

NO• Disproportionation by a {RhNO}⁹ Pincer-Type Complex

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Supporting Information

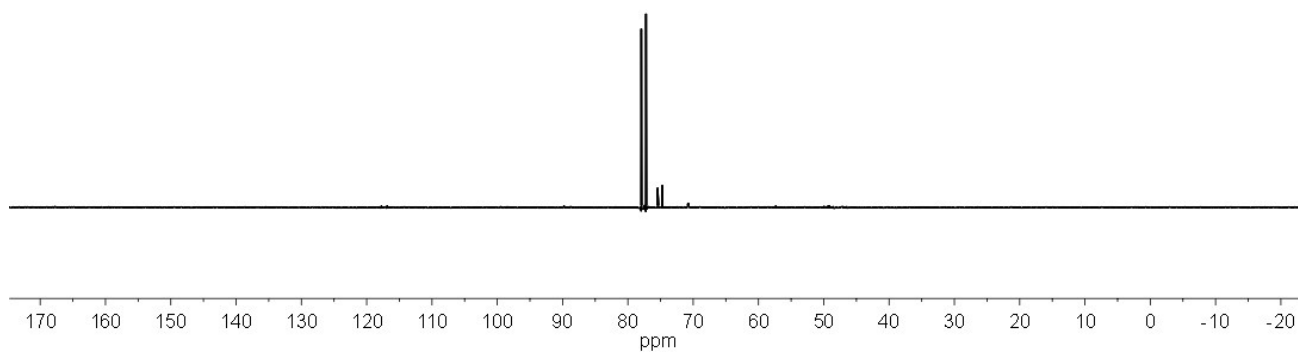


Figure S1. $^{31}\text{P}\{^1\text{H}\}$ NMR of **2** in C_6D_6 . The minor doublet corresponds to the known complex $\text{Rh}(\text{PCP}^t\text{Bu})\text{Cl}(\text{NO})$, obtained as a byproduct from reaction of **2** with a chloride impurity present in the precursor **1**⁺.

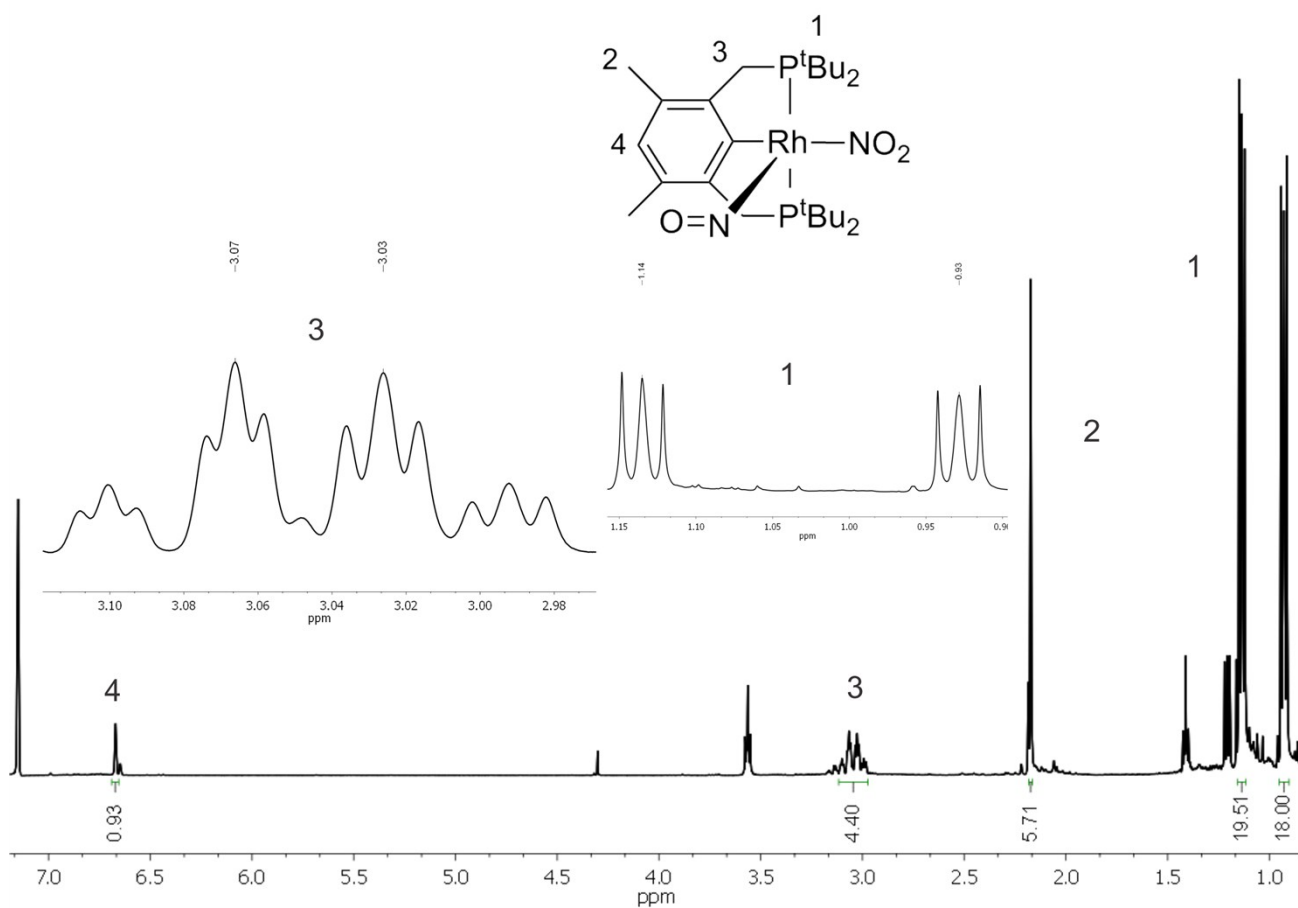


Figure S2. ^1H NMR of **2** in C_6D_6 .

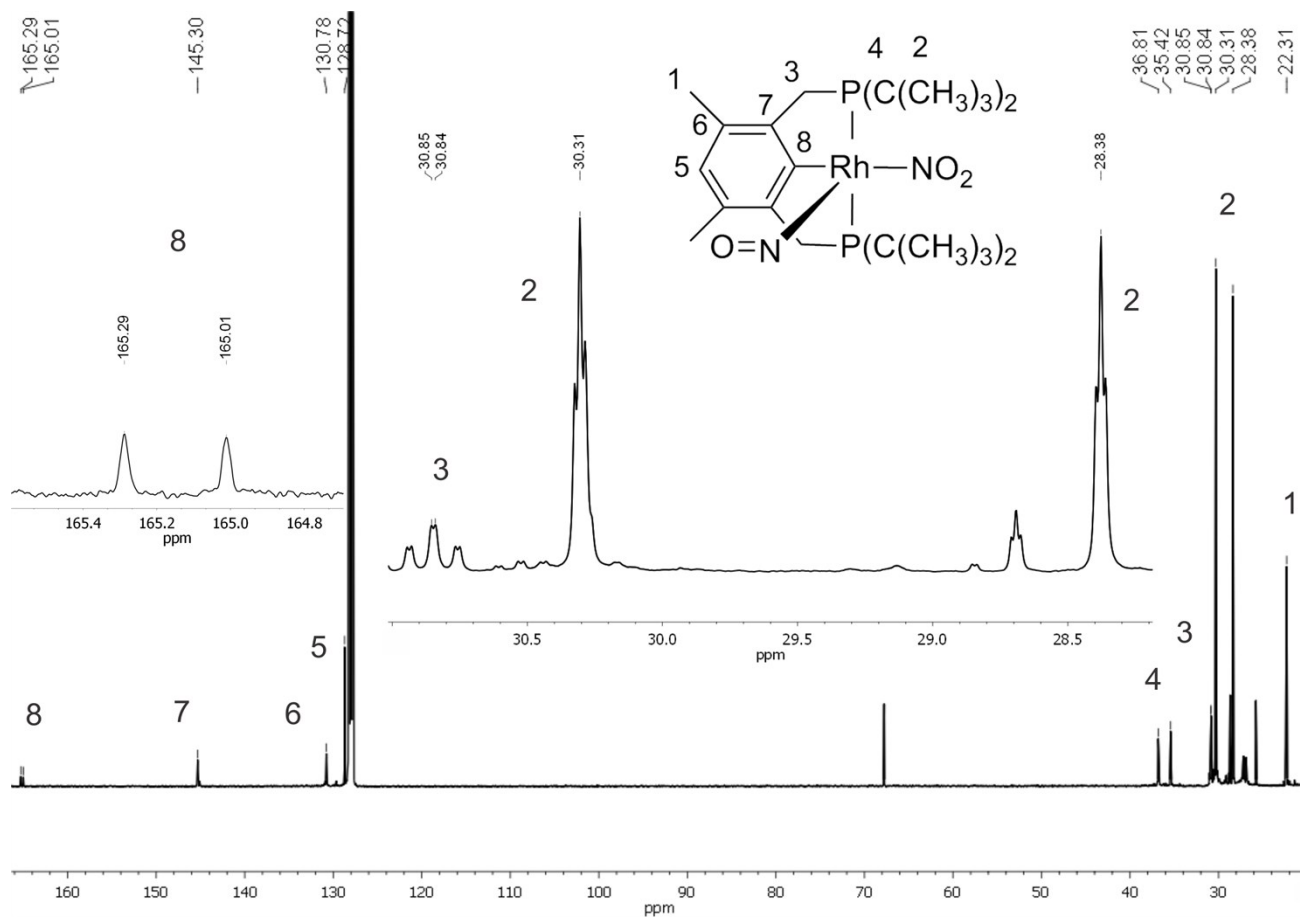


Figure S3. ¹³C{¹H} NMR of **2** in C₆D₆.

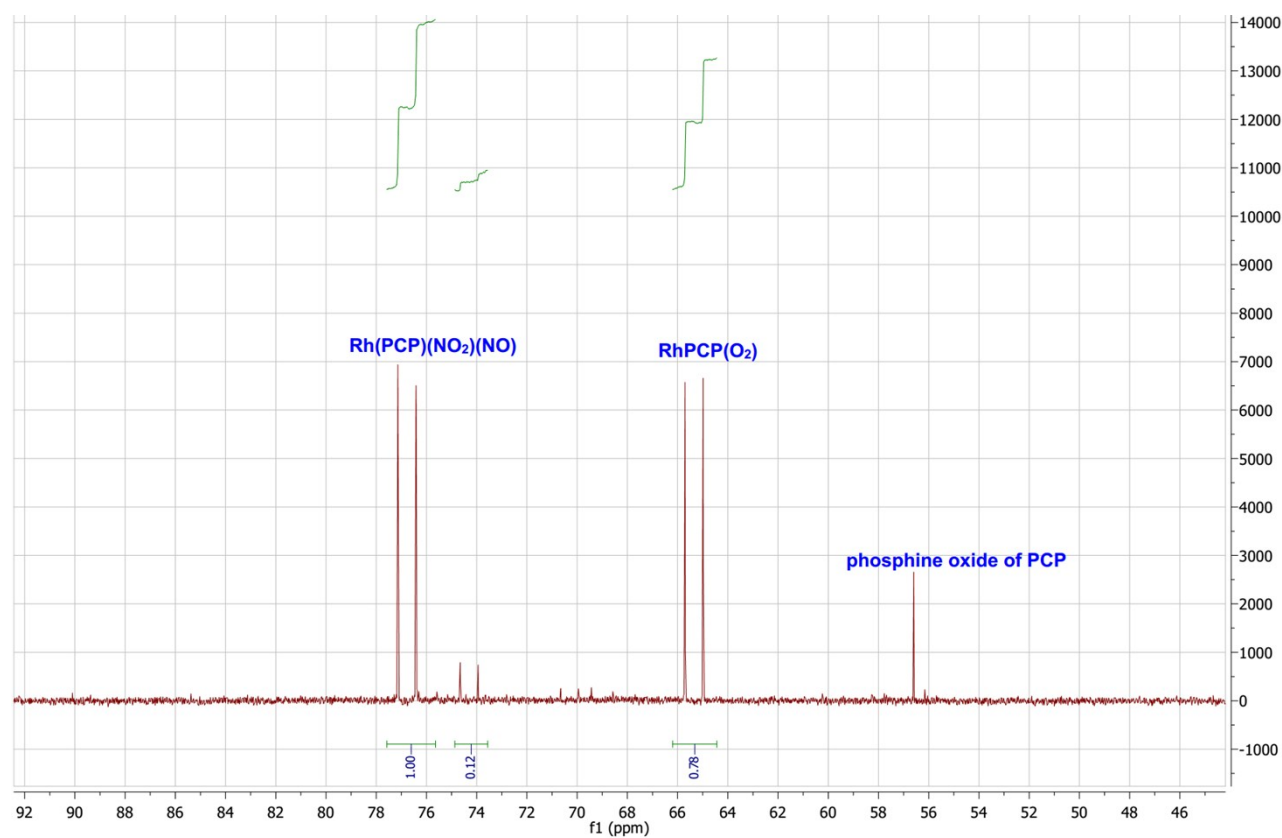


Figure S4. ³¹P{¹H} NMR of the reaction of **1**• with oxygen in C₆D₆.

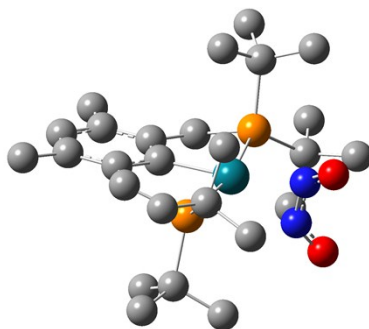


Figure S5. DFT optimized structure of Rh(PCP)(η^2 -N₂O₂) (hydrogen atoms are omitted).

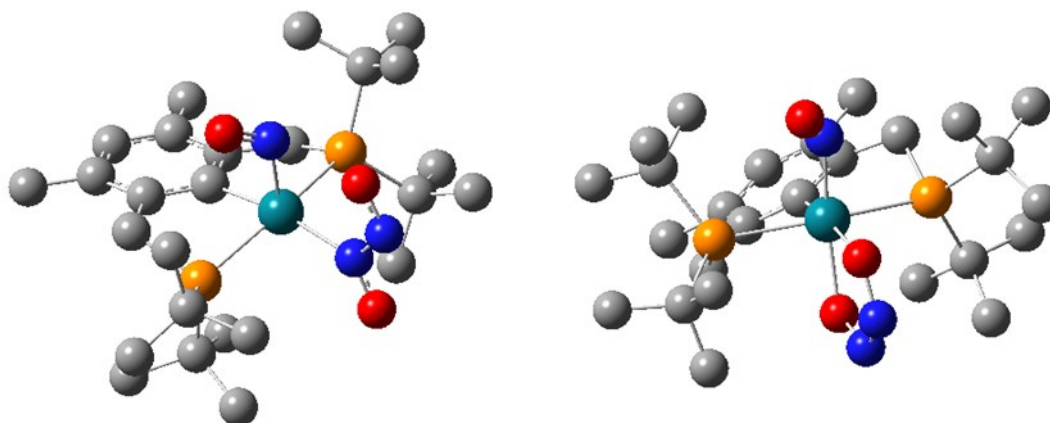


Figure S6. DFT optimized structures of Rh^{III}(NO⁻)(N₂O₂^{•-}) and Rh^{III}(NO[•])(η^2 -N₂O₂²⁻) (hydrogen atoms are omitted).

Cartesian coordinates from optimizations (Angstroms):

[Rh(PCP'Bu)(NO)][•] (1[•])

	X	Y	Z
C	1.21503	2.20124	-0.33617
C	0.00001	1.45162	-0.26833
C	-1.21510	2.20095	-0.33753
			-0.37
C	-1.22433	3.61609	56
C	-0.00028	4.29989	-0.37191
C	1.22394	3.61639	-0.37417
Rh	0.00026	-0.64294	-0.09056
N	-0.00084	-2.54166	0.02501
O	-0.00141	-3.60776	-0.53564
C	-2.53683	1.47489	-0.45718
P	-2.31063	-0.31436	-0.02110
C	-3.39917	-1.24218	-1.30050
C	-4.77375	-0.58795	-1.54917
C	-2.51707	4.39926	-0.44123
C	2.51657	4.39985	-0.43833
C	2.53718	1.47565	-0.45441

P	2.31092	-0.31425	-0.02090
C	2.99969	-0.46991	1.76352
C	4.52392	-0.27973	1.87205
C	3.39892	-1.24033	-1.30197
C	2.58267	-1.20597	-2.61462
C	-2.99906	-0.46736	1.76366
C	-2.28884	0.63507	2.58127
C	4.77385	-0.58652	-1.54977
C	3.59356	-2.70960	-0.88043
C	2.28923	0.63107	2.58288
C	2.59066	-1.83847	2.34534
C	-4.52332	-0.27735	1.87214
C	-2.58961	-1.83495	2.34745
C	-2.58309	-1.21052	-2.61331
C	-3.59469	-2.71064	-0.87652
H	-0.00040	5.39640	-0.39721
H	-2.32032	5.48250	-0.47478
H	-3.16590	4.20831	0.43344
H	-3.11307	4.14195	-1.33577
H	3.16441	4.20902	0.43711
H	2.31963	5.48305	-0.47211
H	3.11368	4.14266	-1.33216
H	3.34230	1.92795	0.15224
H	2.89257	1.51992	-1.50140
H	5.42182	-0.60541	-0.66174
H	4.68712	0.45857	-1.88779
H	5.29414	-1.14337	-2.35039
H	4.07607	-3.26166	-1.70726
H	2.63666	-3.20847	-0.66224
H	4.24784	-2.80498	0.00057
H	2.40559	-0.17689	-2.96940
H	1.59975	-1.68749	-2.48816
H	3.14294	-1.74038	-3.40345
H	2.55186	0.50798	3.64905
H	1.19442	0.55724	2.47840
H	2.58883	1.64664	2.27854
H	2.87560	-1.87863	3.41236
H	3.08417	-2.68082	1.83728
H	1.50138	-1.98733	2.26840
H	4.86365	0.66434	1.41325
H	5.08349	-1.11045	1.41313
H	4.80914	-0.24600	2.93940
H	-2.89026	1.51754	-1.50491
H	-3.34322	1.92775	0.14736
H	-4.80834	-0.24194	2.93949
H	-5.08285	-1.10890	1.41469
H	-4.86331	0.66592	1.41189
H	-2.87454	-1.87370	3.41452
H	-1.50028	-1.98358	2.27069
H	-3.08283	-2.67816	1.84054

H	-2.58891	1.65007	2.27550
H	-1.19402	0.56158	2.47669
H	-2.55123	0.51343	3.64766
H	-1.60039	-1.69230	-2.48617
H	-2.40562	-0.18216	-2.96997
H	-3.14373	-1.74607	-3.40111
H	-4.24859	-2.80417	0.00496
H	-2.63810	-3.20996	-0.65803
H	-4.07805	-3.26360	-1.70225
H	-5.29442	-1.14574	-2.34889
H	-4.68645	0.45657	-1.88880
H	-5.42166	-0.60511	-0.66106

Rh(PCP'Bu)(NO)₂

	X	Y	Z
Rh	0.00991	-0.63647	-0.16978
P	2.33131	-0.17843	0.02921
P	-2.38188	-0.31782	0.09478
N	-0.09085	-1.71704	-1.81725
C	-0.02203	1.51906	-0.04655
C	-1.23576	2.22384	0.20230
C	-1.29785	3.63935	0.13744
C	-0.13251	4.35182	-0.17984
H	-0.17880	5.44577	-0.24580
C	1.09382	3.70821	-0.39792
C	1.13919	2.29588	-0.30968
C	2.32651	4.52284	-0.71970
H	2.08146	5.59289	-0.80920
H	2.79420	4.20619	-1.66911
H	3.10406	4.42650	0.06068
C	-2.58033	4.39579	0.40872
H	-3.37779	4.13711	-0.31222
H	-2.41782	5.48303	0.34013
H	-2.98348	4.18220	1.41477
C	2.46775	1.60076	-0.49774
H	3.28578	2.10751	0.04707
H	2.77163	1.60637	-1.56104
C	2.85711	-0.14522	1.89328
C	3.68155	-1.01569	-1.07302
C	3.19855	-0.94149	-2.54093
H	3.07768	0.09422	-2.89782
H	2.25961	-1.47942	-2.70942
H	3.96999	-1.41211	-3.17696
C	5.05408	-0.31028	-1.01510
H	5.70798	-0.76235	-1.78306
H	5.56121	-0.42487	-0.04881
H	4.98426	0.76588	-1.24294
C	3.82708	-2.49814	-0.67549
H	4.49722	-3.00314	-1.39470

H	2.85748	-3.02044	-0.69173
H	4.27602	-2.61549	0.32373
C	2.59511	-1.51426	2.55178
H	3.17378	-2.32941	2.09120
H	1.52880	-1.78574	2.51235
H	2.88903	-1.45603	3.61538
C	1.95646	0.89797	2.59362
H	2.19004	0.88704	3.67390
H	0.88881	0.66450	2.46202
H	2.12161	1.92154	2.22267
C	4.32908	0.24843	2.12566
H	4.62421	1.16291	1.58571
H	5.02348	-0.56052	1.85285
H	4.47237	0.44649	3.20335
C	-2.48463	1.47081	0.60523
H	-3.40688	1.93169	0.21091
H	-2.59516	1.48678	1.70639
C	-3.25263	-1.22496	1.54987
C	-3.41016	-0.36846	-1.52873
C	-2.71945	0.64069	-2.47576
H	-3.23072	0.61040	-3.45502
H	-1.66025	0.38446	-2.63138
H	-2.76952	1.67549	-2.10151
C	-3.33236	-1.76798	-2.17194
H	-3.84278	-1.73643	-3.15164
H	-3.82871	-2.54099	-1.56639
H	-2.28980	-2.07219	-2.34938
C	-4.89005	0.02573	-1.35621
H	-5.02646	0.97150	-0.80658
H	-5.47064	-0.75854	-0.84623
H	-5.33855	0.16218	-2.35693
C	-4.59885	-0.59559	1.96245
H	-5.37810	-0.71227	1.19629
H	-4.50714	0.47700	2.19819
H	-4.95885	-1.09972	2.87784
C	-3.45462	-2.71185	1.19986
H	-3.76190	-3.26074	2.10813
H	-2.52685	-3.17492	0.82744
H	-4.24610	-2.85559	0.44766
C	-2.27471	-1.12876	2.74520
H	-2.05936	-0.08560	3.03168
H	-1.32175	-1.63375	2.52642
H	-2.73796	-1.61949	3.62067
N	0.08952	-2.43542	0.80312
O	0.52932	-2.72183	-2.03207
O	0.60248	-3.42676	0.35815

Rh(PCP'Bu)(ONNO)

	X	Y	Z
C	1.12808	2.26456	0.10644
C	-0.02430	1.48583	-0.20228
C	-1.22238	2.16494	-0.57074
C	-1.27008	3.57562	-0.65252
C	-0.10571	4.30154	-0.34886
C	1.09053	3.67938	0.03926
Rh	0.00161	-0.55335	0.07342
C	-2.44538	1.33672	-0.89648
P	-2.34308	-0.28646	0.01849
C	-3.56549	-1.43546	-0.91785
C	-5.03361	-1.00248	-0.73708
C	-2.52569	4.31342	-1.06259
C	2.29976	4.52196	0.37891
C	2.39555	1.57920	0.57645
P	2.35294	-0.23593	0.13108
C	3.24822	-1.09005	1.59539
C	4.51673	-0.35418	2.06787
C	3.32905	-0.32457	-1.51476
C	2.59314	0.62176	-2.49133
C	-2.93305	0.07804	1.81278
C	-1.71552	0.67737	2.55581
C	4.79744	0.12152	-1.36955
C	3.28440	-1.75083	-2.10275
C	2.20227	-1.10136	2.73541
C	3.58206	-2.55219	1.24056
C	-4.09939	1.07952	1.90039
C	-3.30520	-1.24587	2.51062
C	-3.20126	-1.35850	-2.42092
C	-3.38394	-2.89872	-0.45968
H	-0.13516	5.39620	-0.41108
H	-2.34892	5.39970	-1.10149
H	-3.35866	4.14161	-0.35636
H	-2.88368	3.99768	-2.05817
H	2.65858	4.33505	1.40677
H	2.06890	5.59549	0.29628
H	3.15133	4.31455	-0.29465
H	2.46822	1.63578	1.67920
H	3.30856	2.06754	0.19312
H	5.39700	-0.60308	-0.79605
H	4.90510	1.11316	-0.89933
H	5.24544	0.18828	-2.37757
H	3.78356	-1.73470	-3.08871
H	2.25156	-2.09360	-2.24934
H	3.81479	-2.48415	-1.47848
H	2.60525	1.67230	-2.16006
H	1.54681	0.31023	-2.63008
H	3.10229	0.57299	-3.47091

H	2.65740	-1.54887	3.63805
H	1.32831	-1.71043	2.45176
H	1.86468	-0.08643	3.01063
H	3.91221	-3.07425	2.15692
H	4.40328	-2.62457	0.51063
H	2.69960	-3.08310	0.85015
H	4.31531	0.68755	2.36557
H	5.30999	-0.34480	1.30633
H	4.91910	-0.87427	2.95639
H	-2.43035	1.06655	-1.96736
H	-3.39494	1.86636	-0.71617
H	-4.37009	1.22356	2.96234
H	-5.00137	0.73444	1.37373
H	-3.81967	2.06794	1.50141
H	-3.45136	-1.05207	3.58872
H	-2.50481	-1.99739	2.40807
H	-4.24301	-1.67654	2.12684
H	-1.39220	1.63576	2.12385
H	-0.85201	-0.01690	2.54240
H	-1.98526	0.84262	3.61579
H	-2.12297	-1.50173	-2.59013
H	-3.51397	-0.40584	-2.87837
H	-3.74355	-2.16272	-2.94906
H	-3.62420	-3.04895	0.60177
H	-2.36114	-3.25968	-0.63615
H	-4.07171	-3.53380	-1.04688
H	-5.67001	-1.62026	-1.39670
H	-5.19700	0.05150	-1.01773
H	-5.39344	-1.14971	0.29329
O	0.03396	-1.46854	-1.69544
N	0.06171	-2.86526	-1.61901
N	0.10622	-3.40436	-0.49631
O	0.08340	-2.62246	0.59986

Rh(PCP^tBu)(NO₂)•

	X	Y	Z
Rh	-0.00187	-0.54640	0.03331
P	-2.32636	-0.24740	0.00665
P	2.31690	-0.27998	0.06963
N	-0.02645	-2.56466	-0.33545
C	0.01164	1.52191	0.01919
C	-1.17742	2.26769	-0.24847
O	-0.11568	-3.25061	-1.36192
C	1.22164	2.25604	0.22776
C	1.24595	3.66916	0.18073
O	0.04659	-3.07888	0.82317
C	-1.16263	3.68138	-0.31345
C	0.05102	4.35173	-0.09741

H	0.06618	5.44752	-0.14535
C	2.49217	1.50924	0.56530
H	2.65600	1.52129	1.65972
H	3.39272	1.97011	0.12214
C	2.51505	4.45343	0.43073
H	2.95028	4.22949	1.42088
H	2.32442	5.53729	0.38808
H	3.29756	4.22648	-0.31640
C	-2.48162	1.54294	-0.49480
H	-2.72807	1.55796	-1.57304
H	-3.33653	2.02899	0.01003
C	-3.10783	-0.34195	1.75340
C	3.14494	-0.37796	-1.65848
C	-3.37708	-1.15072	-1.32260
C	-2.41441	4.47483	-0.61405
H	-2.87207	4.17494	-1.57356
H	-2.19538	5.55262	-0.67082
H	-3.19000	4.33555	0.16134
C	3.30801	-1.21186	1.42298
C	2.39087	-1.19972	2.66829
H	2.15273	-0.17676	3.00538
H	2.90845	-1.71149	3.50016
H	1.44462	-1.72588	2.46717
C	-2.80501	-1.73166	2.35370
H	-3.35870	-2.53701	1.84797
H	-3.10589	-1.73819	3.41706
H	-1.73209	-1.97544	2.29437
C	2.83616	-1.74903	-2.29579
H	3.30730	-2.58297	-1.75395
H	3.23228	-1.75899	-3.32759
H	1.75383	-1.94590	-2.34243
C	3.54659	-2.67692	1.00872
H	2.60635	-3.18193	0.73783
H	3.98335	-3.22373	1.86407
H	4.25572	-2.76438	0.17039
C	4.65117	-0.54123	1.77451
H	5.36498	-0.55265	0.93820
H	5.11502	-1.09336	2.61214
H	4.52717	0.50265	2.10447
C	2.46588	0.71300	-2.51669
H	1.37299	0.57404	-2.54836
H	2.85555	0.64454	-3.54846
H	2.66487	1.73228	-2.14836
C	-4.72122	-0.45501	-1.62301
H	-5.40580	-0.45755	-0.76276
H	-5.22314	-0.99582	-2.44583
H	-4.59225	0.58782	-1.95399
C	-3.63788	-2.61465	-0.91639
H	-2.70946	-3.15156	-0.66913
H	-4.10593	-3.14243	-1.76692

H	-4.33113	-2.69326	-0.06392
C	-2.50707	-1.14090	-2.60231
H	-2.25341	-0.11842	-2.93019
H	-3.07596	-1.61648	-3.42209
H	-1.57108	-1.70295	-2.45985
C	-2.37350	0.72269	2.59953
H	-1.28367	0.55812	2.58859
H	-2.73021	0.65458	3.64319
H	-2.56101	1.74951	2.24587
C	4.66499	-0.13986	-1.63478
H	4.93985	0.80312	-1.13337
H	5.03718	-0.07844	-2.67362
H	5.20444	-0.96492	-1.14394
C	-4.62123	-0.06839	1.78868
H	-4.88945	0.88752	1.30846
H	-4.95403	-0.01050	2.84100
H	-5.19962	-0.87302	1.30850

Rh(PCP'Bu)(NO₂)(NO)

	X	Y	Z
Rh	-0.00076	-0.53553	-0.26758
P	2.36469	-0.25519	0.13416
P	-2.31364	-0.24709	0.07933
N	-0.03604	-2.67368	-0.23959
O	-0.54464	0.41212	-2.82125
N	0.06658	-0.38811	-2.18562
C	-0.01168	1.54068	-0.04261
C	1.16606	2.27119	0.26523
O	0.01771	-3.17745	0.91971
C	-1.21510	2.26018	-0.28459
C	-1.23766	3.67446	-0.27137
O	-0.15583	-3.39958	-1.24303
C	1.15460	3.68917	0.29371
C	-0.04478	4.35900	0.01244
H	-0.05365	5.45563	0.02259
C	-2.48879	1.49003	-0.56935
H	-2.63880	1.38601	-1.66215
H	-3.39132	1.98914	-0.17562
C	-2.50140	4.45425	-0.55943
H	-2.93311	4.19115	-1.54117
H	-2.30449	5.53774	-0.56131
H	-3.28841	4.26456	0.19376
C	2.43813	1.53903	0.64607
H	2.56134	1.55825	1.74520
H	3.34720	2.01793	0.24155
C	3.51927	-0.40331	-1.38969
C	-2.77371	-0.16978	1.94555
C	3.05539	-1.18191	1.66565
C	2.39761	4.48408	0.62560

H	2.79640	4.23108	1.62438
H	2.18942	5.56536	0.61438
H	3.21425	4.29772	-0.09606
C	-3.59512	-1.28492	-0.90951
C	-2.97078	-1.58176	-2.29090
H	-2.77043	-0.66429	-2.86609
H	-3.69181	-2.18295	-2.87366
H	-2.03584	-2.15857	-2.20376
C	3.21801	-1.74424	-2.09518
H	3.47516	-2.61130	-1.46835
H	3.82505	-1.80686	-3.01619
H	2.15705	-1.83232	-2.37568
C	-2.41818	-1.51346	2.62100
H	-3.11152	-2.32161	2.34788
H	-2.47741	-1.38422	3.71666
H	-1.40202	-1.85302	2.36431
C	-3.86110	-2.63248	-0.20992
H	-2.92906	-3.18047	0.00052
H	-4.47129	-3.26218	-0.88164
H	-4.42453	-2.51613	0.72837
C	-4.92043	-0.52272	-1.12176
H	-5.43968	-0.28809	-0.18159
H	-5.59624	-1.15483	-1.72548
H	-4.77179	0.41661	-1.67794
C	-1.91130	0.93458	2.59506
H	-0.83596	0.73965	2.46329
H	-2.13191	0.95068	3.67767
H	-2.12029	1.93628	2.18957
C	4.32477	-0.53824	2.26400
H	5.19153	-0.58815	1.59044
H	4.58946	-1.09021	3.18384
H	4.17378	0.51410	2.55423
C	3.33195	-2.66090	1.32736
H	2.43754	-3.16131	0.92581
H	3.61475	-3.18727	2.25683
H	4.16784	-2.78072	0.61989
C	1.92035	-1.12310	2.71409
H	1.62636	-0.08875	2.96294
H	2.27234	-1.59788	3.64804
H	1.03774	-1.67935	2.35938
C	3.17518	0.76064	-2.34447
H	2.10708	0.79859	-2.59736
H	3.73561	0.61681	-3.28537
H	3.46575	1.74083	-1.93420
C	-4.25919	0.16483	2.17990
H	-4.56361	1.10472	1.68914
H	-4.42662	0.29296	3.26460
H	-4.92858	-0.64006	1.84071
C	5.01583	-0.31648	-1.03739
H	5.26418	0.60409	-0.48322

H	5.60119	-0.30478	-1.97460
H	5.35659	-1.18242	-0.44996

Rh(PCP'Bu)(η^2 -N₂O₂)

	X	Y	Z
C	1.22151	2.26146	-0.42123
C	0.02189	1.55187	-0.10862
C	-1.14852	2.31458	0.18738
C	-1.12461	3.73002	0.17440
C	0.07444	4.37794	-0.15948
C	1.25194	3.67507	-0.46098
Rh	-0.00299	-0.51061	0.01651
N	-0.10213	-2.47002	-0.82212
O	0.30662	-3.12987	-1.80940
C	-2.42630	1.60399	0.57470
P	-2.33064	-0.18760	0.06112
C	-3.17378	-0.22632	-1.66353
C	-4.68500	0.06257	-1.61340
C	-2.34997	4.54882	0.51436
C	2.50832	4.43720	-0.81998
C	2.47372	1.47865	-0.74152
P	2.32435	-0.23416	-0.01338
C	3.02052	-0.04426	1.77912
C	4.29778	0.81361	1.87502
C	3.46770	-1.30280	-1.13372
C	2.90892	-1.18571	-2.57242
C	-3.37536	-1.08062	1.40409
C	-2.45690	-1.15863	2.64701
C	4.93150	-0.82103	-1.11905
C	3.40835	-2.79344	-0.73456
C	1.91024	0.64635	2.60387
C	3.28416	-1.43500	2.39167
C	-4.66687	-0.32374	1.77837
C	-3.72285	-2.51807	0.96878
C	-2.47460	0.85572	-2.51567
C	-2.92610	-1.59463	-2.33369
H	0.09388	5.47451	-0.18120
H	-2.12338	5.62629	0.49310
H	-2.74035	4.30845	1.51916
H	-3.17795	4.37135	-0.19626
H	3.32150	4.26361	-0.09145
H	2.31805	5.52159	-0.84633
H	2.90142	4.14225	-1.80879
H	3.39395	1.98939	-0.41362
H	2.56752	1.34878	-1.83484
H	5.43339	-1.04625	-0.16501
H	5.02445	0.25979	-1.31657
H	5.49134	-1.35012	-1.91163

H	4.07121	-3.35911	-1.41434
H	2.39683	-3.20960	-0.85531
H	3.75478	-2.98023	0.29093
H	3.03090	-0.17722	-2.99932
H	1.84789	-1.47470	-2.62650
H	3.47512	-1.87970	-3.21931
H	2.26937	0.77391	3.64208
H	0.98809	0.04114	2.62267
H	1.64941	1.63815	2.20275
H	3.44793	-1.32006	3.47849
H	4.18781	-1.90901	1.97711
H	2.43042	-2.11857	2.25413
H	4.12426	1.85484	1.55844
H	5.13749	0.40944	1.29109
H	4.61901	0.85050	2.93182
H	-3.32927	2.09827	0.17360
H	-2.54378	1.61027	1.67498
H	-5.16962	-0.86656	2.59930
H	-5.37967	-0.25631	0.94413
H	-4.46635	0.69681	2.14186
H	-4.20159	-3.03992	1.81708
H	-2.82423	-3.09606	0.69959
H	-4.43506	-2.54265	0.12873
H	-2.09419	-0.16683	2.96761
H	-1.58691	-1.80787	2.46390
H	-3.03248	-1.58648	3.48818
H	-1.38473	0.69740	-2.54591
H	-2.65758	1.87629	-2.14267
H	-2.86601	0.79904	-3.54747
H	-3.35756	-2.43284	-1.76624
H	-1.85323	-1.79394	-2.47313
H	-3.40177	-1.58990	-3.33119
H	-5.06771	0.15413	-2.64613
H	-4.91991	1.00622	-1.09370
H	-5.24634	-0.75092	-1.12837
N	-0.00767	-2.61757	0.45631
O	-0.38410	-3.54290	1.22072

Rh^{III}(PCP'Bu)(NO⁻)(N₂O₂^{•-})

	X	Y	Z
C	-1.11974	2.32862	0.17671
C	0.03064	1.56898	-0.16459
C	1.22628	2.26167	-0.50938
C	1.26273	3.67523	-0.56510
C	0.09516	4.38672	-0.24665
C	-1.09183	3.74596	0.13661
Rh	0.00379	-0.51670	-0.16968
N	0.06315	-2.58397	0.29481

O	0.23016	-3.00126	1.46246
C	2.47032	1.45599	-0.82006
P	2.33359	-0.17115	0.07271
C	2.75381	0.19687	1.92801
C	3.87755	1.23976	2.09415
C	2.51500	4.42717	-0.95927
C	-2.30297	4.57244	0.50768
C	-2.36830	1.63163	0.67472
P	-2.37449	-0.16785	0.18000
C	-3.52413	-0.22363	-1.36273
C	-5.00732	0.02963	-1.03444
C	-3.17607	-1.03454	1.69761
C	-2.09117	-1.03646	2.79950
C	3.70308	-1.29478	-0.69793
C	3.61459	-1.21657	-2.23840
C	-4.42256	-0.31045	2.24890
C	-3.52943	-2.49275	1.34531
C	-3.04371	0.88673	-2.32475
C	-3.37212	-1.59453	-2.05557
C	5.12421	-0.85682	-0.28772
C	3.45658	-2.76583	-0.29798
C	1.48361	0.75913	2.60358
C	3.11013	-1.11656	2.65706
H	0.11563	5.48246	-0.28746
H	2.32635	5.51141	-0.99826
H	2.88786	4.11682	-1.95105
H	3.34167	4.26368	-0.24356
H	-3.16486	4.36581	-0.15313
H	-2.08305	5.64891	0.43418
H	-2.64155	4.37031	1.53960
H	-3.29741	2.12861	0.34467
H	-2.39170	1.66216	1.78082
H	-5.27226	-0.32202	1.55343
H	-4.21424	0.73707	2.52047
H	-4.74436	-0.82534	3.17223
H	-3.81574	-3.02778	2.26832
H	-2.67693	-3.02931	0.90063
H	-4.38291	-2.55529	0.65208
H	-1.77630	-0.01591	3.07702
H	-1.20129	-1.61522	2.50519
H	-2.51224	-1.50402	3.70824
H	-3.62871	0.81275	-3.25913
H	-1.98113	0.78331	-2.58545
H	-3.20189	1.89688	-1.91488
H	-3.96848	-1.59151	-2.98594
H	-3.74269	-2.42002	-1.42934
H	-2.32574	-1.80657	-2.32037
H	-5.16448	0.96379	-0.46980
H	-5.45899	-0.80205	-0.47223
H	-5.56743	0.12237	-1.98262

H	3.40752	1.98876	-0.59245
H	2.49238	1.19495	-1.89396
H	5.85590	-1.47484	-0.83909
H	5.32285	-0.99774	0.78460
H	5.32592	0.19609	-0.54602
H	4.24873	-3.39112	-0.74782
H	2.49043	-3.12771	-0.67866
H	3.47703	-2.93420	0.78702
H	3.86152	-0.21674	-2.62971
H	2.62533	-1.50471	-2.61880
H	4.35511	-1.92201	-2.65611
H	0.64601	0.04595	2.53488
H	1.16014	1.71215	2.16137
H	1.70408	0.92475	3.67444
H	4.06934	-1.54655	2.33193
H	2.31823	-1.87359	2.53115
H	3.19992	-0.90340	3.73759
H	4.06175	1.38961	3.17346
H	3.58475	2.21759	1.67836
H	4.83100	0.93767	1.63822
N	-0.09469	-3.65209	-0.67575
O	-0.21534	-3.23621	-1.83520
N	-0.18966	-0.67913	-2.09885
O	0.66649	-0.34564	-2.86002

Rh^{III}(NO•)(η²-N₂O₂²⁻)

	X	Y	Z
C	1.06041	2.16067	0.45383
C	-0.02459	1.40213	-0.03955
C	-1.10663	2.03482	-0.69495
C	-1.12721	3.44402	-0.82821
C	-0.06409	4.17922	-0.27454
C	1.03168	3.57406	0.36488
Rh	-0.00105	-0.65290	0.15939
C	-2.20887	1.14953	-1.24277
P	-2.40771	-0.27170	-0.05474
C	-3.49956	-1.61090	-0.91028
C	-5.01580	-1.33011	-0.89828
C	-2.25066	4.16404	-1.54085
C	2.15118	4.42990	0.91486
C	2.25401	1.42281	1.02772
P	2.41951	-0.22015	0.13629
C	3.59755	-1.27115	1.24962
C	4.68958	-0.40616	1.91352
C	3.26892	0.19544	-1.54780
C	2.40946	1.24952	-2.28176
C	-3.33487	0.48859	1.46733
C	-2.39552	1.42327	2.26324

C	4.68474	0.77036	-1.33611
C	3.34911	-1.04918	-2.45905
C	2.73935	-1.91755	2.35672
C	4.24143	-2.41700	0.44401
C	-4.54508	1.34435	1.02946
C	-3.80079	-0.64742	2.40444
C	-3.06976	-1.71304	-2.39045
C	-3.19921	-2.94859	-0.19741
H	-0.08394	5.27252	-0.35733
H	-2.07339	5.25068	-1.55736
H	-3.22880	3.99906	-1.05321
H	-2.35544	3.82651	-2.58663
H	2.34255	4.22431	1.98232
H	1.91236	5.50049	0.81843
H	3.10406	4.25762	0.38099
H	2.08165	1.15610	2.08897
H	3.18263	2.01576	0.99069
H	5.39453	0.02387	-0.94774
H	4.69463	1.64533	-0.66559
H	5.07166	1.10666	-2.31493
H	3.76789	-0.72764	-3.42985
H	2.35810	-1.48273	-2.65048
H	4.00761	-1.83484	-2.06643
H	2.35794	2.20985	-1.74763
H	1.38861	0.87713	-2.45027
H	2.87865	1.43557	-3.26515
H	3.40303	-2.51619	3.00715
H	1.97508	-2.58708	1.93195
H	2.24200	-1.16994	2.99394
H	4.75254	-3.09498	1.15086
H	4.99970	-2.06282	-0.27012
H	3.48802	-3.00961	-0.09944
H	4.26107	0.35918	2.58026
H	5.34446	0.09730	1.18812
H	5.32559	-1.06113	2.53645
H	-1.86502	0.67701	-2.18061
H	-3.15191	1.67904	-1.44901
H	-5.03800	1.73465	1.93812
H	-5.29824	0.78449	0.46115
H	-4.23331	2.21647	0.43295
H	-4.24779	-0.19776	3.30918
H	-2.96294	-1.28424	2.72622
H	-4.56792	-1.28974	1.94716
H	-2.09837	2.30853	1.68319
H	-1.48217	0.92277	2.60885
H	-2.94557	1.77103	3.15684
H	-1.99242	-1.87699	-2.51633
H	-3.36043	-0.81678	-2.96302
H	-3.59942	-2.57298	-2.83807
H	-3.55444	-2.95176	0.84497

H	-2.12032	-3.17070	-0.19158
H	-3.72300	-3.76255	-0.73010
H	-5.51307	-2.13838	-1.46453
H	-5.27001	-0.38079	-1.39794
H	-5.45492	-1.32751	0.11044
O	0.05273	-0.95432	-1.88617
N	0.24484	-2.27448	-2.24001
N	0.30939	-3.14741	-1.33257
O	0.14297	-2.78154	-0.04997
N	-0.00060	-0.82041	2.06699
O	-0.58661	-1.55291	2.80886

Rh(PCP'Bu)O₂

	X	Y	Z
Rh	-0.01418	-0.60283	-0.02726
C	-0.00208	1.44078	-0.11293
C	1.21419	2.15479	-0.36070
C	1.24053	3.56877	-0.37768
C	0.04628	4.26483	-0.13093
H	0.06472	5.36177	-0.13681
C	-1.17081	3.61270	0.11622
C	-1.19413	2.19678	0.11182
C	2.49228	1.39250	-0.64129
H	3.38349	1.88526	-0.21340
H	2.67020	1.34293	-1.73266
C	-2.51433	1.49548	0.35029
H	-3.31202	1.91860	-0.28588
H	-2.86090	1.65022	1.38924
P	2.30801	-0.36412	-0.04446
C	3.07922	-0.35959	1.71222
C	4.60940	-0.19279	1.73241
H	4.94468	0.69008	1.16231
H	5.12959	-1.07958	1.33773
H	4.94482	-0.05601	2.77676
C	2.67893	-1.66498	2.43321
H	3.11726	-2.55812	1.96508
H	1.58523	-1.79539	2.44097
H	3.03476	-1.62188	3.47898
C	2.43415	0.82045	2.47294
H	2.77331	0.79025	3.52422
H	1.33418	0.75544	2.46199
H	2.71753	1.80148	2.05919
C	3.32534	-1.40065	-1.28665
C	3.44747	-2.84238	-0.75238
H	3.82838	-3.49622	-1.55769
H	2.46802	-3.22769	-0.42306
H	4.15813	-2.91188	0.08747
C	4.71404	-0.81583	-1.61001
H	5.38756	-0.79861	-0.74183

H	4.65111	0.20800	-2.01483
H	5.19049	-1.44204	-2.38638
C	2.47781	-1.43030	-2.58010
H	2.30752	-0.42258	-2.99609
H	1.50268	-1.90495	-2.38895
H	3.02047	-2.01476	-3.34557
P	-2.33094	-0.34014	0.05045
C	-3.27273	-0.62867	-1.59608
C	-2.42746	0.11767	-2.65502
H	-1.40545	-0.28999	-2.70689
H	-2.34749	1.19795	-2.44863
H	-2.90622	-0.00339	-3.64381
C	-3.27677	-2.13239	-1.94102
H	-3.55832	-2.25583	-3.00268
H	-4.01506	-2.68867	-1.34233
H	-2.28132	-2.57850	-1.78121
C	-4.71247	-0.08355	-1.62279
H	-4.77104	0.99376	-1.39503
H	-5.37648	-0.61803	-0.92777
H	-5.12388	-0.21973	-2.63955
C	-3.15904	-1.16331	1.56653
C	-2.29625	-0.73437	2.77715
H	-2.31597	0.35317	2.95799
H	-1.24593	-1.04177	2.64107
H	-2.68779	-1.22768	3.68518
C	-4.62032	-0.74071	1.80159
H	-4.95945	-1.13044	2.77888
H	-5.29897	-1.14877	1.03698
H	-4.74595	0.35496	1.82327
C	-3.04436	-2.69563	1.42899
H	-3.32492	-3.16395	2.39019
H	-2.01007	-2.99261	1.18094
H	-3.72265	-3.09470	0.66013
O	0.13172	-2.70981	0.33937
O	-0.15774	-2.42175	-0.96511
C	2.51100	4.33959	-0.65985
H	3.28601	4.15721	0.10700
H	2.95578	4.05884	-1.63075
H	2.31868	5.42373	-0.68141
C	-2.42002	4.42424	0.37315
H	-3.19424	4.24618	-0.39540
H	-2.88097	4.17409	1.34538
H	-2.19844	5.50292	0.37583

Rh(PCP'Bu)

	X	Y	Z
C	1.19385	1.99962	-0.28040
C	0.00001	1.26360	0.00000
C	-1.19380	1.99967	0.28036
C	-1.19177	3.41442	0.28573
C	0.00006	4.09719	-0.00005
C	1.19187	3.41436	-0.28580
Rh	-0.00002	-0.71877	0.00002
C	-2.47624	1.25970	0.59786
P	-2.29032	-0.50982	0.04301
C	-3.13821	-0.56580	-1.68126
C	-4.66639	-0.39645	-1.66644
C	-2.44787	4.19934	0.59528
C	2.44800	4.19923	-0.59540
C	2.47626	1.25959	-0.59789
P	2.29028	-0.50991	-0.04299
C	3.29742	-1.49290	-1.35626
C	3.48297	-2.95004	-0.89210
C	3.13818	-0.56579	1.68127
C	4.66649	-0.39762	1.66630
C	-3.29746	-1.49277	1.35631
C	-2.40866	-1.49508	2.62061
C	2.75169	-1.89406	2.36582
C	2.50152	0.58283	2.49440
C	2.40906	-1.49440	-2.62086
C	4.66460	-0.87527	-1.70901
C	-4.66424	-0.87466	1.70974
C	-3.48377	-2.94967	0.89170
C	-2.50064	0.58194	-2.49492
C	-2.75272	-1.89470	-2.36515
H	0.00008	5.19371	-0.00007
H	2.24213	5.28120	-0.60568
H	2.87334	3.93002	-1.57867
H	3.24469	4.02261	0.15089
H	-3.24456	4.02272	-0.15100
H	-2.24196	5.28130	0.60553
H	-2.87322	3.93017	1.57856
H	3.36698	1.74327	-0.15750
H	2.65151	1.23897	-1.69027
H	2.25018	-0.47905	-3.02020
H	1.41368	-1.92040	-2.41076
H	2.89799	-2.09296	-3.41166
H	5.12058	-1.44882	-2.53717
H	5.37110	-0.89600	-0.86705
H	4.57179	0.16852	-2.05010
H	3.89254	-3.55356	-1.72255
H	2.52478	-3.40649	-0.58952
H	4.18630	-3.03328	-0.04829
H	3.17623	-2.77439	1.85898
H	1.65392	-2.00497	2.39220

H	3.12478	-1.89491	3.40655
H	2.85055	0.51698	3.54119
H	1.40107	0.51014	2.48160
H	2.77820	1.57754	2.11022
H	4.98134	0.51111	1.12598
H	5.17750	-1.26355	1.21581
H	5.03550	-0.30544	2.70441
H	-3.36694	1.74340	0.15746
H	-2.65150	1.23912	1.69024
H	-2.84963	0.51580	-3.54171
H	-1.40024	0.50846	-2.48199
H	-2.77663	1.57705	-2.11129
H	-3.12583	-1.89579	-3.40587
H	-3.17792	-2.77445	-1.85785
H	-1.65504	-2.00643	-2.39148
H	-4.98057	0.51277	-1.12656
H	-5.17808	-1.26179	-1.21558
H	-5.03527	-0.30448	-2.70461
H	-5.37109	-0.89490	0.86807
H	-4.57086	0.16901	2.05104
H	-5.12012	-1.44822	2.53795
H	-3.89350	-3.55327	1.72203
H	-2.52585	-3.40646	0.58882
H	-4.18727	-3.03229	0.04798
H	-2.24926	-0.47994	3.02028
H	-1.41352	-1.92139	2.41001
H	-2.89755	-2.09375	3.41135