34123	0.13296
P	1.68893	1.06666	1.09275
P	-2.45141	0.35279	-0.74740
C	-0.49408	2.32608	-0.24177
C	-0.85739	5.11016	-0.64852
C	-1.46032	2.82796	-1.14200
C	0.25991	3.28597	0.47205
C	0.08401	4.64901	0.25950
C	-1.63548	4.19238	-1.33928
H	0.68531	5.35935	0.82475
H	-2.39224	4.54028	-2.04036
H	-0.99169	6.17585	-0.80794
C	1.23329	2.80623	1.51112
H	0.74004	2.75267	2.49324
H	2.10077	3.47066	1.62099
C	-2.33357	1.83566	-1.84525
H	-3.30450	2.25550	-2.13557
H	-1.84888	1.46453	-2.76216
C	2.13937	0.28880	2.72439
H	1.13495	0.14054	3.15324
C	2.75793	-1.08565	2.51366
H	2.87324	-1.60003	3.47499
H	3.75508	-1.00997	2.06137
H	2.12951	-1.70531	1.86519
C	2.94853	1.13332	3.69959

H	2.97230	0.63826	4.67804
H	2.52270	2.13016	3.84946
H	3.98602	1.25703	3.37683
C	3.21953	1.20911	0.04377
H	3.39380	0.18053	-0.29315
C	2.90710	2.06058	-1.18131
H	2.00836	1.71345	-1.70149
H	3.75166	2.02018	-1.88003
H	2.74692	3.11156	-0.91168
C	4.47768	1.70959	0.73618
H	4.84804	1.01091	1.49161
H	4.32651	2.68500	1.21519
H	5.27565	1.83458	-0.00704
C	-3.15884	-0.95669	-1.88624
H	-2.25746	-1.31711	-2.40560
C	-3.75847	-2.12296	-1.11187
H	-3.08427	-2.51295	-0.34310
H	-3.99403	-2.94653	-1.79579
H	-4.69427	-1.83566	-0.61806
C	-4.11602	-0.46470	-2.96638
H	-5.04147	-0.05498	-2.55207
H	-4.39531	-1.30689	-3.61125
H	-3.66934	0.30001	-3.60732
C	-3.78274	0.72500	0.51151
H	-3.87752	-0.22750	1.05589
C	-5.14259	1.11020	-0.05292
H	-5.82347	1.36506	0.76812
H	-5.61286	0.30729	-0.62584
H	-5.07390	1.99623	-0.69565
C	-3.30735	1.78674	1.49857
H	-4.03711	1.88644	2.31106
H	-3.20772	2.76564	1.01363
H	-2.32994	1.53860	1.92589
O	0.10141	-1.79248	0.65151
C	0.20811	-1.75437	-1.20855
H	0.30356	-0.87662	-1.86153
H	-0.73856	-2.27075	-1.35145
C	1.36898	-2.71210	-1.36954
C	-0.87880	-2.54702	1.17867

B3

EE = -2262.273920

EE + ZPE = -2261.525430

G° = -2261.599723

Ir	-0.35683	0.12255	0.02329
P	1.47006	1.42418	0.69310
P	-2.09420	-1.46125	-0.01082
C	2.25664	0.28281	1.91380
H	2.88711	-0.38576	1.31316
H	2.91787	0.78850	2.62555
C	-2.41153	-1.55632	1.80653
H	-2.92913	-2.47556	2.11044
H	-3.09233	-0.71903	2.02524
C	1.14760	-0.47128	2.59143
C	-0.94927	-1.80259	3.83651
C	-0.03685	-0.71118	1.85520
C	1.27006	-0.89536	3.90888
C	0.23022	-1.57609	4.52898
C	-1.09724	-1.36620	2.52338
H	2.18919	-0.69413	4.45639
H	0.33517	-1.91623	5.55478
H	-1.77476	-2.31566	4.32673

C	0.94998	2.90991	1.69652
H	0.01694	2.55443	2.15999
C	0.61227	4.09132	0.79567
H	1.52268	4.56013	0.40519
H	0.07312	4.85417	1.36831
H	-0.02069	3.80632	-0.05101
C	1.89248	3.31161	2.82236
H	2.88966	3.57564	2.45450
H	1.99973	2.52215	3.57240
H	1.48994	4.19341	3.33487
C	2.82489	1.85570	-0.49509
H	3.13064	0.84961	-0.81909
C	4.04763	2.52849	0.10999
H	4.84661	2.57312	-0.64019
H	4.44249	1.98439	0.97504
H	3.83285	3.55776	0.41920
C	-1.69311	-3.20645	-0.53644
H	-1.15515	-3.09445	-1.48794
C	-0.74328	-3.86589	0.45764
H	-0.35026	-4.78951	0.01884
H	-1.26538	-4.13443	1.38393
H	0.10251	-3.23244	0.73050
C	-2.89990	-4.11118	-0.74504
H	-2.55209	-5.12437	-0.97920
H	-3.54196	-3.78898	-1.56748
H	-3.51294	-4.18346	0.16188
C	-3.67547	-0.91889	-0.81366
H	-3.70982	0.13674	-0.50276
C	-3.49986	-0.93686	-2.32840
H	-3.45432	-1.95902	-2.72293
H	-2.58822	-0.40614	-2.62725
H	-4.34704	-0.43384	-2.80775
C	-4.97284	-1.57152	-0.35671
H	-5.09104	-2.58906	-0.73698
H	-5.81839	-0.98343	-0.73225
H	-5.06258	-1.60551	0.73434
O	-0.98843	1.31159	-1.68804
C	-2.03724	2.02885	-1.39030
C	-4.42509	3.43180	-0.76730
C	-2.40379	2.32965	-0.05613
C	-2.89695	2.50930	-2.40192
C	-4.05885	3.18758	-2.09120
C	-3.58137	3.00158	0.24522
H	-1.73058	2.04174	0.76069
H	-2.62508	2.29893	-3.43310
H	-4.70334	3.53073	-2.89704
H	-3.83126	3.20112	1.28443
H	-5.34124	3.96516	-0.53594
C	0.73550	-0.85922	-1.45166
H	-0.01730	-1.27563	-2.13000
H	1.22408	-0.04620	-1.99759
C	1.72124	-1.97539	-1.11589
H	1.64007	-2.23676	-0.04771
O	1.34151	-3.09753	-1.91311
H	1.98577	-3.79547	-1.76379
C	3.16363	-1.61672	-1.38889
C	5.81679	-0.88654	-1.87652
C	4.13777	-1.78453	-0.41105
C	3.54650	-1.12593	-2.63774
C	4.85938	-0.75682	-2.87792
C	5.45693	-1.41282	-0.64605
H	3.85605	-2.20550	0.55268

H	2.79645	-1.02513	-3.41828
H	5.14191	-0.36516	-3.85059
H	6.20282	-1.53805	0.13308
H	6.84418	-0.58961	-2.06356
C	2.31123	2.59644	-1.72561
H	3.04251	2.50512	-2.53802
H	2.18025	3.66450	-1.52355
H	1.34917	2.20796	-2.07792

TSB2

EE = -2262.236654

EE + ZPE = -2261.490865

G° = -2261.563732

Imaginary Freq = -158.14

Ir	-0.09709	-0.19094	-0.17878
P	1.39813	1.55644	0.39647
P	-1.93141	-1.62452	-0.00515
C	1.83585	1.04084	2.11644
H	2.60445	0.26089	2.00315
H	2.28690	1.84291	2.71144
C	-2.62335	-1.21690	1.66224
H	-3.11741	-2.07761	2.13175
H	-3.40442	-0.46273	1.48471
C	0.58929	0.48247	2.74903
C	-1.67472	-0.62947	3.91043
C	-0.40010	-0.07155	1.90850
C	0.42918	0.50258	4.13115
C	-0.69999	-0.05435	4.71342
C	-1.53573	-0.63836	2.52628
H	1.19985	0.94729	4.75832
H	-0.82001	-0.04228	5.79270
H	-2.56187	-1.06550	4.36625
C	0.54080	3.19694	0.60761
H	-0.45899	2.87801	0.92700
C	0.38323	3.94324	-0.71243
H	1.30591	4.47098	-0.98179
H	-0.41004	4.69397	-0.61500
H	0.10305	3.27955	-1.53573
C	1.10621	4.10112	1.69392
H	2.14458	4.39143	1.50169
H	1.05404	3.64247	2.68616
H	0.51392	5.02309	1.73316
C	3.04722	1.78390	-0.43400
H	3.43621	0.75774	-0.38057
C	4.04294	2.69062	0.27416
H	5.02594	2.59685	-0.20487
H	4.16925	2.43682	1.33178
H	3.75007	3.74425	0.20709
C	-1.54382	-3.44681	0.05100
H	-0.94753	-3.61526	-0.85589
C	-0.65295	-3.74279	1.25431
H	-0.27070	-4.76804	1.18348
H	-1.21248	-3.66654	2.19448
H	0.20166	-3.06371	1.33190
C	-2.74020	-4.38719	0.05345
H	-2.39536	-5.41521	0.21820
H	-3.28431	-4.37598	-0.89312
H	-3.44872	-4.15266	0.85724
C	-3.32695	-1.30630	-1.18450
H	-3.42657	-0.21538	-1.09119
C	-2.90347	-1.60647	-2.61495
H	-2.66537	-2.66829	-2.76010

H	-2.03217	-1.00767	-2.89659
H	-3.71892	-1.35709	-3.30367
C	-4.68393	-1.90842	-0.84030
H	-4.74273	-2.97285	-1.08030
H	-5.45587	-1.40117	-1.43017
H	-4.95021	-1.78346	0.21441
O	-1.04845	1.02671	-1.56306
C	-2.09036	1.79530	-1.30764
C	-4.31323	3.51071	-0.98224
C	-2.63502	2.04642	-0.03713
C	-2.70302	2.41974	-2.41243
C	-3.78690	3.26079	-2.24648
C	-3.72611	2.89302	0.11173
H	-2.18410	1.56970	0.82895
H	-2.28762	2.22080	-3.39684
H	-4.23206	3.72949	-3.12062
H	-4.12008	3.07070	1.10963
H	-5.16501	4.17108	-0.85658
C	0.83778	-1.06372	-1.92835
H	0.15580	-1.63200	-2.56353
H	1.38865	-0.32073	-2.50312
C	1.64300	-1.92801	-1.04250
H	1.24133	-1.67011	0.05668
O	1.36843	-3.29454	-1.24939
H	1.87560	-3.80484	-0.60924
C	3.12628	-1.67841	-0.91858
C	5.86910	-1.24445	-0.64909
C	3.74270	-1.78427	0.32590
C	3.90538	-1.39009	-2.03500
C	5.26779	-1.16733	-1.89915
C	5.10578	-1.56437	0.46537
H	3.13428	-2.01323	1.20174
H	3.43202	-1.32597	-3.01075
H	5.86505	-0.92928	-2.77424
H	5.57054	-1.63527	1.44399
H	6.93416	-1.06195	-0.54523
C	2.92241	2.14679	-1.90902
H	3.86043	1.91499	-2.42773
H	2.72936	3.21511	-2.04353
H	2.11399	1.60190	-2.40657

B4i

EE = -2262.269025

EE + ZPE = -2261.521887

G° = -2261.594503

Ir	0.44371	-0.03810	-0.72789
P	-0.58437	-0.91481	1.33885
P	2.55590	0.79412	-0.50957
C	-0.37222	-2.71253	0.92912
H	-1.20782	-2.96767	0.26669
H	-0.45072	-3.36588	1.80378
C	3.47762	-0.57996	-1.35786
H	3.33516	-0.41781	-2.43399
H	4.55636	-0.54692	-1.16057
C	0.95955	-2.87146	0.24431
C	3.57159	-3.02388	-0.71380
C	1.71261	-4.03261	0.41375
C	1.49013	-1.77607	-0.47088
C	2.83767	-1.85642	-0.88433
C	3.00181	-4.12578	-0.09036
H	1.28809	-4.86619	0.97096
H	3.57737	-5.03632	0.04563

H	4.61005	-3.06040	-1.03878
C	-2.39744	-0.80792	1.76447
H	-2.84234	-1.15460	0.82371
C	-2.90821	0.60950	1.99702
H	-2.58914	1.30450	1.21427
H	-2.57859	1.01978	2.95635
H	-4.00482	0.59620	2.00477
C	-2.86671	-1.75463	2.86076
H	-2.56624	-2.79233	2.68266
H	-3.96295	-1.73659	2.90747
H	-2.49786	-1.45632	3.84867
C	0.40074	-0.71876	2.92675
H	1.39207	-0.46652	2.53470
C	-0.07484	0.45198	3.77847
H	0.67612	0.67989	4.54503
H	-1.00470	0.20973	4.30399
H	-0.24814	1.36264	3.19537
C	0.56373	-1.97243	3.77547
H	1.08756	-2.77021	3.23958
H	-0.39534	-2.36615	4.12873
H	1.16194	-1.73093	4.66282
C	3.57110	1.05373	1.05029
H	4.45263	1.59284	0.66378
C	2.90275	1.92303	2.10896
H	2.07955	1.39274	2.59416
H	2.50012	2.86112	1.72161
H	3.63304	2.16815	2.88892
C	4.06028	-0.25265	1.66959
H	4.75506	-0.79413	1.02338
H	3.24094	-0.94224	1.90312
H	4.58434	-0.03281	2.60710
C	3.00886	2.29870	-1.52224
H	4.09736	2.18112	-1.66108
C	2.74343	3.62173	-0.81470
H	2.97145	4.44685	-1.49834
H	3.36271	3.76178	0.07477
H	1.68946	3.71734	-0.52625
C	2.33440	2.31013	-2.88596
H	2.70804	3.16372	-3.46342
H	1.24955	2.41822	-2.77316
H	2.53119	1.40809	-3.47314
O	-0.74727	1.73387	-1.17255
C	-1.05056	2.70949	-0.35914
C	-1.82049	4.82269	1.37420
C	-2.07306	3.61956	-0.70920
C	-0.42289	2.91708	0.88406
C	-0.79917	3.95167	1.72711
C	-2.44762	4.64172	0.14355
H	-2.55992	3.49010	-1.67356
H	0.35595	2.21819	1.17258
H	-0.28551	4.06990	2.68073
H	-3.24556	5.31668	-0.15732
H	-2.11975	5.62863	2.03621
C	-1.70755	-1.58993	-2.03264
C	-3.05654	-1.24480	-1.57789
C	-5.62516	-0.61327	-0.69556
C	-3.45784	0.09173	-1.47147
C	-3.96042	-2.25867	-1.24692
C	-5.23692	-1.94090	-0.80927
C	-4.73111	0.39872	-1.02808
H	-2.74334	0.88714	-1.67240
H	-3.65285	-3.29526	-1.33086

H	-5.93196	-2.73563	-0.55633
H	-5.01970	1.44059	-0.92341
H	-6.62320	-0.36575	-0.34690
C	-0.80958	-0.72474	-2.60590
H	-1.13752	0.26739	-2.89336
H	-0.03955	-1.17249	-3.22859
O	-1.43772	-2.90592	-1.95496
H	-0.50677	-3.05587	-2.16523
H	1.15221	0.26174	-2.12639

B4ii

EE = -2262.287455

EE + ZPE = -2261.541456

G° = -2261.614312

Ir	0.08261	-0.24907	0.01158
P	2.30911	-1.02214	0.27096
P	-1.83569	0.63075	-1.06446
C	0.61163	-0.43160	-1.99659
C	1.32062	-0.79926	-4.68947
C	-0.36942	-0.53771	-2.99309
C	1.95754	-0.51972	-2.37913
C	2.30317	-0.70256	-3.71468
C	-0.01497	-0.71534	-4.32706
H	3.35316	-0.76430	-3.99417
H	-0.79103	-0.78631	-5.08675
H	1.59653	-0.93910	-5.73041
C	3.00957	-0.39591	-1.31746
H	3.20463	0.66587	-1.12661
H	3.95375	-0.87996	-1.59194
C	-1.80917	-0.41651	-2.58350
H	-2.44570	-0.02909	-3.38830
H	-2.21829	-1.39206	-2.27759
C	3.32592	-0.24336	1.62548
H	2.77929	0.69472	1.79378
C	3.31436	-1.05953	2.91236
H	3.74658	-0.46392	3.72425
H	3.92410	-1.96639	2.82092
H	2.30836	-1.36391	3.21238
C	4.74885	0.13285	1.22940
H	5.23008	0.64479	2.07116
H	4.77781	0.81618	0.37683
H	5.36286	-0.74058	0.98470
C	2.66497	-2.85052	0.29647
H	2.33979	-3.16402	1.29777
C	1.82656	-3.58440	-0.74290
H	0.75670	-3.39186	-0.61973
H	1.99853	-4.66436	-0.66492
H	2.09420	-3.27755	-1.76127
C	4.13634	-3.20696	0.12773
H	4.77316	-2.77631	0.90439
H	4.51926	-2.88133	-0.84630
H	4.25906	-4.29567	0.17030
C	-3.53566	0.41273	-0.33520
H	-3.40215	-0.49877	0.25660
C	-3.87154	1.53859	0.63393
H	-3.07546	1.70248	1.36928
H	-4.78328	1.29064	1.19009
H	-4.04888	2.48894	0.11887
C	-4.67482	0.13534	-1.30782
H	-4.90319	0.98479	-1.95774
H	-5.58198	-0.09396	-0.73426
H	-4.46994	-0.73100	-1.94424

C	-1.73924	2.38958	-1.68776
H	-1.74632	2.99333	-0.76981
C	-2.91862	2.80464	-2.55948
H	-2.75409	3.82735	-2.91779
H	-3.87648	2.79521	-2.03390
H	-3.00897	2.16882	-3.44850
C	-0.43057	2.67855	-2.41831
H	-0.37263	3.75488	-2.61821
H	-0.39094	2.15861	-3.38311
H	0.44430	2.38869	-1.83210
O	1.29279	1.61341	0.04321
C	-0.27690	0.13675	2.20150
H	-1.03547	0.90079	2.31889
H	0.66497	0.34253	2.70060
C	-0.66658	-1.17934	1.99097
C	1.23780	2.70115	0.76851
C	1.26207	5.12069	2.25654
C	0.06102	3.24323	1.32253
C	2.42994	3.42439	0.99822
C	2.43693	4.60311	1.72053
C	0.07924	4.42635	2.04621
H	-0.87533	2.71368	1.17265
H	3.34825	3.02952	0.56718
H	3.37664	5.12992	1.86892
H	-0.85282	4.81222	2.45318
H	1.27023	6.04515	2.82470
C	-2.09181	-1.62572	1.96737
C	-4.75248	-2.49835	2.00724
C	-2.50154	-2.71200	1.18975
C	-3.03043	-1.01084	2.79144
C	-4.35241	-1.43731	2.80429
C	-3.81739	-3.14296	1.20544
H	-1.78994	-3.19691	0.52395
H	-2.72007	-0.18927	3.43008
H	-5.07052	-0.93878	3.44850
H	-4.11834	-3.97908	0.58183
H	-5.78567	-2.83093	2.01610
O	0.20359	-2.16990	2.40021
H	-0.10187	-3.01521	2.05722
H	-0.53441	-1.66632	-0.32482

TSB3

EE = -2262.231597

EE + ZPE = -2261.488302

G° = -2261.559694

Imaginary Freq = -1331.35

Ir	0.02473	-0.14865	-0.58452
P	-1.14291	-0.72712	1.44853
P	2.39418	-0.53026	-0.60456
C	-1.90518	-2.29580	0.83702
H	-2.73124	-1.98159	0.18629
H	-2.31667	-2.93630	1.62315
C	2.30719	-1.98249	-1.75982
H	2.12093	-1.55843	-2.75502
H	3.25760	-2.53040	-1.80717
C	-0.84495	-2.98839	0.03002
C	1.23387	-4.23064	-1.33927
C	-0.75141	-4.37681	-0.00627
C	0.09971	-2.19310	-0.65411
C	1.17172	-2.84127	-1.29163
C	0.26689	-5.00142	-0.71233
H	-1.48555	-4.97310	0.53205

H	0.32562	-6.08494	-0.74344
H	2.07272	-4.71072	-1.83987
C	-2.58731	0.35251	1.88205
H	-3.15608	0.30618	0.94167
C	-2.19190	1.80995	2.08449
H	-1.58161	2.18155	1.25456
H	-1.63613	1.96582	3.01513
H	-3.09626	2.42765	2.13054
C	-3.48324	-0.16548	2.99693
H	-3.80173	-1.20021	2.83067
H	-4.38907	0.45007	3.05219
H	-2.99603	-0.11099	3.97697
C	-0.22778	-1.23340	3.00877
H	0.73259	-1.57743	2.60049
C	0.05219	-0.05685	3.93646
H	0.77891	-0.35492	4.70158
H	-0.85476	0.26340	4.46047
H	0.45952	0.81666	3.41674
C	-0.83687	-2.39653	3.78030
H	-0.86775	-3.31412	3.18502
H	-1.85179	-2.17812	4.12910
H	-0.22547	-2.60543	4.66656
C	3.47893	-1.16669	0.79263
H	4.49890	-1.14415	0.37518
C	3.42236	-0.25952	2.01486
H	2.43302	-0.30619	2.48354
H	3.62360	0.79009	1.78741
H	4.15437	-0.59287	2.75983
C	3.16357	-2.60280	1.19225
H	3.37484	-3.32184	0.39704
H	2.11128	-2.73291	1.47229
H	3.77320	-2.87981	2.06059
C	3.60867	0.55132	-1.54430
H	4.35732	-0.17736	-1.89788
C	4.32074	1.59945	-0.70004
H	4.98803	2.18698	-1.34092
H	4.93560	1.16028	0.09013
H	3.61210	2.29756	-0.23987
C	2.96673	1.21085	-2.75739
H	3.74488	1.67042	-3.37759
H	2.28138	2.01271	-2.45557
H	2.41109	0.51216	-3.39005
O	0.20561	2.16841	-0.81321
C	0.94163	2.93816	-0.01042
C	2.44354	4.64791	1.64211
C	1.30879	4.22022	-0.44616
C	1.35454	2.53290	1.26085
C	2.08859	3.37931	2.07856
C	2.04605	5.05795	0.37308
H	0.99075	4.53704	-1.43579
H	1.09485	1.52610	1.57355
H	2.39259	3.03352	3.06490
H	2.31665	6.04804	0.01633
H	3.02217	5.30972	2.27826
C	-1.85116	-0.22906	-1.89800
C	-2.94594	0.72204	-1.58730
C	-5.05579	2.46008	-0.93667
C	-2.73812	2.10287	-1.50249
C	-4.23969	0.23617	-1.36665
C	-5.27915	1.09577	-1.04000
C	-3.78002	2.95508	-1.17820
H	-1.74219	2.50784	-1.64156

H	-4.42570	-0.82790	-1.45745
H	-6.27366	0.69177	-0.87246
H	-3.58958	4.02227	-1.10747
H	-5.86804	3.13371	-0.68085
C	-0.66699	0.11317	-2.61803
H	-0.55680	1.13615	-2.97332
H	-0.29107	-0.63452	-3.31716
O	-2.36905	-1.50160	-2.08245
H	-1.63712	-2.12664	-2.13903
H	0.80272	1.05294	-1.44393

Reaction between (PCP)Ir and 1 along path C C2

EE = -2261.058276

EE + ZPE = -2260.331642

G° = -2260.407294

Ir	0.11513	-0.16880	-0.29552
P	0.90970	-2.42993	-0.28032
P	-0.29560	1.08076	1.56418
C	2.64221	-2.00710	-0.79475
H	2.55803	-1.81020	-1.87331
H	3.36692	-2.81917	-0.65410
C	1.21904	2.14608	1.52591
H	1.02281	2.91462	0.76274
H	1.43159	2.65714	2.47278
C	2.01166	0.14402	0.29260
C	4.66939	0.62609	1.04947
C	3.03104	-0.75540	-0.06410
C	2.34111	1.25503	1.08704
C	3.66122	1.48981	1.45351
C	4.34751	-0.49973	0.30467
H	3.89915	2.35855	2.06421
H	5.12724	-1.20290	0.01704
H	5.69933	0.81537	1.33632
O	0.47126	0.01241	-2.40593
C	-0.10650	1.12009	-1.96259
C	0.63793	2.40152	-1.98783
C	2.16963	4.75200	-1.88142
C	2.01721	2.37074	-2.21399
C	0.03875	3.64062	-1.73797
C	0.79691	4.80180	-1.68479
C	2.77216	3.52885	-2.15135
H	2.48237	1.41145	-2.41826
H	-1.03339	3.71175	-1.57082
H	0.30848	5.75244	-1.48916
H	3.84504	3.47654	-2.31329
H	2.76371	5.65944	-1.83450
C	-1.61064	1.10227	-2.15639
H	-1.90319	0.99380	-3.21006
H	-2.11818	1.97064	-1.71836
O	-2.00013	-0.07938	-1.42749
C	-3.28760	-0.26478	-1.03407
C	-5.86061	-0.76079	-0.10466
C	-3.50198	-1.23867	-0.06141
C	-4.35563	0.46119	-1.54617
C	-5.63730	0.20681	-1.07025
C	-4.78383	-1.48656	0.39371
H	-2.63646	-1.75551	0.34752
H	-4.20007	1.21095	-2.31367
H	-6.47025	0.77710	-1.47000
H	-4.94233	-2.24332	1.15607
H	-6.86500	-0.95049	0.25866

C	0.22125	-3.36803	-1.73513
H	0.02932	-2.53387	-2.42819
C	1.15090	-4.35326	-2.43216
H	2.11880	-3.91107	-2.68464
H	0.69049	-4.68073	-3.37214
H	1.33502	-5.25015	-1.83384
C	-1.11311	-4.01124	-1.38784
H	-1.57257	-4.43768	-2.28672
H	-1.82081	-3.28645	-0.97271
H	-0.99685	-4.82855	-0.66529
C	1.06843	-3.60250	1.16472
H	0.02946	-3.73597	1.50511
C	1.66751	-4.96708	0.85716
H	2.65237	-4.87634	0.38312
H	1.03176	-5.57116	0.20521
H	1.80986	-5.52878	1.78867
C	1.85579	-2.92042	2.27659
H	2.91318	-2.81787	2.00498
H	1.80510	-3.51730	3.19462
H	1.47788	-1.91829	2.49661
C	-0.20995	0.29037	3.25535
H	0.83021	-0.07461	3.23782
C	-1.13067	-0.91616	3.36813
H	-1.04127	-1.56423	2.48897
H	-2.18081	-0.61498	3.45837
H	-0.87955	-1.50665	4.25776
C	-0.35459	1.21775	4.45287
H	0.31233	2.08393	4.39888
H	-0.10928	0.67590	5.37434
H	-1.38119	1.58406	4.56200
C	-1.71953	2.29720	1.53486
H	-1.80729	2.49398	0.45533
C	-3.03167	1.68501	2.00614
H	-3.23024	0.71098	1.54935
H	-3.86775	2.34511	1.74597
H	-3.04635	1.56089	3.09479
C	-1.45894	3.63000	2.22561
H	-0.58624	4.14895	1.81895
H	-1.31424	3.51307	3.30422
H	-2.32558	4.28771	2.08469

TSC1/t

EE = -2260.973791

EE + ZPE = -2260.249783

G° = -2260.323020

Imaginary Freq = -330.85

Ir	0.114687	-0.620878	0.431001
P	2.376287	-0.614914	0.868772
P	-1.625116	-0.907643	-1.177649
C	2.908580	-2.349739	0.638548
H	2.805158	-2.828006	1.622948
H	3.958081	-2.457122	0.336614
C	-1.663167	-2.730922	-1.343265
H	-2.231105	-3.096908	-0.474803
H	-2.172618	-3.083863	-2.247224
C	0.659862	-2.406893	-0.491697
C	1.435102	-4.836118	-1.784350
C	1.946615	-2.979521	-0.323703
C	-0.240799	-3.180569	-1.261832
C	0.144420	-4.349884	-1.907527
C	2.321608	-4.153657	-0.968680
H	-0.586880	-4.890817	-2.505113

H	3.327595	-4.540840	-0.816871
H	1.738345	-5.743918	-2.296585
O	0.037629	0.590627	2.145567
C	-1.017676	0.981223	1.500948
C	-2.345966	0.590412	2.058824
C	-4.801961	-0.222791	3.138514
C	-2.458314	-0.619484	2.752222
C	-3.477146	1.398701	1.952943
C	-4.695877	0.993817	2.486332
C	-3.672159	-1.025046	3.274530
H	-1.573568	-1.241681	2.850556
H	-3.426009	2.360074	1.450161
H	-5.563808	1.639978	2.391690
H	-3.741609	-1.974489	3.797221
H	-5.754145	-0.543009	3.550019
C	-0.909626	2.341959	0.853328
H	-0.906673	3.102679	1.654485
H	-1.762781	2.555769	0.195020
O	0.285121	2.411266	0.112244
C	0.538077	3.578981	-0.536563
C	1.219224	5.886124	-1.959218
C	1.614179	3.570569	-1.426337
C	-0.206379	4.745584	-0.378180
C	0.144524	5.888858	-1.088115
C	1.949850	4.714447	-2.125040
H	2.164024	2.645748	-1.569710
H	-1.051962	4.782998	0.297817
H	-0.440881	6.793025	-0.949921
H	2.788881	4.689274	-2.813857
H	1.484600	6.782625	-2.509426
C	2.922690	-0.088366	2.567657
H	2.080643	-0.430344	3.184819
C	4.197335	-0.745497	3.081945
H	4.134737	-1.837462	3.092316
H	4.379364	-0.421987	4.113836
H	5.078967	-0.466958	2.496256
C	2.984376	1.430645	2.681808
H	3.106779	1.715101	3.733103
H	2.067562	1.895652	2.310948
H	3.837978	1.846035	2.133587
C	3.364893	0.385261	-0.350605
H	3.025783	1.414314	-0.166370
C	4.874262	0.320007	-0.157256
H	5.248071	-0.709076	-0.219624
H	5.202890	0.743477	0.794649
H	5.369936	0.887240	-0.954077
C	2.996388	-0.007100	-1.775288
H	3.297936	-1.038649	-1.995200
H	3.513002	0.646660	-2.489310
H	1.918058	0.063748	-1.942756
C	-1.035940	-0.360015	-2.860813
H	-0.114863	-0.958541	-2.940309
C	-0.636495	1.108420	-2.877897
H	-0.023712	1.352773	-2.006362
H	-1.508376	1.773413	-2.874662
H	-0.059547	1.336288	-3.782586
C	-1.929542	-0.718640	-4.038471
H	-2.181911	-1.783206	-4.070971
H	-1.409688	-0.481559	-4.974437
H	-2.862100	-0.144118	-4.037389
C	-3.431093	-0.454204	-0.978810
H	-3.579474	-0.543253	0.106402

C	-3.741393	0.980506	-1.382355
H	-3.015555	1.700177	-0.996348
H	-4.728084	1.267186	-0.999605
H	-3.768417	1.091897	-2.471886
C	-4.408919	-1.406101	-1.659786
H	-4.315282	-2.434492	-1.303175
H	-4.293777	-1.410956	-2.748842
H	-5.433232	-1.079837	-1.442263

C3

EE = -2261.059564

EE + ZPE = -2261.059564

G° = -2260.408300

Ir	0.11700	-0.16558	-0.29278
P	0.98779	-2.40011	-0.28639
P	-0.31294	1.05818	1.57727
C	2.69719	-1.91676	-0.82342
H	2.59108	-1.72017	-1.90010
H	3.45108	-2.70375	-0.69484
C	1.15890	2.18144	1.52062
H	0.92622	2.94284	0.76066
H	1.36473	2.69922	2.46528
C	2.00774	0.21069	0.27324
C	4.65434	0.78147	1.00344
C	3.05261	-0.65337	-0.09565
C	2.30657	1.33094	1.06670
C	3.62173	1.60970	1.41994
C	4.36336	-0.35353	0.25977
H	3.83630	2.48497	2.02988
H	5.16342	-1.02961	-0.03662
H	5.68019	1.00515	1.28000
O	0.44304	0.02710	-2.40350
C	-0.15877	1.11996	-1.95216
C	0.55145	2.42048	-1.98282
C	2.02086	4.81153	-1.88664
C	1.92833	2.42809	-2.22579
C	-0.07730	3.64252	-1.72041
C	0.64993	4.82340	-1.67221
C	2.65247	3.60605	-2.16860
H	2.41739	1.48255	-2.43829
H	-1.14841	3.68440	-1.53846
H	0.13881	5.75985	-1.46649
H	3.72423	3.58322	-2.34428
H	2.59085	5.73449	-1.84385
C	-1.66319	1.06612	-2.13449
H	-1.95962	0.94274	-3.18524
H	-2.18589	1.92689	-1.69971
O	-2.02183	-0.11813	-1.39484
C	-3.30705	-0.34418	-1.01808
C	-5.87296	-0.92413	-0.11781
C	-3.50291	-1.34150	-0.06545
C	-4.38985	0.36384	-1.52445
C	-5.66801	0.06648	-1.06372
C	-4.78101	-1.63045	0.37559
H	-2.62788	-1.84536	0.33891
H	-4.24990	1.13105	-2.27738
H	-6.51265	0.62193	-1.45990
H	-4.92532	-2.40574	1.12193
H	-6.87463	-1.14681	0.23406
C	0.31646	-3.35866	-1.73591
H	0.09459	-2.52981	-2.42648
C	1.26879	-4.31543	-2.44199

H	2.22441	-3.84721	-2.69463
H	0.81366	-4.64850	-3.38255
H	1.47748	-5.21126	-1.85017
C	-0.99580	-4.04068	-1.37925
H	-1.44957	-4.47969	-2.27495
H	-1.72065	-3.33639	-0.95852
H	-0.85064	-4.85455	-0.65811
C	1.20877	-3.56833	1.15465
H	0.18047	-3.73868	1.51050
C	1.85097	-4.91053	0.83627
H	2.82381	-4.78453	0.34590
H	1.22650	-5.53715	0.19491
H	2.02887	-5.46660	1.76504
C	1.98874	-2.85979	2.25518
H	3.03707	-2.71869	1.96637
H	1.97462	-3.45964	3.17256
H	1.57875	-1.87238	2.48417
C	-0.17064	0.27398	3.26728
H	0.88576	-0.04015	3.23905
C	-1.03062	-0.97527	3.39239
H	-0.91980	-1.62090	2.51377
H	-2.09273	-0.72467	3.49385
H	-0.74148	-1.55058	4.28043
C	-0.34742	1.19619	4.46463
H	0.27363	2.09520	4.40139
H	-0.06456	0.66975	5.38427
H	-1.38982	1.51032	4.58493
C	-1.78767	2.21148	1.56278
H	-1.89979	2.39710	0.48335
C	-3.06382	1.54289	2.05545
H	-3.22228	0.55861	1.60471
H	-3.93307	2.16178	1.80289
H	-3.05829	1.42304	3.14479
C	-1.57602	3.55870	2.24194
H	-0.72791	4.10909	1.82451
H	-1.41811	3.45570	3.32005
H	-2.46956	4.17995	2.10383

TSC1

EE = -2261.014554

EE + ZPE = -2260.291273

G° = -2260.364655

Imaginary Freq = -397.18

Ir	0.23927	-0.24193	0.08770
P	2.39323	-1.10690	0.00193
P	-1.61111	0.86856	0.97504
C	3.40807	0.42171	0.04804
H	3.55308	0.68954	-1.00967
H	4.40074	0.28265	0.49458
C	-0.99757	2.60017	1.07597
H	-1.25036	3.08785	0.12367
H	-1.48241	3.17752	1.87306
C	1.19419	1.41362	0.75823
C	2.55685	3.69613	1.74040
C	2.60825	1.50445	0.72375
C	0.49628	2.54989	1.22781
C	1.17144	3.65822	1.72735
C	3.26701	2.62409	1.22018
H	0.60073	4.51131	2.09023
H	4.35444	2.66059	1.18554
H	3.08025	4.56208	2.13451
O	1.61102	0.40104	-2.71853

C	0.44065	0.54372	-2.35360
C	-0.13371	1.93379	-2.27829
C	-1.03428	4.58425	-2.29363
C	0.74412	2.98705	-2.01830
C	-1.45860	2.23619	-2.59167
C	-1.90704	3.55101	-2.59967
C	0.29595	4.29552	-2.00739
H	1.78315	2.75534	-1.80677
H	-2.15576	1.44895	-2.86424
H	-2.94108	3.76502	-2.85461
H	0.98924	5.09706	-1.77038
H	-1.38343	5.61235	-2.29296
C	-0.48942	-0.61104	-2.33205
H	-0.20250	-1.36048	-3.06757
H	-1.55356	-0.40079	-2.29193
O	-0.51421	-1.99887	-1.05543
C	-1.65931	-2.67084	-0.88007
C	-3.97928	-4.18349	-0.43176
C	-2.61711	-2.82103	-1.88885
C	-1.87140	-3.31354	0.34595
C	-3.01362	-4.06328	0.56196
C	-3.76667	-3.56401	-1.65377
H	-2.45654	-2.37488	-2.86447
H	-1.10680	-3.20938	1.11169
H	-3.15384	-4.55685	1.51991
H	-4.50184	-3.66525	-2.44722
H	-4.87883	-4.76471	-0.25822
C	2.96801	-2.14678	-1.42159
H	2.44905	-1.65443	-2.25497
C	4.46010	-2.09986	-1.72030
H	4.81133	-1.07754	-1.88961
H	4.66460	-2.66716	-2.63623
H	5.06753	-2.54024	-0.92358
C	2.44007	-3.56957	-1.28734
H	2.60604	-4.11718	-2.22211
H	1.36454	-3.58014	-1.07901
H	2.95344	-4.12541	-0.49374
C	2.77965	-2.03861	1.57199
H	2.09636	-2.90146	1.53280
C	4.21134	-2.54118	1.69524
H	4.93326	-1.71921	1.61486
H	4.46669	-3.29083	0.94276
H	4.35858	-3.00182	2.67948
C	2.41504	-1.19549	2.78841
H	3.06796	-0.31876	2.87513
H	2.53266	-1.78966	3.70204
H	1.38455	-0.82875	2.74308
C	-1.75430	0.45741	2.79673
H	-0.78273	0.83732	3.15266
C	-1.79961	-1.03683	3.07985
H	-0.95446	-1.55510	2.61516
H	-2.71877	-1.49974	2.70324
H	-1.75748	-1.21415	4.16129
C	-2.84981	1.19035	3.55879
H	-2.83780	2.27155	3.39109
H	-2.71876	1.02737	4.63517
H	-3.84542	0.81553	3.29762
C	-3.31863	0.97008	0.22480
H	-3.08275	0.99323	-0.84999
C	-4.12823	-0.29119	0.49609
H	-3.55757	-1.20360	0.29784
H	-5.01841	-0.31298	-0.14325

H	-4.47546	-0.32770	1.53486
C	-4.11511	2.22856	0.54149
H	-3.56856	3.14338	0.29345
H	-4.40182	2.27849	1.59620
H	-5.04168	2.23072	-0.04591

C4

EE = -2261.093894

EE + ZPE = -2260.368328

G° = -2260.441505

Ir	0.34818	-0.09612	-0.15971
P	-0.81162	1.87596	0.40167
P	1.32078	-2.21746	-0.08446
C	-2.25721	1.21463	1.33091
H	-3.08634	1.15190	0.60846
H	-2.58647	1.88671	2.13339
C	-0.00777	-3.22101	0.69147
H	-0.60680	-3.59901	-0.14925
H	0.36556	-4.08629	1.24780
C	-0.96357	-0.94401	1.15743
C	-2.49205	-2.01830	3.28034
C	-1.94120	-0.17100	1.82724
C	-0.85958	-2.30799	1.52682
C	-1.59892	-2.82200	2.58724
C	-2.67343	-0.70165	2.88334
H	-1.48325	-3.86857	2.86253
H	-3.40602	-0.07797	3.39259
H	-3.06010	-2.42238	4.11288
O	-1.57064	-2.60471	-1.87234
C	-1.72215	-1.39777	-1.80183
C	-3.07715	-0.84776	-1.47930
C	-5.62595	0.09104	-0.85896
C	-3.85664	-1.50380	-0.52886
C	-3.59863	0.26382	-2.13693
C	-4.87343	0.72562	-1.83724
C	-5.11487	-1.02479	-0.20548
H	-3.44707	-2.37728	-0.02904
H	-3.01883	0.75431	-2.91454
H	-5.27843	1.58153	-2.36898
H	-5.70104	-1.52385	0.56023
H	-6.61677	0.45985	-0.61142
C	-0.59001	-0.45199	-1.99061
H	-0.88602	0.52672	-2.37791
H	0.17112	-0.88412	-2.64611
O	1.80853	0.87264	-1.45194
C	2.65224	1.69000	-0.87983
C	4.38373	3.56531	0.36299
C	3.19767	2.77963	-1.59432
C	3.04906	1.56247	0.46843
C	3.88652	2.48589	1.07781
C	4.03567	3.69102	-0.98144
H	2.92185	2.88630	-2.64038
H	2.68870	0.70120	1.03367
H	4.15707	2.35223	2.12308
H	4.42628	4.52413	-1.56083
H	5.04309	4.28701	0.83391
C	-1.49021	2.94729	-0.94844
H	-1.91092	2.19119	-1.62604
C	-2.62788	3.89038	-0.58164
H	-3.42790	3.38703	-0.02847
H	-3.07190	4.29323	-1.50017
H	-2.28855	4.74246	0.01266

C	-0.34576	3.64077	-1.67449
H	-0.72382	4.17005	-2.55647
H	0.41239	2.91948	-1.99995
H	0.15232	4.38124	-1.03702
C	0.12482	2.94163	1.60708
H	1.05272	3.19415	1.07251
C	-0.57357	4.22292	2.03754
H	-1.58058	4.03379	2.42949
H	-0.65341	4.94903	1.22548
H	0.00149	4.69758	2.84125
C	0.49252	2.10689	2.82926
H	-0.39239	1.86084	3.42858
H	1.18209	2.67254	3.46591
H	0.98380	1.16345	2.56836
C	2.70578	-2.18134	1.17314
H	2.39673	-1.35629	1.83556
C	4.04005	-1.80744	0.53850
H	3.96338	-0.95619	-0.14438
H	4.46234	-2.65558	-0.01179
H	4.75892	-1.53689	1.32023
C	2.83264	-3.42836	2.03787
H	1.94260	-3.59920	2.65055
H	3.68185	-3.31037	2.72124
H	3.01733	-4.32739	1.43963
C	1.80963	-3.14578	-1.60708
H	0.82887	-3.21494	-2.10278
C	2.74587	-2.34628	-2.50803
H	2.47828	-1.28467	-2.55457
H	2.71770	-2.75739	-3.52347
H	3.78281	-2.40842	-2.16330
C	2.31947	-4.55753	-1.35612
H	1.62825	-5.15173	-0.74926
H	3.29638	-4.55314	-0.85903
H	2.44773	-5.07909	-2.31184

C5

EE = -2262.285807

EE + ZPE = -2261.542802

G° = -2261.618813

Ir	0.04503	-0.02417	-0.18384
P	-1.61033	-1.66262	0.22743
P	2.15521	0.83257	-0.86647
C	-3.37304	-1.25299	0.64309
H	-3.71223	-0.76042	-0.27862
C	-0.92648	-2.94225	1.39224
H	0.15121	-2.83194	1.21489
C	-4.24811	-2.48079	0.86349
H	-3.99200	-3.00599	1.78973
H	-4.18269	-3.19358	0.03541
H	-5.29654	-2.17162	0.94503
C	-3.50573	-0.25833	1.78950
H	-3.16348	-0.67417	2.74243
H	-4.55899	0.02150	1.91029
H	-2.95156	0.66813	1.60025
C	-1.33198	-4.37700	1.08413
H	-0.83655	-5.04495	1.79867
H	-1.01997	-4.68995	0.08329
H	-2.41001	-4.54469	1.17901
C	-1.16928	-2.59067	2.85378
H	-0.54520	-3.23076	3.48761
H	-2.21180	-2.75765	3.14965
H	-0.89887	-1.55642	3.08769

C	3.17754	1.74292	0.38709
H	3.20546	1.00394	1.20242
C	2.51941	2.99702	0.94477
H	3.07105	3.32975	1.83139
H	1.48820	2.81598	1.26487
H	2.52096	3.82169	0.22429
C	4.60953	2.01637	-0.05365
H	5.18784	2.39075	0.79856
H	4.65661	2.78169	-0.83653
H	5.11563	1.11820	-0.42118
C	2.22703	1.66261	-2.53287
H	1.38730	1.18874	-3.05921
C	1.94793	3.15735	-2.44045
H	2.80920	3.70000	-2.03506
H	1.08150	3.39096	-1.81208
H	1.74931	3.56248	-3.43877
C	3.48440	1.38729	-3.34704
H	4.39333	1.73882	-2.84828
H	3.41407	1.91381	-4.30618
H	3.60247	0.32328	-3.57085
C	3.02498	-0.76899	-1.08847
H	3.25707	-1.10077	-0.06787
H	3.95986	-0.68269	-1.65065
C	-1.64924	-2.47044	-1.42273
H	-2.23534	-1.79886	-2.06535
H	-2.14050	-3.44937	-1.41369
C	0.68753	-1.58593	-1.37746
C	1.56812	-3.67571	-3.03769
C	2.04549	-1.72014	-1.71041
C	-0.21264	-2.55438	-1.85491
C	0.23392	-3.58992	-2.67142
C	2.47200	-2.74370	-2.55114
H	-0.47698	-4.33321	-3.02687
H	3.52701	-2.82185	-2.80700
H	1.90566	-4.47696	-3.68796
O	1.26522	-0.90570	1.38891
C	1.58966	-0.38338	2.54878
C	2.46086	0.68587	5.02887
C	2.81528	-0.76876	3.13582
C	0.80664	0.53818	3.27146
C	1.24108	1.05782	4.48270
C	3.23736	-0.24304	4.34300
H	3.41892	-1.49927	2.60161
H	-0.16238	0.83573	2.88028
H	0.60685	1.76639	5.01011
H	4.19081	-0.56215	4.75697
H	2.79555	1.09992	5.97427
C	-0.93518	0.84838	-1.90116
H	-0.76955	0.18835	-2.75947
H	-0.45446	1.81117	-2.09992
C	-2.39175	1.03417	-1.74707
O	-3.20030	0.23023	-2.19042
C	-2.91439	2.21976	-0.97990
C	-4.00947	4.33272	0.48356
C	-4.28436	2.27607	-0.72511
C	-2.10486	3.25348	-0.50862
C	-2.64703	4.30165	0.21927
C	-4.82906	3.31917	0.00448
H	-4.90604	1.47630	-1.11613
H	-1.03643	3.24220	-0.70263
H	-2.00418	5.09794	0.58173
H	-5.89679	3.34581	0.19971

H	-4.43303	5.15116	1.05773
H	-0.89970	1.08197	0.84796
H	-0.15753	1.48993	0.74615

TSC3i

EE = -2262.246488

EE + ZPE = -2261.505954

G° = -2261.580427

Imaginary Freq = -696.55

Ir	0.13412	-0.15737	0.05316
P	-1.19692	1.70031	0.65247
P	1.96932	-1.62992	0.13381
C	-2.97130	1.86159	0.12118
H	-3.43258	1.00335	0.63025
C	-0.27065	3.28968	0.37360
H	0.76922	2.94385	0.44415
C	-3.67226	3.11668	0.62392
H	-3.28228	4.02018	0.14330
H	-3.58264	3.23926	1.70806
H	-4.74142	3.06050	0.38769
C	-3.15578	1.67002	-1.37909
H	-2.80122	2.53697	-1.94566
H	-4.22039	1.53735	-1.60700
H	-2.61948	0.78805	-1.74542
C	-0.49226	4.36371	1.42932
H	0.11931	5.23841	1.17817
H	-0.18571	4.03230	2.42605
H	-1.53324	4.70048	1.48156
C	-0.47841	3.83231	-1.03540
H	0.27461	4.60021	-1.24677
H	-1.46395	4.29954	-1.14997
H	-0.36609	3.05963	-1.80255
C	3.03508	-1.75310	-1.37970
H	3.27105	-0.68940	-1.54008
C	2.28103	-2.23858	-2.60971
H	2.86781	-2.01931	-3.50866
H	1.31461	-1.73593	-2.71278
H	2.11146	-3.32049	-2.58263
C	4.33998	-2.51249	-1.18631
H	4.97791	-2.37645	-2.06709
H	4.16661	-3.58934	-1.07912
H	4.90650	-2.16808	-0.31532
C	1.63841	-3.30553	0.87561
H	0.86656	-3.06664	1.62169
C	1.03941	-4.26255	-0.14781
H	1.81137	-4.65542	-0.81869
H	0.27264	-3.79003	-0.77305
H	0.58222	-5.12091	0.35760
C	2.79703	-3.95103	1.62389
H	3.66242	-4.13159	0.97820
H	2.47713	-4.92180	2.02109
H	3.12249	-3.34565	2.47460
C	3.03220	-0.76103	1.36722
H	3.53253	0.02915	0.78974
H	3.80782	-1.40587	1.79375
C	-1.27159	1.48973	2.48816
H	-2.04734	0.73405	2.67542
H	-1.57894	2.40474	3.00690
C	0.86057	0.27752	2.01679
C	1.81759	0.81550	4.59773
C	2.14555	-0.13075	2.40614
C	0.08299	1.00241	2.93302

C	0.56624	1.27340	4.21173
C	2.60867	0.11782	3.69529
H	-0.04378	1.84073	4.91246
H	3.60375	-0.21248	3.98843
H	2.18418	1.01597	5.60024
O	1.65247	1.14480	-0.50342
C	2.00287	1.58448	-1.70123
C	2.93290	2.67953	-4.13209
C	3.14674	2.40607	-1.74577
C	1.34490	1.32161	-2.91078
C	1.81055	1.86565	-4.10052
C	3.59610	2.94269	-2.93779
H	3.65493	2.61171	-0.80653
H	0.45740	0.69662	-2.89817
H	1.27537	1.64843	-5.02175
H	4.47858	3.57750	-2.93529
H	3.28631	3.10151	-5.06726
C	-1.36563	-1.72457	0.96438
H	-0.98272	-1.55563	1.96994
H	-1.15437	-2.75920	0.67038
C	-2.84777	-1.47707	0.97811
O	-3.38476	-1.00573	1.96036
C	-3.64969	-1.78669	-0.24230
C	-5.23899	-2.23400	-2.48605
C	-5.00515	-1.45362	-0.22863
C	-3.10459	-2.36202	-1.39079
C	-3.89623	-2.58223	-2.50750
C	-5.79491	-1.67294	-1.34228
H	-5.41384	-1.01519	0.67655
H	-2.05344	-2.63298	-1.43429
H	-3.46208	-3.02369	-3.39862
H	-6.84694	-1.40644	-1.32359
H	-5.85598	-2.40245	-3.36337
H	-1.05793	-1.22733	-0.27641
H	-0.36493	-0.41253	-1.51376

TSC3ii

EE = -2262.256238

EE + ZPE = -2261.515152

G° = -2261.588302

Imaginary Freq = -1359.38

Ir	-0.06464	0.01513	-0.09021
P	-1.72387	-1.63749	0.23132
P	1.94727	1.00184	-0.87750
C	-3.47104	-1.29520	0.76114
H	-3.84198	-0.70008	-0.08391
C	-1.00701	-3.03996	1.24086
H	0.07050	-2.89027	1.09415
C	-4.35217	-2.53329	0.86646
H	-4.06434	-3.17589	1.70489
H	-4.33680	-3.13519	-0.04782
H	-5.39109	-2.22714	1.03647
C	-3.54662	-0.43068	2.01410
H	-3.24612	-0.98062	2.91144
H	-4.57860	-0.09193	2.16428
H	-2.91627	0.46185	1.93358
C	-1.37181	-4.43186	0.74223
H	-0.88519	-5.17820	1.38153
H	-1.03170	-4.61068	-0.28187
H	-2.44975	-4.62170	0.78694
C	-1.28239	-2.89899	2.73247
H	-0.65176	-3.60734	3.28230

H	-2.32340	-3.13562	2.97910
H	-1.04341	-1.89893	3.09881
C	3.10272	1.83065	0.31500
H	3.19875	1.03791	1.06840
C	2.49011	3.03393	1.01788
H	3.08747	3.28200	1.90324
H	1.46729	2.83098	1.35360
H	2.47022	3.92043	0.37584
C	4.49943	2.13155	-0.20809
H	5.14004	2.43286	0.62977
H	4.50162	2.95496	-0.93146
H	4.96833	1.25980	-0.67598
C	1.85455	1.98112	-2.46656
H	0.97963	1.54529	-2.96506
C	1.57552	3.45802	-2.21510
H	2.47062	3.97280	-1.84864
H	0.77374	3.62702	-1.48792
H	1.28057	3.94624	-3.15058
C	3.03812	1.80589	-3.40958
H	3.98680	2.11305	-2.95747
H	2.88320	2.43022	-4.29765
H	3.13818	0.77334	-3.75598
C	2.83422	-0.54007	-1.35608
H	3.23216	-0.94860	-0.41637
H	3.68986	-0.36008	-2.01470
C	-1.84110	-2.29591	-1.48431
H	-2.45999	-1.57222	-2.03283
H	-2.33388	-3.27234	-1.54110
C	0.48882	-1.39124	-1.50755
C	1.27126	-3.32451	-3.40093
C	1.82031	-1.47178	-1.95789
C	-0.43283	-2.33144	-2.00858
C	-0.03559	-3.28896	-2.93729
C	2.19687	-2.41812	-2.90687
H	-0.76248	-4.01032	-3.30614
H	3.23019	-2.45474	-3.24752
H	1.56988	-4.06484	-4.13696
O	0.71695	-0.63197	2.06424
C	1.97087	-0.55560	2.51200
C	4.62721	-0.39292	3.39997
C	2.92072	-1.49960	2.10337
C	2.36566	0.44786	3.40381
C	3.68188	0.52746	3.83443
C	4.23207	-1.41406	2.54189
H	2.60188	-2.28903	1.42486
H	1.62332	1.16808	3.73959
H	3.97166	1.31933	4.52012
H	4.95611	-2.15340	2.21029
H	5.65578	-0.32734	3.73932
C	-1.11637	1.03654	-1.62352
H	-1.00465	0.49742	-2.57092
H	-0.66635	2.02794	-1.72402
C	-2.57248	1.19198	-1.37102
O	-3.39313	0.47358	-1.92151
C	-3.05606	2.24745	-0.42232
C	-4.07542	4.13513	1.36046
C	-4.42724	2.32900	-0.18089
C	-2.20395	3.13974	0.22771
C	-2.71016	4.07600	1.11557
C	-4.93534	3.26229	0.70618
H	-5.07901	1.63810	-0.70710
H	-1.13283	3.08648	0.06176

H	-2.03668	4.76070	1.62179
H	-6.00434	3.31283	0.88919
H	-4.47025	4.86636	2.05947
H	-0.46646	1.14346	1.28685
H	0.06868	0.45158	1.78814

C6i

EE = -1877.574998

EE + ZPE = -1876.969717

G° = -1877.035945

Ir	0.24447	-0.02780	-0.14006
P	2.39572	-0.88396	0.01611
P	-1.60178	1.41742	-0.16878
C	3.34133	0.58093	0.61544
H	4.38012	0.58373	0.26146
H	3.38374	0.48926	1.71043
C	-0.83089	2.91199	-0.92335
H	-0.86680	2.75348	-2.01170
H	-1.38448	3.83468	-0.71207
C	1.24168	1.76705	-0.11704
C	2.59977	4.24080	-0.01452
C	2.60459	1.83736	0.23432
C	0.59472	2.97454	-0.45302
C	1.26177	4.19107	-0.37762
C	3.26542	3.06174	0.27897
H	0.73148	5.10888	-0.62448
H	4.31719	3.08866	0.55859
H	3.12103	5.19192	0.03247
O	-0.63393	-1.77285	0.57603
C	-1.78702	-2.30676	0.22601
C	-4.23324	-3.51047	-0.49317
C	-2.19801	-2.37471	-1.11606
C	-2.63481	-2.86430	1.19808
C	-3.83650	-3.45164	0.83852
C	-3.39891	-2.97113	-1.46467
H	-1.53698	-1.95202	-1.87104
H	-2.31851	-2.82070	2.23732
H	-4.47522	-3.87246	1.61104
H	-3.68769	-3.01646	-2.51205
H	-5.17358	-3.97692	-0.76882
C	3.10041	-1.32397	-1.64352
H	2.97606	-0.37359	-2.18664
C	4.56527	-1.72796	-1.69510
H	5.22391	-1.03540	-1.16118
H	4.90129	-1.76098	-2.73790
H	4.71166	-2.73172	-1.28102
C	2.22277	-2.38284	-2.29945
H	2.55923	-2.57506	-3.32449
H	1.17150	-2.08137	-2.32884
H	2.28003	-3.33382	-1.75535
C	2.77477	-2.25218	1.21426
H	2.47216	-3.16912	0.68694
C	4.23914	-2.35528	1.62560
H	4.55740	-1.46018	2.17248
H	4.92381	-2.49684	0.78776
H	4.36809	-3.20483	2.30612
C	1.89018	-2.09242	2.44739
H	2.09285	-1.14039	2.95632
H	2.10762	-2.89229	3.16469
H	0.82956	-2.12887	2.18667
C	-1.95797	1.96765	1.57414
H	-0.97744	2.38784	1.84896

C	-2.23273	0.78605	2.49725
H	-1.47403	0.00109	2.39517
H	-3.20611	0.32723	2.29338
H	-2.23843	1.12241	3.54040
C	-3.00235	3.06313	1.72997
H	-2.80544	3.92977	1.09056
H	-3.00921	3.41990	2.76665
H	-4.01105	2.69800	1.50974
C	-3.19115	1.14811	-1.10545
H	-2.85002	0.54312	-1.95964
C	-4.19746	0.31911	-0.31706
H	-3.75037	-0.56885	0.13772
H	-4.99448	-0.02676	-0.98464
H	-4.66863	0.91612	0.47154
C	-3.83882	2.41958	-1.64063
H	-3.17801	2.98975	-2.29934
H	-4.16533	3.08208	-0.83193
H	-4.73034	2.15418	-2.22101
H	0.55967	0.38557	-1.60384

C6ii

EE = -1954.917758

EE + ZPE = -1954.279519

G° = -1954.347331

Ir	-0.28884	-0.14222	0.19725
P	1.22705	1.61076	0.43072
P	-2.35525	-1.12133	0.03855
C	3.08222	1.57773	0.47985
H	3.29423	1.22046	-0.54031
C	0.52408	2.47994	1.93790
H	-0.53310	2.16135	1.91443
C	3.73907	2.93996	0.65454
H	3.56857	3.34373	1.65930
H	3.38542	3.67580	-0.07445
H	4.82398	2.84631	0.52646
C	3.64016	0.55402	1.46057
H	3.61441	0.92579	2.49007
H	4.68662	0.33868	1.21447
H	3.08746	-0.38990	1.42669
C	0.53285	4.00086	1.87802
H	0.07661	4.40677	2.78895
H	-0.03883	4.38239	1.02701
H	1.55081	4.40079	1.81554
C	1.12996	1.96088	3.23480
H	0.54321	2.31782	4.08910
H	2.15307	2.32889	3.37071
H	1.15037	0.86701	3.27016
C	-3.34867	-0.52357	1.50491
H	-2.89654	0.46656	1.67965
C	-3.09349	-1.37586	2.74105
H	-3.48524	-0.87074	3.63113
H	-2.02573	-1.56124	2.89711
H	-3.60456	-2.34292	2.66924
C	-4.83532	-0.30616	1.26136
H	-5.30648	0.05766	2.18222
H	-5.34796	-1.23110	0.97584
H	-5.01901	0.44267	0.48524
C	-2.62843	-2.93176	-0.27505
H	-2.16178	-3.03268	-1.26905
C	-1.85420	-3.81921	0.69000
H	-2.34389	-3.86900	1.66786
H	-0.83580	-3.45096	0.84946

H	-1.80174	-4.84175	0.29941
C	-4.08513	-3.35724	-0.38792
H	-4.58993	-3.30015	0.58295
H	-4.14714	-4.39991	-0.72115
H	-4.64964	-2.74875	-1.10168
C	-3.12410	-0.29687	-1.42451
H	-4.21977	-0.30083	-1.40828
H	-2.82118	-0.90467	-2.29139
C	0.82490	2.71973	-0.98459
H	1.44094	2.33534	-1.81136
H	1.10273	3.76651	-0.81673
C	-1.23395	1.29779	-1.04034
C	-2.64598	3.34245	-2.37852
C	-2.53606	1.08528	-1.54262
C	-0.62817	2.53978	-1.32834
C	-1.33630	3.55203	-1.96982
C	-3.23775	2.10215	-2.18315
H	-0.85615	4.50974	-2.16417
H	-4.24996	1.92243	-2.54209
H	-3.19764	4.13833	-2.87036
C	0.39747	-1.24555	-1.43959
H	-0.18191	-0.93109	-2.31461
H	0.25528	-2.31308	-1.24599
C	1.82206	-0.88753	-1.68091
O	2.11896	0.07584	-2.36971
C	2.91025	-1.72649	-1.08446
C	5.02892	-3.20636	-0.03940
C	4.21705	-1.49489	-1.51369
C	2.67622	-2.71597	-0.13013
C	3.73170	-3.44673	0.39313
C	5.27053	-2.23047	-0.99825
H	4.37939	-0.72531	-2.26233
H	1.67007	-2.87574	0.24312
H	3.54214	-4.20456	1.14708
H	6.28324	-2.04580	-1.34379
H	5.85353	-3.78196	0.37073
H	0.42488	-1.25803	1.22490

TSC4i

EE = -1877.529042

EE + ZPE = -1876.926851

G° = -1876.993426

Imaginary Freq = -1219.57

Ir	0.25274	-0.04002	-0.16517
P	2.34132	-1.00100	-0.03013
P	-1.53144	1.46597	-0.02826
C	3.43947	0.30589	-0.71743
H	3.62410	0.02945	-1.76543
H	4.41976	0.34712	-0.22555
C	-0.83113	2.92814	-0.90252
H	-1.10486	2.80670	-1.96047
H	-1.25980	3.87972	-0.56507
C	1.29757	1.63467	-0.59769
C	2.78678	4.02601	-0.88486
C	2.71120	1.62152	-0.67939
C	0.66278	2.88683	-0.77041
C	1.40114	4.05917	-0.88941
C	3.43401	2.80289	-0.80229
H	0.88102	5.00872	-0.99996
H	4.52089	2.76076	-0.84444
H	3.35860	4.94518	-0.96888
O	-0.70689	-2.12961	-0.22721

C	-2.01536	-2.39494	-0.27426
C	-4.72767	-3.11210	-0.34287
C	-2.66263	-2.85695	0.87782
C	-2.75512	-2.28271	-1.45672
C	-4.09445	-2.64023	-1.48534
C	-3.99977	-3.21861	0.83620
H	-2.08287	-2.93907	1.79313
H	-2.25339	-1.92922	-2.35505
H	-4.64901	-2.55520	-2.41628
H	-4.48080	-3.58746	1.73818
H	-5.77424	-3.39776	-0.37168
C	2.73048	-2.56180	-0.95980
H	2.17157	-2.39845	-1.89411
C	4.19236	-2.79549	-1.31650
H	4.64129	-1.94880	-1.84452
H	4.27025	-3.66823	-1.97564
H	4.80500	-3.00336	-0.43463
C	2.11598	-3.76134	-0.24931
H	2.19578	-4.65228	-0.88226
H	1.05796	-3.59302	-0.02531
H	2.64362	-3.98168	0.68657
C	2.86874	-1.23127	1.74152
H	2.15762	-1.97853	2.12348
C	4.28915	-1.73155	1.95878
H	5.02719	-1.08428	1.46934
H	4.43938	-2.75128	1.59596
H	4.52281	-1.72940	3.03014
C	2.64011	0.07599	2.49332
H	3.29780	0.87131	2.12110
H	2.85594	-0.06140	3.55897
H	1.60792	0.42989	2.39329
C	-1.61715	2.05905	1.74116
H	-0.58651	2.42968	1.87083
C	-1.82299	0.90590	2.71704
H	-1.12147	0.08647	2.52295
H	-2.83576	0.49434	2.65118
H	-1.67520	1.25292	3.74668
C	-2.57023	3.20954	2.02984
H	-2.43148	4.05693	1.35106
H	-2.40380	3.57939	3.04866
H	-3.61732	2.89342	1.97166
C	-3.25418	1.27868	-0.71852
H	-3.07134	0.67729	-1.62268
C	-4.15737	0.47061	0.20238
H	-3.68562	-0.45353	0.54898
H	-5.07281	0.18827	-0.32912
H	-4.45732	1.05745	1.07788
C	-3.93063	2.57939	-1.13389
H	-3.35497	3.14340	-1.87267
H	-4.11607	3.23510	-0.27700
H	-4.90453	2.35193	-1.58354
H	-0.30016	-1.21221	-1.17549

TSC4ii

EE = -1954.909601

EE + ZPE = -1954.272204

G° = -1954.340105

Imaginary Freq = -683.18

Ir	-0.48706	0.05796	-0.39762
P	0.82414	1.96755	-0.09050
P	-2.25706	-1.40683	-0.07771
C	2.41314	2.37209	-0.98552

H	2.28531	1.82281	-1.92887
C	1.03280	2.31252	1.73620
H	-0.02386	2.36535	2.04172
C	2.62468	3.84732	-1.30232
H	2.72424	4.45378	-0.39557
H	1.81836	4.27134	-1.90665
H	3.55386	3.96348	-1.87333
C	3.64088	1.79858	-0.28885
H	3.94563	2.42016	0.56058
H	4.48144	1.76335	-0.99127
H	3.49175	0.77948	0.07755
C	1.69637	3.63610	2.09118
H	1.60114	3.81700	3.16859
H	1.24371	4.49124	1.58005
H	2.76701	3.63021	1.86140
C	1.67030	1.15706	2.49542
H	1.62158	1.34717	3.57438
H	2.72634	1.02478	2.23513
H	1.14720	0.21790	2.28963
C	-2.35281	-1.98867	1.69647
H	-2.48265	-1.02062	2.20723
C	-1.04492	-2.59667	2.18463
H	-1.11763	-2.84025	3.25116
H	-0.21469	-1.89760	2.04951
H	-0.80232	-3.52574	1.65455
C	-3.53054	-2.88550	2.05084
H	-3.60600	-2.98214	3.14039
H	-3.39897	-3.89664	1.64956
H	-4.48962	-2.50012	1.69137
C	-2.65623	-2.83466	-1.22405
H	-2.42052	-2.38262	-2.20079
C	-1.72988	-4.02599	-1.02039
H	-1.93612	-4.53329	-0.07097
H	-0.67378	-3.74602	-1.03351
H	-1.88519	-4.76235	-1.81726
C	-4.10794	-3.29861	-1.25841
H	-4.39217	-3.81493	-0.33697
H	-4.24170	-4.01079	-2.08167
H	-4.81598	-2.48145	-1.41911
C	-3.74657	-0.32961	-0.20947
H	-4.55962	-0.65547	0.45190
H	-4.11787	-0.42932	-1.23923
C	-0.34672	3.30890	-0.56348
H	-0.28684	3.39974	-1.65668
H	-0.08394	4.28599	-0.14065
C	-1.99391	1.46947	-0.16052
C	-4.00563	3.38785	0.38512
C	-3.34289	1.09746	0.02118
C	-1.72143	2.85592	-0.17130
C	-2.70670	3.79337	0.11742
C	-4.32378	2.04189	0.31128
H	-2.45694	4.85253	0.12033
H	-5.35127	1.71796	0.46641
H	-4.77125	4.12059	0.62264
C	0.99452	-1.56544	-1.07710
H	0.42701	-1.52246	-2.01442
H	0.92375	-2.56786	-0.64440
C	2.40152	-1.19324	-1.36270
O	2.70446	-0.49536	-2.31226
C	3.47139	-1.69987	-0.44144
C	5.54898	-2.52100	1.22642
C	4.79873	-1.59068	-0.85625

C	3.19871	-2.22816	0.81983
C	4.23353	-2.62817	1.65325
C	5.83032	-2.00530	-0.03359
H	4.99102	-1.16436	-1.83618
H	2.17368	-2.31382	1.17019
H	4.01150	-3.02564	2.63872
H	6.85957	-1.92362	-0.36932
H	6.35810	-2.83935	1.87681
H	0.66298	-0.94079	0.21221

Reaction between (PCP)Co and 1 along pathway

A

Cobalt catalyst

EE = -1610.577162

EE + ZPE = -1610.075474

G° = -1610.134208

P	-2.17530	0.49199	-0.10542
P	2.17530	0.49199	0.10541
C	-2.34830	-1.19196	-0.84444
H	-2.34859	-1.04542	-1.93425
H	-3.28710	-1.70048	-0.58681
C	2.34830	-1.19196	0.84444
H	3.28710	-1.70048	0.58682
H	2.34859	-1.04541	1.93425
C	0.00000	-1.22285	-0.00000
C	-0.00000	-4.05009	0.00001
C	-1.13115	-1.95929	-0.40743
C	1.13115	-1.95929	0.40743
C	1.12992	-3.35019	0.39879
C	-1.12992	-3.35019	-0.39878
H	2.02183	-3.89097	0.71208
H	-2.02183	-3.89097	-0.71207
H	-0.00000	-5.13618	0.00001
C	-3.15644	1.61017	-1.23437
H	-2.46100	1.70624	-2.08294
C	-3.07771	0.42702	1.52970
H	-2.96267	1.44791	1.92440
C	3.07772	0.42701	-1.52970
H	2.96269	1.44790	-1.92440
C	3.15643	1.61018	1.23437
H	2.46098	1.70625	2.08294
C	4.47763	1.08401	1.77783
H	4.37712	0.09326	2.23109
H	4.85516	1.76162	2.55357
H	5.24742	1.02028	1.00408
C	3.31437	2.98557	0.60244
H	4.01078	2.95793	-0.24436
H	3.71428	3.70262	1.32834
H	2.35836	3.37783	0.23610
C	4.55841	0.08016	-1.48669
H	4.74051	-0.85737	-0.94771
H	5.16285	0.86184	-1.01978
H	4.93792	-0.05842	-2.50648
C	2.32881	-0.52237	-2.45860
H	2.41144	-1.56052	-2.11433
H	2.75175	-0.47101	-3.46879
H	1.26212	-0.28122	-2.50718
C	-2.32880	-0.52236	2.45860
H	-2.41143	-1.56052	2.11433
H	-2.75173	-0.47099	3.46879
H	-1.26211	-0.28121	2.50718
C	-4.55840	0.08016	1.48670

H	-4.74050	-0.85737	0.94773
H	-5.16284	0.86184	1.01979
H	-4.93791	-0.05841	2.50649
C	-3.31438	2.98556	-0.60244
H	-3.71430	3.70262	-1.32834
H	-2.35838	3.37782	-0.23611
H	-4.01079	2.95792	0.24437
C	-4.47764	1.08399	-1.77783
H	-4.37713	0.09325	-2.23109
H	-4.85518	1.76160	-2.55357
H	-5.24742	1.02026	-1.00407
Co	0.00000	0.66402	-0.00001

TSA1

EE = -2302.605645

EE + ZPE = -2301.859455

G° = -2301.930205

Imaginary Freq = -523.16

P	-1.96320	0.14305	0.86939
P	1.87428	1.34394	-0.64558
C	-3.07027	1.43895	0.15893
H	-3.94497	1.68565	0.77160
H	-3.43591	1.04218	-0.79810
C	1.58116	3.16235	-0.43727
H	1.90546	3.67300	-1.35240
H	2.19301	3.57846	0.37559
C	0.11491	3.39977	-0.22718
C	-2.59513	3.90876	0.10307
C	-0.34738	4.70875	-0.09811
C	-0.76616	2.30405	-0.19617
C	-2.13734	2.60092	-0.01364
C	-1.69897	4.96713	0.05733
H	0.36290	5.53385	-0.12281
H	-2.05349	5.98940	0.15398
H	-3.65756	4.09933	0.24585
C	3.08803	1.35140	-2.09125
H	2.41993	1.58610	-2.93466
C	3.70463	-0.01529	-2.35466
H	2.94890	-0.72808	-2.68498
H	4.21018	-0.41400	-1.46559
H	4.45776	0.06132	-3.14787
C	4.18513	2.41471	-2.06988
H	5.00049	2.14456	-1.39488
H	3.83623	3.41070	-1.78684
H	4.61808	2.49720	-3.07416
C	2.85471	0.79989	0.85416
H	2.94490	-0.28687	0.71063
C	4.24626	1.37750	1.05459
H	4.63282	1.05398	2.02951
H	4.24484	2.47469	1.05348
H	4.95825	1.03642	0.29872
C	1.99708	1.02379	2.09097
H	1.01938	0.55377	1.96319
H	1.83877	2.09246	2.28898
H	2.48203	0.58510	2.97208
C	-3.06975	-1.35334	1.02425
H	-3.37132	-1.49855	-0.02258
C	-2.32661	-2.60877	1.46317
H	-2.93629	-3.49533	1.24824
H	-2.13148	-2.60442	2.54091
H	-1.37216	-2.73134	0.94213
C	-4.33854	-1.16513	1.84463

H	-4.99254	-2.03567	1.71088
H	-4.90907	-0.27937	1.54876
H	-4.12173	-1.09016	2.91579
C	-1.62525	0.80082	2.59942
H	-0.82688	1.52742	2.40458
C	-1.06898	-0.26658	3.53373
H	-1.85782	-0.93561	3.89548
H	-0.62161	0.21032	4.41438
H	-0.29230	-0.87828	3.06194
C	-2.76579	1.55913	3.26587
H	-3.64590	0.93173	3.43752
H	-3.07324	2.43454	2.68682
H	-2.43029	1.92315	4.24502
C	0.01708	-1.21023	-1.68804
C	0.94301	-2.43090	-1.57809
H	1.95633	-2.06879	-1.75195
H	0.70283	-3.15464	-2.36620
O	0.86117	-3.09601	-0.32643
C	1.89089	-2.92938	0.55354
C	3.89453	-2.55523	2.45882
C	1.56344	-2.79416	1.89905
C	3.22927	-2.92139	0.16816
C	4.22040	-2.72628	1.12125
C	2.55993	-2.60673	2.84246
H	0.51608	-2.82811	2.18270
H	3.50320	-3.07293	-0.87100
H	5.26072	-2.71546	0.80860
H	2.28673	-2.48579	3.88708
H	4.67356	-2.39907	3.19788
O	0.55301	-0.55110	-2.82964
H	0.22775	0.35732	-2.81620
C	-1.41850	-1.59001	-1.96640
C	-4.05768	-2.28929	-2.64100
C	-1.90735	-2.87432	-1.72575
C	-2.28082	-0.66706	-2.56922
C	-3.58230	-1.00763	-2.89592
C	-3.21172	-3.21908	-2.05792
H	-1.26832	-3.62079	-1.26407
H	-1.93008	0.34004	-2.78311
H	-4.22796	-0.26961	-3.36347
H	-3.56304	-4.22834	-1.86205
H	-5.07492	-2.56022	-2.90593
H	0.37889	-0.91738	-0.21077
Co	-0.17602	0.43798	-0.44514

A2

EE = -2302.617824

EE + ZPE = -2301.871333

G° = -2301.943598

P	-1.78734	-0.80535	1.04357
P	0.90806	2.20005	-0.35484
C	-3.42335	-0.12267	0.51843
H	-4.19108	-0.16948	1.30146
H	-3.77683	-0.75048	-0.31307
C	-0.25615	3.35635	-1.20946
H	-0.10874	3.19442	-2.28743
H	-0.05015	4.41820	-1.01970
C	-1.64710	2.95043	-0.79968
C	-4.21389	2.19406	-0.05086
C	-2.70118	3.85396	-0.90278
C	-1.84756	1.64179	-0.30971
C	-3.16588	1.28229	0.04524

C	-3.98123	3.47783	-0.52198
H	-2.52116	4.86050	-1.27635
H	-4.80035	4.18804	-0.59280
H	-5.21972	1.89907	0.24279
C	2.50461	2.28587	-1.31683
H	2.29958	1.56988	-2.12363
C	3.66932	1.76121	-0.48327
H	3.41942	0.84652	0.06832
H	4.01059	2.50383	0.24641
H	4.52419	1.52681	-1.12887
C	2.84048	3.61553	-1.98191
H	3.03668	4.41451	-1.26158
H	2.04519	3.95576	-2.65155
H	3.74617	3.49774	-2.58964
C	1.26212	3.02479	1.28928
H	1.90707	2.29559	1.80260
C	1.98785	4.36207	1.21804
H	2.07529	4.78447	2.22643
H	1.43136	5.09004	0.61515
H	2.99773	4.28461	0.81061
C	-0.01321	3.19199	2.10564
H	-0.58080	2.26381	2.18387
H	-0.67644	3.94157	1.65722
H	0.23716	3.53285	3.11736
C	-2.00349	-2.64911	1.03670
H	-2.00950	-2.84638	-0.03951
C	-0.77821	-3.34580	1.61111
H	-0.80986	-4.41584	1.37107
H	-0.73794	-3.25852	2.70386
H	0.14971	-2.93601	1.19429
C	-3.30428	-3.21762	1.58673
H	-3.38163	-4.27317	1.29646
H	-4.18585	-2.70807	1.18388
H	-3.35694	-3.17659	2.67807
C	-1.68680	-0.19880	2.81279
H	-1.95302	0.86130	2.68108
C	-0.27445	-0.27041	3.38034
H	0.01512	-1.30718	3.58778
H	-0.22129	0.27978	4.32818
H	0.46619	0.14469	2.69025
C	-2.68311	-0.80480	3.79128
H	-2.41508	-1.83566	4.04604
H	-3.71165	-0.80224	3.41772
H	-2.67264	-0.23119	4.72604
C	0.34897	-0.76322	-1.60297
C	1.77977	-1.27125	-1.60280
H	2.44879	-0.40548	-1.60316
H	1.97045	-1.83926	-2.52980
O	2.04471	-2.08982	-0.47816
C	3.27635	-2.00026	0.08370
C	5.73712	-1.82035	1.37161
C	3.34510	-2.08689	1.47165
C	4.44029	-1.83605	-0.66128
C	5.66331	-1.74364	-0.01092
C	4.57172	-1.99950	2.10775
H	2.41910	-2.20387	2.02696
H	4.39031	-1.78320	-1.74446
H	6.56851	-1.61424	-0.59692
H	4.61745	-2.05981	3.19105
H	6.69612	-1.74543	1.87375
O	0.36182	0.22307	-2.62898
H	-0.53406	0.56516	-2.72243

C	-0.66657	-1.82739	-1.92231
C	-2.57462	-3.79182	-2.58695
C	-0.36359	-3.18948	-1.83752
C	-1.94831	-1.47794	-2.36491
C	-2.88958	-2.44192	-2.68726
C	-1.30500	-4.15667	-2.16574
H	0.61515	-3.50289	-1.49055
H	-2.23442	-0.43005	-2.43584
H	-3.87572	-2.13537	-3.02487
H	-1.03727	-5.20692	-2.09130
H	-3.30934	-4.54831	-2.84433
H	0.79196	-0.36016	0.52590
Co	-0.32472	0.36091	-0.12472

TSA2

EE = -2302.590675

EE + ZPE = -2301.844352

G° = -2301.915067

Imaginary Freq = -408.28

P	-0.81156	-0.54841	1.33880
P	2.63109	0.09234	-0.54270
C	-1.19642	-2.30885	0.92025
H	-2.05773	-2.27515	0.24113
H	-1.49619	-2.90238	1.79049
C	3.10248	-1.48252	-1.38807
H	3.00943	-1.31222	-2.46814
H	4.13945	-1.78029	-1.19129
C	0.01767	-2.87199	0.25120
C	2.41322	-3.83462	-0.77992
C	0.34300	-4.22227	0.36231
C	0.87325	-1.97907	-0.41517
C	2.10053	-2.48357	-0.88844
C	1.52639	-4.71009	-0.17141
H	-0.33332	-4.89244	0.88999
H	1.77300	-5.76375	-0.08148
H	3.37150	-4.19635	-1.14820
C	-2.51671	0.03392	1.84386
H	-3.09058	-0.27581	0.96182
C	-2.67158	1.54244	1.96317
H	-2.26881	2.07137	1.09431
H	-2.17204	1.94584	2.85090
H	-3.73696	1.79279	2.04574
C	-3.13236	-0.68012	3.04062
H	-3.09726	-1.76984	2.94866
H	-4.18955	-0.39779	3.11969
H	-2.65554	-0.39985	3.98600
C	0.22689	-0.67836	2.89905
H	1.23745	-0.72475	2.47874
C	0.13621	0.58268	3.75053
H	0.92906	0.58006	4.50870
H	-0.81802	0.63926	4.28411
H	0.24021	1.50144	3.16292
C	0.04347	-1.92792	3.74802
H	0.25887	-2.84192	3.18540
H	-0.96582	-2.00919	4.16392
H	0.74181	-1.89594	4.59390
C	3.76419	0.08153	0.96431
H	4.74856	0.34745	0.54415
C	3.37928	1.12400	2.00679
H	2.46925	0.82914	2.53598
H	3.20529	2.11874	1.58989
H	4.17431	1.21094	2.75670

C	3.88449	-1.29288	1.61437
H	4.36231	-2.03017	0.96451
H	2.91061	-1.70554	1.90337
H	4.49140	-1.21365	2.52433
C	3.46455	1.38224	-1.61192
H	4.47789	0.96708	-1.74683
C	3.58604	2.75284	-0.95819
H	4.01064	3.46183	-1.67795
H	4.24303	2.75041	-0.08482
H	2.60586	3.14223	-0.65759
C	2.80997	1.52662	-2.97813
H	3.44221	2.15394	-3.61746
H	1.83694	2.01508	-2.87208
H	2.66279	0.57419	-3.49622
O	0.09744	1.80605	-1.24696
C	-0.26268	2.87450	-0.54525
C	-0.92618	5.15342	0.96251
C	-1.06141	3.88804	-1.09279
C	0.21116	3.03972	0.76318
C	-0.10651	4.16740	1.49908
C	-1.39422	5.00240	-0.33569
H	-1.39991	3.80959	-2.12172
H	0.82915	2.24807	1.17969
H	0.28010	4.27042	2.51056
H	-2.02168	5.77230	-0.77634
H	-1.18751	6.03153	1.54356
C	-1.25478	-0.36455	-2.16159
C	-2.65515	-0.64247	-1.75579
C	-5.33136	-1.20822	-1.06965
C	-3.50887	0.35511	-1.26572
C	-3.18655	-1.92837	-1.90412
C	-4.49941	-2.20758	-1.55617
C	-4.82688	0.07855	-0.93784
H	-3.13677	1.36466	-1.10228
H	-2.54941	-2.70876	-2.30689
H	-4.87929	-3.21815	-1.67766
H	-5.45986	0.87755	-0.56054
H	-6.36109	-1.42681	-0.80511
C	-0.96923	0.95566	-2.55749
H	-1.73596	1.72034	-2.49087
H	-0.24543	1.08215	-3.35534
O	-0.70612	-1.36587	-2.98358
H	-0.11297	-1.90321	-2.44664
H	1.13052	-0.14663	-1.91888
Co	0.43227	-0.09163	-0.63508

A3

EE = -1917.953319

EE + ZPE = -1917.348186

G° = -1917.412108

P	-2.17399	-0.32900	0.05010
P	1.94641	1.09154	0.58045
C	-2.56616	0.65704	-1.45813
H	-3.62694	0.91865	-1.55928
H	-2.30859	0.01781	-2.31651
C	1.49002	2.87385	0.40875
H	1.20246	3.24425	1.39982
H	2.33067	3.48870	0.06132
C	-1.67190	1.86592	-1.39180
C	-0.01454	4.08613	-1.21214
C	-1.98986	3.03499	-2.07748
C	-0.50468	1.78003	-0.61090

C	0.30037	2.92814	-0.50966
C	-1.15633	4.14027	-1.99962
H	-2.89527	3.07787	-2.68005
H	-1.40206	5.04841	-2.54201
H	0.63178	4.95843	-1.13230
C	-3.22348	0.40723	1.39114
H	-2.94461	1.46911	1.29891
C	-2.79670	-0.07834	2.77171
H	-1.70979	-0.04533	2.89948
H	-3.12003	-1.10909	2.94909
H	-3.25529	0.54676	3.54625
C	-4.72797	0.27938	1.20596
H	-5.06441	0.58318	0.20947
H	-5.24577	0.91403	1.93463
H	-5.06316	-0.74868	1.38105
C	-2.67657	-2.07068	-0.34129
H	-1.88280	-2.36361	-1.04750
C	-2.56418	-2.97886	0.87730
H	-2.61582	-4.02724	0.56248
H	-3.39358	-2.80934	1.57440
H	-1.61686	-2.82625	1.40457
C	-4.01869	-2.22779	-1.04361
H	-4.10585	-1.60271	-1.93786
H	-4.85660	-1.98881	-0.38157
H	-4.14323	-3.27011	-1.36019
C	3.34421	0.95441	-0.64925
H	4.03088	1.76507	-0.35336
C	4.09011	-0.37016	-0.58349
H	3.41670	-1.21893	-0.74992
H	4.60163	-0.51578	0.37205
H	4.85295	-0.39777	-1.37027
C	2.84504	1.22480	-2.06182
H	2.31754	2.17895	-2.15519
H	2.16414	0.43092	-2.38779
H	3.69315	1.23788	-2.75602
C	2.78977	0.88299	2.22813
H	3.82123	1.24471	2.09047
C	2.80766	-0.58945	2.63018
H	3.38489	-0.71115	3.55418
H	3.24327	-1.24180	1.86850
H	1.78793	-0.95114	2.79465
C	2.12265	1.69937	3.32617
H	2.57232	1.44868	4.29356
H	1.05297	1.46296	3.39463
H	2.22921	2.77842	3.18490
O	0.40397	-1.64671	0.99105
C	0.90507	-2.31539	-0.00526
C	2.06702	-3.68325	-2.19773
C	1.58908	-3.53640	0.17331
C	0.80643	-1.82767	-1.33013
C	1.38783	-2.49100	-2.40175
C	2.15219	-4.19548	-0.90292
H	1.67022	-3.92821	1.18390
H	0.23287	-0.90484	-1.53093
H	1.30104	-2.07509	-3.40275
H	2.67832	-5.13176	-0.73320
H	2.51566	-4.21240	-3.03176
H	-0.34387	0.83289	1.47271
Co	-0.02495	0.12843	0.26655

TSA3

EE = -1917.908672

EE + ZPE = -1917.306131

G° = -1917.370184

Imaginary Freq = -1265.98

P	-1.98748	-1.11557	-0.09932
P	1.29330	1.72958	0.38069
C	-2.90887	-0.08991	-1.32387
H	-3.98888	-0.28508	-1.35352
H	-2.50346	-0.33103	-2.31669
C	0.15950	3.07456	0.95568
H	-0.01162	2.92442	2.02759
H	0.58923	4.07682	0.82109
C	-2.58074	1.32154	-0.92044
C	-1.97401	3.90720	-0.10726
C	-3.44244	2.37279	-1.22257
C	-1.38383	1.53910	-0.20665
C	-1.11422	2.85975	0.19864
C	-3.13901	3.66552	-0.82340
H	-4.35818	2.17657	-1.77729
H	-3.81192	4.48334	-1.06414
H	-1.73319	4.91845	0.21535
C	-3.10481	-1.10294	1.38668
H	-3.37304	-0.03585	1.42887
C	-2.32724	-1.43750	2.65252
H	-1.45120	-0.78905	2.75557
H	-1.97596	-2.47524	2.65081
H	-2.96416	-1.30473	3.53502
C	-4.38211	-1.92062	1.27420
H	-4.94665	-1.70126	0.36201
H	-5.03833	-1.70329	2.12545
H	-4.17401	-2.99613	1.29619
C	-1.85865	-2.81992	-0.83457
H	-1.03504	-2.67090	-1.55222
C	-1.39358	-3.85265	0.18508
H	-1.15174	-4.79295	-0.32366
H	-2.18198	-4.07493	0.91396
H	-0.50302	-3.51377	0.72192
C	-3.08121	-3.30404	-1.60247
H	-3.41037	-2.59264	-2.36600
H	-3.92755	-3.50035	-0.93705
H	-2.84531	-4.24594	-2.11231
C	2.04722	2.53193	-1.14080
H	2.24178	3.56988	-0.82564
C	3.36591	1.90734	-1.57151
H	3.24523	0.84835	-1.82521
H	4.14446	1.98415	-0.80729
H	3.73568	2.42076	-2.46686
C	1.06520	2.54405	-2.30489
H	0.12891	3.05771	-2.07034
H	0.80941	1.51984	-2.60391
H	1.52223	3.04198	-3.16849
C	2.71218	1.78382	1.60078
H	3.33091	2.64243	1.29651
C	3.54874	0.51060	1.55625
H	4.45456	0.63665	2.16057
H	3.85311	0.20999	0.54983
H	2.98555	-0.32737	1.98310
C	2.22815	2.01360	3.02677
H	3.06372	1.88942	3.72527
H	1.46050	1.27954	3.30656
H	1.81556	3.01382	3.18139
O	0.82462	-1.59833	0.62889
C	1.95906	-1.95424	0.02017

C	4.31842	-2.80435	-1.23423
C	2.85919	-2.79604	0.68534
C	2.24907	-1.56839	-1.29268
C	3.42009	-1.98847	-1.90781
C	4.02372	-3.21030	0.06380
H	2.62067	-3.10105	1.70088
H	1.52735	-0.94073	-1.81382
H	3.62897	-1.67669	-2.92815
H	4.71382	-3.85785	0.59762
H	5.23354	-3.13078	-1.71755
H	0.61981	-0.43343	1.31235
Co	-0.15252	0.08403	0.12718

Reaction between (PCP)Co and 1 along pathway B

B2

EE = -2302.639011

EE + ZPE = -2301.888926

G° = -2301.963932

P	-2.60922	-0.67250	-0.31595
P	0.70305	1.91993	0.67744
C	-3.49809	0.44348	-1.48539
H	-3.11080	0.22351	-2.48907
H	-4.58684	0.30776	-1.51214
C	-0.36802	3.37249	1.04657
H	0.13616	4.34027	0.92139
H	-0.64680	3.29138	2.10711
C	-3.09330	1.81562	-1.03132
C	-2.38156	4.32200	-0.10584
C	-1.89322	1.92385	-0.29137
C	-3.90145	2.91620	-1.29992
C	-3.54259	4.17811	-0.85122
C	-1.58445	3.21896	0.18184
H	-4.81882	2.78131	-1.87171
H	-4.16663	5.03963	-1.07102
H	-2.09585	5.30338	0.27076
C	-3.54564	-0.51555	1.30242
H	-3.03754	0.35049	1.74720
C	-3.27025	-1.71591	2.19762
H	-3.76167	-2.62673	1.83565
H	-3.64677	-1.52701	3.21007
H	-2.19682	-1.92481	2.27439
C	-5.02701	-0.18215	1.21364
H	-5.61094	-0.96586	0.72099
H	-5.19767	0.75752	0.67874
H	-5.43602	-0.05874	2.22446
C	-3.00043	-2.38885	-0.96727
H	-2.44763	-3.06697	-0.30061
C	-4.46882	-2.79279	-0.97131
H	-4.58417	-3.77759	-1.44230
H	-5.07511	-2.08647	-1.55136
H	-4.89647	-2.85926	0.03172
C	1.97466	2.53664	-0.54658
H	2.60392	1.64968	-0.71189
C	1.25963	2.86515	-1.85246
H	1.98930	3.04904	-2.65148
H	0.64476	3.76813	-1.75029
H	0.58571	2.05903	-2.16333
C	2.87613	3.68688	-0.12542
H	3.48345	4.01597	-0.97899

H	3.56746	3.40986	0.67524
H	2.29898	4.55746	0.20975
C	1.62725	1.62426	2.27988
H	0.86934	1.07289	2.86051
C	2.81475	0.70394	2.04532
H	3.62941	1.22566	1.52829
H	2.54841	-0.16284	1.43235
H	3.22066	0.33563	2.99620
C	2.02694	2.84711	3.09527
H	2.78826	3.44863	2.59049
H	2.45165	2.52796	4.05558
H	1.17837	3.50092	3.31579
O	0.79115	-1.18075	-0.16220
C	0.51181	-2.33383	0.53669
C	-0.09495	-4.54347	2.11168
C	0.19673	-3.54428	-0.06676
C	0.53196	-2.22559	1.92348
C	0.23160	-3.32844	2.70338
C	-0.10809	-4.64244	0.73023
H	0.16842	-3.64099	-1.14705
H	0.76889	-1.26432	2.36838
H	0.24591	-3.23538	3.78492
H	-0.36008	-5.58517	0.25401
H	-0.33315	-5.40597	2.72498
C	1.20526	-1.27833	-1.52029
H	0.44650	-1.78189	-2.12943
H	1.27290	-0.24321	-1.87073
C	2.54049	-1.98630	-1.71609
H	2.49447	-2.98349	-1.24746
O	2.62979	-2.10022	-3.12250
H	3.50978	-2.41728	-3.34092
C	3.71110	-1.24688	-1.12667
C	5.89319	0.11644	-0.05480
C	4.33632	-1.71264	0.02447
C	4.19269	-0.09318	-1.74263
C	5.27590	0.58708	-1.20751
C	5.42286	-1.03502	0.55992
H	3.96265	-2.61499	0.50535
H	3.71051	0.26495	-2.64993
H	5.64186	1.48779	-1.69184
H	5.90359	-1.40715	1.45951
H	6.74458	0.64650	0.36104
C	-2.43815	-2.53426	-2.37673
H	-1.43698	-2.10351	-2.47899
H	-3.08136	-2.02852	-3.10633
H	-2.38736	-3.59051	-2.66795
Co	-0.71130	0.41222	-0.04228

TSB1

EE = -2302.593518

EE + ZPE = -2301.847332

G° = -2301.920507

Imaginary Freq = -538.91

P	-2.49072	0.40350	-0.48480
P	1.48449	1.08727	1.11722
C	0.99445	2.82156	1.52452
H	1.84471	3.49158	1.70946
H	0.41269	2.76878	2.45693
C	-1.48677	2.68579	-1.29584
C	-0.01446	4.60670	0.05101
C	-0.58426	2.25844	-0.30072
C	-1.62472	4.02870	-1.62934

C	-0.87284	4.99156	-0.96942
C	0.11730	3.26391	0.39073
H	-2.33042	4.32465	-2.40382
H	-0.97234	6.04020	-1.23436
H	0.55305	5.35948	0.59624
C	-3.47950	1.33651	0.79886
H	-2.94163	2.29476	0.80761
C	-3.30838	0.71640	2.17919
H	-3.77160	-0.27415	2.25200
H	-3.77154	1.35562	2.94056
H	-2.24445	0.60723	2.42198
C	-4.93591	1.62817	0.47328
H	-5.55627	0.72583	0.48782
H	-5.05450	2.10975	-0.50299
H	-5.34929	2.31303	1.22374
C	-3.55757	-0.98339	-1.16546
H	-2.82408	-1.61658	-1.68999
C	-4.17431	-1.83303	-0.06201
H	-4.58620	-2.75671	-0.48561
H	-4.99889	-1.30808	0.43225
H	-3.44573	-2.12105	0.70134
C	3.12457	1.27171	0.25339
H	3.34034	0.25519	-0.09293
C	2.93963	2.15879	-0.97221
H	3.84566	2.12895	-1.58959
H	2.76449	3.20357	-0.68918
H	2.09383	1.84408	-1.59194
C	4.30329	1.75466	1.08382
H	5.17172	1.90492	0.42898
H	4.59959	1.03336	1.85053
H	4.09878	2.71408	1.57517
C	1.77591	0.29198	2.78208
H	0.73362	0.14521	3.11283
C	2.41370	-1.08082	2.62839
H	3.45224	-1.00039	2.28381
H	1.86639	-1.69549	1.90675
H	2.42672	-1.60556	3.59128
C	2.47896	1.12437	3.84637
H	3.54347	1.25194	3.63274
H	2.40344	0.61723	4.81625
H	2.03886	2.11928	3.96354
O	0.15819	-1.55829	0.19221
C	-0.69112	-2.51624	0.60908
C	-2.29773	-4.56183	1.66663
C	-1.14778	-3.55707	-0.20545
C	-1.07705	-2.50436	1.95589
C	-1.85891	-3.52044	2.47688
C	-1.94219	-4.56464	0.32709
H	-0.89439	-3.58306	-1.26019
H	-0.73602	-1.68062	2.57721
H	-2.13448	-3.49516	3.52748
H	-2.28618	-5.36398	-0.32337
H	-2.91317	-5.35649	2.07519
C	0.18578	-1.02454	-1.56391
H	-0.79518	-1.32643	-1.92653
H	0.44952	0.00870	-1.85635
C	1.22630	-2.01020	-2.06169
H	0.97906	-3.01284	-1.68402
O	1.03410	-1.96291	-3.46802
H	1.69965	-2.52396	-3.87646
C	2.65762	-1.73458	-1.68330
C	5.34725	-1.34239	-1.04993

C	3.22910	-2.38671	-0.59423
C	3.44756	-0.88674	-2.45516
C	4.78570	-0.69311	-2.14094
C	4.56426	-2.18912	-0.27502
H	2.61461	-3.05807	0.00204
H	3.00355	-0.38333	-3.30998
H	5.39308	-0.03160	-2.75217
H	4.99853	-2.70660	0.57555
H	6.39532	-1.19484	-0.80747
C	-4.60709	-0.56753	-2.18841
H	-4.17106	-0.05583	-3.05096
H	-5.36622	0.09033	-1.75377
H	-5.12595	-1.45848	-2.56367
Co	-0.33091	0.36755	0.06579
C	-2.38047	1.62759	-1.87201
H	-3.34426	2.02670	-2.21124
H	-1.92134	1.09858	-2.72175

B3

EE = -2302.656725

EE + ZPE = -2301.907954

G° = -2301.980527

P	1.18586	1.36362	0.67715
P	-2.16758	-1.46330	-0.21297
C	1.91941	0.26432	1.96138
H	2.57097	-0.43615	1.42518
H	2.54482	0.78693	2.69256
C	-2.75408	-1.42635	1.53510
H	-3.32716	-2.31656	1.82533
H	-3.43540	-0.56735	1.62230
C	0.74428	-0.42940	2.58521
C	-1.50569	-1.59784	3.71476
C	-0.38224	-0.65193	1.76716
C	0.74406	-0.79334	3.92707
C	-0.37642	-1.38994	4.49022
C	-1.51790	-1.22601	2.37247
H	1.62515	-0.60523	4.53825
H	-0.37185	-1.68070	5.53658
H	-2.39244	-2.04908	4.15646
C	0.62111	2.87602	1.62742
H	-0.38452	2.58042	1.95873
C	0.47338	4.09044	0.71933
H	1.45146	4.50821	0.45455
H	-0.08588	4.87417	1.24275
H	-0.07221	3.86551	-0.20228
C	1.44118	3.21028	2.86551
H	2.48928	3.42037	2.62508
H	1.41175	2.41126	3.61236
H	1.02893	4.11055	3.33679
C	2.60668	1.78386	-0.44146
H	2.95542	0.77614	-0.71258
C	3.77416	2.49689	0.22451
H	4.60993	2.56813	-0.48250
H	4.13994	1.96285	1.10849
H	3.51319	3.51823	0.52349
C	-1.80505	-3.25970	-0.55534
H	-1.15076	-3.25004	-1.43635
C	-1.01644	-3.88236	0.59178
H	-0.65171	-4.86696	0.27871
H	-1.64885	-4.02888	1.47576
H	-0.15585	-3.28446	0.89711
C	-3.02982	-4.11569	-0.84804

H	-2.71768	-5.16093	-0.96015
H	-3.54135	-3.82831	-1.76931
H	-3.75653	-4.08361	-0.02687
C	-3.58453	-0.89468	-1.26772
H	-3.59783	0.17998	-1.03002
C	-3.22556	-1.02281	-2.74319
H	-3.14285	-2.07058	-3.05678
H	-2.28249	-0.51093	-2.95772
H	-4.00686	-0.56006	-3.35693
C	-4.96717	-1.44793	-0.94715
H	-5.09474	-2.47981	-1.28337
H	-5.72213	-0.84381	-1.46407
H	-5.19961	-1.41009	0.12238
O	-0.94161	1.02881	-1.69344
C	-1.66872	2.06941	-1.39990
C	-3.17770	4.37507	-0.73241
C	-2.29257	2.21536	-0.13916
C	-1.85450	3.11947	-2.32465
C	-2.59380	4.23860	-1.99134
C	-3.01757	3.35161	0.19027
H	-2.19830	1.41054	0.60074
H	-1.38667	3.02085	-3.30082
H	-2.71545	5.03063	-2.72634
H	-3.46942	3.43072	1.17629
H	-3.75443	5.25960	-0.48314
C	0.68924	-0.99356	-1.25424
H	0.01008	-1.42325	-1.99714
H	1.21865	-0.18085	-1.75512
C	1.63754	-2.08417	-0.77916
H	1.52425	-2.24758	0.30732
O	1.27304	-3.27835	-1.47507
H	1.87997	-3.97293	-1.20361
C	3.09378	-1.76989	-1.04646
C	5.76765	-1.12252	-1.54209
C	4.04882	-1.87692	-0.04181
C	3.50630	-1.38227	-2.32212
C	4.82895	-1.05459	-2.56703
C	5.37812	-1.54588	-0.28168
H	3.74605	-2.21671	0.94723
H	2.77038	-1.32797	-3.12040
H	5.13393	-0.74335	-3.56175
H	6.10844	-1.62176	0.51831
H	6.80290	-0.85683	-1.73278
C	2.16298	2.47351	-1.72792
H	2.95815	2.38914	-2.47899
H	1.97293	3.53994	-1.56940
H	1.24825	2.03092	-2.13900
Co	-0.49573	0.03180	-0.05577

TSB2

EE = -2302.634573

EE + ZPE = -2301.887053

G° = -2301.958985

Imaginary Freq = -136.75

P	1.35206	1.55329	0.30430
P	-1.79280	-1.59831	-0.00094
C	1.84625	1.03777	2.00858
H	2.56946	0.21821	1.88859
H	2.34577	1.82322	2.58670
C	-2.70132	-0.92097	1.45911
H	-3.34253	-1.66188	1.95096
H	-3.35107	-0.11523	1.09631

C	0.56685	0.56499	2.64078
C	-1.84248	-0.27349	3.74002
C	-0.42317	0.04484	1.78612
C	0.35158	0.66845	4.01189
C	-0.85119	0.24553	4.56055
C	-1.63490	-0.37465	2.36687
H	1.12746	1.08015	4.65497
H	-1.01838	0.32533	5.63084
H	-2.78819	-0.59709	4.17086
C	0.51713	3.19981	0.55844
H	-0.47094	2.89449	0.92231
C	0.31139	3.94812	-0.75323
H	1.23420	4.44530	-1.07397
H	-0.44840	4.72538	-0.61390
H	-0.03344	3.29050	-1.55642
C	1.14130	4.09688	1.61792
H	2.17061	4.37999	1.37359
H	1.13658	3.63634	2.61058
H	0.55879	5.02322	1.68916
C	2.96350	1.77016	-0.60098
H	3.33007	0.73457	-0.59622
C	4.01539	2.62314	0.09338
H	4.97126	2.52352	-0.43675
H	4.18551	2.32195	1.13217
H	3.74859	3.68574	0.08234
C	-1.46790	-3.36678	0.51115
H	-0.95975	-3.80120	-0.35777
C	-0.52213	-3.45437	1.70412
H	-0.28231	-4.50649	1.90159
H	-0.97807	-3.04484	2.61294
H	0.41651	-2.91511	1.54709
C	-2.73449	-4.15958	0.81215
H	-2.47071	-5.20259	1.02511
H	-3.44927	-4.16570	-0.01373
H	-3.24939	-3.77589	1.70026
C	-2.92512	-1.66827	-1.47892
H	-2.63871	-0.75243	-2.01157
C	-2.59621	-2.83851	-2.39993
H	-2.94507	-3.79637	-1.99983
H	-1.52273	-2.93066	-2.59627
H	-3.09560	-2.69028	-3.36377
C	-4.41099	-1.57919	-1.16292
H	-4.75887	-2.40891	-0.53627
H	-4.98499	-1.60860	-2.09683
H	-4.66347	-0.63923	-0.66215
O	-0.96604	0.94215	-1.56359
C	-2.10303	1.58456	-1.40548
C	-4.55824	2.99579	-1.26677
C	-2.66134	1.96838	-0.17264
C	-2.82176	1.93803	-2.56822
C	-4.01584	2.62984	-2.49568
C	-3.86547	2.65840	-0.11367
H	-2.13380	1.71625	0.74209
H	-2.39740	1.64698	-3.52580
H	-4.53755	2.88492	-3.41488
H	-4.26321	2.93918	0.85908
H	-5.49777	3.53600	-1.21309
C	0.79451	-0.94729	-1.75473
H	0.09241	-1.45463	-2.41673
H	1.36704	-0.19616	-2.29447
C	1.56404	-1.86158	-0.87853
H	1.22085	-1.60899	0.18979

O	1.20683	-3.21134	-1.13600
H	1.67555	-3.76772	-0.50529
C	3.06514	-1.70157	-0.83778
C	5.83538	-1.38997	-0.71862
C	3.73629	-1.78130	0.37875
C	3.80270	-1.50880	-2.00304
C	5.17833	-1.34718	-1.94300
C	5.11399	-1.61924	0.44404
H	3.16301	-1.94900	1.29103
H	3.28321	-1.46614	-2.95672
H	5.74352	-1.18312	-2.85560
H	5.62277	-1.66738	1.40197
H	6.91134	-1.25288	-0.67353
C	2.79396	2.18672	-2.05861
H	3.68542	1.89865	-2.62882
H	2.68279	3.27108	-2.15216
H	1.92230	1.72706	-2.53427
Co	-0.11005	-0.10935	-0.20051

Reaction between (PCP)Co and 1 along pathway

C

C2

EE = -2301.446401

EE + ZPE = -2300.720163

G° = -2300.795873

P	0.20885	-1.85782	-1.22397
P	2.25447	1.46868	0.59403
C	1.64812	-2.89391	-1.71640
H	1.70093	-2.86774	-2.81393
H	1.54216	-3.94974	-1.43252
C	3.96520	1.18112	-0.01247
H	4.08749	1.78924	-0.92007
H	4.75249	1.47859	0.69254
C	2.76538	-0.89911	-0.69526
C	5.24687	-2.30760	-0.72219
C	2.87093	-2.23646	-1.14299
C	3.99334	-0.28213	-0.35032
C	5.20002	-0.97390	-0.34614
C	4.07913	-2.92713	-1.13894
H	6.11369	-0.45884	-0.05307
H	4.10508	-3.96199	-1.47796
H	6.18659	-2.85213	-0.70952
O	-0.38886	1.21952	-0.91914
C	-1.46402	1.54663	-0.39770
C	-2.26470	2.62681	-0.96887
C	-3.70639	4.74817	-2.06150
C	-1.78565	3.30495	-2.09683
C	-3.47852	3.02585	-0.39922
C	-4.19128	4.08057	-0.94518
C	-2.50193	4.35576	-2.63646
H	-0.84293	2.98752	-2.53071
H	-3.87477	2.49373	0.45938
H	-5.13336	4.38228	-0.49843
H	-2.12271	4.87667	-3.51008
H	-4.26767	5.57466	-2.48619
C	-1.89089	0.84015	0.86293
H	-1.98805	1.55085	1.70317
H	-1.08689	0.12913	1.09556
O	-3.11362	0.16596	0.63333
C	-3.41154	-0.88182	1.44893
C	-4.09723	-3.13134	2.93731
C	-2.77756	-1.12816	2.66243

C	-4.40046	-1.74902	0.98846
C	-4.73772	-2.86526	1.73135
C	-3.12560	-2.25748	3.39534
H	-2.01294	-0.45830	3.04162
H	-4.87755	-1.52811	0.03849
H	-5.50378	-3.54007	1.36185
H	-2.62272	-2.44877	4.33851
H	-4.35874	-4.01193	3.51434
C	-0.96940	-1.96840	-2.67392
H	-0.51168	-1.24860	-3.37032
C	-1.07519	-3.30839	-3.39100
H	-0.10018	-3.71315	-3.67702
H	-1.66008	-3.18721	-4.31137
H	-1.58386	-4.06168	-2.78304
C	-2.34716	-1.44009	-2.29640
H	-2.99173	-1.39382	-3.18217
H	-2.30791	-0.43665	-1.86294
H	-2.84145	-2.09480	-1.56775
C	-0.57681	-2.79136	0.19449
H	-1.39829	-2.14028	0.52573
C	-1.16237	-4.16250	-0.10772
H	-0.42812	-4.82719	-0.57971
H	-2.04256	-4.11026	-0.75409
H	-1.47791	-4.63995	0.82877
C	0.43863	-2.88495	1.32783
H	1.23673	-3.59715	1.08431
H	-0.05192	-3.23346	2.24516
H	0.92010	-1.92056	1.52165
C	2.43281	0.99662	2.39686
H	2.94482	0.02674	2.28944
C	1.09299	0.73676	3.07076
H	0.50845	0.00084	2.51049
H	0.49575	1.65284	3.15975
H	1.24570	0.34756	4.08484
C	3.30187	1.90561	3.25341
H	4.27116	2.12270	2.79450
H	3.49899	1.42929	4.22158
H	2.80305	2.85907	3.46205
C	1.98689	3.31656	0.45757
H	1.73328	3.40323	-0.61133
C	0.77667	3.78431	1.25644
H	-0.11124	3.17143	1.06971
H	0.52114	4.81718	0.99168
H	0.97804	3.76743	2.33397
C	3.19141	4.20716	0.73033
H	4.06822	3.91398	0.14601
H	3.47421	4.19934	1.78739
H	2.95347	5.24526	0.46621
Co	1.07306	0.06696	-0.61446

TSC1/t

EE = -2301.430666

EE + ZPE = -2300.704601

G° = -2300.777515

Imaginary Freq = -511.65

P	-2.00861	-1.42056	-0.34293
P	1.89629	-0.03791	1.18439
C	-1.43109	-2.94020	-1.23568
H	-1.43080	-2.66140	-2.30008
H	-2.12239	-3.78714	-1.12634
C	2.97058	-1.42452	0.58199
H	3.57452	-1.01734	-0.24354

H	3.67735	-1.76043	1.35336
C	0.76344	-2.23983	-0.26768
C	1.77984	-4.84742	-0.54797
C	-0.02543	-3.27259	-0.79881
C	2.08778	-2.54352	0.08333
C	2.58877	-3.83782	-0.04504
C	0.47470	-4.56463	-0.93250
H	3.61343	-4.06175	0.25012
H	-0.15413	-5.35823	-1.33470
H	2.16709	-5.85836	-0.64223
O	-0.40315	0.09679	-2.96365
C	0.02157	1.10243	-2.43074
C	1.47686	1.39200	-2.35852
C	4.21471	1.88787	-2.45941
C	2.37104	0.35171	-2.62201
C	1.96745	2.67978	-2.13779
C	3.33143	2.92698	-2.19867
C	3.73246	0.59812	-2.66159
H	1.97018	-0.64535	-2.78304
H	1.28523	3.49196	-1.90684
H	3.70604	3.93310	-2.03624
H	4.42303	-0.21621	-2.85983
H	5.28241	2.08139	-2.50257
C	-0.96163	2.16820	-1.97189
H	-1.96697	1.73570	-2.03711
H	-0.91249	3.02610	-2.66455
O	-0.66935	2.56916	-0.64909
C	-1.71315	3.00117	0.11459
C	-3.77308	3.79069	1.80582
C	-1.64295	2.71812	1.47567
C	-2.80494	3.68815	-0.40181
C	-3.83030	4.07861	0.45126
C	-2.67057	3.11268	2.31437
H	-0.78162	2.16850	1.84254
H	-2.86116	3.91827	-1.46111
H	-4.68320	4.61383	0.04507
H	-2.61316	2.87906	3.37359
H	-4.58069	4.09428	2.46366
C	-3.36771	-0.74704	-1.43065
H	-2.77008	-0.23592	-2.20068
C	-4.26082	-1.74702	-2.15342
H	-3.68545	-2.45593	-2.75524
H	-4.93206	-1.21113	-2.83637
H	-4.88982	-2.32131	-1.46742
C	-4.18318	0.29067	-0.67005
H	-4.77710	0.90160	-1.36133
H	-3.55036	0.97130	-0.08729
H	-4.88560	-0.18465	0.02490
C	-2.82500	-2.04539	1.22164
H	-3.11648	-1.11646	1.73853
C	-4.05539	-2.92375	1.05215
H	-3.83998	-3.80178	0.43122
H	-4.89955	-2.39160	0.60679
H	-4.38386	-3.29632	2.03044
C	-1.78902	-2.76099	2.08175
H	-1.47628	-3.70492	1.61939
H	-2.21361	-2.99434	3.06547
H	-0.88487	-2.16100	2.22320
C	1.64577	-0.50680	2.97901
H	1.41096	-1.57894	2.87926
C	0.42384	0.19139	3.56260
H	-0.46553	0.05292	2.93291

H	0.59374	1.27110	3.66560
H	0.19514	-0.20028	4.56135
C	2.84592	-0.36311	3.90106
H	3.74767	-0.83447	3.49814
H	2.63457	-0.83194	4.86993
H	3.07227	0.69124	4.09690
C	3.00168	1.45218	1.03047
H	3.02919	1.53759	-0.06396
C	2.32450	2.70988	1.55348
H	1.32783	2.83914	1.11638
H	2.91958	3.59459	1.29272
H	2.22572	2.69830	2.64643
C	4.44424	1.34286	1.50262
H	4.93491	0.43320	1.14127
H	4.52878	1.36286	2.59345
H	5.01724	2.19638	1.11612
Co	-0.03662	-0.42848	0.11653

C3

EE = -2301.464590

EE + ZPE = -2300.737502

G° = -2300.808691

P	1.08058	2.27919	-0.26460
P	-0.52146	-1.09691	1.35580
C	-0.42747	3.28358	-0.63877
H	-0.57669	3.17136	-1.72087
H	-0.32143	4.35357	-0.41820
C	-2.34309	-0.79793	1.40918
H	-2.79695	-1.39990	0.60932
H	-2.81203	-1.09284	2.35581
C	-1.46753	1.26934	0.37442
C	-3.69178	2.74856	1.23371
C	-1.56242	2.64169	0.10240
C	-2.49197	0.66308	1.11155
C	-3.59430	1.39882	1.53685
C	-2.67105	3.36815	0.52432
H	-4.38061	0.90797	2.10752
H	-2.72940	4.43305	0.30450
H	-4.55202	3.32262	1.56546
O	-0.42736	0.63077	-2.20079
C	-0.78409	-0.59237	-1.94419
C	-2.20126	-1.00226	-1.98084
C	-4.92608	-1.67275	-1.92643
C	-3.18654	-0.01247	-2.06218
C	-2.61322	-2.33797	-1.90675
C	-3.96048	-2.66832	-1.87859
C	-4.52893	-0.34412	-2.02488
H	-2.87056	1.02358	-2.13198
H	-1.88067	-3.13999	-1.86061
H	-4.25601	-3.71206	-1.81939
H	-5.27509	0.44399	-2.06905
H	-5.98034	-1.93042	-1.89820
C	0.32677	-1.58900	-2.20158
H	0.64662	-1.60411	-3.25362
H	0.09811	-2.60988	-1.87423
O	1.38620	-1.06041	-1.38513
C	2.46503	-1.82389	-1.07324
C	4.70504	-3.27886	-0.29801
C	3.28632	-1.34987	-0.05299
C	2.76206	-3.02261	-1.71048
C	3.88271	-3.74249	-1.31168
C	4.40190	-2.07370	0.32633

H	3.00380	-0.42660	0.44595
H	2.13740	-3.39444	-2.51466
H	4.11104	-4.67976	-1.80988
H	5.03353	-1.69935	1.12637
H	5.57649	-3.84945	0.00484
C	2.17224	2.52664	-1.75728
H	1.69400	1.82603	-2.45817
C	2.16570	3.90907	-2.39785
H	1.15537	4.26903	-2.61026
H	2.70156	3.86725	-3.35423
H	2.66785	4.65937	-1.77996
C	3.59310	2.04765	-1.49845
H	4.17639	2.08061	-2.42601
H	3.62176	1.01633	-1.13414
H	4.11328	2.68111	-0.76933
C	1.88774	3.13514	1.18938
H	2.72192	2.46828	1.46067
C	2.44182	4.52881	0.93071
H	1.67004	5.19966	0.53452
H	3.28127	4.52876	0.23125
H	2.79779	4.96824	1.87088
C	0.90598	3.17468	2.35495
H	0.08864	3.87783	2.15556
H	1.41555	3.50836	3.26659
H	0.45186	2.20005	2.55171
C	-0.01090	-0.58026	3.07945
H	-0.49743	0.40714	3.13106
C	1.49180	-0.36475	3.18933
H	1.86109	0.25763	2.36709
H	2.04163	-1.31261	3.16736
H	1.73768	0.13841	4.13256
C	-0.53877	-1.41460	4.23736
H	-1.62242	-1.56029	4.19344
H	-0.31808	-0.91174	5.18685
H	-0.06430	-2.40073	4.28077
C	-0.35376	-2.96258	1.22008
H	-0.39216	-3.11325	0.13024
C	0.99008	-3.48777	1.70990
H	1.83811	-2.91640	1.32250
H	1.12263	-4.52799	1.38912
H	1.04669	-3.47945	2.80394
C	-1.49879	-3.76342	1.82848
H	-2.46860	-3.50163	1.39609
H	-1.56178	-3.62870	2.91314
H	-1.33460	-4.83252	1.64419
Co	0.00246	0.25695	-0.31824

TSC2

EE = -2301.409002

EE + ZPE = -2300.684602

G° = -2300.755617

Imaginary Freq = -396.51

P	0.41496	-2.52259	-0.05028
P	-0.31567	1.66216	0.96183
C	2.24287	-2.56130	0.04802
H	2.59468	-2.53187	-0.99280
H	2.65088	-3.46460	0.51915
C	1.41449	2.24899	1.14385
H	1.68740	2.78025	0.22192
H	1.54780	2.95141	1.97593
C	1.75423	-0.19738	0.74901
C	4.35237	-0.00945	1.87706

C	2.64807	-1.29191	0.74531
C	2.25057	1.00991	1.28348
C	3.51723	1.09601	1.85336
C	3.91811	-1.19667	1.30736
H	3.85688	2.04520	2.26460
H	4.57604	-2.06403	1.29153
H	5.34018	0.05651	2.32391
O	1.43542	-1.03278	-2.52688
C	0.87480	0.02422	-2.21707
C	1.68814	1.28517	-2.11855
C	3.35799	3.53371	-2.09021
C	3.05524	1.15751	-1.86681
C	1.18208	2.55640	-2.39343
C	2.00940	3.67214	-2.38162
C	3.87753	2.26905	-1.83575
H	3.45363	0.16607	-1.67615
H	0.13546	2.69373	-2.64933
H	1.59600	4.65057	-2.60871
H	4.93243	2.14907	-1.60780
H	4.00561	4.40504	-2.07390
C	-0.59256	0.13720	-2.24975
H	-1.03469	-0.49852	-3.01506
H	-1.01489	1.13378	-2.19332
O	-1.70868	-0.67165	-0.99024
C	-2.97102	-0.22652	-0.92387
C	-5.66552	0.53768	-0.69396
C	-3.57559	0.56433	-1.90768
C	-3.75199	-0.65173	0.15911
C	-5.07776	-0.27343	0.27017
C	-4.90662	0.94081	-1.78086
H	-3.02128	0.87773	-2.78432
H	-3.28754	-1.29346	0.90246
H	-5.65953	-0.61789	1.12064
H	-5.35417	1.55763	-2.55509
H	-6.70436	0.83720	-0.60459
C	-0.11499	-3.58405	-1.48115
H	0.00311	-2.88047	-2.31529
C	0.77523	-4.78476	-1.77261
H	1.81340	-4.48880	-1.94992
H	0.42253	-5.28855	-2.68085
H	0.76648	-5.52508	-0.96627
C	-1.58531	-3.96568	-1.37016
H	-1.92223	-4.42280	-2.30776
H	-2.21545	-3.09119	-1.17923
H	-1.76249	-4.69868	-0.57436
C	-0.18465	-3.36628	1.50587
H	-1.27991	-3.26422	1.44940
C	0.16567	-4.84295	1.63136
H	1.24988	-5.00141	1.58335
H	-0.30059	-5.46059	0.86032
H	-0.17077	-5.22254	2.60398
C	0.30467	-2.61414	2.73827
H	1.39013	-2.71334	2.85667
H	-0.16706	-3.02506	3.63873
H	0.08468	-1.54428	2.68811
C	-0.75034	1.38091	2.76273
H	0.13489	0.80759	3.08120
C	-1.96952	0.49019	2.94739
H	-1.87989	-0.42986	2.36091
H	-2.89505	0.98879	2.63885
H	-2.07725	0.21167	4.00282
C	-0.83695	2.62174	3.64007

H	0.03979	3.26978	3.54849
H	-0.90885	2.32131	4.69238
H	-1.72727	3.21878	3.41682
C	-1.29517	3.12089	0.31500
H	-1.18870	3.00480	-0.77547
C	-2.77886	3.01486	0.64558
H	-3.18286	2.01703	0.45315
H	-3.35118	3.72284	0.03483
H	-2.97110	3.26476	1.69456
C	-0.74465	4.49237	0.68305
H	0.29250	4.62692	0.36188
H	-0.79223	4.67399	1.76168
H	-1.34481	5.27130	0.19659
Co	-0.04395	-0.33932	0.00347

C4

EE = -2301.472065

EE + ZPE = -2300.745935

G° = -2300.818786

P	-1.08864	-1.25462	0.96130
P	2.62515	0.73890	-0.58093
C	-0.62963	-2.96976	0.51261
H	-1.07713	-3.17271	-0.47046
H	-1.00843	-3.72152	1.21331
C	3.57904	-0.76260	-1.01694
H	3.53244	-0.88445	-2.10882
H	4.64023	-0.68912	-0.75208
C	1.51211	-1.80670	-0.05172
C	2.94964	-4.18739	0.45609
C	0.86195	-2.98036	0.38045
C	2.88653	-1.91271	-0.34055
C	3.59634	-3.07831	-0.06256
C	1.57783	-4.14118	0.65286
H	4.66475	-3.11607	-0.26631
H	1.04974	-5.02216	1.01251
H	3.50617	-5.09226	0.68056
O	-0.72102	-2.35715	-2.59030
C	-0.83497	-1.15963	-2.38788
C	-2.19040	-0.52675	-2.46362
C	-4.78279	0.49045	-2.47400
C	-3.26098	-1.32650	-2.86647
C	-2.42914	0.79330	-2.08197
C	-3.72259	1.29552	-2.08006
C	-4.54958	-0.82124	-2.87437
H	-3.05135	-2.35220	-3.15450
H	-1.61034	1.40889	-1.72091
H	-3.90068	2.31436	-1.74793
H	-5.37817	-1.44909	-3.18815
H	-5.79481	0.88466	-2.46922
C	0.33889	-0.31667	-2.06899
H	0.22627	0.72363	-2.39068
H	1.21669	-0.78998	-2.51672
O	-0.04504	1.74465	-0.01065
C	-0.87641	2.44389	0.71910
C	-2.69074	4.01747	2.22867
C	-0.97332	2.32482	2.11970
C	-1.69968	3.41579	0.11016
C	-2.59029	4.17324	0.84940
C	-1.86198	3.09640	2.85327
H	-0.32271	1.62047	2.63066
H	-1.61118	3.55621	-0.96549
H	-3.21400	4.90534	0.34197

H	-1.90472	2.97404	3.93307
H	-3.38856	4.61630	2.80454
C	-2.94488	-1.14555	0.76171
H	-3.04747	-0.83915	-0.28333
C	-3.68674	-2.46810	0.90570
H	-3.31212	-3.23334	0.21944
H	-4.74394	-2.30590	0.66182
H	-3.64546	-2.87098	1.92335
C	-3.57456	-0.04897	1.60770
H	-4.62775	0.05976	1.32329
H	-3.09078	0.92186	1.46195
H	-3.54824	-0.28483	2.67902
C	-0.75143	-1.14531	2.80068
H	-1.30421	-0.24399	3.09945
C	-1.25970	-2.32527	3.61510
H	-0.72095	-3.24520	3.35916
H	-2.32969	-2.50591	3.48346
H	-1.08606	-2.13888	4.68177
C	0.72821	-0.91294	3.09038
H	1.33341	-1.78885	2.83118
H	0.86878	-0.70900	4.15899
H	1.13587	-0.05918	2.53561
C	3.46769	1.32772	0.97338
H	3.44934	0.40060	1.57119
C	2.68492	2.39995	1.71888
H	1.63579	2.13867	1.86072
H	2.70218	3.35332	1.18060
H	3.13922	2.57055	2.70167
C	4.91954	1.75713	0.80396
H	5.52349	1.04816	0.22989
H	5.38468	1.86075	1.79106
H	4.98338	2.73550	0.31604
C	2.85259	1.93411	-1.98093
H	2.24309	1.46247	-2.76636
C	2.24915	3.29914	-1.67391
H	1.23969	3.20959	-1.25942
H	2.20695	3.89889	-2.59014
H	2.86976	3.85004	-0.95752
C	4.27520	2.05221	-2.51375
H	4.73234	1.08177	-2.73080
H	4.92750	2.58643	-1.81748
H	4.26315	2.62443	-3.44872
Co	0.60391	-0.08767	-0.12266

C5

EE = -2302.657671

EE + ZPE = -2301.912443

G° = -2301.985082

P	-1.42548	-1.70400	0.07624
P	2.10449	0.91070	-0.72312
C	-3.22476	-1.36145	0.40655
H	-3.54266	-0.89802	-0.53679
C	-0.76782	-2.95146	1.29469
H	0.31269	-2.79348	1.19863
C	-4.06224	-2.61961	0.60249
H	-3.83274	-3.12491	1.54634
H	-3.93018	-3.33810	-0.21258
H	-5.12426	-2.34906	0.62887
C	-3.45200	-0.35628	1.52961
H	-3.12625	-0.73690	2.50268
H	-4.52191	-0.12796	1.60447
H	-2.94013	0.59617	1.34650

C	-1.08543	-4.40263	0.95975
H	-0.62461	-5.04765	1.71729
H	-0.67836	-4.70451	-0.00966
H	-2.15998	-4.61410	0.96563
C	-1.14041	-2.62003	2.73408
H	-0.53038	-3.22724	3.41262
H	-2.19045	-2.84915	2.94980
H	-0.94974	-1.57376	2.99009
C	2.86617	1.99279	0.58290
H	2.87303	1.30849	1.44454
C	2.01292	3.19290	0.97109
H	2.42990	3.65808	1.87152
H	0.98367	2.90774	1.21418
H	1.98685	3.95623	0.18637
C	4.30502	2.40116	0.29516
H	4.73090	2.88753	1.18021
H	4.37019	3.11839	-0.53057
H	4.94301	1.54473	0.05551
C	2.33845	1.66424	-2.41833
H	1.60635	1.10932	-3.02015
C	1.96444	3.14106	-2.46094
H	2.72340	3.76007	-1.96986
H	1.00098	3.35685	-1.98697
H	1.89663	3.47625	-3.50176
C	3.70540	1.43714	-3.05238
H	4.51975	1.86992	-2.46215
H	3.72695	1.91669	-4.03822
H	3.91626	0.37529	-3.20616
C	3.14501	-0.59879	-0.75114
H	3.28774	-0.87609	0.30004
H	4.12533	-0.45139	-1.21398
C	-1.34903	-2.53882	-1.55613
H	-1.90879	-1.90701	-2.25830
H	-1.80008	-3.53679	-1.55866
C	0.91523	-1.55071	-1.29092
C	2.08047	-3.62679	-2.77596
C	2.30564	-1.62750	-1.44639
C	0.12275	-2.56544	-1.84732
C	0.70814	-3.59444	-2.58067
C	2.87727	-2.64817	-2.20202
H	0.07837	-4.37681	-2.99979
H	3.95830	-2.68211	-2.32483
H	2.53005	-4.42354	-3.36077
O	1.11314	-0.69822	1.32983
C	1.23251	-0.20664	2.53884
C	1.67119	0.74498	5.17941
C	2.32851	-0.64310	3.31856
C	0.35511	0.71342	3.14884
C	0.58015	1.17387	4.43959
C	2.53919	-0.17712	4.60218
H	3.00084	-1.37117	2.86986
H	-0.52530	1.05900	2.61545
H	-0.12236	1.88110	4.87408
H	3.39636	-0.53949	5.16448
H	1.83872	1.11180	6.18661
C	-0.75124	0.67024	-1.97680
H	-0.48275	0.00151	-2.79783
H	-0.26576	1.63754	-2.11683
C	-2.21044	0.84041	-1.95493
O	-2.97237	0.03189	-2.47066
C	-2.81347	2.02283	-1.24019
C	-4.06364	4.10976	0.13648

C	-4.19946	2.04865	-1.08861
C	-2.06692	3.07720	-0.71354
C	-2.68515	4.11164	-0.02808
C	-4.82111	3.07828	-0.40261
H	-4.77155	1.23450	-1.52317
H	-0.98778	3.09736	-0.83218
H	-2.08893	4.92305	0.37835
H	-5.90074	3.07944	-0.28735
H	-4.54751	4.91670	0.67832
H	-0.91719	0.85513	0.60779
H	-0.26720	1.34140	0.47248
Co	0.11212	-0.08113	-0.26311

TSC3i

EE = -2302.628673

EE + ZPE = -2301.887337

G° = -2301.960180

Imaginary Freq = -972.11

P	-0.95189	-1.78591	-0.57620
P	1.99999	1.50783	-0.18173
C	-2.78060	-1.89974	-0.24498
H	-3.17965	-1.15938	-0.95153
C	-0.06973	-3.29292	0.08101
H	0.96014	-2.91989	0.15516
C	-3.40344	-3.24247	-0.60627
H	-3.07793	-4.04176	0.06700
H	-3.17240	-3.54450	-1.63281
H	-4.49469	-3.17402	-0.52409
C	-3.15657	-1.45264	1.16192
H	-2.79561	-2.14819	1.92650
H	-4.24794	-1.39499	1.25289
H	-2.75117	-0.46134	1.39324
C	-0.09118	-4.49710	-0.85061
H	0.47548	-5.31334	-0.38699
H	0.37792	-4.28615	-1.81601
H	-1.10578	-4.86984	-1.03120
C	-0.52085	-3.68198	1.48510
H	0.19204	-4.40074	1.90528
H	-1.50355	-4.16712	1.47779
H	-0.55590	-2.83291	2.17375
C	2.63075	2.04560	1.47840
H	2.80068	1.06714	1.95215
C	1.58933	2.77736	2.31463
H	1.91269	2.80614	3.36115
H	0.62003	2.26914	2.28592
H	1.45202	3.81218	1.98351
C	3.95454	2.79656	1.44281
H	4.32818	2.93278	2.46434
H	3.84436	3.79526	1.00487
H	4.72612	2.26029	0.88113
C	1.95249	2.94732	-1.37264
H	1.31084	2.55844	-2.17590
C	1.27206	4.16928	-0.76674
H	1.93981	4.69065	-0.07213
H	0.35624	3.92400	-0.21686
H	1.00585	4.88174	-1.55571
C	3.28327	3.32693	-2.00943
H	4.03291	3.62070	-1.26705
H	3.13402	4.18232	-2.67938
H	3.69543	2.51250	-2.61181
C	3.30492	0.39942	-0.84931
H	3.59053	-0.25003	-0.01167

H	4.19776	0.92890	-1.19676
C	-0.79923	-1.89328	-2.41092
H	-1.50635	-1.16380	-2.82962
H	-1.06330	-2.87716	-2.81385
C	1.26233	-0.67937	-1.74677
C	2.67234	-1.70219	-3.94956
C	2.62722	-0.40610	-1.91893
C	0.63201	-1.51874	-2.67717
C	1.33611	-2.02598	-3.76767
C	3.31961	-0.89819	-3.02164
H	0.83289	-2.67991	-4.47771
H	4.37596	-0.66553	-3.14522
H	3.21482	-2.08987	-4.80683
O	1.41302	-0.86538	0.99334
C	1.34226	-1.03749	2.29682
C	1.36415	-1.60602	5.06874
C	2.38627	-1.77850	2.89073
C	0.32190	-0.57503	3.14402
C	0.34074	-0.86080	4.50278
C	2.38949	-2.05861	4.24378
H	3.17759	-2.14074	2.23800
H	-0.49823	-0.00692	2.71503
H	-0.47032	-0.49494	5.12783
H	3.20513	-2.64215	4.66343
H	1.36715	-1.82854	6.13071
C	-1.05260	1.43546	-1.42692
H	-0.54638	1.04012	-2.30514
H	-0.80530	2.49471	-1.30893
C	-2.52569	1.25399	-1.58693
O	-2.98505	0.58656	-2.49467
C	-3.43800	1.86236	-0.57093
C	-5.22806	2.84919	1.32351
C	-4.80020	1.57448	-0.66497
C	-2.98673	2.66397	0.47868
C	-3.87797	3.15396	1.42100
C	-5.68947	2.06092	0.27613
H	-5.13404	0.95424	-1.49108
H	-1.93256	2.90688	0.57874
H	-3.51676	3.77312	2.23582
H	-6.74636	1.82638	0.19726
H	-5.92396	3.22883	2.06537
H	-0.90981	1.12035	-0.10919
H	-0.59439	0.73851	0.93511
Co	0.25525	0.08786	-0.19930

TSC3ii

EE = -2302.630366

EE + ZPE = -2301.889215

G° = -2301.962125

Imaginary Freq = -1158.31

P	-1.60421	-1.64355	0.26243
P	1.86387	0.90632	-0.96841
C	-3.33718	-1.30423	0.84256
H	-3.76287	-0.78407	-0.02504
C	-0.82106	-2.95723	1.34783
H	0.24603	-2.80157	1.14863
C	-4.18002	-2.55075	1.08022
H	-3.84133	-3.12076	1.95144
H	-4.18568	-3.21984	0.21369
H	-5.21897	-2.25635	1.27056
C	-3.37685	-0.34967	2.03032
H	-3.00465	-0.81751	2.94715

H	-4.41105	-0.03600	2.21601
H	-2.78790	0.55561	1.84497
C	-1.17582	-4.38758	0.96197
H	-0.65475	-5.07676	1.63749
H	-0.86411	-4.63581	-0.05640
H	-2.24770	-4.59231	1.05622
C	-1.04376	-2.72877	2.83830
H	-0.37162	-3.38549	3.40352
H	-2.06618	-2.97970	3.14216
H	-0.82327	-1.70189	3.13442
C	2.87861	2.00555	0.13623
H	3.02211	1.34263	1.00182
C	2.11585	3.22665	0.63201
H	2.65418	3.68016	1.47279
H	1.11296	2.96159	0.98501
H	2.01378	3.99184	-0.14481
C	4.25919	2.37437	-0.38827
H	4.83114	2.86387	0.40915
H	4.20819	3.07620	-1.22800
H	4.83272	1.49843	-0.70760
C	1.84202	1.60135	-2.70550
H	1.00213	1.06498	-3.16477
C	1.52489	3.09248	-2.73159
H	2.38334	3.68847	-2.40306
H	0.67012	3.36598	-2.10400
H	1.28916	3.40210	-3.75575
C	3.07963	1.30214	-3.54160
H	3.99165	1.72546	-3.10792
H	2.95520	1.74697	-4.53612
H	3.23019	0.22865	-3.68553
C	2.86804	-0.62684	-1.11559
H	3.17326	-0.88967	-0.09344
H	3.78147	-0.50160	-1.70617
C	-1.74441	-2.44112	-1.38807
H	-2.35503	-1.76758	-2.00387
H	-2.23319	-3.42092	-1.36901
C	0.56632	-1.52844	-1.36050
C	1.48985	-3.62136	-2.99804
C	1.92655	-1.64707	-1.68683
C	-0.31549	-2.51038	-1.84617
C	0.14769	-3.54494	-2.65389
C	2.37908	-2.67709	-2.50824
H	-0.55018	-4.29857	-3.01429
H	3.43696	-2.74279	-2.75687
H	1.84376	-4.42425	-3.63790
O	0.63570	-0.40740	1.83469
C	1.76939	-0.18919	2.49835
C	4.17866	0.23792	3.86837
C	2.79886	-1.13607	2.44511
C	1.95235	0.95700	3.28123
C	3.14819	1.16589	3.95103
C	3.98876	-0.91924	3.12141
H	2.63689	-2.03827	1.85818
H	1.14356	1.68118	3.34599
H	3.27477	2.06456	4.54877
H	4.77821	-1.66369	3.06618
H	5.11293	0.40531	4.39412
C	-1.11720	0.79941	-1.71531
H	-0.99101	0.17152	-2.60137
H	-0.63699	1.76632	-1.86976
C	-2.55929	0.99436	-1.47487
O	-3.39701	0.23534	-1.94404

C	-3.02745	2.14423	-0.62929
C	-4.01950	4.19883	0.97971
C	-4.38631	2.21764	-0.32583
C	-2.17589	3.13061	-0.13229
C	-2.66757	4.15051	0.66706
C	-4.88024	3.23201	0.47681
H	-5.04093	1.45422	-0.73522
H	-1.11443	3.09638	-0.35458
H	-1.99256	4.90971	1.05059
H	-5.93967	3.27230	0.71109
H	-4.40299	4.99439	1.61155
H	-0.56640	1.14823	0.80425
H	-0.03744	0.57020	1.43404
Co	-0.06828	-0.05195	-0.21754

C6ii

EE = -1995.293734

EE + ZPE = -1994.655612

G° = -1994.721824

P	1.03245	1.56911	0.42116
P	-2.24265	-1.20069	0.05419
C	2.88386	1.62301	0.55175
H	3.15802	1.32034	-0.47127
C	0.23018	2.31701	1.94514
H	-0.80852	1.95584	1.85983
C	3.46056	3.00855	0.80939
H	3.22830	3.35892	1.82168
H	3.09864	3.75659	0.09723
H	4.55324	2.97524	0.72403
C	3.45986	0.59319	1.51564
H	3.36035	0.91482	2.55729
H	4.52925	0.45885	1.31467
H	2.97750	-0.38339	1.41215
C	0.16919	3.83769	1.97066
H	-0.33792	4.16933	2.88498
H	-0.39031	4.24085	1.12158
H	1.16832	4.28693	1.96830
C	0.81058	1.75644	3.23663
H	0.15730	2.01007	4.07995
H	1.79467	2.18845	3.45001
H	0.91664	0.66700	3.20595
C	-3.20806	-0.65581	1.55499
H	-3.34764	0.41253	1.32172
C	-2.38026	-0.75955	2.83000
H	-2.91422	-0.29186	3.66571
H	-1.40279	-0.27752	2.72726
H	-2.19131	-1.80427	3.10127
C	-4.57970	-1.28679	1.74082
H	-5.12754	-0.75382	2.52699
H	-4.49653	-2.33158	2.06040
H	-5.19227	-1.25386	0.83448
C	-2.35490	-3.03365	-0.20644
H	-1.68795	-3.16172	-1.07385
C	-1.75053	-3.78985	0.96791
H	-2.41222	-3.75444	1.84192
H	-0.78167	-3.37085	1.26091
H	-1.60985	-4.84569	0.71111
C	-3.72101	-3.58244	-0.59539
H	-4.42586	-3.55323	0.24008
H	-3.62173	-4.63140	-0.89876
H	-4.16805	-3.04094	-1.43467
C	0.62739	2.74150	-0.93558

H	1.26594	2.42705	-1.77405
H	0.85058	3.79096	-0.71160
C	-1.35551	1.22780	-0.99455
C	-2.86428	3.20037	-2.33837
C	-2.65156	0.96038	-1.48124
C	-0.81223	2.49621	-1.28757
C	-1.56554	3.47310	-1.93209
C	-3.40082	1.93866	-2.12867
H	-1.12968	4.45070	-2.13121
H	-4.40707	1.71253	-2.47737
H	-3.45182	3.96656	-2.83614
C	0.33186	-1.15995	-1.45487
H	-0.27474	-0.84382	-2.30922
H	0.21912	-2.22690	-1.24881
C	1.73178	-0.76178	-1.67832
O	2.02428	0.22427	-2.34199
C	2.83636	-1.58980	-1.08588
C	4.98055	-3.03882	-0.04340
C	4.14256	-1.31364	-1.48769
C	2.61710	-2.60966	-0.16039
C	3.68362	-3.32544	0.36130
C	5.20854	-2.03300	-0.97374
H	4.29440	-0.52098	-2.21423
H	1.60951	-2.81182	0.18811
H	3.50322	-4.10831	1.09178
H	6.22080	-1.81171	-1.29873
H	5.81442	-3.60200	0.36528
H	0.34524	-1.09814	1.02854
Co	-0.36017	-0.11766	0.08199
C	-3.18899	-0.43831	-1.32947
H	-4.27655	-0.47150	-1.18332
H	-2.96970	-1.02990	-2.23148

TSC4ii

EE = -1995.288371

EE + ZPE = -1994.650822

G° = -1994.716867

Imaginary Freq = -540.47

P	0.46370	1.97260	-0.00368
P	-1.90498	-1.59278	-0.17165
C	2.08719	2.71793	-0.55635
H	2.16182	2.34033	-1.58527
C	0.31868	2.10679	1.86122
H	-0.70677	1.73030	2.00078
C	2.12600	4.24103	-0.59858
H	2.00136	4.68603	0.39456
H	1.36543	4.66792	-1.25728
H	3.10263	4.56555	-0.97837
C	3.29055	2.18522	0.21091
H	3.39970	2.69530	1.17531
H	4.20615	2.37019	-0.36271
H	3.24265	1.10956	0.40318
C	0.39642	3.50738	2.45120
H	0.17571	3.46627	3.52503
H	-0.32045	4.20013	2.00093
H	1.40034	3.93420	2.34755
C	1.26619	1.17110	2.60552
H	0.90399	1.00712	3.62760
H	2.27075	1.59788	2.68228
H	1.35879	0.19467	2.11998
C	-2.29313	-1.72004	1.65323
H	-2.69595	-0.70993	1.82985

C	-1.04620	-1.87327	2.51166
H	-1.30224	-1.76510	3.57246
H	-0.29991	-1.11570	2.25932
H	-0.58457	-2.85967	2.38867
C	-3.35500	-2.73553	2.05038
H	-3.63271	-2.58528	3.10055
H	-2.98391	-3.76294	1.96338
H	-4.27140	-2.65268	1.45836
C	-1.73680	-3.30861	-0.89463
H	-1.30826	-3.08794	-1.88545
C	-0.73374	-4.16478	-0.13153
H	-1.14532	-4.49706	0.82808
H	0.20502	-3.63996	0.07273
H	-0.49027	-5.06516	-0.70704
C	-3.03713	-4.07162	-1.11367
H	-3.52253	-4.33173	-0.16821
H	-2.82837	-5.01065	-1.64075
H	-3.75564	-3.51164	-1.71837
C	-0.77703	3.19888	-0.59159
H	-0.53604	3.38477	-1.64818
H	-0.73420	4.16711	-0.07978
C	-2.14489	1.11994	-0.52540
C	-4.51715	2.67155	-0.45502
C	-3.42425	0.53165	-0.61902
C	-2.11210	2.52935	-0.49264
C	-3.27621	3.28960	-0.43732
C	-4.58907	1.29216	-0.56798
H	-3.21016	4.37512	-0.39361
H	-5.55844	0.80046	-0.62452
H	-5.42552	3.26494	-0.40311
C	0.91313	-1.08369	-1.46846
H	0.35572	-0.80321	-2.37930
H	0.87348	-2.16651	-1.31702
C	2.30917	-0.61211	-1.60885
O	2.62030	0.25931	-2.40135
C	3.36803	-1.22847	-0.74027
C	5.42440	-2.25912	0.83769
C	4.70177	-0.97260	-1.05692
C	3.07849	-2.00959	0.37826
C	4.10142	-2.51590	1.16721
C	5.72346	-1.48827	-0.27937
H	4.90670	-0.35261	-1.92445
H	2.04637	-2.20537	0.65711
H	3.86462	-3.11226	2.04296
H	6.75833	-1.28777	-0.53953
H	6.22464	-2.65897	1.45321
H	0.60801	-0.69569	0.11661
Co	-0.47859	0.02761	-0.55089
C	-3.49992	-0.95282	-0.82619
H	-4.38837	-1.41057	-0.37312
H	-3.52628	-1.18371	-1.90053