

Electronic Supplementary Information

Distinct Electronic Effect on Borane and Boryl Nickel Complexes for Catalyzing H₂ Activation

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1. DFT benchmarking for the calculation of borane-nickel catalyst¹⁻⁶

The DFT benchmarking was performed by using M06-L, ω B97XD, PBE0, and M06-2X functionals. Selected parameters of the optimized geometries in comparison to the crystal structure of **A-CAT** were shown in **Table S1**.

Table S1. Selected bond lengths and angles in the crystal and optimized structures of **A-Cat** using different DFT functional.

A-Cat	X-Ray	M06L	PBE0	ω B97XD	M06-2X
RMS	0.0	5.468	5.469	5.480	5.520
B-Ni/Å	2.201	2.170	2.119	2.155	2.111
Ni-P ^I / Å	2.260	2.213	2.216	2.209	2.315
P ^I -Ni-P ^{2/o}	120	118	121	115	116

2. Absolute energies of all optimized structures

Table S2. The absolute energies of all optimized structures

Species	ZPE	Hc	Gc	E/(hartree)	H/(hartree)	G/(hartree)	Solvation Energy/(hartree)
A-Cat-G							
H ₂	0.009991	0.013296	-0.001498	-1.160086	-1.156781	-1.171575	-1.171122
CH ₃	0.708516	0.75395	0.630033	-2614.365	-2614.319	-2614.443	-2617.161
Cl	0.595968	0.640015	0.517338	-3875.266	-3875.222	-3875.345	-3878.013
CN	0.62048	0.666309	0.53997	-2773.223	-2773.178	-2773.304	-2775.979
NH ₂	0.676861	0.721139	0.601511	-2662.52	-2662.476	-2662.595	-2665.305
NO ₂	0.633553	0.681285	0.55076	-3109.979	-3109.931	-3110.062	-3112.859
OCH ₃	0.723646	0.771249	0.643287	-2839.942	-2839.894	-2840.022	-2842.82
H	0.625368	0.665397	0.553792	-2496.505	-2496.465	-2496.576	-2499.193
A-RC-G							
CH ₃	0.724714	0.771115	0.646109	-2615.541	-2615.495	-2615.62	-2618.357
Cl	0.612372	0.656476	0.535797	-3876.443	-3876.399	-3876.52	-3879.21
CN	0.636973	0.683681	0.555042	-2774.4	-2774.354	-2774.482	-2777.176
NH ₂	0.692118	0.737627	0.615571	-2663.696	-2663.651	-2663.773	-2666.5
NO ₂	0.649541	0.698363	0.565288	-3111.155	-3111.107	-3111.24	-3114.054
OCH ₃	0.739761	0.788504	0.658126	-2841.117	-2841.068	-2841.199	-2844.014
H	0.640898	0.682376	0.567457	-2497.682	-2497.64	-2497.755	-2500.389
A-TS-G							
CH ₃	0.719992	0.766081	0.641009	-2615.495	-2615.449	-2615.574	-2618.31
Cl	0.608634	0.653146	0.529694	-3876.398	-3876.353	-3876.477	-3879.165
CN	0.633368	0.67864	0.555744	-2774.354	-2774.309	-2774.432	-2777.128
NH ₂	0.688621	0.733494	0.612835	-2663.651	-2663.606	-2663.726	-2666.455
NO ₂	0.645928	0.694193	0.562404	-3111.111	-3111.062	-3111.194	-3114.007
OCH ₃	0.735931	0.784011	0.655049	-2841.072	-2841.024	-2841.153	-2843.97

H	0.637981	0.678532	0.566048	-2497.631	-2497.591	-2497.703	-2500.34
A-PC-G							
CH ₃	0.724925	0.771191	0.643591	-2615.525	-2615.478	-2615.606	-2618.347
Cl	0.614248	0.658579	0.535993	-3876.43	-3876.385	-3876.508	-3879.204
CN	0.638761	0.684677	0.559529	-2774.389	-2774.343	-2774.468	-2777.169
NH ₂	0.692784	0.738021	0.614609	-2663.677	-2663.632	-2663.755	-2666.488
NO ₂	0.652017	0.700038	0.568685	-3111.144	-3111.096	-3111.228	-3114.049
OCH ₃	0.741023	0.788889	0.661264	-2841.101	-2841.053	-2841.181	-2844.005
H	0.642301	0.683138	0.568078	-2497.665	-2497.625	-2497.74	-2500.381
B-Cat-G							
CH ₃	0.702723	0.748768	0.623586	-2631.018	-2630.972	-2631.098	-2633.848
CN	0.617209	0.663356	0.536267	-2789.919	-2789.873	-2790	-2792.704
Cl	0.591318	0.636106	0.51221	-3891.935	-3891.89	-3892.014	-3894.712
NH ₂	0.670959	0.71618	0.594094	-2679.158	-2679.113	-2679.235	-2681.979
NO ₂	0.629673	0.677766	0.546078	-3126.694	-3126.646	-3126.778	-3129.606
OCH ₃	0.718268	0.766585	0.636317	-2856.586	-2856.537	-2856.668	-2859.498
H	0.61964	0.660268	0.547268	-2513.158	-2513.118	-2513.231	-2515.882
B-RC-G							
CH ₃	0.718546	0.765678	0.639529	-2632.192	-2632.145	-2632.271	-2635.039
CN	0.633305	0.680408	0.553166	-2791.089	-2791.042	-2791.169	-2793.894
Cl	0.606873	0.652634	0.527587	-3893.109	-3893.063	-3893.188	-3895.903
NH ₂	0.686382	0.732919	0.608518	-2680.333	-2680.286	-2680.411	-2683.172
NO ₂	0.645771	0.694872	0.562189	-3127.865	-3127.816	-3127.949	-3130.798
OCH ₃	0.733794	0.783241	0.651845	-2857.761	-2857.711	-2857.843	-2860.691
H	0.636094	0.677703	0.564064	-2514.334	-2514.292	-2514.406	-2517.076
B-TS-G							
CH ₃	0.716151	0.762358	0.638627	-2632.171	-2632.125	-2632.248	-2635.017
CN	0.63106	0.677202	0.552908	-2791.071	-2791.025	-2791.15	-2793.87
Cl	0.604296	0.649459	0.525509	-3893.089	-3893.044	-3893.168	-3895.883
NH ₂	0.683281	0.728977	0.607113	-2680.316	-2680.27	-2680.392	-2683.154
NO ₂	0.64297	0.691252	0.560798	-3127.844	-3127.796	-3127.926	-3130.768
OCH ₃	0.731853	0.780228	0.652186	-2857.742	-2857.694	-2857.822	-2860.672
H	0.633094	0.674286	0.560012	-2514.312	-2514.27	-2514.385	-2517.052
B-PC-G							
CH ₃	0.717893	0.7646	0.638524	-2632.179	-2632.133	-2632.259	-2635.027
CN	0.633309	0.67978	0.552966	-2791.08	-2791.033	-2791.16	-2793.883
Cl	0.606572	0.651806	0.52743	-3893.094	-3893.049	-3893.174	-3895.89
NH ₂	0.685934	0.731785	0.609085	-2680.323	-2680.277	-2680.4	-2683.163
NO ₂	0.646644	0.695032	0.564061	-3127.859	-3127.811	-3127.942	-3130.794
OCH ₃	0.733914	0.782585	0.653014	-2857.749	-2857.7	-2857.83	-2860.679
H	0.635327	0.676602	0.562624	-2514.32	-2514.278	-2514.392	-2517.062

3. The free energy and the distance and the Fuzzy bond order of all optimized structures

Table S3. The free energy and the distance and Fuzzy bond order of B and Ni of all optimized structures

	The free energy/(kcal/mol)	the distance of B-Ni/(Å)	B-Ni Fuzzy bond order
A-TS-NH ₂	21.40	2.21899	0.48523
A-TS-OCH ₃	21.64	2.21961	0.48308
A-TS-CH ₃	21.84	2.22341	0.48366
A-TS-H	23.68	2.22298	0.48818
A-TS-Cl	20.88	2.22196	0.48648
A-TS-CN	24.75	2.2274	0.48683
A-TS-NO ₂	22.22	2.23127	0.48362
B-TS-NH ₂	6.1	2.30533	0.45477
B-TS-OCH ₃	8.9	2.32015	0.43955
B-TS-CH ₃	11.6	2.36847	0.40791
B-TS-H	9.8	2.34915	0.42219
B-TS-Cl	9.3	2.35379	0.42203
B-TS-CN	14.4	2.42135	0.36506
B-TS-NO ₂	15.9	2.40802	0.36906

4. Physical and electronic structures of nickel-hydrogen and nickel-hydride species

The reaction barriers of **A-RC-G** and **B-RC-G** were -6.0 ~ -0.5 kcal/mol (Table 1), which suggested that both the borane-nickel and boryl-nickel catalysts improved the process of hydrogen coordination. Meanwhile, the reaction barriers of **A-PC-G** and **B-PC-G** were -0.2 ~ 6.5 kcal/mol, leading to the hydrogenation activity of both systems. Comparing the two catalysts, we found that the boryl-nickel catalyst had higher energy (5.2 kcal/mol) than the borane-nickel catalyst (-0.2 kcal/mol). The dihydride complex **B-PC** may had higher potential activity in hydrogenation reactions.

The distance of B-H¹ in **A-PC** was 1.295 Å, which was similar to that in **B-PC** (1.289 Å). While, the distance of Ni-H¹ in **A-PC** was 1.637 Å, which was shorter than that in **B-PC** (1.778 Å). The results indicated that the Ni-H¹ showed different features in the two systems. The orbital energy of Ni-H¹ in **A-PC** was -0.43 eV, which had lower activity than that in **B-PC** (-0.15 eV). The orbital components of B-H¹-Ni in **A-PC** were B: 29.1%, H¹: 39.2%, and Ni:17.3%, respectively. However, the orbital components of B-H¹-Ni in **B-PC** were B: 31.2%, H¹: 39.6%, and Ni:11.1%, respectively. These results were also consistent with the activity of two complexes, which indicated that **B-PC** was superior for further hydrogenation reaction. Besides, the Fuzzy bond order of Ni-H¹ in **A-PC** was 0.385, which was stronger than that in **B-PC** (0.313).

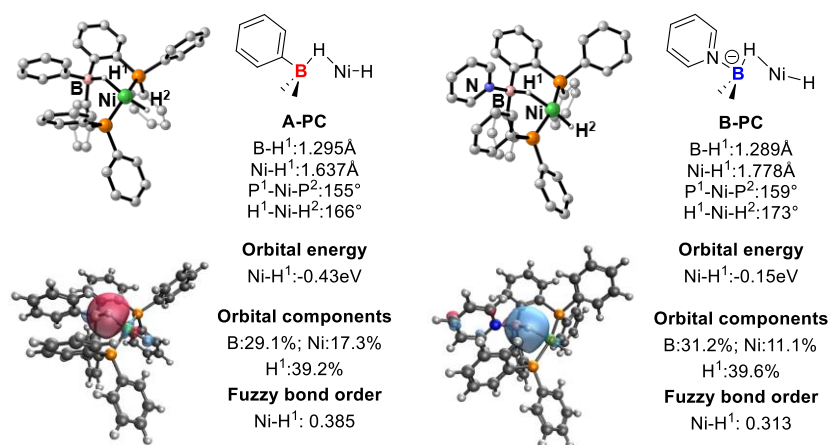


Figure S1. Structures of **A-PC** and **B-PC**, the orbital energy, the orbital components of the B-H¹-Ni bond, and the Fuzzy bond order of Ni-H¹. (Hydrogen atoms on phenyl and pyridine are omitted)

5. The Cartesian coordinates (xyz) for all structure

A-Cat-H

C	2.54837	-1.17215	1.01233
C	-1.85902	-3.07122	-0.15993
H	-2.56148	-2.84907	0.64209
C	0.41160	-3.05605	-1.02360
H	1.48327	-2.98561	-0.84527
C	-1.02332	-1.21892	3.47940
H	-0.25727	-1.85034	3.92653
C	-1.98663	-0.13376	1.56164
C	-2.99439	0.14591	3.74801
C	-2.30861	-3.67216	-1.32181
H	-3.35981	-3.92650	-1.43305
C	-2.98004	0.41367	2.38347
H	-3.74716	1.05150	1.94690
C	-1.41291	-3.90710	-2.37549
C	-0.06439	-3.61137	-2.22433
H	0.63472	-3.83955	-3.02622
C	1.93602	-2.81528	2.65131
H	1.18881	-3.43791	3.14223
C	-1.99913	-0.66049	4.29735
H	-1.98956	-0.85862	5.36647
C	3.89100	-1.29875	1.37983
H	4.65133	-0.70932	0.87015
C	3.27195	-2.94578	3.02054
H	3.55162	-3.65147	3.79923
C	4.25409	-2.18774	2.38516
Ni	-0.02490	-0.85120	-0.79442
P	-1.82741	0.29054	-0.20792
P	1.93606	-0.02671	-0.27453
B	0.02965	-1.77479	1.16813
C	1.93837	1.59543	0.57708
C	1.79849	1.68477	1.96756
C	1.95781	2.77723	-0.17608
C	1.69489	2.92787	2.58701
H	1.77093	0.77754	2.56780
C	1.86428	4.01579	0.44596
H	2.05295	2.72391	-1.25949
C	1.73210	4.09535	1.83076
H	1.59017	2.98115	3.66745
H	1.88002	4.92147	-0.15490
H	1.65043	5.06460	2.31579
C	3.33329	0.12348	-1.45209
C	3.31311	-0.67440	-2.60276
C	4.43171	0.96457	-1.23206

C	4.36907	-0.63876	-3.50874
H	2.45520	-1.32264	-2.78096
C	5.48469	1.00334	-2.14026
H	4.45410	1.59646	-0.34700
C	5.45580	0.20130	-3.27915
H	4.34058	-1.26217	-4.39820
H	6.33114	1.66036	-1.95818
H	6.27789	0.23425	-3.98907
C	-3.53634	0.11300	-0.86816
C	-4.42975	-0.81718	-0.31868
C	-3.93620	0.82087	-2.00998
C	-5.68242	-1.02571	-0.88934
H	-4.15037	-1.36650	0.57675
C	-5.18789	0.61274	-2.57769
H	-3.26869	1.55582	-2.45260
C	-6.06687	-0.31353	-2.02153
H	-6.36231	-1.74508	-0.44014
H	-5.47903	1.18201	-3.45649
H	-7.04537	-0.47540	-2.46489
C	-1.58535	2.10965	-0.31516
C	-1.13985	2.60778	-1.54915
C	-1.79638	3.01467	0.72937
C	-0.98026	3.97370	-1.75609
H	-0.90744	1.90774	-2.35195
C	-1.60552	4.38019	0.53115
H	-2.09727	2.65345	1.70884
C	-1.21928	4.86596	-0.71419
H	-0.64862	4.33844	-2.72497
H	-1.76137	5.06825	1.35838
H	-1.08194	5.93344	-0.86585
H	-1.77118	-4.34526	-3.30349
H	-3.76831	0.57302	4.38026
H	5.29794	-2.29492	2.66831
C	-0.49753	-2.71701	0.02661
C	1.53787	-1.92829	1.63818
C	-1.00488	-1.00710	2.08950

A-Cat-CH₃

C	-2.61667	0.52873	1.16264
C	0.33953	2.46758	0.90503
C	1.67531	2.94806	0.89800
H	2.38347	2.50180	1.59495
C	-1.65802	1.04193	2.05563
C	0.93536	0.15536	2.21967

C	-0.57510	3.10871	0.01416	H	-1.95287	-2.29319	-2.31546
H	-1.64304	2.92696	0.12112	C	-1.55730	-4.63615	0.11140
C	0.94596	-0.15581	3.59181	H	-1.42198	-4.21951	2.21935
H	0.14989	0.23144	4.22621	H	-1.70831	-4.73065	-2.03658
C	1.96236	-0.42026	1.43694	H	-1.44421	-5.71040	0.23194
C	2.99526	-1.44305	3.39643	C	-3.27680	0.17617	-1.63989
C	2.09198	3.95002	0.04479	C	-3.24814	1.31989	-2.44722
H	3.12570	4.29139	0.06908	C	-4.34573	-0.71910	-1.77533
C	2.97875	-1.18244	2.02692	C	-4.26528	1.56758	-3.36454
H	3.77842	-1.58220	1.40230	H	-2.41260	2.01329	-2.35024
C	1.20571	4.50371	-0.90175	C	-5.35980	-0.47391	-2.69604
C	-0.12100	4.08067	-0.89513	H	-4.37365	-1.61685	-1.16157
H	-0.82583	4.53984	-1.58772	C	-5.32173	0.66918	-3.49162
C	-2.12763	1.45968	3.31202	H	-4.22896	2.45802	-3.98624
H	-1.42833	1.88360	4.03181	H	-6.18266	-1.17738	-2.79325
C	1.94592	-0.92760	4.16730	H	-6.11213	0.85649	-4.21340
H	1.92213	-1.13286	5.23678	C	3.55181	0.23916	-0.88188
C	-3.96907	0.44656	1.50489	C	4.37855	0.99009	-0.03385
H	-4.68693	0.05066	0.78624	C	4.02605	-0.07023	-2.16367
C	-3.47293	1.37822	3.65243	C	5.63599	1.41352	-0.45377
H	-3.80321	1.72388	4.63115	H	4.04330	1.22290	0.97335
C	-4.42041	0.87421	2.75311	C	5.28373	0.35113	-2.58095
Ni	-0.00757	1.01184	-0.54859	H	3.41454	-0.66359	-2.83852
P	1.83674	-0.19855	-0.37193	C	6.09405	1.09819	-1.72943
P	-1.92032	-0.04700	-0.42662	H	6.26236	1.98683	0.22505
B	-0.13712	1.15157	1.61534	H	5.63424	0.08778	-3.57567
C	1.68650	5.54198	-1.86684	H	7.07684	1.42679	-2.05609
H	2.44669	5.13768	-2.54503	C	1.66864	-1.87531	-1.10794
H	0.87093	5.93399	-2.48029	C	1.26789	-1.93435	-2.45171
H	2.15228	6.38764	-1.34884	C	1.90007	-3.07671	-0.43115
C	4.08134	-2.26439	4.02076	C	1.17508	-3.15028	-3.12021
H	3.68928	-3.19524	4.44574	H	1.01929	-1.00917	-2.97251
H	4.85095	-2.53369	3.29285	C	1.77578	-4.29622	-1.09223
H	4.57160	-1.72998	4.84134	H	2.16363	-3.06421	0.62270
C	-5.87312	0.81610	3.11617	C	1.43675	-4.33751	-2.44102
H	-6.31653	1.81733	3.16378	H	0.87858	-3.17056	-4.16579
H	-6.44715	0.24082	2.38497	H	1.94647	-5.22072	-0.54591
H	-6.02779	0.35825	4.09857	H	1.35101	-5.29191	-2.95408
C	-1.85419	-1.86429	-0.20213				
C	-1.69162	-2.42424	1.07156	A-Cat-Cl			
C	-1.84552	-2.71355	-1.31679	C	-2.65827	0.03210	1.05087
C	-1.54264	-3.80029	1.22386	C	0.22177	2.04553	1.42497
H	-1.68660	-1.77982	1.94849	C	1.53650	2.55209	1.58472
C	-1.70863	-4.08762	-1.16019	H	2.26472	1.94118	2.11523

C	-1.73103	0.29514	2.07715
C	0.89126	-0.52886	2.04527
C	-0.71622	2.89126	0.75781
H	-1.77379	2.63569	0.77044
C	0.87694	-1.21833	3.27069
H	0.04869	-1.05899	3.95911
C	1.96016	-0.81860	1.16506
C	2.96144	-2.29491	2.78257
C	1.92345	3.78674	1.09715
H	2.93568	4.15479	1.22989
C	3.00066	-1.67642	1.53978
H	3.83824	-1.85635	0.87009
C	0.99008	4.54710	0.38040
C	-0.31942	4.12185	0.21010
H	-1.03103	4.75679	-0.30908
C	-2.22899	0.34849	3.38804
H	-1.55508	0.57306	4.21364
C	1.89247	-2.08742	3.65046
H	1.86764	-2.59600	4.60903
C	-4.01715	-0.16016	1.30990
H	-4.72115	-0.35399	0.50454
C	-3.57885	0.16150	3.67045
H	-3.95207	0.22321	4.68776
C	-4.46237	-0.08924	2.62350
Ni	-0.03081	1.03196	-0.38902
P	1.87928	-0.08401	-0.50721
P	-1.90500	-0.07173	-0.61270
B	-0.20873	0.56141	1.71070
Cl	1.47959	6.09025	-0.26914
Cl	-6.16087	-0.30843	2.96818
Cl	4.26048	-3.35966	3.25508
C	3.58487	0.54361	-0.79148
C	4.35967	1.02084	0.27525
C	4.09925	0.65948	-2.08985
C	5.60892	1.59079	0.05009
H	3.99368	0.92374	1.29407
C	5.34805	1.22897	-2.31272
H	3.52609	0.28643	-2.93519
C	6.10796	1.69900	-1.24443
H	6.19663	1.94291	0.89373
H	5.73125	1.29976	-3.32716
H	7.08397	2.14236	-1.41946
C	1.78976	-1.47652	-1.70195
C	1.40104	-1.14571	-3.00891

C	2.06875	-2.81434	-1.40729
C	1.35758	-2.11137	-4.00899
H	1.12217	-0.11656	-3.23643
C	1.99456	-3.78634	-2.40218
H	2.33096	-3.10717	-0.39447
C	1.65974	-3.43684	-3.70696
H	1.07003	-1.83103	-5.01901
H	2.20177	-4.82354	-2.15226
H	1.61339	-4.19784	-4.48150
C	-3.21691	0.47381	-1.76451
C	-4.24431	-0.35626	-2.23054
C	-3.19232	1.81541	-2.16673
C	-5.22478	0.15005	-3.07887
H	-4.26784	-1.40241	-1.93312
C	-4.17641	2.32155	-3.00920
H	-2.38525	2.45697	-1.81230
C	-5.19320	1.48753	-3.46785
H	-6.01740	-0.50174	-3.43638
H	-4.14564	3.36365	-3.31453
H	-5.95877	1.87811	-4.13253
C	-1.78742	-1.87868	-0.88196
C	-1.69274	-2.75837	0.20385
C	-1.66487	-2.39400	-2.17977
C	-1.49562	-4.12038	-0.00506
H	-1.77719	-2.37764	1.21926
C	-1.47785	-3.75600	-2.38434
H	-1.71753	-1.72277	-3.03529
C	-1.39288	-4.62400	-1.29799
H	-1.43029	-4.78943	0.84867
H	-1.38416	-4.13817	-3.39766
H	-1.24173	-5.68786	-1.46042

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C	-2.66118	0.12397	1.12788
C	0.30897	2.03788	1.48160
C	1.64743	2.48478	1.63990
H	2.34540	1.84629	2.17802
C	-1.71503	0.37082	2.14347
C	0.86232	-0.56389	2.10014
C	-0.59802	2.92190	0.81426
H	-1.66655	2.71982	0.84559
C	0.80754	-1.26347	3.31979
H	-0.01722	-1.07312	4.00366
C	1.92065	-0.88984	1.21707

C	2.85723	-2.44025	2.83006	H	2.31573	-3.14646	-0.42092
C	2.09066	3.68287	1.12105	C	1.61789	-3.37123	-3.73502
H	3.12308	3.99596	1.24319	H	1.02192	-1.72515	-4.99338
C	2.91742	-1.79259	1.58904	H	2.17242	-4.80510	-2.22796
H	3.75127	-1.99769	0.92119	H	1.56343	-4.10827	-4.53160
C	1.20208	4.48900	0.37398	C	-3.25631	0.55007	-1.68066
C	-0.13894	4.11159	0.23728	C	-4.28864	-0.28013	-2.13571
H	-0.82404	4.76616	-0.29482	C	-3.23720	1.89350	-2.07702
C	-2.18945	0.46111	3.46207	C	-5.28098	0.22920	-2.96805
H	-1.49378	0.67616	4.27136	H	-4.30760	-1.32735	-1.84186
C	1.77814	-2.18095	3.68947	C	-4.23337	2.40191	-2.90357
H	1.71957	-2.69891	4.64209	H	-2.42682	2.53581	-1.73226
C	-4.01724	-0.01869	1.41076	C	-5.25555	1.56853	-3.35125
H	-4.73598	-0.19912	0.61435	H	-6.07833	-0.42128	-3.31666
C	-3.53731	0.32152	3.76255	H	-4.20807	3.44515	-3.20477
H	-3.88985	0.40921	4.78589	H	-6.03095	1.96137	-4.00282
C	-4.46333	0.08201	2.73527	C	-1.82706	-1.81055	-0.80844
Ni	-0.01849	1.04837	-0.32967	C	-1.74391	-2.69019	0.27798
P	1.86441	-0.11988	-0.43873	C	-1.69435	-2.32449	-2.10591
P	-1.93523	-0.00350	-0.54676	C	-1.54233	-4.05191	0.07042
B	-0.18667	0.57500	1.76538	H	-1.84101	-2.31106	1.29276
C	1.66295	5.70075	-0.21546	C	-1.50357	-3.68611	-2.30908
C	-5.85115	-0.05335	3.03552	H	-1.74127	-1.65305	-2.96155
C	3.87305	-3.36784	3.20487	C	-1.42565	-4.55396	-1.22188
N	2.04271	6.69374	-0.70295	H	-1.48553	-4.72168	0.92401
N	-6.98838	-0.16777	3.27998	H	-1.40130	-4.06808	-3.32145
N	4.70528	-4.13030	3.50888	H	-1.27080	-5.61728	-1.38321
C	3.55860	0.54083	-0.69425	A-Cat-NH₂			
C	4.37684	0.89400	0.38741	C	-2.62380	0.51527	1.16156
C	4.00567	0.82914	-1.99118	C	0.29892	2.47927	0.88954
C	5.60646	1.51175	0.17671	C	1.63625	2.95355	0.83545
H	4.06209	0.66915	1.40328	H	2.36530	2.49712	1.50335
C	5.23320	1.44683	-2.19884	C	-1.66899	1.03041	2.05897
H	3.39487	0.55734	-2.84873	C	0.93658	0.18289	2.21331
C	6.03718	1.79452	-1.11544	C	-0.63093	3.13098	0.02331
H	6.22937	1.76844	1.02910	H	-1.69400	2.92717	0.13845
H	5.56346	1.65610	-3.21248	C	0.95214	-0.13972	3.58307
H	6.99519	2.27924	-1.27874	H	0.14926	0.23128	4.21884
C	1.77044	-1.47314	-1.67386	C	1.97530	-0.38175	1.43449
C	1.37301	-1.10124	-2.96719	C	3.01486	-1.39381	3.39086
C	2.04861	-2.81988	-1.42183	C	2.03836	3.96527	-0.01087
C	1.31743	-2.03649	-3.99498	H	3.07594	4.29396	-0.02554
H	1.09314	-0.06574	-3.16238	C	2.99964	-1.13393	2.01579
C	1.96415	-3.76085	-2.44462				

H	3.79855	-1.53317	1.39034
C	1.11817	4.53708	-0.91589
C	-0.21634	4.11498	-0.88252
H	-0.93991	4.58413	-1.54789
C	-2.15271	1.42159	3.31833
H	-1.46446	1.84648	4.04841
C	1.95603	-0.89770	4.16622
H	1.93083	-1.11387	5.23310
C	-3.97399	0.40234	1.49176
H	-4.68451	0.00749	0.76571
C	-3.49414	1.31599	3.66297
H	-3.83424	1.64907	4.64231
C	-4.43050	0.80659	2.75112
Ni	-0.00769	1.00251	-0.55051
P	1.84796	-0.18106	-0.38050
P	-1.91136	-0.04638	-0.42738
B	-0.15085	1.16416	1.61587
N	1.54505	5.47601	-1.84094
N	-5.78710	0.76771	3.06830
N	4.00283	-2.19276	3.95692
H	0.82947	6.08450	-2.20595
H	2.38485	5.97567	-1.59472
H	-5.98225	0.69873	4.05528
H	-6.31674	0.08814	2.54408
H	4.16313	-2.03445	4.93954
H	4.86812	-2.22263	3.44008
C	3.56856	0.24948	-0.88841
C	4.39336	1.01158	-0.04787
C	4.04907	-0.07359	-2.16458
C	5.65145	1.43217	-0.46866
H	4.05506	1.25532	0.95590
C	5.30749	0.34434	-2.58330
H	3.44070	-0.67486	-2.83506
C	6.11482	1.10254	-1.73895
H	6.27479	2.01483	0.20540
H	5.66066	0.07002	-3.57421
H	7.09804	1.42903	-2.06680
C	1.69693	-1.87680	-1.08280
C	1.32530	-1.97013	-2.43345
C	1.90431	-3.06226	-0.37053
C	1.24395	-3.20259	-3.07246
H	1.08957	-1.05865	-2.98310
C	1.78942	-4.29798	-1.00245
H	2.14042	-3.02490	0.68909

C	1.48448	-4.37341	-2.35761
H	0.97126	-3.24831	-4.12391
H	1.94009	-5.20830	-0.42700
H	1.40572	-5.34027	-2.84816
C	-1.84362	-1.86500	-0.20790
C	-1.68775	-2.42802	1.06541
C	-1.82675	-2.71195	-1.32438
C	-1.54054	-3.80455	1.21545
H	-1.68337	-1.78405	1.94278
C	-1.69253	-4.08654	-1.17015
H	-1.92588	-2.28898	-2.32290
C	-1.55000	-4.63819	0.10118
H	-1.42235	-4.22587	2.21044
H	-1.68561	-4.72747	-2.04817
H	-1.43677	-5.71274	0.21982
C	-3.26603	0.17434	-1.64539
C	-4.32819	-0.72675	-1.79426
C	-3.24282	1.32535	-2.44259
C	-5.34087	-0.48032	-2.71640
H	-4.35136	-1.63113	-1.18995
C	-4.25843	1.57462	-3.36119
H	-2.41158	2.02269	-2.33593
C	-5.30850	0.67051	-3.50079
H	-6.15785	-1.18932	-2.82428
H	-4.22590	2.47097	-3.97475
H	-6.09764	0.85924	-4.22371

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C	-2.66434	-0.09448	0.89068
C	0.26562	1.73909	1.76497
C	1.59204	2.15581	2.06674
H	2.26698	1.43820	2.52913
C	-1.78650	-0.01827	1.99339
C	0.78104	-0.94880	1.87095
C	-0.62632	2.71977	1.21074
H	-1.69690	2.52842	1.18718
C	0.66904	-1.89360	2.90950
H	-0.15934	-1.81523	3.61093
C	1.84514	-1.11954	0.95014
C	2.64061	-3.02503	2.17327
C	2.04838	3.42158	1.76863
H	3.06135	3.74015	1.98523
C	2.78924	-2.13246	1.12034
H	3.64013	-2.23827	0.45430

C	1.18044	4.30280	1.10573
C	-0.14320	3.98143	0.83901
H	-0.78212	4.72752	0.37857
C	-2.33683	-0.17083	3.27767
H	-1.69188	-0.09887	4.15159
C	1.58232	-2.92524	3.07131
H	1.49805	-3.64959	3.87377
C	-4.03136	-0.29964	1.06112
H	-4.71682	-0.34725	0.22028
C	-3.69736	-0.37673	3.46734
H	-4.13417	-0.47807	4.45426
C	-4.52581	-0.43573	2.35163
Ni	0.00021	1.15794	-0.20509
P	1.86434	-0.00825	-0.49830
P	-1.85427	0.08586	-0.74255
B	-0.23966	0.25627	1.75100
N	-5.96616	-0.64370	2.54492
O	-6.36965	-0.78193	3.69829
O	-6.67658	-0.66851	1.54140
N	1.67481	5.61851	0.70755
O	2.81914	5.92398	1.04597
O	0.91958	6.33979	0.05211
N	3.61495	-4.10862	2.33017
O	3.48929	-4.84930	3.30361
O	4.49221	-4.21091	1.47334
C	3.57534	0.64706	-0.55100
C	4.35283	0.75058	0.61010
C	4.08633	1.16294	-1.74989
C	5.60946	1.34797	0.57006
H	3.98194	0.34621	1.54854
C	5.34071	1.75953	-1.78630
H	3.50373	1.08515	-2.66513
C	6.10616	1.85605	-0.62613
H	6.20283	1.40991	1.47801
H	5.72363	2.14682	-2.72607
H	7.08627	2.32303	-0.65589
C	1.78933	-1.03409	-2.01595
C	1.37106	-0.36085	-3.17411
C	2.13287	-2.38567	-2.11344
C	1.34815	-1.00434	-4.40651
H	1.05499	0.68046	-3.10006
C	2.08431	-3.03576	-3.34383
H	2.42534	-2.94668	-1.23057
C	1.70955	-2.34629	-4.49322

H	1.03519	-0.46130	-5.29409
H	2.34413	-4.08941	-3.40062
H	1.68428	-2.85768	-5.45169
C	-1.62385	-1.65396	-1.26549
C	-1.38339	-2.65038	-0.31081
C	-1.55943	-1.99246	-2.62343
C	-1.09164	-3.95316	-0.70363
H	-1.43347	-2.41198	0.74895
C	-1.28439	-3.29922	-3.01215
H	-1.72883	-1.23075	-3.38167
C	-1.04851	-4.28337	-2.05490
H	-0.91070	-4.71307	0.05208
H	-1.24243	-3.54548	-4.06982
H	-0.82713	-5.30180	-2.36203
C	-3.15856	0.73178	-1.84461
C	-4.17254	-0.06856	-2.38711
C	-3.15742	2.10598	-2.11353
C	-5.16678	0.49975	-3.17687
H	-4.17644	-1.13907	-2.19309
C	-4.15429	2.67274	-2.90185
H	-2.36479	2.72789	-1.69781
C	-5.15901	1.86915	-3.43399
H	-5.95127	-0.12788	-3.59013
H	-4.14305	3.73974	-3.10499
H	-5.93603	2.30942	-4.05250

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C	-2.74356	0.03086	0.94475
C	0.33562	1.53048	1.98504
C	1.70901	1.76267	2.24415
H	2.30026	0.94104	2.64643
C	-1.86598	-0.07028	2.04636
C	0.63229	-1.16595	1.80578
C	-0.42082	2.64700	1.49304
H	-1.50814	2.59825	1.48179
C	0.46579	-2.19827	2.74035
H	-0.37092	-2.14578	3.43633
C	1.70076	-1.31875	0.88274
C	2.41045	-3.37733	1.94936
C	2.33530	2.96775	1.97971
H	3.39628	3.07894	2.17702
C	2.58526	-2.39287	0.97303
H	3.43089	-2.48719	0.29565
C	1.59797	3.99225	1.35987

C	0.22615	3.83947	1.13833
H	-0.32456	4.67908	0.72250
C	-2.45257	-0.32618	3.29112
H	-1.82190	-0.39486	4.17709
C	1.32834	-3.28802	2.82788
H	1.15775	-4.05121	3.58048
C	-4.12149	-0.10596	1.08204
H	-4.79160	-0.01407	0.23014
C	-3.83126	-0.46605	3.45259
H	-4.23829	-0.64461	4.44256
C	-4.67160	-0.35401	2.34225
Ni	0.03177	1.17606	-0.04251
P	1.79327	-0.08144	-0.46330
P	-1.88834	0.33869	-0.64494
B	-0.30404	0.11092	1.83333
O	2.13199	5.18098	0.97002
O	-6.03049	-0.46851	2.38747
O	3.33236	-4.38049	1.95380
C	3.52598	5.34360	1.13605
H	3.76880	6.32125	0.71943
H	3.81443	5.32243	2.19493
H	4.09047	4.56808	0.60208
C	-6.60657	-0.71840	3.64957
H	-6.39767	0.09109	4.36200
H	-7.68276	-0.78296	3.48757
H	-6.24985	-1.66338	4.08134
C	3.17303	-5.38859	2.92806
H	2.22133	-5.92342	2.80909
H	3.99699	-6.08734	2.78232
H	3.22018	-4.98149	3.94680
C	3.53017	0.52660	-0.42409
C	4.34247	0.39464	0.70982
C	4.01027	1.29430	-1.49519
C	5.59281	1.00597	0.76795
H	4.00030	-0.19951	1.55337
C	5.25863	1.90202	-1.43806
H	3.40098	1.41217	-2.38885
C	6.05583	1.76474	-0.30235
H	6.20768	0.88288	1.65618
H	5.61077	2.48559	-2.28490
H	7.03141	2.24118	-0.25632
C	1.74486	-0.98647	-2.06531
C	1.45973	-0.21101	-3.19991
C	1.94892	-2.35886	-2.23511

C	1.45483	-0.77383	-4.47169
H	1.22121	0.84521	-3.07337
C	1.92000	-2.92708	-3.50634
H	2.10722	-2.99744	-1.37160
C	1.69477	-2.13654	-4.62886
H	1.24341	-0.15111	-5.33713
H	2.07117	-3.99818	-3.61612
H	1.68154	-2.58366	-5.61957
C	-1.79148	-1.33213	-1.38872
C	-1.65453	-2.45968	-0.56848
C	-1.69319	-1.49456	-2.77739
C	-1.44374	-3.71827	-1.12444
H	-1.71473	-2.35058	0.51211
C	-1.49836	-2.75518	-3.33013
H	-1.77142	-0.62687	-3.43015
C	-1.37331	-3.87186	-2.50610
H	-1.33868	-4.58056	-0.47046
H	-1.42799	-2.86304	-4.40952
H	-1.21141	-4.85463	-2.94126
C	-3.11948	1.21783	-1.67565
C	-4.17668	0.58419	-2.34169
C	-3.00596	2.61108	-1.75804
C	-5.09884	1.33069	-3.06909
H	-4.26888	-0.49893	-2.29371
C	-3.93173	3.35753	-2.48023
H	-2.17730	3.10217	-1.24802
C	-4.97888	2.71720	-3.13845
H	-5.91488	0.82875	-3.58205
H	-3.83200	4.43814	-2.53583
H	-5.69949	3.29732	-3.70866

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C	2.55948	-1.10730	1.04856
C	-1.79689	-3.05335	-0.16355
H	-2.54051	-2.68209	0.53900
C	0.50146	-3.21220	-0.88249
H	1.56168	-3.03340	-0.70891
C	-1.03440	-1.19135	3.48150
H	-0.26441	-1.82067	3.92367
C	-2.00632	-0.08830	1.58560
C	-3.01909	0.15469	3.76932
C	-2.19002	-3.86985	-1.20892
H	-3.23951	-4.12712	-1.33171
C	-3.01092	0.43702	2.40833

H	-3.78482	1.07142	1.97868	C	-5.67785	-1.00536	-0.89449
C	-1.23643	-4.35264	-2.11564	H	-4.20043	-1.26992	0.64091
C	0.10120	-4.02351	-1.95277	C	-5.10293	0.50901	-2.67060
H	0.84589	-4.40606	-2.64693	H	-3.17153	1.42680	-2.54855
C	1.91521	-2.73291	2.68579	C	-6.01445	-0.36509	-2.08269
H	1.16119	-3.35249	3.16984	H	-6.38223	-1.68492	-0.42175
C	-2.01535	-0.65131	4.30543	H	-5.35663	1.02184	-3.59478
H	-2.00360	-0.86349	5.37190	H	-6.98093	-0.54218	-2.54621
C	3.89924	-1.23886	1.42186	C	-1.59183	2.12285	-0.33161
H	4.66756	-0.65989	0.91215	C	-1.12967	2.59675	-1.56887
C	3.24742	-2.87042	3.06650	C	-1.84597	3.04814	0.68502
H	3.51529	-3.57571	3.84979	C	-0.99349	3.96018	-1.80658
C	4.24336	-2.12393	2.43712	H	-0.86080	1.87909	-2.34420
Ni	-0.02091	-0.79306	-0.88020	C	-1.67988	4.41178	0.45534
P	-1.82417	0.30811	-0.17912	H	-2.16197	2.70348	1.66594
P	1.92058	0.00697	-0.24168	C	-1.27571	4.87305	-0.79395
B	0.03991	-1.67302	1.14681	H	-0.64702	4.30770	-2.77658
H	-0.55807	-0.81390	-2.49097	H	-1.86931	5.11764	1.26016
H	0.26093	-0.75443	-2.55748	H	-1.15829	5.93909	-0.97053
C	1.87725	1.63854	0.59097	H	-1.54454	-4.99030	-2.94036
C	1.70436	1.73325	1.97723	H	-3.79271	0.56982	4.40979
C	1.90341	2.81549	-0.16836	H	5.28297	-2.23940	2.73240
C	1.57852	2.97847	2.58763	C	-0.44085	-2.69563	0.04854
H	1.66923	0.82823	2.58054	C	-1.01357	-0.95563	2.09506
C	1.78649	4.05694	0.44491	C	1.53514	-1.84620	1.66545
H	2.02316	2.75668	-1.24899				
C	1.62439	4.14235	1.82588	A-RC-CH₃			
H	1.44944	3.03649	3.66517	C	-2.59959	0.47912	1.17520
H	1.80745	4.95949	-0.16039	C	0.29510	2.44432	0.72490
H	1.52588	5.11340	2.30405	C	1.62333	2.93822	0.64910
C	3.31918	0.17379	-1.41778	H	2.39141	2.43376	1.23246
C	3.34219	-0.65818	-2.54295	C	-1.61081	1.03668	2.00075
C	4.39199	1.04822	-1.20220	C	0.99965	0.23248	2.18265
C	4.41048	-0.61738	-3.43393	C	-0.67290	3.15078	-0.03842
H	2.50788	-1.34041	-2.71028	H	-1.72200	2.87416	0.05702
C	5.45623	1.09478	-2.09739	C	1.04333	0.05992	3.57879
H	4.38556	1.70096	-0.33223	H	0.24951	0.48278	4.19176
C	5.46694	0.26325	-3.21484	C	2.03333	-0.38608	1.44927
H	4.41445	-1.26805	-4.30414	C	3.12823	-1.18673	3.47101
H	6.27957	1.78222	-1.92182	C	1.96070	4.04147	-0.11008
H	6.29727	0.30252	-3.91477	H	2.99303	4.38856	-0.13155
C	-3.51475	0.10082	-0.87883	C	3.08509	-1.05882	2.08407
C	-4.44061	-0.77632	-0.29767	H	3.88291	-1.49758	1.48362
C	-3.86607	0.73504	-2.07808	C	0.98974	4.71670	-0.87512

C	-0.32178	4.25623	-0.82443
H	-1.09047	4.77512	-1.39600
C	-2.03940	1.53400	3.24317
H	-1.32173	2.00851	3.91124
C	2.07560	-0.62457	4.20558
H	2.07502	-0.72474	5.29028
C	-3.94254	0.41926	1.55698
H	-4.68172	-0.01099	0.88055
C	-3.37335	1.47438	3.62843
H	-3.67363	1.88208	4.59299
C	-4.35111	0.91708	2.79330
Ni	-0.00666	0.87614	-0.72614
P	1.84923	-0.27868	-0.35435
P	-1.91873	-0.14510	-0.39289
B	-0.11147	1.12130	1.47629
H	0.53103	1.39310	-2.25498
H	-0.28054	1.29702	-2.35132
C	1.37147	5.89648	-1.71380
H	2.05979	5.61069	-2.51772
H	0.49828	6.36283	-2.17783
H	1.88626	6.66240	-1.12342
C	4.24714	-1.91169	4.15460
H	3.88152	-2.76586	4.73509
H	4.97976	-2.28908	3.43655
H	4.77785	-1.26119	4.85842
C	-5.78885	0.87705	3.21392
H	-6.21123	1.88431	3.30257
H	-6.40231	0.32677	2.49572
H	-5.91168	0.39972	4.19190
C	-1.83985	-1.95585	-0.13692
C	-1.68833	-2.49702	1.14563
C	-1.81450	-2.81738	-1.24126
C	-1.53301	-3.87029	1.31635
H	-1.69661	-1.84007	2.01325
C	-1.67039	-4.18838	-1.06640
H	-1.91374	-2.40764	-2.24541
C	-1.52922	-4.71930	0.21372
H	-1.42021	-4.27703	2.31792
H	-1.65579	-4.84255	-1.93436
H	-1.40857	-5.79106	0.34871
C	-3.29569	0.05647	-1.59056
C	-3.30942	1.21203	-2.38053
C	-4.35458	-0.85290	-1.70815
C	-4.35346	1.45578	-3.26721

H	-2.48538	1.92098	-2.29121
C	-5.39499	-0.61317	-2.60147
H	-4.35589	-1.75681	-1.10295
C	-5.39641	0.54009	-3.38263
H	-4.34870	2.35682	-3.87446
H	-6.20737	-1.33009	-2.68790
H	-6.20777	0.72288	-4.08206
C	3.51852	0.21956	-0.95590
C	4.37572	0.97880	-0.14731
C	3.91919	-0.04948	-2.27186
C	5.59033	1.44997	-0.63762
H	4.10180	1.18646	0.88347
C	5.13474	0.41726	-2.75935
H	3.28316	-0.64572	-2.92090
C	5.97549	1.17301	-1.94563
H	6.23980	2.03174	0.01139
H	5.42694	0.18533	-3.78022
H	6.92430	1.53916	-2.32757
C	1.71707	-1.99437	-0.99696
C	1.34145	-2.14930	-2.34085
C	1.94352	-3.14348	-0.23327
C	1.27415	-3.40973	-2.92386
H	1.08731	-1.26736	-2.92814
C	1.84432	-4.40711	-0.81042
H	2.18494	-3.05386	0.82251
C	1.53448	-4.54443	-2.15973
H	0.99693	-3.50586	-3.97072
H	2.01279	-5.28946	-0.19795
H	1.46806	-5.53237	-2.60797

A-RC-OCH₃

C	-2.70336	0.39141	0.83402
C	0.32123	2.24814	0.98337
C	1.69105	2.59717	1.03599
H	2.38432	1.88721	1.48325
C	-1.77655	0.78738	1.81782
C	0.73757	-0.26834	2.01003
C	-0.53966	3.21504	0.39253
H	-1.60942	3.01326	0.36667
C	0.60404	-0.74161	3.32427
H	-0.22412	-0.38033	3.93271
C	1.79708	-0.82549	1.25460
C	2.55841	-2.14030	3.13882
C	2.18387	3.80655	0.57313

H	3.24586	4.01855	0.64561
C	2.70892	-1.71947	1.81576
H	3.54862	-2.10748	1.24379
C	1.29728	4.73002	-0.00273
C	-0.06343	4.42991	-0.09002
H	-0.72859	5.16368	-0.53535
C	-2.30407	1.13966	3.06512
H	-1.63628	1.47668	3.85772
C	1.48396	-1.65978	3.89192
H	1.33251	-1.98690	4.91580
C	-4.07362	0.35795	1.06520
H	-4.77983	0.06374	0.29227
C	-3.67512	1.11565	3.32523
H	-4.04114	1.41921	4.30095
C	-4.56486	0.72577	2.32055
Ni	0.04584	0.98830	-0.76006
P	1.81445	-0.33123	-0.49840
P	-1.86432	-0.07259	-0.71737
B	-0.23391	0.84709	1.43090
H	0.69896	1.78914	-2.10584
H	-0.11730	1.88320	-2.19000
O	1.67262	5.94180	-0.49545
O	-5.92065	0.67644	2.46579
O	3.49094	-3.02472	3.59292
C	3.04371	6.26978	-0.42105
H	3.14383	7.26229	-0.86081
H	3.39946	6.29747	0.61715
H	3.66330	5.56009	-0.98463
C	-6.44236	1.04953	3.72095
H	-6.19919	2.09087	3.97190
H	-7.52476	0.94375	3.64593
H	-6.07229	0.40126	4.52692
C	3.34178	-3.48378	4.91856
H	2.39155	-4.01566	5.06097
H	4.16754	-4.17227	5.09846
H	3.39359	-2.66087	5.64387
C	3.54751	0.19587	-0.82555
C	4.41311	0.59550	0.20070
C	3.98453	0.33036	-2.15094
C	5.67336	1.11214	-0.09042
H	4.10516	0.49148	1.23825
C	5.24399	0.84038	-2.44057
H	3.33248	0.02516	-2.96714
C	6.09429	1.23780	-1.41027

H	6.32986	1.41043	0.72317
H	5.56333	0.92710	-3.47591
H	7.07851	1.63916	-1.63595
C	1.70329	-1.84738	-1.53241
C	1.29711	-1.65816	-2.86246
C	2.00655	-3.14334	-1.10621
C	1.25266	-2.72342	-3.75545
H	0.99570	-0.66174	-3.18662
C	1.93861	-4.21333	-1.99470
H	2.27915	-3.32600	-0.07108
C	1.58014	-4.00602	-3.32364
H	0.94546	-2.55314	-4.78425
H	2.16644	-5.21644	-1.64243
H	1.53728	-4.84375	-4.01485
C	-1.70266	-1.89463	-0.56017
C	-1.52853	-2.48116	0.69916
C	-1.63771	-2.71197	-1.69663
C	-1.30454	-3.84972	0.81856
H	-1.57435	-1.86423	1.59320
C	-1.43149	-4.08154	-1.57340
H	-1.75358	-2.27236	-2.68544
C	-1.26443	-4.65577	-0.31526
H	-1.17195	-4.28635	1.80536
H	-1.38915	-4.69975	-2.46642
H	-1.09637	-5.72567	-0.22188
C	-3.15034	0.11717	-2.01131
C	-4.18557	-0.81187	-2.18214
C	-3.13466	1.26297	-2.81279
C	-5.17542	-0.59900	-3.13640
H	-4.20726	-1.70893	-1.56739
C	-4.12641	1.47803	-3.76598
H	-2.33231	1.98845	-2.67812
C	-5.14678	0.54517	-3.93084
H	-5.97141	-1.32848	-3.26015
H	-4.09952	2.37207	-4.38289
H	-5.91810	0.70777	-4.67870

A-RC-NH₂

C	-2.60386	0.46607	1.15404
C	0.22389	2.47804	0.65488
C	1.54605	2.95968	0.47742
H	2.35273	2.43431	0.98448
C	-1.62760	1.05046	1.97776
C	1.00116	0.31118	2.16307

C	-0.78607	3.21323	-0.02373
H	-1.82510	2.91630	0.11293
C	1.05395	0.17394	3.56310
H	0.25975	0.60764	4.16823
C	2.04045	-0.32411	1.44979
C	3.14190	-1.05838	3.48819
C	1.84528	4.07823	-0.27572
H	2.87753	4.40806	-0.38321
C	3.09691	-0.97588	2.09281
H	3.89175	-1.43406	1.50373
C	0.81914	4.78477	-0.93335
C	-0.50034	4.33704	-0.79403
H	-1.30273	4.87307	-1.29821
C	-2.08215	1.54871	3.20989
H	-1.38317	2.04388	3.88311
C	2.08760	-0.48226	4.21405
H	2.08988	-0.55553	5.30053
C	-3.94717	0.37662	1.51687
H	-4.67080	-0.07462	0.83765
C	-3.41552	1.46952	3.59149
H	-3.73529	1.88647	4.54527
C	-4.37316	0.88200	2.74987
Ni	-0.00756	0.85918	-0.74444
P	1.85904	-0.26787	-0.35901
P	-1.89553	-0.18108	-0.39433
B	-0.13131	1.16489	1.44787
H	0.51685	1.36811	-2.28156
H	-0.30305	1.43202	-2.31626
N	1.12197	5.86636	-1.74567
N	-5.72092	0.86820	3.10553
N	4.15454	-1.76256	4.13412
H	0.36676	6.51553	-1.90037
H	1.99030	6.33353	-1.53712
H	-5.88905	0.87583	4.09984
H	-6.26193	0.14880	2.65073
H	4.32260	-1.47506	5.08598
H	5.01582	-1.82787	3.61345
C	3.53054	0.23191	-0.96195
C	4.37644	1.02085	-0.16916
C	3.94266	-0.06377	-2.26868
C	5.58715	1.49583	-0.66541
H	4.09576	1.24882	0.85586
C	5.15493	0.40569	-2.76223
H	3.31667	-0.68246	-2.90629

C	5.98280	1.19181	-1.96439
H	6.22624	2.10159	-0.02782
H	5.45418	0.15273	-3.77616
H	6.92866	1.56063	-2.35130
C	1.75720	-2.00217	-0.95874
C	1.39037	-2.18905	-2.30103
C	1.99062	-3.13280	-0.16983
C	1.33974	-3.46151	-2.85872
H	1.12862	-1.32173	-2.90645
C	1.90733	-4.40907	-0.72184
H	2.22205	-3.01845	0.88587
C	1.60752	-4.57755	-2.06990
H	1.06947	-3.58227	-3.90496
H	2.07970	-5.27685	-0.08976
H	1.55366	-5.57534	-2.49788
C	-1.78837	-1.98314	-0.07804
C	-1.63017	-2.47590	1.22351
C	-1.73992	-2.88463	-1.14964
C	-1.45125	-3.83890	1.44501
H	-1.64658	-1.78785	2.06649
C	-1.57324	-4.24577	-0.92419
H	-1.83871	-2.51426	-2.16899
C	-1.42983	-4.72810	0.37479
H	-1.33142	-4.20575	2.46127
H	-1.54033	-4.93015	-1.76828
H	-1.28979	-5.79193	0.54919
C	-3.27173	-0.03800	-1.60372
C	-4.29418	-0.98538	-1.74212
C	-3.31944	1.12085	-2.38810
C	-5.32914	-0.78051	-2.65110
H	-4.27155	-1.89202	-1.14143
C	-4.35759	1.32993	-3.28963
H	-2.52535	1.86066	-2.28096
C	-5.36278	0.37559	-3.42709
H	-6.11175	-1.52786	-2.75416
H	-4.37760	2.23414	-3.89205
H	-6.16904	0.53042	-4.13912

A-RC-CN

C	-2.63208	0.16483	1.11396
C	0.30991	2.14503	1.24006
C	1.64854	2.61453	1.31575
H	2.39427	1.97623	1.78560
C	-1.66801	0.52336	2.07342

C	0.89755	-0.39177	2.11493	H	5.38807	1.57596	-3.41497
C	-0.63560	3.01582	0.62545	H	6.91558	2.24734	-1.57233
H	-1.68927	2.74510	0.63789	C	1.78389	-1.65994	-1.54659
C	0.83620	-0.94590	3.40699	C	1.40657	-1.40415	-2.87398
H	0.01239	-0.67607	4.06381	C	2.06089	-2.97813	-1.17178
C	1.95737	-0.82454	1.28428	C	1.37134	-2.42685	-3.81538
C	2.87532	-2.19330	3.05881	H	1.12305	-0.39300	-3.16482
C	2.02941	3.84414	0.82283	C	1.99906	-4.00542	-2.10992
H	3.06040	4.17745	0.89550	H	2.31075	-3.21304	-0.14124
C	2.94942	-1.68486	1.75553	C	1.67468	-3.73158	-3.43539
H	3.78343	-1.97100	1.11832	H	1.09099	-2.20573	-4.84172
C	1.07281	4.67493	0.19629	H	2.20856	-5.02552	-1.79949
C	-0.25619	4.25563	0.10356	H	1.63900	-4.53545	-4.16565
H	-0.99135	4.90525	-0.36298	C	-3.25126	0.34281	-1.69733
C	-2.11737	0.74920	3.38524	C	-4.28965	-0.53975	-2.02328
H	-1.41159	1.06422	4.15186	C	-3.27746	1.64258	-2.21600
C	1.79544	-1.82733	3.87868	C	-5.33029	-0.12527	-2.84910
H	1.72765	-2.23658	4.88229	H	-4.27772	-1.55559	-1.63358
C	-3.98071	0.03261	1.43317	C	-4.32103	2.05673	-3.03760
H	-4.71187	-0.23389	0.67302	H	-2.46791	2.32925	-1.96636
C	-3.45648	0.62097	3.72617	C	-5.34830	1.17206	-3.35573
H	-3.79080	0.81288	4.74149	H	-6.13050	-0.81752	-3.09573
C	-4.39975	0.25881	2.75056	H	-4.32972	3.06856	-3.43298
Ni	0.00684	1.00747	-0.54888	H	-6.16200	1.49222	-4.00022
P	1.87169	-0.20991	-0.42705	C	-1.77772	-1.91153	-0.67259
P	-1.90479	-0.09341	-0.53774	C	-1.70637	-2.72385	0.46517
B	-0.15134	0.69081	1.62000	C	-1.64568	-2.50092	-1.93687
H	0.57823	1.85007	-1.91239	C	-1.52139	-4.09830	0.33817
H	-0.22773	1.76397	-2.05166	H	-1.80148	-2.28183	1.45454
C	1.46197	5.93803	-0.33509	C	-1.46828	-3.87359	-2.05968
C	-5.77796	0.13119	3.09495	H	-1.68822	-1.87928	-2.82941
C	3.87740	-3.08693	3.53750	C	-1.40682	-4.67639	-0.92236
N	1.78189	6.97320	-0.77533	H	-1.47649	-4.71815	1.22921
N	-6.90743	0.02235	3.37534	H	-1.36580	-4.31565	-3.04706
N	4.70131	-3.81909	3.92673	H	-1.26628	-5.74937	-1.01999
C	3.54063	0.47365	-0.77311				
C	4.41154	0.85390	0.25573	A-RC-NO₂			
C	3.91203	0.74846	-2.09653	C	-2.66113	-0.12112	0.91333
C	5.61912	1.48513	-0.03174	C	0.21264	1.89914	1.33918
H	4.15309	0.64884	1.29137	C	1.53130	2.39182	1.53320
C	5.11788	1.37674	-2.38180	H	2.27983	1.71551	1.93975
H	3.25674	0.46151	-2.91579	C	-1.71397	0.11965	1.92692
C	5.97534	1.75147	-1.34947	C	0.90185	-0.68766	1.89517
H	6.28228	1.76641	0.78171	C	-0.74545	2.82037	0.82344

H	-1.79150	2.52659	0.76886
C	0.86966	-1.39659	3.11196
H	0.02489	-1.26509	3.78417
C	1.99561	-0.93987	1.03379
C	2.97591	-2.42451	2.63663
C	1.88727	3.69121	1.23879
H	2.89349	4.06260	1.39488
C	3.04532	-1.77792	1.41037
H	3.90783	-1.94445	0.77139
C	0.91437	4.54609	0.70512
C	-0.39079	4.13185	0.49367
H	-1.11226	4.83833	0.09898
C	-2.17727	0.15557	3.25342
H	-1.48445	0.37484	4.06351
C	1.89015	-2.25582	3.49126
H	1.87253	-2.79558	4.43157
C	-4.01146	-0.31631	1.19274
H	-4.74861	-0.49053	0.41422
C	-3.51836	-0.03746	3.55787
H	-3.88974	0.00465	4.57548
C	-4.41625	-0.27410	2.52046
Ni	-0.02519	0.99848	-0.58869
P	1.88446	-0.14507	-0.59728
P	-1.90652	-0.14496	-0.74608
B	-0.20093	0.39101	1.51828
H	0.52889	2.01236	-1.84202
H	-0.27286	1.92260	-1.99660
N	-5.83473	-0.47936	2.83770
O	-6.16383	-0.43283	4.02177
O	-6.60219	-0.68863	1.89982
N	1.28041	5.92219	0.37562
O	2.43053	6.28171	0.63111
O	0.41869	6.63797	-0.13780
N	4.06403	-3.32565	3.02864
O	3.98988	-3.85803	4.13472
O	4.97989	-3.49060	2.22369
C	3.52256	0.64012	-0.85902
C	4.35421	0.98395	0.21474
C	3.90755	1.02478	-2.15083
C	5.53540	1.68914	0.00125
H	4.08917	0.68775	1.22626
C	5.08792	1.72615	-2.36193
H	3.28517	0.76515	-3.00385
C	5.90485	2.06555	-1.28549

H	6.16800	1.94128	0.84759
H	5.37069	2.00878	-3.37200
H	6.82490	2.61846	-1.45059
C	1.85826	-1.47574	-1.85737
C	1.48172	-1.11018	-3.15879
C	2.18125	-2.81233	-1.60343
C	1.49503	-2.04043	-4.19218
H	1.16058	-0.08772	-3.35547
C	2.16740	-3.74805	-2.63427
H	2.43342	-3.13351	-0.59683
C	1.84483	-3.36290	-3.93194
H	1.21447	-1.73519	-5.19670
H	2.41333	-4.78402	-2.41773
H	1.84695	-4.09514	-4.73482
C	-1.70324	-1.92727	-1.09805
C	-1.53772	-2.85208	-0.06005
C	-1.58975	-2.36796	-2.42312
C	-1.27489	-4.18932	-0.34353
H	-1.61808	-2.52787	0.97549
C	-1.33604	-3.70568	-2.70179
H	-1.70791	-1.65759	-3.23966
C	-1.17763	-4.62020	-1.66320
H	-1.15418	-4.89711	0.47191
H	-1.25226	-4.03218	-3.73495
H	-0.97311	-5.66434	-1.88323
C	-3.24190	0.39398	-1.87212
C	-4.24297	-0.46816	-2.33873
C	-3.28938	1.74712	-2.22807
C	-5.26431	0.01788	-3.14930
H	-4.21462	-1.52231	-2.07174
C	-4.31483	2.23248	-3.03232
H	-2.51020	2.41852	-1.86653
C	-5.30142	1.36638	-3.49712
H	-6.03421	-0.65883	-3.50900
H	-4.33965	3.28424	-3.30204
H	-6.09912	1.74130	-4.13213

A-RC-CI

C	-2.63369	0.12816	1.02245
C	0.27864	2.14971	1.15473
C	1.61438	2.62174	1.22133
H	2.36975	1.97454	1.66345
C	-1.68322	0.50753	1.98427
C	0.89321	-0.37800	2.04563

C	-0.67115	3.02942	0.56779
H	-1.72196	2.74588	0.56714
C	0.83524	-0.91621	3.34330
H	0.00800	-0.64576	3.99637
C	1.95944	-0.81440	1.22862
C	2.86889	-2.14421	3.01360
C	1.98731	3.87178	0.76372
H	3.01582	4.21202	0.83125
C	2.95854	-1.66742	1.71246
H	3.79580	-1.96157	1.08448
C	1.01241	4.69690	0.18907
C	-0.30846	4.29245	0.08358
H	-1.04675	4.95583	-0.35538
C	-2.15234	0.73725	3.28692
H	-1.46192	1.06747	4.06180
C	1.80024	-1.78688	3.83293
H	1.73651	-2.18531	4.84053
C	-3.98852	-0.02184	1.32616
H	-4.71000	-0.30639	0.56434
C	-3.49670	0.59584	3.61712
H	-3.84974	0.79275	4.62459
C	-4.40343	0.21437	2.63021
Ni	0.00822	0.98004	-0.63433
P	1.87766	-0.22562	-0.49220
P	-1.88165	-0.13877	-0.61663
B	-0.16601	0.69039	1.53942
H	0.57793	1.85059	-1.97789
H	-0.23324	1.78802	-2.10682
Cl	1.47765	6.27561	-0.39105
Cl	-6.09325	0.04618	3.03767
Cl	4.09727	-3.22458	3.62210
C	3.55253	0.45023	-0.83987
C	4.41546	0.85041	0.18835
C	3.93844	0.69803	-2.16452
C	5.62689	1.47375	-0.10038
H	4.14711	0.66441	1.22512
C	5.14867	1.31724	-2.45165
H	3.29016	0.39618	-2.98394
C	5.99762	1.71149	-1.41961
H	6.28273	1.77028	0.71385
H	5.42907	1.49370	-3.48655
H	6.94188	2.19960	-1.64361
C	1.81548	-1.69700	-1.58911
C	1.45378	-1.46709	-2.92566

C	2.09133	-3.00782	-1.18844
C	1.43468	-2.50592	-3.84960
H	1.16798	-0.46228	-3.23596
C	2.04535	-4.05160	-2.10919
H	2.32674	-3.22337	-0.15031
C	1.73801	-3.80287	-3.44354
H	1.16532	-2.30381	-4.88298
H	2.25232	-5.06582	-1.77760
H	1.71388	-4.61989	-4.15979
C	-3.23330	0.24453	-1.79356
C	-4.25699	-0.66437	-2.09186
C	-3.28426	1.52720	-2.35077
C	-5.30664	-0.29405	-2.92713
H	-4.22673	-1.66728	-1.67113
C	-4.33627	1.89794	-3.18302
H	-2.48730	2.23513	-2.12112
C	-5.34855	0.98681	-3.47282
H	-6.09477	-1.00793	-3.15062
H	-4.36337	2.89742	-3.60838
H	-6.16887	1.27355	-4.12495
C	-1.73305	-1.95932	-0.72744
C	-1.65645	-2.75757	0.41980
C	-1.59564	-2.56400	-1.98390
C	-1.46388	-4.13260	0.30921
H	-1.75249	-2.30306	1.40346
C	-1.41175	-3.93703	-2.09078
H	-1.63994	-1.95327	-2.88392
C	-1.34753	-4.72607	-0.94398
H	-1.41404	-4.74097	1.20810
H	-1.30553	-4.39001	-3.07296
H	-1.20137	-5.79960	-1.02867

A-TS-H

C	2.30463	-1.80615	0.12484
C	-1.64727	-2.63275	0.29868
C	-2.72231	-2.44229	1.18211
H	-2.67701	-1.62423	1.90048
C	1.07649	-2.44411	0.45057
C	-0.45835	-0.36934	1.26112
C	-1.75771	-3.70437	-0.60680
H	-0.94320	-3.88456	-1.30958
C	0.21134	-0.42548	2.51099
H	0.79730	-1.31547	2.73348
C	-1.18468	0.84759	0.98928

C	-0.61975	1.72679	3.18767	H	3.82828	3.05914	4.10871
C	-3.84089	-3.27099	1.16955	C	-3.43161	0.23043	-0.78529
H	-4.65504	-3.09181	1.86876	C	-4.45444	0.45723	0.14530
C	-1.22642	1.87703	1.95461	C	-3.58978	-0.77257	-1.74596
H	-1.77263	2.79102	1.73446	C	-5.62508	-0.29114	0.09603
C	-3.92077	-4.32355	0.26243	H	-4.32276	1.21319	0.91773
C	-2.87109	-4.53775	-0.63002	C	-4.75852	-1.52628	-1.78811
H	-2.92289	-5.35633	-1.34476	H	-2.77594	-0.97786	-2.43883
C	1.16194	-3.78086	0.87448	C	-5.77709	-1.28250	-0.87162
H	0.24104	-4.30096	1.13228	H	-6.41257	-0.11343	0.82360
C	0.11171	0.56825	3.46572	H	-4.86499	-2.31791	-2.52428
H	0.61293	0.45462	4.42367	H	-6.68495	-1.87937	-0.89830
C	3.51865	-2.50009	0.19803	C	-2.25743	2.91030	-0.76489
H	4.44037	-2.00165	-0.09964	C	-1.16319	3.78827	-0.73833
C	2.37226	-4.46177	0.97054	C	-3.54218	3.44078	-0.92161
H	2.38718	-5.49613	1.30578	C	-1.34889	5.16085	-0.82160
C	3.55908	-3.82374	0.62399	H	-0.15844	3.36948	-0.66681
Ni	0.09479	0.12660	-0.82086	C	-3.72494	4.81890	-1.02677
P	-1.85336	1.13289	-0.71120	H	-4.40286	2.77938	-0.97035
P	2.26404	-0.05134	-0.42533	C	-2.63492	5.68094	-0.96829
B	-0.35309	-1.70639	0.34991	H	-0.49010	5.82576	-0.79164
H	-0.34006	-1.37583	-1.11407	H	-4.72760	5.21809	-1.15411
H	0.09993	-0.69680	-2.04384	H	-2.78296	6.75413	-1.05021
C	3.67392	0.08001	-1.58025	H	-0.70681	2.51330	3.93353
C	4.64554	1.07882	-1.45405	H	4.50813	-4.35100	0.67732
C	3.74166	-0.79642	-2.67301	H	-4.79381	-4.97163	0.24844
C	5.66525	1.19444	-2.39533				
H	4.60917	1.76570	-0.61188	A-TS-CH₃			
C	4.76447	-0.68233	-3.60661	C	2.29492	-1.67507	0.11059
H	2.99175	-1.57810	-2.78104	C	-1.65829	-2.45078	0.38395
C	5.72977	0.31472	-3.47106	C	-2.73719	-2.20429	1.24530
H	6.41513	1.97264	-2.28134	H	-2.68504	-1.35622	1.92800
H	4.80847	-1.37340	-4.44416	C	1.06683	-2.27926	0.48821
H	6.52749	0.40450	-4.20315	C	-0.41598	-0.14150	1.19203
C	2.81611	0.91497	1.03023	C	-1.78570	-3.56092	-0.47207
C	3.80622	0.46617	1.91212	H	-0.96887	-3.79328	-1.15672
C	2.19704	2.14351	1.27499	C	0.30921	-0.11279	2.41282
C	4.16733	1.23558	3.01332	H	0.86927	-1.00443	2.68933
H	4.28390	-0.49644	1.74361	C	-1.10550	1.08010	0.85342
C	2.56104	2.91639	2.37408	C	-0.36680	2.15179	2.92939
H	1.39883	2.46732	0.60759	C	-3.87652	-3.00419	1.24497
C	3.54678	2.46253	3.24518	H	-4.70241	-2.77041	1.91661
H	4.93257	0.87514	3.69572	C	-1.03782	2.19441	1.71749
H	2.05986	3.86352	2.55763	H	-1.55111	3.11267	1.43837

C	-3.99579	-4.08900	0.37557	H	-4.28720	1.42877	0.83828
C	-2.92103	-4.35956	-0.48078	C	-4.76669	-1.43309	-1.73148
H	-2.98688	-5.20228	-1.16863	H	-2.78906	-0.92538	-2.42776
C	1.15550	-3.59333	0.97769	C	-5.77393	-1.14120	-0.81679
H	0.23712	-4.09442	1.27939	H	-6.38424	0.10809	0.82937
C	0.31085	0.96796	3.26778	H	-4.88431	-2.25850	-2.42868
H	0.86090	0.91683	4.20639	H	-6.68420	-1.73562	-0.80346
C	3.50220	-2.37801	0.19481	C	-2.22964	3.03161	-1.00101
H	4.42429	-1.90391	-0.14543	C	-1.12976	3.89987	-1.07623
C	2.36114	-4.27570	1.08697	C	-3.51586	3.56114	-1.14777
H	2.37283	-5.29344	1.47550	C	-1.31008	5.26477	-1.24939
C	3.56204	-3.68214	0.68789	H	-0.12624	3.47816	-1.00502
Ni	0.09378	0.21303	-0.92007	C	-3.69411	4.93005	-1.34232
P	-1.83521	1.25790	-0.83619	H	-4.38188	2.90553	-1.11918
P	2.25839	0.04723	-0.54320	C	-2.59750	5.78464	-1.38484
B	-0.35789	-1.53726	0.37454	H	-0.44676	5.92293	-1.29572
H	-0.37897	-1.28999	-1.10823	H	-4.69845	5.32810	-1.46005
H	0.07330	-0.67549	-2.09711	H	-2.74220	6.85079	-1.53596
C	3.60537	0.07792	-1.77814	C	4.86213	-4.42110	0.77810
C	4.91956	0.45631	-1.48148	H	5.08734	-4.71871	1.80821
C	3.28935	-0.30968	-3.08663	H	4.84567	-5.34190	0.18502
C	5.89878	0.43438	-2.47179	H	5.69688	-3.81300	0.41932
H	5.17641	0.77137	-0.47226	C	-5.24491	-4.91474	0.32848
C	4.27019	-0.33937	-4.07120	H	-5.74274	-4.83216	-0.64597
H	2.26143	-0.57848	-3.32515	H	-5.04183	-5.98018	0.48327
C	5.57772	0.03346	-3.76543	H	-5.96456	-4.59922	1.08942
H	6.91580	0.73195	-2.23020	C	-0.35101	3.32833	3.85349
H	4.01192	-0.64342	-5.08196	H	-0.90388	3.12268	4.77709
H	6.34299	0.01846	-4.53683	H	0.67325	3.57955	4.15150
C	2.88294	1.08473	0.83283	H	-0.79575	4.21343	3.39090
C	3.75544	0.61097	1.81973				
C	2.41911	2.40187	0.91810	A-TS-Cl			
C	4.16149	1.44137	2.86031	C	2.30034	-1.56786	0.05902
H	4.10084	-0.42006	1.78237	C	-1.64799	-2.28956	0.40012
C	2.82824	3.23381	1.95599	C	-2.73801	-1.99730	1.23387
H	1.70951	2.76044	0.17323	H	-2.70023	-1.11218	1.86772
C	3.69987	2.75436	2.93027	C	1.07062	-2.13110	0.49411
H	4.83634	1.06019	3.62229	C	-0.39213	0.05462	1.09877
H	2.45127	4.25227	2.01184	C	-1.75709	-3.44335	-0.39643
H	4.01351	3.39937	3.74715	H	-0.93127	-3.70985	-1.05621
C	-3.41986	0.36292	-0.82659	C	0.34971	0.14301	2.30514
C	-4.43115	0.63791	0.10376	H	0.91723	-0.73054	2.62007
C	-3.59484	-0.68341	-1.73742	C	-1.08172	1.25831	0.69781
C	-5.60595	-0.10667	0.10172	C	-0.32154	2.40095	2.69068

C	-3.87991	-2.79231	1.26950
H	-4.71879	-2.53983	1.91091
C	-1.01343	2.41994	1.49662
H	-1.52394	3.32742	1.18909
C	-3.94545	-3.91084	0.44789
C	-2.88614	-4.25322	-0.38731
H	-2.95466	-5.13262	-1.02003
C	1.14098	-3.41371	1.06163
H	0.22099	-3.87969	1.40965
C	0.37192	1.26335	3.11113
H	0.93181	1.27827	4.04070
C	3.50120	-2.27787	0.15854
H	4.43041	-1.85541	-0.21775
C	2.33138	-4.12060	1.19709
H	2.35054	-5.10993	1.64352
C	3.50708	-3.54375	0.73280
Ni	0.11242	0.29931	-1.03318
P	-1.81629	1.35530	-0.99887
P	2.28194	0.12625	-0.67338
B	-0.34561	-1.37843	0.34976
H	-0.37558	-1.20693	-1.14289
H	0.06642	-0.66000	-2.15345
C	3.62326	0.08702	-1.91029
C	4.94873	0.42925	-1.61901
C	3.29361	-0.32243	-3.20844
C	5.92732	0.34793	-2.60653
H	5.21409	0.76160	-0.61740
C	4.27427	-0.41021	-4.18991
H	2.25756	-0.56296	-3.44156
C	5.59315	-0.07507	-3.88994
H	6.95358	0.61570	-2.37088
H	4.00749	-0.73114	-5.19307
H	6.35847	-0.13808	-4.65847
C	2.90767	1.20344	0.66845
C	3.74519	0.75166	1.69484
C	2.46336	2.53050	0.69238
C	4.12725	1.61079	2.72158
H	4.08008	-0.28323	1.70398
C	2.84833	3.38965	1.71658
H	1.78326	2.87386	-0.08653
C	3.67714	2.92927	2.73621
H	4.77178	1.24597	3.51694
H	2.47953	4.41171	1.73191
H	3.96334	3.59425	3.54659

C	-3.39856	0.46126	-0.94135
C	-4.40059	0.76785	-0.01017
C	-3.58714	-0.60828	-1.82235
C	-5.58081	0.03216	0.01498
H	-4.24711	1.57804	0.70109
C	-4.76394	-1.34967	-1.78721
H	-2.79059	-0.87146	-2.51572
C	-5.76337	-1.02515	-0.87468
H	-6.35297	0.27315	0.74080
H	-4.89456	-2.19240	-2.46057
H	-6.67698	-1.61253	-0.84053
C	-2.20744	3.11873	-1.24314
C	-1.10789	3.97795	-1.39039
C	-3.49734	3.64401	-1.37296
C	-1.29178	5.33474	-1.61705
H	-0.10293	3.55805	-1.33276
C	-3.67877	5.00331	-1.62090
H	-4.36291	2.99249	-1.28982
C	-2.58192	5.85131	-1.73423
H	-0.42973	5.98813	-1.71828
H	-4.68531	5.39927	-1.72420
H	-2.72969	6.91039	-1.92571
Cl	5.01316	-4.41849	0.86564
Cl	-5.39812	-4.88651	0.43933
Cl	-0.29686	3.83068	3.69162

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C	2.27173	-1.64070	0.10485
C	-1.68376	-2.34100	0.44094
C	-2.76061	-2.05124	1.29527
H	-2.69894	-1.18336	1.94995
C	1.03834	-2.20784	0.53325
C	-0.39978	-0.01945	1.16326
C	-1.81269	-3.47549	-0.38315
H	-0.99451	-3.73548	-1.05441
C	0.35564	0.05609	2.36314
H	0.89616	-0.83261	2.68220
C	-1.06640	1.19723	0.75369
C	-0.22878	2.35925	2.72779
C	-3.91062	-2.82701	1.31690
H	-4.73857	-2.57340	1.97307
C	-0.94424	2.36312	1.53471
H	-1.42667	3.28218	1.21389
C	-4.02191	-3.93488	0.46509

C	-2.95289	-4.26221	-0.38439
H	-3.03691	-5.12204	-1.04273
C	1.09645	-3.50119	1.08078
H	0.17210	-3.96338	1.42082
C	0.42512	1.18518	3.14821
H	1.00072	1.19094	4.06877
C	3.46164	-2.36167	0.19600
H	4.39257	-1.93549	-0.17333
C	2.27997	-4.21441	1.20423
H	2.28693	-5.21056	1.63693
C	3.47899	-3.64894	0.75139
Ni	0.09420	0.24415	-0.97220
P	-1.83566	1.29836	-0.93049
P	2.26552	0.05710	-0.62375
B	-0.37248	-1.44330	0.40477
H	-0.39654	-1.26608	-1.09934
H	0.03251	-0.74704	-2.06917
C	3.59364	0.00424	-1.87181
C	4.92497	0.32923	-1.58689
C	3.25027	-0.40100	-3.16760
C	5.89666	0.23367	-2.57961
H	5.20009	0.65875	-0.58702
C	4.22449	-0.50255	-4.15422
H	2.20991	-0.62772	-3.39555
C	5.54930	-0.18567	-3.86084
H	6.92767	0.48688	-2.34974
H	3.94826	-0.82020	-5.15571
H	6.30966	-0.26047	-4.63296
C	2.90683	1.13305	0.70978
C	3.72166	0.67267	1.75062
C	2.50430	2.47416	0.70683
C	4.11926	1.53617	2.76776
H	4.02876	-0.37037	1.77860
C	2.90572	3.33775	1.72150
H	1.84418	2.82668	-0.08516
C	3.70831	2.86764	2.75783
H	4.74534	1.16506	3.57469
H	2.56942	4.37102	1.71959
H	4.00386	3.53650	3.56127
C	-3.42738	0.42727	-0.84082
C	-4.39918	0.74072	0.11999
C	-3.66214	-0.62196	-1.73580
C	-5.59485	0.03129	0.16250
H	-4.21126	1.53593	0.83967

C	-4.85575	-1.33505	-1.68507
H	-2.89203	-0.88939	-2.45703
C	-5.82412	-1.00536	-0.74084
H	-6.34358	0.27758	0.91051
H	-5.02490	-2.15903	-2.37270
H	-6.74937	-1.57349	-0.69403
C	-2.19348	3.06593	-1.17858
C	-1.08041	3.89229	-1.39567
C	-3.47473	3.62441	-1.23609
C	-1.24071	5.25279	-1.61924
H	-0.08573	3.44434	-1.39664
C	-3.63281	4.98679	-1.48125
H	-4.35137	2.99724	-1.09867
C	-2.52118	5.80324	-1.66368
H	-0.36924	5.88202	-1.77615
H	-4.63225	5.41012	-1.52831
H	-2.65098	6.86508	-1.85190
C	4.70645	-4.36743	0.85075
C	-5.23207	-4.68563	0.42914
C	-0.10988	3.55501	3.49608
N	0.01949	4.53732	4.11637
N	5.71615	-4.95025	0.93649
N	-6.23916	-5.27892	0.38739

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C	2.37751	-1.59334	0.08645
C	-1.54893	-2.48729	0.39696
C	-2.64285	-2.25108	1.24609
H	-2.61727	-1.38792	1.91112
C	1.16813	-2.23432	0.46632
C	-0.38140	-0.13581	1.17470
C	-1.65402	-3.61676	-0.43511
H	-0.83112	-3.84724	-1.11294
C	0.34091	-0.08832	2.39764
H	0.96697	-0.94277	2.64847
C	-1.16154	1.04342	0.88484
C	-0.51762	2.08514	2.99824
C	-3.76359	-3.07035	1.26594
H	-4.59973	-2.83912	1.92521
C	-1.19856	2.12255	1.78237
H	-1.78049	3.00781	1.53439
C	-3.85064	-4.17598	0.41174
C	-2.76872	-4.44366	-0.43857
H	-2.81784	-5.29915	-1.11133

C	1.30724	-3.55229	0.93388
H	0.40892	-4.08746	1.23754
C	0.26078	0.95049	3.29640
H	0.81932	0.91510	4.23013
C	3.60711	-2.25138	0.14403
H	4.51170	-1.74486	-0.19521
C	2.52814	-4.20802	1.01845
H	2.57654	-5.23054	1.39019
C	3.70525	-3.56776	0.61348
Ni	0.11380	0.22022	-0.93432
P	-1.84371	1.22140	-0.82175
P	2.28073	0.13484	-0.55012
B	-0.27745	-1.53740	0.36246
H	-0.32518	-1.28153	-1.12180
H	0.10866	-0.60851	-2.15557
C	3.64456	0.22300	-1.76565
C	4.93365	0.67052	-1.45578
C	3.36744	-0.19114	-3.07511
C	5.92655	0.69057	-2.43284
H	5.16020	1.00711	-0.44631
C	4.36196	-0.17890	-4.04618
H	2.35743	-0.51327	-3.32453
C	5.64478	0.26274	-3.72691
H	6.92347	1.04304	-2.18035
H	4.13322	-0.50389	-5.05774
H	6.42017	0.28188	-4.48820
C	2.85169	1.16729	0.85261
C	3.75931	0.71523	1.81756
C	2.28766	2.43938	0.99872
C	4.10007	1.52347	2.89819
H	4.17975	-0.28489	1.73396
C	2.62684	3.24757	2.07935
H	1.54774	2.77081	0.27032
C	3.53335	2.78965	3.03188
H	4.80227	1.15900	3.64365
H	2.15818	4.22127	2.19403
H	3.79126	3.41446	3.88306
C	-3.38556	0.25084	-0.86750
C	-4.44948	0.51687	0.00494
C	-3.47891	-0.83203	-1.74665
C	-5.59328	-0.27336	-0.01956
H	-4.37376	1.34538	0.70788
C	-4.61883	-1.63016	-1.76022
H	-2.63352	-1.06571	-2.39141

C	-5.67799	-1.34808	-0.90273
H	-6.41261	-0.06138	0.66288
H	-4.66999	-2.49006	-2.42243
H	-6.55918	-1.98389	-0.90509
C	-2.36401	2.96626	-0.97725
C	-1.36945	3.95147	-0.86585
C	-3.65499	3.36155	-1.34720
C	-1.66564	5.29146	-1.07215
H	-0.35285	3.64723	-0.61651
C	-3.94595	4.70544	-1.57441
H	-4.43699	2.61698	-1.46645
C	-2.95885	5.67421	-1.42982
H	-0.88351	6.03890	-0.96957
H	-4.95301	4.99291	-1.86522
H	-3.18922	6.72103	-1.60770
N	4.94449	-4.19382	0.72635
H	4.90409	-5.20129	0.70238
H	5.64601	-3.84259	0.09224
N	-5.01684	-4.94252	0.34920
H	-4.86785	-5.88980	0.03410
H	-5.55822	-4.93223	1.20086
N	-0.54577	3.16232	3.86710
H	-1.33057	3.78619	3.76529
H	-0.34317	2.94966	4.83104

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C	-2.26097	-1.56401	-0.04870
C	1.71203	-2.19046	-0.38042
C	2.78381	-1.85162	-1.22470
H	2.69638	-0.97754	-1.86759
C	-1.01660	-2.10531	-0.48406
C	0.37714	0.12558	-1.03017
C	1.86765	-3.33652	0.42474
H	1.05244	-3.63239	1.08425
C	-0.36531	0.22114	-2.23699
H	-0.86282	-0.67432	-2.60332
C	0.99601	1.34626	-0.56010
C	0.12971	2.53534	-2.47600
C	3.96263	-2.58406	-1.24463
H	4.80022	-2.31072	-1.87665
C	0.82733	2.54225	-1.28585
H	1.25169	3.47800	-0.93601
C	4.07792	-3.68567	-0.40424
C	3.03329	-4.08572	0.42530

H	3.16276	-4.95466	1.06051
C	-1.05003	-3.38209	-1.07341
H	-0.11533	-3.82154	-1.41488
C	-0.46797	1.37891	-2.97784
H	-1.01860	1.42109	-3.91024
C	-3.44286	-2.29188	-0.18295
H	-4.39381	-1.91142	0.18040
C	-2.22444	-4.10381	-1.23860
H	-2.23893	-5.08476	-1.70024
C	-3.41177	-3.54461	-0.78361
Ni	-0.11877	0.30161	1.12051
P	1.79973	1.39453	1.11382
P	-2.28489	0.09773	0.75685
B	0.38075	-1.32423	-0.32368
H	0.39771	-1.20534	1.18519
H	-0.06227	-0.74459	2.16426
C	-3.61495	-0.03391	1.99508
C	-4.95421	0.25516	1.70849
C	-3.26678	-0.46611	3.28060
C	-5.92904	0.09728	2.68961
H	-5.23300	0.60471	0.71645
C	-4.24421	-0.62885	4.25595
H	-2.22087	-0.66418	3.51007
C	-5.57659	-0.34775	3.96085
H	-6.96635	0.32138	2.45840
H	-3.96473	-0.96649	5.24997
H	-6.33955	-0.47045	4.72406
C	-2.93027	1.23435	-0.52114
C	-3.72962	0.82266	-1.59441
C	-2.54515	2.57820	-0.43935
C	-4.12809	1.73693	-2.56547
H	-4.02276	-0.22121	-1.68410
C	-2.94832	3.49234	-1.40797
H	-1.89581	2.89417	0.37666
C	-3.73461	3.07069	-2.47736
H	-4.73950	1.40405	-3.39954
H	-2.62178	4.52749	-1.34459
H	-4.02725	3.77782	-3.24816
C	3.43327	0.62906	0.89014
C	4.27557	1.02327	-0.15928
C	3.84409	-0.39374	1.75061
C	5.51597	0.41891	-0.32829
H	3.94965	1.80174	-0.84758
C	5.08379	-1.00253	1.57356

H	3.18159	-0.72096	2.54936
C	5.92168	-0.59455	0.53886
H	6.16175	0.72789	-1.14563
H	5.38998	-1.80760	2.23636
H	6.88032	-1.08391	0.39254
C	2.08667	3.16435	1.42592
C	0.95395	3.93049	1.73788
C	3.34314	3.77870	1.41911
C	1.06890	5.29027	1.99407
H	-0.01820	3.43743	1.78318
C	3.45687	5.13898	1.69583
H	4.23438	3.19675	1.20202
C	2.32391	5.89720	1.97415
H	0.18289	5.87474	2.22410
H	4.43733	5.60699	1.69026
H	2.41797	6.95844	2.18558
O	5.39219	-5.43528	0.32843
O	6.29496	-3.94737	-0.98882
O	-5.69788	-3.75473	-0.53426
O	-4.60394	-5.40333	-1.45563
O	0.43476	4.81617	-2.70455
O	-0.65344	3.75730	-4.27145
N	-0.03548	3.79725	-3.20862
N	5.34451	-4.41237	-0.35583
N	-4.66483	-4.29079	-0.93441

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C	-2.26754	1.57299	0.05602
C	1.69485	2.19222	0.50188
C	2.75487	1.84838	1.36056
H	2.66229	0.96095	1.98592
C	-1.03107	2.09906	0.52319
C	0.36760	-0.13156	1.10420
C	1.88118	3.34659	-0.27298
H	1.08482	3.65779	-0.95023
C	-0.40909	-0.23084	2.28496
H	-0.99014	0.64012	2.58253
C	1.08264	-1.33319	0.73612
C	0.25722	-2.49775	2.70625
C	3.92442	2.58912	1.42806
H	4.74412	2.30016	2.08053
C	0.99904	-2.48680	1.53019
H	1.51583	-3.39902	1.24565
C	4.08727	3.71105	0.61219

C	3.04996	4.10380	-0.23604	C	4.76398	1.29672	-1.70931
H	3.14941	4.97686	-0.87372	H	2.77519	0.84643	-2.41410
C	-1.09346	3.36406	1.12261	C	5.78043	0.94135	-0.82802
H	-0.16823	3.80583	1.48908	H	6.39741	-0.41146	0.73109
C	-0.45046	-1.35064	3.09310	H	4.87802	2.16491	-2.35356
H	-1.05529	-1.34226	3.99379	H	6.69175	1.53211	-0.78420
C	-3.45380	2.29683	0.16911	C	2.20236	-3.18678	-1.21596
H	-4.38936	1.91696	-0.23630	C	1.09882	-4.04290	-1.35258
C	-2.27562	4.08714	1.27120	C	3.48701	-3.71718	-1.37376
H	-2.25525	5.06136	1.74979	C	1.27362	-5.39830	-1.59312
C	-3.46770	3.55170	0.78470	H	0.09573	-3.62094	-1.27747
Ni	-0.08235	-0.31276	-1.04335	C	3.66019	-5.07539	-1.63482
P	1.81821	-1.42139	-0.95605	H	4.35662	-3.06989	-1.30207
P	-2.26096	-0.08478	-0.75298	C	2.55951	-5.91961	-1.73526
B	0.36974	1.32274	0.38753	H	0.40705	-6.04730	-1.68552
H	0.43167	1.18084	-1.09981	H	4.66389	-5.47323	-1.75871
H	0.01907	0.61067	-2.18531	H	2.70025	-6.97789	-1.93712
C	-3.56863	0.06454	-2.01946	O	-4.68337	4.16566	0.85342
C	-4.62640	-0.84368	-2.13027	O	0.26129	-3.66453	3.40344
C	-3.45631	1.09299	-2.96644	O	5.29798	4.33992	0.69991
C	-5.55577	-0.72032	-3.16092	C	-4.72046	5.43503	1.46698
H	-4.72820	-1.64612	-1.40335	H	-5.76007	5.76148	1.43194
C	-4.38789	1.21675	-3.98885	H	-4.39079	5.39210	2.51374
H	-2.63648	1.80506	-2.88861	H	-4.09527	6.16429	0.93457
C	-5.44095	0.30839	-4.09045	C	5.50186	5.44399	-0.15018
H	-6.37533	-1.43061	-3.23261	H	6.51247	5.80316	0.04800
H	-4.29199	2.02354	-4.71056	H	5.41947	5.16364	-1.21026
H	-6.16873	0.40446	-4.89142	H	4.78755	6.25460	0.04864
C	-2.97443	-1.23010	0.48796	C	-0.52954	-3.71536	4.57447
C	-4.03713	-0.88395	1.33101	H	-1.58790	-3.52403	4.35244
C	-2.39856	-2.49804	0.61115	H	-0.41846	-4.72440	4.97145
C	-4.51068	-1.78996	2.27466	H	-0.18922	-2.99265	5.32688
H	-4.48635	0.10383	1.25616				
C	-2.87123	-3.40628	1.55502	A-PC-H			
H	-1.54325	-2.74678	-0.01716	C	2.28994	-1.67287	0.32576
C	-3.92957	-3.05266	2.38760	C	-2.63708	-2.61153	1.18323
H	-5.33531	-1.51016	2.92506	H	-2.74734	-1.83234	1.93872
H	-2.39942	-4.38165	1.64920	C	-1.41702	-3.63616	-0.60258
H	-4.30155	-3.75833	3.12651	H	-0.54349	-3.66831	-1.25447
C	3.41138	-0.54148	-0.90142	C	-0.20435	-0.61997	2.80202
C	4.43118	-0.87952	-0.00123	H	0.37100	-1.52373	2.97910
C	3.58638	0.55691	-1.74877	C	-1.32732	0.70099	1.17840
C	5.61330	-0.14669	0.02645	C	-1.31172	1.37453	3.51546
H	4.28852	-1.71048	0.68791	C	-3.64556	-3.56506	1.03998

H	-4.52402	-3.52363	1.68011
C	-1.68105	1.58948	2.19914
H	-2.27195	2.46152	1.93692
C	-3.53351	-4.56251	0.07692
C	-2.40994	-4.59600	-0.74883
H	-2.31515	-5.36732	-1.50955
C	1.11115	-3.53267	1.25888
H	0.14993	-3.92090	1.57664
C	-0.53605	0.23843	3.81747
H	-0.20166	0.02527	4.82647
C	3.45842	-2.45118	0.38814
H	4.38025	-2.00753	0.02501
C	2.25288	-4.26822	1.38043
H	2.19840	-5.25512	1.82622
C	3.47682	-3.72182	0.92206
Ni	0.31679	0.42805	-1.45916
P	-1.60476	1.04387	-0.59559
P	2.24134	-0.08668	-0.54164
B	-0.29508	-1.58123	0.48097
C	2.32852	1.18691	0.78209
C	2.68412	0.87679	2.09824
C	2.05053	2.51757	0.44595
C	2.75337	1.87792	3.06517
H	2.90726	-0.15665	2.36061
C	2.12954	3.51606	1.41183
H	1.75624	2.74646	-0.57895
C	2.47535	3.19843	2.72474
H	3.02252	1.62322	4.08728
H	1.91241	4.54684	1.13919
H	2.52975	3.97891	3.47916
C	3.89058	0.04815	-1.31642
C	3.99935	-0.26748	-2.67518
C	5.03118	0.45509	-0.61484
C	5.23263	-0.20175	-3.31573
H	3.10439	-0.54890	-3.22619
C	6.26441	0.51954	-1.25706
H	4.94837	0.72054	0.43754
C	6.36641	0.18864	-2.60647
H	5.30730	-0.44686	-4.37165
H	7.14656	0.83129	-0.70421
H	7.32900	0.24447	-3.10786
C	-3.08006	0.04083	-0.99259
C	-3.02043	-0.84212	-2.07292
C	-4.25304	0.11153	-0.22967

C	-4.11483	-1.64355	-2.38796
H	-2.09765	-0.90938	-2.64828
C	-5.34834	-0.68126	-0.54987
H	-4.29952	0.78868	0.62216
C	-5.27734	-1.56279	-1.62818
H	-4.05276	-2.34239	-3.21765
H	-6.25263	-0.62547	0.05044
H	-6.12779	-2.19522	-1.86844
C	-2.21497	2.76340	-0.60600
C	-3.44342	3.13597	-1.16246
C	-1.34283	3.76965	-0.16434
C	-3.79896	4.48012	-1.25071
H	-4.12613	2.37661	-1.53304
C	-1.70602	5.10783	-0.24030
H	-0.37565	3.49070	0.24846
C	-2.93727	5.46832	-0.78593
H	-4.75721	4.75280	-1.68489
H	-1.02073	5.87228	0.11719
H	-3.21871	6.51546	-0.85482
H	-4.31818	-5.30660	-0.03448
H	-1.63016	2.05818	4.29567
H	4.40558	-4.27642	1.00220
C	-1.49620	-2.62618	0.37239
N	-0.56680	-0.42328	1.50521
H	-0.18736	-1.03968	-0.64999
H	0.79071	1.62426	-2.29849
N	1.06931	-2.25766	0.74370

A-PC-CH₃

C	-2.37905	1.46080	0.48138
C	1.47596	2.40915	0.44674
C	2.66399	2.35391	1.18583
H	2.81266	1.53799	1.89414
C	-1.14509	1.99014	0.90344
C	0.65515	0.07477	1.52329
C	1.35200	3.48510	-0.44910
H	0.43770	3.57395	-1.03854
C	0.28756	0.13262	2.87662
H	-0.33953	0.96016	3.20813
C	1.45991	-1.03878	1.15945
C	1.50021	-1.89789	3.43545
C	3.67211	3.30502	1.03148
H	4.58846	3.22252	1.61618
C	1.86662	-1.99699	2.09113

H	2.46932	-2.84502	1.76550	C	-3.36051	-2.60943	-0.12912
C	3.54204	4.35362	0.12036	C	-4.12880	-2.20408	2.51319
C	2.35240	4.43380	-0.61322	H	-3.36382	-0.20442	2.27711
H	2.21976	5.24854	-1.32511	C	-3.96445	-3.63755	0.58290
C	-1.22212	3.14568	1.70055	H	-3.04264	-2.77159	-1.15755
H	-0.29225	3.59954	2.04159	C	-4.35067	-3.43646	1.90751
C	0.69743	-0.81738	3.80726	H	-4.42026	-2.04435	3.54774
H	0.38811	-0.72323	4.84758	H	-4.12846	-4.60025	0.10639
C	-3.60261	2.05498	0.81875	H	-4.81882	-4.24215	2.46628
H	-4.53553	1.62366	0.45170	C	3.23743	-0.21512	-1.02720
C	-2.43190	3.73054	2.05147	C	4.45314	-0.39841	-0.35550
H	-2.43847	4.62702	2.67036	C	3.12081	0.80807	-1.97083
C	-3.65098	3.20090	1.60921	C	5.54124	0.41616	-0.64713
Ni	-0.26642	-0.50082	-0.94786	H	4.53938	-1.17569	0.40216
P	1.77348	-1.21690	-0.62934	C	4.20976	1.62589	-2.25742
P	-2.33386	-0.05862	-0.51654	H	2.15882	0.97715	-2.45125
B	0.28813	1.31940	0.54769	C	5.42013	1.42592	-1.60059
H	0.22111	1.03307	-0.72359	H	6.48197	0.27125	-0.12273
H	-0.72149	-1.80741	-1.44531	H	4.10533	2.43305	-2.97735
C	-4.95250	3.85521	1.95926	H	6.26927	2.06818	-1.81914
H	-5.03986	4.84839	1.50466	C	2.24543	-2.95446	-0.89575
H	-5.80603	3.26335	1.61803	C	1.31272	-3.94230	-0.54608
H	-5.05612	3.99687	3.04032	C	3.46255	-3.34054	-1.46415
C	4.65299	5.33445	-0.10094	C	1.60708	-5.28569	-0.73560
H	5.34336	5.36373	0.74708	H	0.35225	-3.64347	-0.12770
H	5.24685	5.07472	-0.98754	C	3.74836	-4.68978	-1.66519
H	4.27710	6.34957	-0.26409	H	4.19008	-2.58755	-1.75500
C	1.93403	-2.93211	4.42903	C	2.82725	-5.66348	-1.29652
H	1.43379	-3.89214	4.25682	H	0.87917	-6.04152	-0.45331
H	3.01006	-3.12601	4.37056	H	4.69672	-4.97651	-2.11154
H	1.70587	-2.62523	5.45321	H	3.05294	-6.71490	-1.45226
C	-3.45846	0.21337	-1.92553				
C	-4.82747	-0.06950	-1.86889	A-PC-Cl			
C	-2.91952	0.76480	-3.09364	C	-2.38838	1.53226	0.09552
C	-5.64440	0.20747	-2.96166	C	1.55247	2.25201	0.24624
H	-5.24930	-0.51542	-0.97011	C	2.22418	2.51294	1.45013
C	-3.73875	1.04368	-4.18208	H	1.86146	2.05368	2.37048
H	-1.85031	0.96663	-3.13932	C	-1.14166	2.07400	0.47220
C	-5.10225	0.76533	-4.11670	C	0.44723	0.01722	1.19032
H	-6.70665	-0.01585	-2.91147	C	2.07443	2.85943	-0.90454
H	-3.31181	1.47017	-5.08554	H	1.59381	2.67472	-1.86535
H	-5.74140	0.97802	-4.96917	C	-0.09425	0.05624	2.48528
C	-3.15184	-1.35794	0.46817	H	-0.71132	0.90956	2.76602
C	-3.53239	-1.16614	1.79902	C	1.23111	-1.12917	0.87945

C	0.87467	-2.05700	3.06818
C	3.35922	3.31857	1.51487
H	3.86950	3.49902	2.45641
C	1.43799	-2.16043	1.80144
H	2.01472	-3.04236	1.53596
C	3.84885	3.87558	0.33952
C	3.21221	3.65878	-0.87724
H	3.61633	4.09385	-1.78644
C	-1.18343	3.31718	1.12054
H	-0.24557	3.78176	1.42145
C	0.10665	-0.95336	3.42116
H	-0.33759	-0.89720	4.41034
C	-3.59891	2.18934	0.33810
H	-4.54670	1.76081	0.01955
C	-2.37321	3.99016	1.38354
H	-2.37285	4.95601	1.87962
C	-3.57715	3.41749	0.98648
Ni	-0.31586	-0.53277	-1.23821
P	1.70069	-1.31193	-0.87770
P	-2.36799	-0.10397	-0.70770
B	0.25500	1.29404	0.19786
H	0.23062	1.00990	-1.06415
H	-0.80601	-1.82087	-1.73653
Cl	-5.07965	4.25347	1.29297
Cl	5.31542	4.83371	0.37824
Cl	1.11755	-3.34222	4.22542
C	-3.68261	-0.08830	-1.96464
C	-5.01224	-0.39834	-1.65645
C	-3.34613	0.28042	-3.27191
C	-5.99251	-0.32341	-2.64179
H	-5.27560	-0.70348	-0.64547
C	-4.32898	0.35627	-4.25284
H	-2.30740	0.49930	-3.51221
C	-5.65243	0.05572	-3.93789
H	-7.02294	-0.56440	-2.39673
H	-4.06091	0.64229	-5.26586
H	-6.41913	0.11199	-4.70551
C	-2.93991	-1.29373	0.55169
C	-3.36360	-0.89465	1.82300
C	-2.91693	-2.65910	0.23526
C	-3.76058	-1.84633	2.75967
H	-3.37722	0.16049	2.08398
C	-3.31911	-3.60412	1.17078
H	-2.57129	-2.97337	-0.74793

C	-3.73868	-3.19918	2.43709
H	-4.08258	-1.52578	3.74669
H	-3.29689	-4.65971	0.91519
H	-4.04162	-3.93938	3.17229
C	3.21233	-0.35272	-1.18150
C	4.03668	0.06485	-0.13148
C	3.54005	-0.00608	-2.49736
C	5.17012	0.82674	-0.39670
H	3.77048	-0.18374	0.89376
C	4.68122	0.74471	-2.75854
H	2.89248	-0.31623	-3.31542
C	5.49378	1.16575	-1.70822
H	5.79291	1.17055	0.42472
H	4.92870	1.01344	-3.78168
H	6.37247	1.77273	-1.90905
C	2.18977	-3.05168	-1.08090
C	1.19288	-4.03337	-1.14400
C	3.53499	-3.43667	-1.10356
C	1.53768	-5.37783	-1.21380
H	0.14774	-3.72852	-1.13210
C	3.87516	-4.78450	-1.18141
H	4.31544	-2.68122	-1.05331
C	2.87932	-5.75530	-1.23412
H	0.75827	-6.13335	-1.25863
H	4.92169	-5.07488	-1.19726
H	3.14736	-6.80643	-1.29315

A-PC-CN

C	-2.37734	1.59975	0.12862
C	1.54820	2.35601	0.32614
C	2.66466	2.12890	1.14445
H	2.67501	1.26561	1.80829
C	-1.13741	2.13278	0.54850
C	0.46505	0.07002	1.23801
C	1.59825	3.48430	-0.51341
H	0.74490	3.70133	-1.15576
C	-0.04285	0.12034	2.54771
H	-0.63309	0.98694	2.84253
C	1.21712	-1.09196	0.90077
C	0.91169	-2.02038	3.11847
C	3.78540	2.94715	1.10852
H	4.65014	2.73158	1.73009
C	1.43449	-2.11589	1.82126
H	1.99237	-3.00526	1.53903

C	3.81873	4.04659	0.24026	H	-2.60246	-4.57488	1.23869
C	2.70264	4.31993	-0.56664	H	-3.47427	-3.83408	3.44386
H	2.72428	5.17539	-1.23602	C	3.25892	-0.32756	-1.05708
C	-1.18978	3.35805	1.23225	C	4.37173	-0.62557	-0.25869
H	-0.25862	3.80463	1.57562	C	3.31531	0.75315	-1.94188
C	0.16509	-0.88917	3.47522	C	5.52532	0.14347	-0.35458
H	-0.25257	-0.81897	4.47555	H	4.32726	-1.45410	0.44644
C	-3.58330	2.26323	0.34448	C	4.47006	1.52501	-2.03037
H	-4.52187	1.84256	-0.01136	H	2.43570	1.00665	-2.53089
C	-2.38034	4.03156	1.47123	C	5.57371	1.22115	-1.23799
H	-2.38395	4.98232	1.99653	H	6.38316	-0.08841	0.27023
C	-3.59239	3.49247	1.01794	H	4.49952	2.37942	-2.70076
Ni	-0.28052	-0.40907	-1.24397	H	6.46627	1.83842	-1.29411
P	1.70443	-1.24726	-0.86056	C	2.09514	-3.00206	-1.12217
P	-2.33275	-0.04051	-0.66890	C	1.09480	-3.94738	-0.85225
B	0.27006	1.36703	0.27740	C	3.32669	-3.43628	-1.62127
H	0.27006	1.11826	-0.99304	C	1.33432	-5.30014	-1.05112
H	-0.75466	-1.68532	-1.78201	H	0.12900	-3.60955	-0.47761
C	-4.82242	4.17990	1.23504	C	3.55758	-4.79426	-1.83242
C	4.99573	4.84295	0.13758	H	4.10743	-2.71489	-1.84644
C	1.11360	-3.07901	4.05091	C	2.56762	-5.72669	-1.54378
N	-5.83376	4.73766	1.41524	H	0.55616	-6.02446	-0.82783
N	5.97326	5.47689	0.03511	H	4.51743	-5.12063	-2.22215
N	1.27357	-3.95263	4.81134	H	2.75180	-6.78487	-1.70547
C	-3.71212	-0.10598	-1.84844				
C	-5.01350	-0.43568	-1.45120	A-PC-NH₂			
C	-3.45625	0.20338	-3.18907	C	2.41997	-1.39074	0.54406
C	-6.04615	-0.44000	-2.38387	C	-1.41785	-2.39155	0.53388
H	-5.21315	-0.69675	-0.41356	C	-2.64246	-2.30274	1.21025
C	-4.49193	0.20010	-4.11682	H	-2.81605	-1.46210	1.88334
H	-2.43881	0.43458	-3.49831	C	1.19776	-1.92540	0.98924
C	-5.78642	-0.12083	-3.71465	C	-0.63895	-0.01711	1.55401
H	-7.05417	-0.69706	-2.07151	C	-1.27350	-3.49581	-0.32300
H	-4.28699	0.43913	-5.15621	H	-0.33443	-3.61603	-0.86722
H	-6.59407	-0.12919	-4.44109	C	-0.25923	-0.00756	2.90754
C	-2.76075	-1.22319	0.65521	H	0.41406	-0.78944	3.25925
C	-3.25996	-0.81477	1.89642	C	-1.49415	1.04779	1.16496
C	-2.53371	-2.58781	0.42844	C	-1.57217	1.96735	3.41092
C	-3.52240	-1.75424	2.89100	C	-3.66310	-3.23146	1.03194
H	-3.43096	0.24070	2.09452	H	-4.61057	-3.11251	1.55753
C	-2.79273	-3.52129	1.42480	C	-1.95010	2.01377	2.06446
H	-2.14027	-2.90969	-0.53405	H	-2.58487	2.82873	1.71757
C	-3.28492	-3.10575	2.66084	C	-3.50268	-4.30496	0.14990
H	-3.90418	-1.42340	3.85281	C	-2.27850	-4.43300	-0.52050

H	-2.13182	-5.26426	-1.20991
C	1.30662	-3.06701	1.80210
H	0.38912	-3.53241	2.16106
C	-0.70499	0.94366	3.81552
H	-0.37640	0.90572	4.85307
C	3.65912	-1.95919	0.86083
H	4.57864	-1.52376	0.46651
C	2.52476	-3.63456	2.14828
H	2.55521	-4.51982	2.78196
C	3.72925	-3.09455	1.67277
Ni	0.26623	0.51605	-0.90740
P	-1.79922	1.17784	-0.63090
P	2.34179	0.10073	-0.49350
B	-0.24539	-1.28793	0.62480
H	-0.17051	-1.02645	-0.66188
H	0.68578	1.83543	-1.40979
N	4.95774	-3.64119	2.04443
H	4.91825	-4.62367	2.27003
H	5.70584	-3.45283	1.39431
N	-4.56323	-5.17806	-0.12023
H	-4.26455	-6.09415	-0.42187
H	-5.22146	-5.25860	0.64100
N	-1.98037	2.95679	4.30296
H	-2.83909	3.42023	4.04836
H	-1.99390	2.66704	5.26884
C	3.41396	-0.26908	-1.92377
C	4.69464	0.26246	-2.09793
C	2.90832	-1.16387	-2.87646
C	5.45564	-0.09447	-3.20963
H	5.09580	0.95700	-1.36349
C	3.67305	-1.52426	-3.97880
H	1.90811	-1.57456	-2.74227
C	4.94823	-0.98643	-4.14936
H	6.44920	0.32640	-3.33905
H	3.27174	-2.21956	-4.71088
H	5.54315	-1.26130	-5.01591
C	3.19132	1.43103	0.41825
C	3.66734	1.25770	1.72109
C	3.32396	2.68511	-0.19531
C	4.28600	2.31336	2.38785
H	3.55123	0.29700	2.21591
C	3.95351	3.73085	0.46834
H	2.92439	2.83513	-1.19672
C	4.43770	3.54649	1.76274

H	4.64958	2.16707	3.40135
H	4.05884	4.69496	-0.02179
H	4.92375	4.36635	2.28428
C	-3.23791	0.13725	-1.02617
C	-4.47911	0.33542	-0.40781
C	-3.06541	-0.94972	-1.88684
C	-5.53516	-0.53140	-0.66722
H	-4.61064	1.16507	0.28528
C	-4.11869	-1.82497	-2.13199
H	-2.08506	-1.12634	-2.32547
C	-5.35360	-1.61351	-1.52632
H	-6.49582	-0.37343	-0.18396
H	-3.96745	-2.69014	-2.77149
H	-6.16945	-2.30854	-1.70614
C	-2.30639	2.89910	-0.93952
C	-1.42219	3.91821	-0.55509
C	-3.49682	3.24286	-1.58632
C	-1.73917	5.24975	-0.78775
H	-0.48147	3.65389	-0.07390
C	-3.80496	4.58030	-1.83041
H	-4.18568	2.46507	-1.90503
C	-2.93278	5.58497	-1.42730
H	-1.04923	6.02942	-0.47639
H	-4.73159	4.83301	-2.33889
H	-3.17548	6.62703	-1.61694

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C	2.43959	-1.42726	0.05081
C	-1.49340	-2.18714	0.23201
C	-2.15459	-2.41643	1.45179
H	-1.77457	-1.94498	2.35800
C	1.19957	-1.97859	0.45036
C	-0.41337	0.08277	1.09607
C	-2.02144	-2.81461	-0.90854
H	-1.53548	-2.65704	-1.87049
C	0.14086	0.09115	2.38950
H	0.77270	-0.74320	2.69119
C	-1.22374	1.20418	0.74558
C	-0.86832	2.19502	2.90069
C	-3.30404	-3.19110	1.53364
H	-3.83340	-3.34663	2.46736
C	-1.44176	2.25499	1.63549
H	-2.03032	3.12643	1.36513
C	-3.81293	-3.74668	0.36447

C	-3.17530	-3.58203	-0.86126
H	-3.61106	-4.02768	-1.74870
C	1.24842	-3.20522	1.13302
H	0.31458	-3.66572	1.44964
C	-0.07422	1.12380	3.29152
H	0.36503	1.12538	4.28322
C	3.65068	-2.06995	0.30215
H	4.60329	-1.65999	-0.02299
C	2.44291	-3.85942	1.40686
H	2.47371	-4.80888	1.92980
C	3.63365	-3.28087	0.98261
Ni	0.33632	0.56317	-1.33129
P	-1.69849	1.32916	-1.01653
P	2.40044	0.18783	-0.79934
B	-0.20275	-1.22250	0.14605
H	-0.17759	-0.98683	-1.12063
H	0.80742	1.84195	-1.86329
N	4.90326	-3.96129	1.25438
N	-1.09299	3.29884	3.83579
N	-5.09248	-4.45009	0.40853
O	4.85743	-5.02443	1.87081
O	5.93439	-3.42192	0.85374
O	-5.57499	-4.82527	-0.66212
O	-5.62531	-4.60521	1.50833
O	-1.81670	4.22254	3.46427
O	-0.54239	3.23335	4.93477
C	3.70277	0.14330	-2.06435
C	5.03704	0.44223	-1.76455
C	3.35462	-0.24007	-3.36432
C	6.01178	0.33946	-2.75242
H	5.30884	0.75921	-0.75952
C	4.33274	-0.34242	-4.34761
H	2.31235	-0.44953	-3.59779
C	5.66100	-0.05483	-4.04123
H	7.04614	0.56920	-2.51456
H	4.05730	-0.63973	-5.35528
H	6.42399	-0.13366	-4.81025
C	2.96253	1.41431	0.42694
C	3.40522	1.05499	1.70374
C	2.91802	2.77042	0.07391
C	3.79925	2.03647	2.61032
H	3.43769	0.00825	1.99499
C	3.31662	3.74523	0.97999
H	2.56060	3.05474	-0.91409

C	3.75475	3.37979	2.25193
H	4.13666	1.74708	3.60152
H	3.27814	4.79304	0.69664
H	4.05518	4.14300	2.96396
C	-2.19970	3.05666	-1.26796
C	-1.20944	4.04019	-1.38157
C	-3.54804	3.43210	-1.27449
C	-1.56342	5.37996	-1.48269
H	-0.16266	3.74109	-1.38463
C	-3.89681	4.77517	-1.38403
H	-4.32297	2.67458	-1.18665
C	-2.90744	5.74889	-1.48483
H	-0.79012	6.13802	-1.56598
H	-4.94475	5.05993	-1.38595
H	-3.18280	6.79642	-1.56684
C	-3.19906	0.34153	-1.28107
C	-4.03090	-0.02383	-0.21653
C	-3.51198	-0.08084	-2.57852
C	-5.15556	-0.80947	-0.44936
H	-3.78144	0.28881	0.79561
C	-4.64194	-0.85879	-2.80661
H	-2.86084	0.18968	-3.40761
C	-5.46087	-1.23009	-1.74194
H	-5.78406	-1.11089	0.38493
H	-4.87569	-1.18931	-3.81469
H	-6.32483	-1.86619	-1.91427

A-PC-OCH₃

C	-2.32238	1.55243	0.07538
C	1.61842	2.19376	0.36791
C	2.71939	1.93851	1.20251
H	2.69829	1.06879	1.85945
C	-1.07683	2.03582	0.53328
C	0.45224	-0.07596	1.23307
C	1.72556	3.32008	-0.45937
H	0.89266	3.56813	-1.11915
C	-0.09186	-0.04924	2.52376
H	-0.67348	0.82397	2.81887
C	1.18778	-1.25215	0.90858
C	0.79490	-2.21563	3.09116
C	3.85751	2.73231	1.19787
H	4.71221	2.50540	1.82982
C	1.35822	-2.29698	1.81528
H	1.90178	-3.19972	1.54771

C	3.93949	3.82698	0.33544	C	-2.90292	-1.28173	0.40694
C	2.85729	4.13360	-0.49197	C	-3.29759	-0.93259	1.70147
H	2.89180	4.98528	-1.16491	C	-2.91944	-2.63166	0.02877
C	-1.12932	3.23567	1.25316	C	-3.70626	-1.91634	2.59956
H	-0.19608	3.65717	1.62397	H	-3.27795	0.10956	2.00968
C	0.05886	-1.08414	3.44423	C	-3.33293	-3.60910	0.92561
H	-0.40284	-1.00350	4.42359	H	-2.59195	-2.90941	-0.97173
C	-3.52307	2.22263	0.30391	C	-3.72524	-3.25304	2.21552
H	-4.47038	1.84608	-0.07692	H	-4.00424	-1.63342	3.60595
C	-2.31570	3.92450	1.50646	H	-3.34129	-4.65212	0.62098
H	-2.28631	4.85431	2.06607	H	-4.04014	-4.01869	2.91961
C	-3.52408	3.41926	1.02432	C	3.28574	-0.51287	-1.01838
Ni	-0.24709	-0.50627	-1.28285	C	4.39898	-0.86013	-0.24165
P	1.70331	-1.39194	-0.84202	C	3.35780	0.59659	-1.86517
P	-2.29787	-0.04603	-0.79568	C	5.56873	-0.11337	-0.32353
B	0.31825	1.24236	0.29171	H	4.34080	-1.70907	0.43778
H	0.33396	0.99312	-0.99286	C	4.52749	1.34647	-1.93913
H	-0.74912	-1.77115	-1.84036	H	2.47605	0.89115	-2.43118
O	-4.74165	4.01082	1.19548	C	5.63166	0.99284	-1.16921
O	5.12109	4.51839	0.35798	H	6.42629	-0.38291	0.28674
O	1.00688	-3.28966	3.90516	H	4.56541	2.22426	-2.57869
C	-4.76035	5.23318	1.89831	H	6.53585	1.59484	-1.20959
H	-5.80198	5.55338	1.92705	C	2.05096	-3.15307	-1.13548
H	-4.39027	5.11989	2.92636	C	1.01836	-4.07137	-0.89459
H	-4.15990	6.00293	1.39499	C	3.26918	-3.61802	-1.63909
C	5.24744	5.58071	-0.55608	C	1.21283	-5.42590	-1.12789
H	6.24719	5.99331	-0.41479	H	0.06214	-3.70920	-0.51929
H	5.14173	5.23982	-1.59658	C	3.45592	-4.97743	-1.88420
H	4.50539	6.37101	-0.37685	H	4.07484	-2.91751	-1.84219
C	0.38702	-3.25629	5.17071	C	2.43325	-5.88296	-1.62550
H	-0.70573	-3.17753	5.08499	H	0.40815	-6.12832	-0.92835
H	0.64226	-4.19591	5.66178	H	4.40655	-5.32596	-2.27821
H	0.74949	-2.42007	5.78374	H	2.58171	-6.94249	-1.81522
C	-3.59631	0.02025	-2.06980				
C	-4.93575	-0.27010	-1.78594	B-Cat-H			
C	-3.23768	0.40880	-3.36518	C	-2.61080	1.56265	0.28644
C	-5.90226	-0.15590	-2.78098	C	1.38925	3.21134	1.91417
H	-5.21719	-0.59065	-0.78462	H	0.56940	3.87900	2.17445
C	-4.20634	0.52430	-4.35660	C	2.26100	1.31393	0.73185
H	-2.19160	0.61058	-3.58814	C	3.67605	2.50745	2.28671
C	-5.53935	0.24361	-4.06474	C	3.47888	1.45564	1.38883
H	-6.94020	-0.38228	-2.55337	H	4.28254	0.74581	1.18858
H	-3.91953	0.82520	-5.36038	C	-1.91955	3.73338	1.06262
H	-6.29520	0.33048	-4.84035	H	-1.15681	4.49093	1.23643

C	2.61664	3.37878	2.54665
H	2.74837	4.18826	3.26448
C	-3.93130	1.85779	0.61352
H	-4.70720	1.11248	0.43865
C	-3.24530	4.04954	1.33142
H	-3.49321	5.03764	1.71947
C	-4.26455	3.11445	1.12545
Ni	-0.04425	0.52544	-1.18834
P	1.92520	-0.02624	-0.48257
P	-2.02151	0.01341	-0.47875
B	-0.12395	2.01689	0.09290
C	-1.81154	-1.16129	0.92120
C	-2.16594	-0.84468	2.23788
C	-1.21135	-2.40536	0.67394
C	-1.94003	-1.75297	3.27086
H	-2.61311	0.12359	2.45158
C	-1.01798	-3.32409	1.69788
H	-0.86869	-2.63398	-0.33525
C	-1.37803	-2.99793	3.00457
H	-2.20954	-1.48411	4.29017
H	-0.54198	-4.27761	1.48284
H	-1.19679	-3.70318	3.81298
C	-3.52694	-0.63603	-1.30993
C	-4.20174	0.23187	-2.18998
C	-3.96700	-1.96552	-1.23345
C	-5.28110	-0.20985	-2.94491
H	-3.87815	1.26919	-2.25858
C	-5.04556	-2.40691	-1.99406
H	-3.46775	-2.65684	-0.55774
C	-5.71066	-1.53372	-2.85455
H	-5.79275	0.48424	-3.60896
H	-5.37646	-3.44005	-1.90553
H	-6.55324	-1.88066	-3.44802
C	3.41390	0.09132	-1.55204
C	3.50046	1.27785	-2.30434
C	4.41933	-0.86950	-1.71216
C	4.54627	1.48397	-3.19486
H	2.72382	2.03192	-2.17653
C	5.46691	-0.66096	-2.60695
H	4.39173	-1.78203	-1.12135
C	5.53405	0.51256	-3.35630
H	4.59278	2.40847	-3.76673
H	6.24165	-1.41810	-2.71173
H	6.35223	0.67118	-4.05521

C	2.20877	-1.55378	0.49111
C	2.29514	-2.79484	-0.16889
C	2.16476	-1.56988	1.89679
C	2.40484	-3.98506	0.53826
H	2.26859	-2.81713	-1.25798
C	2.24564	-2.76528	2.60317
H	2.06489	-0.63284	2.43876
C	2.38530	-3.97946	1.93526
H	2.49157	-4.92578	-0.00244
H	2.19852	-2.74504	3.69030
H	2.45465	-4.91161	2.49121
H	4.63963	2.64617	2.77231
H	-5.30017	3.36644	1.34184
C	-1.54300	2.47813	0.51974
C	1.17165	2.19797	0.95092

B-Cat-CH₃

C	-2.61238	1.36926	-0.10546
C	1.38345	3.43427	0.95524
H	0.55396	4.12743	1.08495
C	2.27479	1.33544	0.22697
C	3.71360	2.89906	1.40994
C	3.50259	1.65723	0.79429
H	4.32300	0.93763	0.74386
C	-1.96639	3.66514	0.16088
H	-1.22449	4.46245	0.14830
C	2.62256	3.77295	1.48490
H	2.75236	4.73291	1.98842
C	-3.92760	1.69876	0.20744
H	-4.68714	0.91502	0.23607
C	-3.29012	3.99763	0.41323
H	-3.55590	5.03967	0.60175
C	-4.30141	3.02611	0.45447
Ni	-0.05520	0.07065	-1.38180
P	1.94202	-0.26615	-0.62007
P	-2.00219	-0.30514	-0.51295
B	-0.14801	1.81562	-0.47924
C	-1.75713	-1.12228	1.11576
C	-2.05489	-0.49754	2.33282
C	-1.19403	-2.40723	1.14855
C	-1.81494	-1.14746	3.54215
H	-2.47281	0.50678	2.32821
C	-0.98972	-3.06919	2.35264
H	-0.89463	-2.87601	0.21143

C	-1.29513	-2.43807	3.55748	H	-5.81541	4.23394	1.41171
H	-2.04156	-0.64027	4.47785	H	-6.25115	3.71346	-0.21065
H	-0.54967	-4.06339	2.35237	H	-6.30078	2.55870	1.11508
H	-1.10381	-2.94269	4.50223				
C	-3.51626	-1.13724	-1.14347	B-Cat-Cl			
C	-4.18690	-0.51348	-2.21310	C	-2.56669	1.16620	-0.19916
C	-3.97921	-2.39073	-0.71881	C	1.44058	3.35209	0.51785
C	-5.28059	-1.11670	-2.82132	H	0.61189	4.05298	0.59827
H	-3.84667	0.46465	-2.54970	C	2.32629	1.18590	-0.00999
C	-5.07378	-2.99405	-1.33039	C	3.74810	2.85667	0.95308
H	-3.48476	-2.89118	0.11079	C	3.57241	1.55625	0.48375
C	-5.73210	-2.36256	-2.38578	H	4.40174	0.85106	0.49339
H	-5.78803	-0.61007	-3.63990	C	-1.92058	3.48207	-0.20325
H	-5.42344	-3.96021	-0.97146	H	-1.18452	4.27396	-0.32824
H	-6.58652	-2.83606	-2.86367	C	2.68612	3.75868	0.97818
C	3.46550	-0.44432	-1.63367	H	2.83940	4.75895	1.37549
C	3.64484	0.53534	-2.62869	C	-3.88162	1.51392	0.09329
C	4.42068	-1.46328	-1.53234	H	-4.64831	0.75083	0.21039
C	4.73171	0.48537	-3.49324	C	-3.23775	3.85165	0.03330
H	2.91292	1.33828	-2.71018	H	-3.51964	4.89951	0.10244
C	5.50915	-1.51164	-2.39975	C	-4.21003	2.86451	0.19739
H	4.32372	-2.21786	-0.75613	Ni	-0.04547	-0.25816	-1.39365
C	5.66988	-0.54112	-3.38750	P	1.97057	-0.50358	-0.64961
H	4.85033	1.25489	-4.25326	P	-1.97382	-0.54372	-0.46283
H	6.24396	-2.30751	-2.29396	B	-0.11568	1.58125	-0.68914
H	6.52091	-0.58011	-4.06357	C	-1.77145	-1.24491	1.22220
C	2.18762	-1.50846	0.70853	C	-2.07906	-0.53526	2.38888
C	2.22087	-2.87584	0.37584	C	-1.22401	-2.53148	1.34958
C	2.19959	-1.17229	2.07267	C	-1.86029	-1.10328	3.64276
C	2.34051	-3.85608	1.35245	H	-2.48868	0.46913	2.31192
H	2.15081	-3.16647	-0.67206	C	-1.03654	-3.10918	2.59881
C	2.28476	-2.15755	3.05207	H	-0.92400	-3.06940	0.45071
H	2.14380	-0.12669	2.36480	C	-1.34974	-2.39332	3.75303
C	2.37686	-3.50224	2.70300	H	-2.09625	-0.53212	4.53792
H	2.38613	-4.90360	1.06063	H	-0.60370	-4.10385	2.67296
H	2.28084	-1.86775	4.10093	H	-1.17483	-2.83268	4.73262
H	2.45095	-4.26840	3.47137	C	-3.48565	-1.38780	-1.07626
C	-1.56584	2.33422	-0.11870	C	-4.10370	-0.82217	-2.20655
C	1.16494	2.21898	0.26524	C	-4.00190	-2.58729	-0.56938
C	5.06065	3.28518	1.93944	C	-5.20553	-1.42903	-2.79610
H	5.70785	3.70814	1.15872	H	-3.71713	0.11311	-2.60806
H	4.98216	4.04203	2.72770	C	-5.10431	-3.19513	-1.16389
H	5.59739	2.42463	2.35417	H	-3.54618	-3.03917	0.30917
C	-5.73049	3.39954	0.70542	C	-5.71218	-2.62098	-2.27941

H	-5.67492	-0.96751	-3.66227	C	-3.24175	3.95277	0.05449
H	-5.49819	-4.11885	-0.74500	H	-3.49718	5.00859	0.11571
H	-6.57356	-3.09737	-2.74137	C	-4.28732	2.99734	0.12535
C	3.45270	-0.79395	-1.69480	Ni	-0.06450	-0.15384	-1.28819
C	3.52824	0.02590	-2.83524	P	1.99645	-0.35938	-0.62426
C	4.46797	-1.73397	-1.48396	P	-2.01539	-0.42792	-0.38574
C	4.57752	-0.09982	-3.73658	B	-0.13160	1.66434	-0.45589
H	2.74465	0.76521	-2.99976	C	-1.80447	-1.13992	1.28830
C	5.51653	-1.86250	-2.39282	C	-2.09023	-0.41529	2.45054
H	4.44995	-2.35828	-0.59412	C	-1.27003	-2.43129	1.41667
C	5.57470	-1.05108	-3.52398	C	-1.86678	-0.97711	3.70558
H	4.61830	0.54697	-4.61012	H	-2.48548	0.59440	2.36701
H	6.29955	-2.59509	-2.20824	C	-1.07806	-3.00175	2.66914
H	6.39464	-1.15422	-4.23083	H	-0.98812	-2.98400	0.52108
C	2.22745	-1.56299	0.82222	C	-1.37365	-2.27381	3.82018
C	2.37414	-2.95597	0.68302	H	-2.08810	-0.39717	4.59831
C	2.10249	-1.04884	2.12463	H	-0.66083	-4.00262	2.74642
C	2.46095	-3.78631	1.79385	H	-1.20287	-2.71019	4.80144
H	2.41411	-3.39026	-0.31508	C	-3.46053	-1.32698	-1.06854
C	2.15734	-1.88566	3.23320	C	-4.02991	-0.79677	-2.23825
H	1.95672	0.01920	2.26701	C	-3.99200	-2.50933	-0.54243
C	2.35662	-3.25553	3.08062	C	-5.10711	-1.42410	-2.85186
H	2.59472	-4.85733	1.65426	H	-3.62985	0.12790	-2.65085
H	2.04348	-1.45962	4.22769	C	-5.06796	-3.13971	-1.16317
H	2.40474	-3.90623	3.95049	H	-3.57374	-2.92954	0.36925
C	-1.52427	2.12577	-0.33954	C	-5.62944	-2.60134	-2.31825
C	1.21343	2.06719	-0.03385	H	-5.54291	-0.99132	-3.74912
Cl	5.33828	3.38003	1.50258	H	-5.47594	-4.05183	-0.73355
Cl	-5.88379	3.33472	0.48998	H	-6.47080	-3.09397	-2.79899
B-Cat-CN				C	3.46012	-0.63462	-1.69892
C	-2.62246	1.26103	-0.15016	C	3.55503	0.22224	-2.80731
C	1.42540	3.40122	0.74271	C	4.45397	-1.60047	-1.51186
H	0.58657	4.08289	0.86244	C	4.61331	0.11509	-3.70066
C	2.34362	1.26678	0.11115	H	2.78532	0.97886	-2.95507
C	3.78701	2.94177	1.10457	C	5.51041	-1.71223	-2.41429
C	3.59018	1.64875	0.56977	H	4.41147	-2.25987	-0.64847
H	4.43376	0.96189	0.51063	C	5.59310	-0.85856	-3.51059
C	-1.92638	3.56859	-0.08370	H	4.67377	0.79154	-4.54974
H	-1.16641	4.34399	-0.15053	H	6.27859	-2.46455	-2.25110
C	2.66572	3.80461	1.18560	H	6.41931	-0.94753	-4.21165
H	2.79654	4.79086	1.62545	C	2.19909	-1.57651	0.72433
C	-3.94069	1.62929	0.03062	C	2.20922	-2.94848	0.41761
H	-4.72414	0.87458	0.07954	C	2.22082	-1.20098	2.07517
				C	2.29216	-3.90675	1.42027

H	2.15596	-3.26293	-0.62396
C	2.28031	-2.16348	3.07847
H	2.19059	-0.14593	2.33641
C	2.33073	-3.51823	2.75922
H	2.31497	-4.96173	1.15623
H	2.28771	-1.84905	4.11932
H	2.38505	-4.26647	3.54628
C	-1.54166	2.19857	-0.20287
C	1.19983	2.12321	0.15200
C	5.06080	3.36020	1.55138
C	-5.63259	3.40178	0.27082
N	6.11761	3.70799	1.92966
N	-6.75077	3.74134	0.39893

B-Cat-NH₂

C	-2.39765	1.49059	-0.15305
C	1.71560	2.97426	1.69193
H	0.87314	3.52510	2.10900
C	2.61827	1.23361	0.31853
C	4.11625	2.65156	1.58531
C	3.90798	1.59528	0.68326
H	4.76362	1.04330	0.29168
C	-1.35528	3.59712	0.33533
H	-0.46619	4.19580	0.53321
C	3.00150	3.32498	2.09737
H	3.15284	4.12855	2.81903
C	-3.63476	2.12198	-0.23674
H	-4.52889	1.54820	-0.48163
C	-2.58180	4.24296	0.23211
H	-2.65675	5.32198	0.37104
C	-3.74228	3.50597	-0.04214
Ni	0.05440	-0.31209	-0.70576
P	2.19324	-0.26811	-0.67108
P	-2.08926	-0.31327	-0.43663
B	0.09778	1.36925	0.27968
C	-2.42788	-1.09810	1.18500
C	-3.58076	-0.80524	1.92720
C	-1.49643	-1.99926	1.71626
C	-3.79914	-1.40662	3.16529
H	-4.30798	-0.10134	1.52517
C	-1.71927	-2.60926	2.94623
H	-0.58639	-2.20937	1.15111
C	-2.87377	-2.31246	3.67644
H	-4.69514	-1.16417	3.73387

H	-0.98461	-3.31077	3.33501
H	-3.04507	-2.78106	4.64338
C	-3.63437	-0.77604	-1.36996
C	-3.96236	-0.07734	-2.54954
C	-4.35718	-1.95260	-1.10263
C	-4.97837	-0.50842	-3.39192
H	-3.40673	0.82679	-2.79789
C	-5.37163	-2.38886	-1.94744
H	-4.12115	-2.52852	-0.20947
C	-5.69786	-1.66837	-3.09716
H	-5.21578	0.06544	-4.28663
H	-5.92256	-3.29515	-1.70046
H	-6.49252	-2.00891	-3.75693
C	3.76244	-0.50082	-1.61867
C	4.01470	0.43266	-2.64349
C	4.64336	-1.59100	-1.50158
C	5.09415	0.29559	-3.50098
H	3.34193	1.28325	-2.75594
C	5.71501	-1.74121	-2.37977
H	4.49094	-2.31928	-0.70788
C	5.95312	-0.80261	-3.38155
H	5.27159	1.04446	-4.27077
H	6.38343	-2.59369	-2.26679
H	6.79394	-0.92209	-4.06074
C	2.18945	-1.60546	0.58392
C	2.06373	-2.94021	0.15856
C	2.10294	-1.33142	1.95740
C	1.85861	-3.96658	1.08218
H	2.11121	-3.16403	-0.90550
C	1.89498	-2.35701	2.87518
H	2.16629	-0.30158	2.29940
C	1.77350	-3.67828	2.44158
H	1.75451	-4.99185	0.73350
H	1.80547	-2.12101	3.93334
H	1.60171	-4.47643	3.16098
C	-1.21683	2.20646	0.17568
C	1.47295	1.92219	0.78882
N	5.41014	2.96479	2.02449
H	6.12320	2.71976	1.35274
H	5.51226	3.92838	2.30829
N	-4.99457	4.13114	-0.07727
H	-4.95230	5.10028	-0.35682
H	-5.67031	3.63120	-0.63688

B-Cat-NO₂

C	-2.58324	1.06417	-0.21263
C	1.54141	3.20664	0.56584
H	0.68668	3.85110	0.75314
C	2.49985	1.08544	-0.05429
C	3.93306	2.86462	0.67490
C	3.76876	1.54233	0.23384
H	4.65104	0.91667	0.12813
C	-1.75082	3.32505	-0.31462
H	-0.94174	4.04452	-0.40868
C	2.79899	3.68528	0.85129
H	2.95364	4.68848	1.23467
C	-3.88593	1.51433	-0.17542
H	-4.73523	0.83703	-0.14271
C	-3.04425	3.79277	-0.29418
H	-3.26657	4.85378	-0.34246
C	-4.13099	2.89759	-0.21473
Ni	-0.02038	-0.60906	-0.94531
P	2.12111	-0.59953	-0.56820
P	-2.06801	-0.66270	-0.21285
B	-0.04257	1.33243	-0.34379
C	-2.20789	-1.26141	1.51358
C	-3.38184	-1.07224	2.25416
C	-1.12040	-1.90366	2.11209
C	-3.46353	-1.52164	3.56696
H	-4.22814	-0.56194	1.79838
C	-1.20385	-2.35590	3.42776
H	-0.20213	-2.03594	1.53997
C	-2.37463	-2.16573	4.15487
H	-4.37630	-1.36352	4.13591
H	-0.34593	-2.84852	3.87938
H	-2.43987	-2.51255	5.18341
C	-3.41013	-1.57573	-1.05839
C	-3.93571	-1.05357	-2.24930
C	-3.87174	-2.81727	-0.60582
C	-4.91308	-1.74685	-2.95412
H	-3.59007	-0.08545	-2.60554
C	-4.84755	-3.51142	-1.31629
H	-3.47661	-3.23499	0.31762
C	-5.37255	-2.97811	-2.49001
H	-5.32316	-1.31984	-3.86563
H	-5.20409	-4.46909	-0.94501
H	-6.14045	-3.51655	-3.03947
C	3.40386	-1.06890	-1.78602

C	3.11062	-0.87236	-3.14091
C	4.67209	-1.54349	-1.42933
C	4.06507	-1.13510	-4.11832
H	2.12481	-0.50159	-3.41816
C	5.62492	-1.80954	-2.40837
H	4.91166	-1.70236	-0.38009
C	5.32379	-1.60575	-3.75295
H	3.82527	-0.97319	-5.16612
H	6.60896	-2.16918	-2.11863
H	6.07101	-1.81151	-4.51514
C	2.48401	-1.64946	0.88279
C	2.72157	-3.02553	0.73849
C	2.37224	-1.12120	2.17749
C	2.85008	-3.84518	1.85493
H	2.80949	-3.45465	-0.25822
C	2.49965	-1.94373	3.29049
H	2.17873	-0.05820	2.30443
C	2.73814	-3.30937	3.13652
H	3.03845	-4.90803	1.72243
H	2.41087	-1.51410	4.28523
H	2.83791	-3.95052	4.00861
C	-1.44192	1.92819	-0.27001
C	1.31816	1.88602	0.06353
N	5.22958	3.36061	0.96294
N	-5.46039	3.38410	-0.19226
O	-6.39769	2.55501	-0.12709
O	-5.64427	4.62215	-0.23219
O	6.20902	2.59534	0.81042
O	5.33885	4.54205	1.36140

B-Cat-OCH₃

C	-2.65739	1.04081	-0.34624
C	1.26914	3.26211	0.50885
H	0.40544	3.91993	0.59791
C	2.25335	1.15599	-0.05096
C	3.60895	2.88279	0.94822
C	3.47501	1.58142	0.44892
H	4.34172	0.92202	0.46140
C	-2.03665	3.35628	-0.44273
H	-1.30145	4.14920	-0.57315
C	2.49608	3.72386	0.98759
H	2.57136	4.72749	1.39840
C	-3.98026	1.39399	-0.11596
H	-4.75132	0.63878	0.02395

C	-3.37168	3.72707	-0.28293	H	2.58143	-3.40075	-0.39232
H	-3.63862	4.78068	-0.28769	C	2.62643	-1.90765	3.16780
C	-4.34779	2.74465	-0.10291	H	2.21262	-0.02066	2.23753
Ni	-0.06826	-0.41036	-1.38359	C	2.87926	-3.26574	2.99255
P	1.97017	-0.55817	-0.69400	H	3.04169	-4.85596	1.53933
P	-2.01360	-0.67544	-0.46959	H	2.59451	-1.48533	4.17059
B	-0.19578	1.44419	-0.75367	H	3.05802	-3.91133	3.84926
C	-1.65839	-1.14705	1.27468	C	-1.62196	2.00844	-0.49508
C	-2.09256	-0.39804	2.37435	C	1.10524	1.98902	-0.06933
C	-0.90237	-2.30417	1.51225	O	4.86598	3.23385	1.38065
C	-1.78222	-0.79863	3.67251	O	-5.69033	3.00161	0.08148
H	-2.67191	0.50759	2.20896	C	5.00728	4.52392	1.91309
C	-0.62115	-2.72190	2.80749	H	4.37202	4.67863	2.79786
H	-0.51446	-2.86192	0.65977	H	6.05437	4.62699	2.20535
C	-1.05483	-1.96430	3.89404	H	4.76132	5.30522	1.17866
H	-2.11492	-0.19610	4.51531	C	-6.06403	4.35081	0.12567
H	-0.02452	-3.61700	2.96585	H	-7.14304	4.37138	0.29460
H	-0.80898	-2.27306	4.90804	H	-5.56396	4.89418	0.94233
C	-3.54038	-1.65030	-0.80294	H	-5.83927	4.87740	-0.81483
C	-4.32059	-1.30200	-1.92279				
C	-3.89119	-2.81190	-0.09717	B-RC-H			
C	-5.41194	-2.07234	-2.30465	C	-2.54705	1.62437	0.15680
H	-4.06964	-0.40120	-2.48102	C	1.38947	3.32922	1.72549
C	-4.98166	-3.58378	-0.48293	H	0.57952	4.03446	1.90749
H	-3.30836	-3.10564	0.77307	C	2.25917	1.35059	0.68731
C	-5.75143	-3.22073	-1.58851	C	3.63265	2.58066	2.24417
H	-6.00613	-1.77297	-3.16595	C	3.44987	1.48978	1.39145
H	-5.24090	-4.47072	0.09218	H	4.24176	0.75025	1.26829
H	-6.60500	-3.82399	-1.88808	C	-1.87215	3.86293	0.71164
C	3.40908	-0.74970	-1.82031	H	-1.11410	4.63839	0.81454
C	3.38573	0.04680	-2.98182	C	2.59207	3.49501	2.40829
C	4.49278	-1.61952	-1.64138	H	2.71754	4.33776	3.08768
C	4.39651	-0.04486	-3.93127	C	-3.87064	1.93470	0.44422
H	2.55491	0.73772	-3.12427	H	-4.64396	1.17400	0.33718
C	5.50196	-1.71195	-2.59540	C	-3.20439	4.19401	0.94405
H	4.55701	-2.22068	-0.73839	H	-3.46363	5.21351	1.22870
C	5.45894	-0.92952	-3.74898	C	-4.21225	3.23601	0.82476
H	4.35703	0.58187	-4.81996	Ni	-0.00868	0.52891	-1.38147
H	6.33564	-2.39188	-2.42965	P	1.87995	-0.02797	-0.46842
H	6.24902	-1.00155	-4.49289	P	-1.89906	0.02831	-0.46209
C	2.43303	-1.58144	0.76050	B	-0.07512	2.03585	-0.09526
C	2.62738	-2.96874	0.60690	H	0.01219	0.63388	-3.02504
C	2.40728	-1.07737	2.07363	H	0.06858	-0.20913	-2.88138
C	2.87014	-3.79278	1.69752	C	-1.82648	-1.00667	1.05602

C	-1.66101	-0.43305	2.32461	H	-5.25093	3.50151	1.00983
C	-1.82548	-2.40703	0.95950	C	1.19233	2.27307	0.81052
C	-1.53364	-1.23188	3.45765	C	-1.49364	2.56781	0.29139
H	-1.63831	0.65118	2.41990				
C	-1.70893	-3.20314	2.09165	B-RC-CH₃			
H	-1.92364	-2.87160	-0.02060	C	-2.53534	1.36422	-0.01721
C	-1.56664	-2.61979	3.35051	C	1.46268	3.58740	0.65591
H	-1.40917	-0.76328	4.43192	H	0.64064	4.29582	0.73875
H	-1.70906	-4.28653	1.99017	C	2.33536	1.43044	0.10651
H	-1.46325	-3.24349	4.23576	C	3.79827	3.08329	1.11689
C	-3.35396	-0.71221	-1.32701	C	3.57334	1.79065	0.62103
C	-3.39270	-0.58888	-2.72103	H	4.39063	1.06694	0.62969
C	-4.41785	-1.36243	-0.68723	C	-1.91572	3.67694	0.04890
C	-4.46285	-1.08953	-3.45593	H	-1.19217	4.48244	-0.06391
H	-2.55750	-0.09703	-3.21904	C	2.71603	3.96742	1.12763
C	-5.48534	-1.87410	-1.42112	H	2.86102	4.96976	1.53435
H	-4.40050	-1.47568	0.39516	C	-3.84452	1.69503	0.31320
C	-5.51221	-1.73775	-2.80736	H	-4.59450	0.90653	0.40537
H	-4.47365	-0.98386	-4.53856	C	-3.23724	4.01052	0.33198
H	-6.30097	-2.37971	-0.90826	H	-3.51515	5.05993	0.44632
H	-6.34516	-2.13997	-3.37997	C	-4.22703	3.03452	0.48338
C	3.42911	-0.13035	-1.46362	Ni	-0.04158	0.02708	-1.46765
C	3.47061	0.65097	-2.62737	P	1.90723	-0.23193	-0.56168
C	4.55694	-0.89315	-1.13371	P	-1.91399	-0.30795	-0.42966
C	4.60437	0.67460	-3.43185	B	-0.10293	1.79101	-0.55723
H	2.58695	1.23619	-2.88433	H	-0.17397	-0.22680	-3.09461
C	5.68917	-0.87834	-1.94523	H	-0.05780	-1.01369	-2.78339
H	4.54288	-1.50814	-0.23606	C	-1.80690	-1.19779	1.17788
C	5.71880	-0.09318	-3.09529	C	-2.38887	-0.74085	2.36562
H	4.61733	1.28896	-4.32952	C	-1.08817	-2.40155	1.20437
H	6.55519	-1.47884	-1.67380	C	-2.27313	-1.48007	3.54143
H	6.60441	-0.08089	-3.72674	H	-2.93327	0.20118	2.36457
C	2.03240	-1.50041	0.61943	C	-1.00332	-3.15657	2.36807
C	2.18187	-2.77480	0.04459	H	-0.57954	-2.72331	0.29519
C	1.84401	-1.42773	2.00825	C	-1.59419	-2.69571	3.54331
C	2.17964	-3.92235	0.82681	H	-2.72319	-1.10650	4.45920
H	2.30288	-2.85702	-1.03500	H	-0.43787	-4.08542	2.36816
C	1.81965	-2.58018	2.78820	H	-1.50658	-3.27260	4.46180
H	1.71225	-0.45732	2.48068	C	-3.40575	-1.10228	-1.15889
C	1.99508	-3.83269	2.20818	C	-4.03912	-0.44450	-2.22857
H	2.31186	-4.89462	0.35610	C	-3.88710	-2.36246	-0.78127
H	1.65703	-2.49417	3.86087	C	-5.12006	-1.02377	-2.88279
H	1.97596	-4.73116	2.82063	H	-3.67439	0.53450	-2.53587
H	4.57282	2.71363	2.77587	C	-4.96659	-2.94327	-1.44047

H	-3.41682	-2.89095	0.04488	C	3.48489	1.61880	0.47436
C	-5.59133	-2.27729	-2.49307	H	4.31827	0.92611	0.57529
H	-5.59988	-0.49325	-3.70282	C	-1.96526	3.45478	-0.66926
H	-5.32832	-3.91919	-1.12232	H	-1.23899	4.23601	-0.88760
H	-6.43621	-2.73043	-3.00668	C	2.56509	3.84580	0.76615
C	3.39901	-0.66324	-1.55940	H	2.69755	4.87365	1.09388
C	3.29207	-0.50870	-2.94746	C	-3.89620	1.50438	-0.12702
C	4.62346	-1.09514	-1.03139	H	-4.65479	0.75442	0.08555
C	4.37370	-0.76948	-3.78298	C	-3.29700	3.82603	-0.50912
H	2.33587	-0.17819	-3.35326	H	-3.60223	4.86609	-0.59157
C	5.70445	-1.36670	-1.86657	C	-4.24938	2.85017	-0.22820
H	4.72335	-1.23386	0.04343	Ni	-0.06368	-0.36231	-1.54115
C	5.58427	-1.20268	-3.24468	P	1.90106	-0.50289	-0.63115
H	4.26978	-0.64304	-4.85838	P	-1.88198	-0.54673	-0.38693
H	6.64589	-1.70605	-1.43902	B	-0.13601	1.50101	-0.87328
H	6.42934	-1.41546	-3.89581	H	-0.14282	-0.87463	-3.10731
C	2.14894	-1.26862	0.93945	H	-0.03147	-1.60079	-2.67121
C	2.52861	-2.61832	0.84820	C	-1.67112	-0.94923	1.39528
C	1.79437	-0.77420	2.20607	C	-1.49251	0.04545	2.36590
C	2.60083	-3.42321	1.97989	C	-1.58017	-2.29100	1.79747
H	2.78133	-3.03559	-0.12574	C	-1.26310	-0.29231	3.69738
C	1.85418	-1.58275	3.33462	H	-1.53771	1.09311	2.07392
H	1.46862	0.26033	2.29960	C	-1.35996	-2.62646	3.12685
C	2.27014	-2.90918	3.23415	H	-1.68915	-3.07742	1.05210
H	2.91572	-4.46083	1.88175	C	-1.20604	-1.62759	4.08758
H	1.56599	-1.17413	4.30115	H	-1.13181	0.49676	4.43481
H	2.31691	-3.54085	4.11831	H	-1.29144	-3.67389	3.41309
C	1.23126	2.31591	0.09058	H	-1.02301	-1.88950	5.12723
C	-1.51182	2.33844	-0.15026	C	-3.35462	-1.57991	-0.80166
C	-5.65025	3.40166	0.77606	C	-3.49072	-2.00698	-2.12720
H	-5.74398	4.46039	1.03979	C	-4.35242	-1.92818	0.11837
H	-6.30981	3.22355	-0.08368	C	-4.59646	-2.75165	-2.52811
H	-6.06388	2.81631	1.60638	H	-2.70756	-1.74760	-2.83906
C	5.15378	3.49916	1.60136	C	-5.45670	-2.67741	-0.27913
H	5.83901	3.71747	0.77137	H	-4.25559	-1.61258	1.15566
H	5.10164	4.40209	2.21865	C	-5.58244	-3.08948	-1.60403
H	5.63212	2.71409	2.19825	H	-4.68535	-3.07495	-3.56284
B-RC-CI				H	-6.22344	-2.93761	0.44752
C	-2.57163	1.15176	-0.34973	H	-6.44455	-3.67571	-1.91344
C	1.34439	3.39704	0.27123	C	3.39069	-0.89607	-1.64130
H	0.50925	4.09534	0.25048	C	3.29860	-0.63981	-3.01628
C	2.26560	1.20679	-0.05130	C	4.59622	-1.39768	-1.13423
C	3.62692	2.95145	0.85896	C	4.38095	-0.87039	-3.85851
				H	2.35458	-0.25682	-3.40521

C	5.67751	-1.63705	-1.97881	H	-0.03062	-1.69156	-2.35834
H	4.68241	-1.61082	-0.07044	C	-1.77818	-0.93374	1.41569
C	5.57469	-1.37228	-3.34227	C	-1.65227	0.02191	2.43184
H	4.29175	-0.66428	-4.92288	C	-1.68492	-2.29045	1.75995
H	6.60658	-2.02735	-1.56883	C	-1.46946	-0.36934	3.75460
H	6.42064	-1.55841	-4.00018	H	-1.70176	1.07944	2.18025
C	2.19318	-1.50361	0.87924	C	-1.51183	-2.67937	3.08282
C	2.40627	-2.88746	0.75465	H	-1.76006	-3.04597	0.97917
C	2.04956	-0.97513	2.17070	C	-1.40748	-1.72028	4.08840
C	2.50069	-3.70358	1.87398	H	-1.37833	0.38845	4.52938
H	2.50059	-3.32195	-0.23980	H	-1.44270	-3.73690	3.32796
C	2.12401	-1.79814	3.29078	H	-1.26194	-2.02435	5.12235
H	1.87099	0.09006	2.29899	C	-3.35197	-1.44456	-0.92208
C	2.35815	-3.16279	3.15315	C	-3.46527	-1.65280	-2.30216
H	2.67904	-4.76978	1.74886	C	-4.34323	-1.96547	-0.08092
H	1.99568	-1.36389	4.27998	C	-4.54106	-2.35842	-2.83076
H	2.41652	-3.80245	4.03060	H	-2.69209	-1.24984	-2.95593
C	1.15891	2.07728	-0.19355	C	-5.41616	-2.67885	-0.60887
C	-1.55301	2.10369	-0.61847	H	-4.26939	-1.81242	0.99366
Cl	-5.93655	3.31902	-0.03154	C	-5.51775	-2.87736	-1.98377
Cl	5.18051	3.52082	1.46441	H	-4.61494	-2.50835	-3.90514
B-RC-CN				H	-6.17887	-3.07637	0.05664
C	-2.57612	1.25874	-0.28772	H	-6.35680	-3.43443	-2.39375
C	1.42191	3.49204	0.31335	C	3.40448	-0.88649	-1.56892
H	0.58806	4.19019	0.31722	C	3.32260	-0.68734	-2.95292
C	2.33823	1.29541	-0.02151	C	4.59306	-1.39728	-1.03235
C	3.76062	3.06286	0.81609	C	4.40320	-0.98006	-3.77897
C	3.57268	1.71536	0.43340	H	2.39242	-0.29698	-3.36584
H	4.41072	1.02212	0.49034	C	5.67219	-1.69637	-1.85965
C	-1.90051	3.55273	-0.54959	H	4.66795	-1.56667	0.04005
H	-1.15160	4.31762	-0.74181	C	5.58060	-1.48724	-3.23384
C	2.65353	3.93726	0.75205	H	4.32444	-0.81740	-4.85127
H	2.78298	4.96904	1.07177	H	6.59005	-2.08988	-1.42915
C	-3.89078	1.63360	-0.10745	H	6.42489	-1.72135	-3.87779
H	-4.66561	0.88813	0.06428	C	2.12192	-1.41790	0.93430
C	-3.21774	3.94494	-0.41189	C	2.31870	-2.80356	0.81748
H	-3.48363	4.99787	-0.47664	C	1.93503	-0.87994	2.21528
C	-4.24319	3.00188	-0.17735	C	2.35508	-3.61730	1.94330
Ni	-0.05588	-0.27842	-1.44301	H	2.45005	-3.24245	-0.17041
P	1.93933	-0.39572	-0.57299	C	1.96183	-1.69849	3.33950
P	-1.92706	-0.43680	-0.34401	H	1.76447	0.18859	2.32878
B	-0.10525	1.58716	-0.71756	C	2.17810	-3.06823	3.21279
H	-0.13075	-1.06900	-2.91393	H	2.51852	-4.68673	1.82865
				H	1.80995	-1.25939	4.32267

H	2.19811	-3.70442	4.09413	C	-4.37104	-1.80301	-0.19873
C	1.21030	2.15710	-0.12500	C	-4.62025	-2.06903	-2.95750
C	-1.51408	2.18471	-0.50369	H	-2.75160	-0.98899	-3.06065
C	-5.58739	3.41710	-0.02736	C	-5.45862	-2.48631	-0.73863
C	5.02238	3.52391	1.26311	H	-4.27826	-1.70108	0.88083
N	-6.70161	3.76390	0.10503	C	-5.58906	-2.62012	-2.11905
N	6.06745	3.90588	1.63739	H	-4.71134	-2.17253	-4.03667
B-RC-NH₂				H	-6.21048	-2.91294	-0.07715
C	-2.57420	1.37325	-0.19706	H	-6.43799	-3.15516	-2.53942
C	1.32781	3.47543	0.80123	C	3.40127	-0.53413	-1.61186
H	0.49733	4.17924	0.84751	C	3.32177	-0.14114	-2.95533
C	2.24363	1.34889	0.21334	C	4.61528	-1.05745	-1.14509
C	3.61593	2.94923	1.40303	C	4.41796	-0.26019	-3.80249
C	3.44163	1.67993	0.83200	H	2.37300	0.25882	-3.31486
H	4.26124	0.95934	0.86716	C	5.71117	-1.18674	-1.99527
C	-1.96640	3.68693	-0.21236	H	4.69431	-1.37839	-0.10802
H	-1.23730	4.48921	-0.32334	C	5.61915	-0.78565	-3.32586
C	2.53604	3.84002	1.38688	H	4.33449	0.05068	-4.84194
H	2.65151	4.81979	1.85223	H	6.64379	-1.59933	-1.61467
C	-3.89782	1.70446	0.06168	H	6.47635	-0.88464	-3.98858
H	-4.65055	0.92188	0.17193	C	2.19170	-1.43981	0.81060
C	-3.30108	4.03442	-0.02153	C	2.48463	-2.78908	0.54537
H	-3.59315	5.08462	0.02077	C	1.94576	-1.07521	2.14408
C	-4.28560	3.05068	0.12731	C	2.56821	-3.72369	1.56873
Ni	-0.05049	-0.02708	-1.50352	H	2.65163	-3.10060	-0.48529
P	1.88859	-0.28024	-0.58548	C	2.00752	-2.01750	3.16665
P	-1.89920	-0.32027	-0.44120	H	1.69837	-0.04275	2.37978
B	-0.13209	1.75234	-0.62523	C	2.32832	-3.34361	2.89130
H	-0.11815	-0.17846	-3.13529	H	2.81447	-4.75774	1.33436
H	-0.02801	-0.99253	-2.86096	H	1.79282	-1.70931	4.18823
C	-1.75062	-0.95491	1.27902	H	2.37777	-4.07741	3.69281
C	-1.62822	-0.10239	2.38467	C	1.14674	2.23801	0.15400
C	-1.62424	-2.33733	1.49234	C	-1.55191	2.34528	-0.33207
C	-1.41806	-0.61826	3.66236	N	-5.62601	3.40217	0.38495
H	-1.69758	0.97412	2.23791	H	-5.87939	4.28273	-0.04190
C	-1.42658	-2.85066	2.76657	H	-6.26985	2.68693	0.07563
H	-1.67859	-3.01150	0.63857	N	4.82298	3.28997	2.03591
C	-1.32824	-1.99251	3.86283	H	5.61024	2.77593	1.66617
H	-1.32683	0.06288	4.50638	H	5.01620	4.28082	2.00237
H	-1.32634	-3.92527	2.90504	B-RC-NO₂			
H	-1.15956	-2.39387	4.85978	C	-2.57817	1.05746	-0.32314
C	-3.38533	-1.25160	-1.02926	C	1.47877	3.32480	0.18524
C	-3.52795	-1.40044	-2.41520	H	0.63615	4.00922	0.23849

C	2.40874	1.13132	-0.16036
C	3.84298	2.93343	0.49544
C	3.67024	1.57882	0.17241
H	4.53827	0.92567	0.18141
C	-1.86039	3.34050	-0.59902
H	-1.09590	4.09080	-0.78378
C	2.73096	3.79799	0.50786
H	2.89512	4.83181	0.79340
C	-3.89428	1.44475	-0.19786
H	-4.69946	0.73173	-0.04230
C	-3.17219	3.74947	-0.50188
H	-3.44977	4.79541	-0.58224
C	-4.20263	2.81239	-0.29077
Ni	-0.05697	-0.55552	-1.37635
P	1.98256	-0.56387	-0.60835
P	-1.94985	-0.62983	-0.29826
B	-0.08458	1.37383	-0.64846
H	-0.50647	-1.64174	-2.58591
H	0.31208	-1.74408	-2.52263
C	-1.76484	-1.09083	1.46272
C	-1.83771	-0.13415	2.48111
C	-1.48153	-2.42134	1.80378
C	-1.65223	-0.50542	3.81019
H	-2.04428	0.90313	2.22751
C	-1.30809	-2.79016	3.13202
H	-1.39719	-3.17129	1.01843
C	-1.39591	-1.83328	4.14123
H	-1.71714	0.24894	4.59045
H	-1.08240	-3.82490	3.37835
H	-1.24963	-2.12000	5.18003
C	-3.35418	-1.67696	-0.84610
C	-3.53782	-1.84821	-2.22324
C	-4.28064	-2.24997	0.03301
C	-4.61768	-2.57383	-2.71327
H	-2.82015	-1.39945	-2.90970
C	-5.35830	-2.98280	-0.45724
H	-4.15799	-2.11811	1.10547
C	-5.52862	-3.14800	-1.82918
H	-4.74747	-2.69364	-3.78583
H	-6.07231	-3.41886	0.23679
H	-6.37168	-3.71992	-2.20865
C	3.41001	-1.18925	-1.57537
C	3.31583	-1.17609	-2.97121
C	4.60329	-1.62317	-0.98352

C	4.38932	-1.57725	-3.76051
H	2.38587	-0.84180	-3.43029
C	5.67582	-2.02757	-1.77242
H	4.68729	-1.64696	0.10097
C	5.57128	-2.00518	-3.16140
H	4.30154	-1.55919	-4.84387
H	6.59804	-2.35749	-1.30083
H	6.41080	-2.32131	-3.77539
C	2.09078	-1.53931	0.93393
C	2.22557	-2.93445	0.86684
C	1.94670	-0.93884	2.19148
C	2.24027	-3.70374	2.02465
H	2.33289	-3.41622	-0.10395
C	1.95624	-1.71256	3.34683
H	1.82898	0.14049	2.26007
C	2.10913	-3.09517	3.27123
H	2.35484	-4.78292	1.95242
H	1.83607	-1.23004	4.31366
H	2.11477	-3.69566	4.17757
C	1.25251	1.96901	-0.19792
C	-1.48912	1.96429	-0.51526
N	-5.54988	3.24700	-0.18091
N	5.13550	3.42503	0.82476
O	-5.78866	4.47230	-0.25717
O	-6.43998	2.38596	-0.00703
O	6.09585	2.62441	0.81885
O	5.25561	4.63647	1.10919

B-RC-OCH₃

C	-2.61903	1.00341	-0.46114
C	1.18521	3.31105	0.18019
H	0.32610	3.97933	0.12439
C	2.18801	1.15747	-0.09871
C	3.46784	2.95487	0.86951
C	3.36511	1.61578	0.47263
H	4.22126	0.95919	0.62062
C	-2.07561	3.29049	-0.93052
H	-1.36959	4.07598	-1.19908
C	2.37100	3.80563	0.72781
H	2.42504	4.84176	1.05090
C	-3.94557	1.34195	-0.24614
H	-4.69201	0.59795	0.02659
C	-3.42029	3.64157	-0.78249
H	-3.72421	4.67352	-0.93669

C	-4.35558	2.66868	-0.42974	H	2.62703	-3.35749	-0.27408
Ni	-0.07920	-0.53096	-1.55780	C	2.27715	-1.84122	3.26070
P	1.89648	-0.57650	-0.66609	H	1.94293	0.03591	2.27474
P	-1.86097	-0.66907	-0.35688	C	2.55187	-3.19766	3.12118
B	-0.19618	1.36303	-0.99853	H	2.90015	-4.79463	1.71041
H	-0.17507	-1.00712	-3.12651	H	2.14665	-1.40938	4.25113
H	-0.05579	-1.74683	-2.70313	H	2.64748	-3.83451	3.99775
C	-1.55894	-0.84599	1.45144	C	1.06054	1.99300	-0.28872
C	-1.25621	0.26824	2.24724	C	-1.62807	1.96369	-0.80237
C	-1.49932	-2.11685	2.04517	O	-5.70059	2.90990	-0.24742
C	-0.95148	0.11932	3.59761	O	4.68067	3.33255	1.39486
H	-1.26362	1.26137	1.80030	C	-6.12819	4.22990	-0.44151
C	-1.19824	-2.26362	3.39343	H	-7.20647	4.23820	-0.26744
H	-1.69495	-2.99820	1.43659	H	-5.64808	4.93028	0.25918
C	-0.93350	-1.14434	4.18224	H	-5.92698	4.58559	-1.46350
H	-0.72734	1.00022	4.19585	C	4.79173	4.66594	1.81733
H	-1.15428	-3.25978	3.82922	H	4.07510	4.90804	2.61625
H	-0.69296	-1.26058	5.23684	H	5.80664	4.78761	2.20132
C	-3.31104	-1.79341	-0.58236	H	4.63208	5.37617	0.99250
C	-3.44331	-2.42356	-1.82476				
C	-4.28659	-2.03400	0.39463	B-TS-H			
C	-4.52193	-3.26159	-2.09202	C	-2.28874	1.41665	0.65633
H	-2.67260	-2.24980	-2.57565	C	-1.21510	2.33047	0.77062
C	-5.36164	-2.88003	0.13419	C	1.49752	2.55980	0.29727
H	-4.19078	-1.56020	1.36999	C	1.87765	3.86132	0.68246
C	-5.48377	-3.49392	-1.11088	H	1.12457	4.64476	0.75571
H	-4.60828	-3.74172	-3.06438	C	2.54045	1.60534	0.18876
H	-6.10939	-3.05825	0.90431	C	4.20993	3.22095	0.83280
H	-6.32344	-4.15530	-1.31339	C	3.86586	1.91501	0.47574
C	3.38721	-0.88676	-1.70501	H	4.63568	1.14836	0.38753
C	3.25876	-0.63061	-3.07772	C	-1.41969	3.43374	1.62272
C	4.62696	-1.32649	-1.22273	H	-0.60812	4.14088	1.78667
C	4.33574	-0.80305	-3.93986	C	3.21056	4.18990	0.92068
H	2.28910	-0.29324	-3.44617	H	3.47568	5.21374	1.18179
C	5.70348	-1.50864	-2.08756	C	-3.49399	1.60181	1.32616
H	4.74392	-1.53520	-0.16097	H	-4.29455	0.87031	1.21707
C	5.56359	-1.24571	-3.44818	C	-2.63614	3.64519	2.26805
H	4.21648	-0.59799	-5.00182	H	-2.77018	4.52194	2.90059
H	6.65853	-1.85253	-1.69514	C	-3.68033	2.73268	2.12263
H	6.40610	-1.38512	-4.12234	Ni	0.00724	0.51564	-1.38574
C	2.28905	-1.54609	0.84644	P	1.88191	0.01067	-0.42499
C	2.54326	-2.92382	0.72200	P	-1.87289	0.00038	-0.44067
C	2.15632	-1.02189	2.14124	B	0.07671	2.00939	-0.08071
C	2.68819	-3.73468	1.83869	H	0.08753	1.01056	-2.82239

H	-0.02965	-0.33181	-2.68393
C	-3.39788	-0.18494	-1.45894
C	-3.34691	0.34555	-2.75326
C	-4.59002	-0.77308	-1.01799
C	-4.46663	0.30913	-3.57898
H	-2.40265	0.77565	-3.08860
C	-5.70847	-0.81685	-1.84728
H	-4.63520	-1.21034	-0.02159
C	-5.65096	-0.27059	-3.12766
H	-4.41249	0.72609	-4.58233
H	-6.62860	-1.27685	-1.49200
H	-6.52547	-0.30377	-3.77401
C	-2.02447	-1.42876	0.70527
C	-1.81346	-1.30561	2.08636
C	-2.19689	-2.71879	0.17725
C	-1.79570	-2.42846	2.90836
H	-1.65636	-0.31905	2.51759
C	-2.19275	-3.83760	1.00079
H	-2.33544	-2.83654	-0.89668
C	-1.99320	-3.69892	2.37478
H	-1.61724	-2.30718	3.97499
H	-2.33956	-4.82515	0.56771
H	-1.97751	-4.57484	3.01948
C	3.30809	-0.71433	-1.34294
C	3.30276	-0.56453	-2.73464
C	4.38149	-1.38299	-0.74126
C	4.35268	-1.05469	-3.50497
H	2.44550	-0.07047	-3.19226
C	5.42762	-1.88344	-1.51300
H	4.38866	-1.51905	0.33918
C	5.41726	-1.71730	-2.89617
H	4.33476	-0.93158	-4.58570
H	6.25347	-2.40491	-1.03320
H	6.23347	-2.11056	-3.49873
C	1.86317	-1.05453	1.07419
C	1.58914	-2.42374	0.92361
C	1.99660	-0.54540	2.37197
C	1.48432	-3.25721	2.02851
H	1.43913	-2.82705	-0.07710
C	1.87609	-1.38060	3.48125
H	2.19743	0.51467	2.51271
C	1.62829	-2.73944	3.31621
H	1.25826	-4.31202	1.88692
H	1.98206	-0.96290	4.48058

H	1.52766	-3.38982	4.18258
H	-4.62968	2.89842	2.62824
H	5.24839	3.48321	1.02431

B-TS-CH₃

C	-2.31806	1.40962	0.08697
C	-1.21587	2.29241	0.01312
C	1.51800	2.33624	-0.37710
C	1.92146	3.68406	-0.33351
H	1.18873	4.47432	-0.49085
C	2.54196	1.37342	-0.19464
C	4.24877	3.07764	0.05519
C	3.86308	1.72887	0.04525
H	4.61773	0.95330	0.19011
C	-1.42022	3.58231	0.53719
H	-0.59099	4.28765	0.56409
C	3.25614	4.03988	-0.14926
H	3.54136	5.09289	-0.15762
C	-3.54363	1.79770	0.61398
H	-4.36686	1.08232	0.66241
C	-2.65779	3.98488	1.03339
H	-2.78878	5.00010	1.41103
C	-3.74364	3.10615	1.07546
Ni	0.03185	-0.06367	-1.51170
P	1.87180	-0.32183	-0.40122
P	-1.89297	-0.26744	-0.54360
B	0.09860	1.72701	-0.65181
H	0.13813	0.06944	-3.02354
H	0.02364	-1.18465	-2.58627
C	-3.38803	-0.73387	-1.51638
C	-3.28848	-0.61337	-2.90776
C	-4.59924	-1.16879	-0.96352
C	-4.37732	-0.90293	-3.72472
H	-2.33028	-0.29865	-3.32220
C	-5.68634	-1.46786	-1.78145
H	-4.68225	-1.28942	0.11548
C	-5.57928	-1.33144	-3.16389
H	-4.28475	-0.80533	-4.80419
H	-6.62017	-1.80916	-1.33882
H	-6.42852	-1.56678	-3.80193
C	-2.10462	-1.29530	0.96523
C	-1.88361	-0.77709	2.25020
C	-2.31988	-2.67805	0.84186
C	-1.89476	-1.60683	3.36695

H	-1.69310	0.28744	2.37285	C	3.47792	1.65833	0.43407
C	-2.34566	-3.50301	1.95962	H	4.31981	0.97930	0.55061
H	-2.46835	-3.10470	-0.14909	C	-1.98367	3.42394	-0.79726
C	-2.13531	-2.97145	3.23223	H	-1.26072	4.19564	-1.05763
H	-1.70517	-1.18170	4.35057	C	2.53655	3.88422	0.67521
H	-2.52525	-4.56956	1.83688	H	2.66179	4.92051	0.97696
H	-2.14125	-3.61805	4.10691	C	-3.90453	1.49132	-0.15936
C	3.32154	-1.25811	-1.05576	H	-4.66030	0.74821	0.08475
C	3.37319	-1.45121	-2.44104	C	-3.31817	3.79599	-0.65550
C	4.36218	-1.76240	-0.26616	H	-3.63180	4.82738	-0.79280
C	4.44656	-2.11673	-3.02541	C	-4.26203	2.82771	-0.32600
H	2.54056	-1.08068	-3.03930	Ni	-0.07474	-0.40861	-1.54602
C	5.43158	-2.43867	-0.84940	P	1.88295	-0.50072	-0.62282
H	4.32619	-1.63028	0.81422	P	-1.86150	-0.55580	-0.32793
C	5.47794	-2.61416	-2.23059	B	-0.14898	1.45221	-0.87296
H	4.47331	-2.25936	-4.10360	H	-0.31714	-0.43553	-3.04484
H	6.23168	-2.82951	-0.22352	H	-0.05928	-1.66389	-2.45330
H	6.31223	-3.14387	-2.68565	C	-1.67626	-0.88989	1.47101
C	1.80159	-0.97308	1.31825	C	-1.52616	0.13894	2.41055
C	1.46788	-2.32475	1.50293	C	-1.54969	-2.21559	1.91490
C	1.96036	-0.16928	2.45404	C	-1.28320	-0.14977	3.75120
C	1.33097	-2.85922	2.77636	H	-1.60153	1.17571	2.08718
H	1.29518	-2.95138	0.62885	C	-1.31275	-2.50213	3.25298
C	1.80884	-0.70425	3.73266	H	-1.63602	-3.02756	1.19456
H	2.20677	0.88373	2.33386	C	-1.18345	-1.46996	4.18144
C	1.50305	-2.05092	3.90060	H	-1.17480	0.66529	4.46382
H	1.05919	-3.90611	2.89466	H	-1.21198	-3.53765	3.57134
H	1.93519	-0.06135	4.60185	H	-0.98893	-1.69423	5.22775
H	1.37691	-2.46666	4.89801	C	-3.30372	-1.62828	-0.73751
C	5.68405	3.46607	0.24449	C	-3.36517	-2.14088	-2.03762
H	6.29931	3.20350	-0.62563	C	-4.33974	-1.92637	0.15684
H	5.79120	4.54430	0.40177	C	-4.44641	-2.92028	-2.44044
H	6.13524	2.95821	1.10519	H	-2.53850	-1.92098	-2.71339
C	-5.08258	3.54612	1.58547	C	-5.41846	-2.71008	-0.24422
H	-5.01222	4.48211	2.14899	H	-4.29225	-1.54821	1.17688
H	-5.79492	3.71477	0.76773	C	-5.47507	-3.20568	-1.54527
H	-5.53608	2.79409	2.24082	H	-4.48281	-3.31287	-3.45418
B-TS-Cl				H	-6.21727	-2.93360	0.45975
C	-2.57576	1.13550	-0.36095	H	-6.31745	-3.81871	-1.85781
C	1.32048	3.41209	0.18902	C	3.35444	-0.93363	-1.64091
H	0.47935	4.10199	0.14454	C	3.19702	-0.86360	-3.03003
C	2.26129	1.22038	-0.08016	C	4.60314	-1.29232	-1.11865
C	3.60417	2.99953	0.78830	C	4.26917	-1.12798	-3.87706
				H	2.20996	-0.60852	-3.41741

C	5.67334	-1.56489	-1.96673	H	0.01318	-1.66241	-2.12859
H	4.73029	-1.37500	-0.04040	C	-1.86563	-1.06691	1.35842
C	5.50973	-1.47838	-3.34767	C	-2.16072	-0.28384	2.47985
H	4.13406	-1.07029	-4.95478	C	-1.47813	-2.40171	1.55378
H	6.63799	-1.84529	-1.54879	C	-2.08512	-0.82544	3.76215
H	6.34634	-1.69192	-4.00941	H	-2.45734	0.75444	2.34595
C	2.19712	-1.46920	0.90569	C	-1.41333	-2.94134	2.83100
C	2.42760	-2.85045	0.79829	H	-1.21152	-3.00847	0.68962
C	2.05605	-0.92082	2.18776	C	-1.71892	-2.15551	3.94195
C	2.53700	-3.64818	1.93000	H	-2.32024	-0.20311	4.62269
H	2.52057	-3.29719	-0.19034	H	-1.10082	-3.97466	2.96395
C	2.15182	-1.72448	3.32066	H	-1.65455	-2.57614	4.94293
H	1.86092	0.14369	2.29991	C	-3.30374	-1.35341	-1.06225
C	2.39981	-3.08848	3.20065	C	-3.29044	-1.60419	-2.43827
H	2.72540	-4.71431	1.82083	C	-4.39559	-1.78659	-0.30021
H	2.02614	-1.27698	4.30419	C	-4.35939	-2.25832	-3.04419
H	2.47338	-3.71362	4.08752	H	-2.41804	-1.28686	-3.00889
C	1.15020	2.08021	-0.23512	C	-5.46174	-2.44500	-0.90695
C	-1.56909	2.08301	-0.67275	H	-4.40270	-1.61260	0.77488
Cl	5.14739	3.59345	1.39325	C	-5.44633	-2.67844	-2.28049
Cl	-5.94859	3.29932	-0.14461	H	-4.34018	-2.44910	-4.11462
B-TS-CN				H	-6.30655	-2.77554	-0.30706
C	-2.50492	1.28385	-0.22035	H	-6.27883	-3.19391	-2.75376
C	1.52593	3.54032	0.19684	C	3.39951	-1.03788	-1.43388
H	0.69647	4.24317	0.19855	C	3.26196	-1.16944	-2.82036
C	2.41644	1.32317	-0.07353	C	4.62531	-1.36349	-0.83864
C	3.87465	3.11952	0.61963	C	4.33530	-1.59476	-3.59841
C	3.67090	1.75759	0.31572	H	2.29231	-0.93779	-3.26125
H	4.50984	1.06698	0.37243	C	5.69600	-1.79328	-1.61707
C	-1.82251	3.57030	-0.52439	H	4.73566	-1.29378	0.24217
H	-1.07295	4.32571	-0.74829	C	5.55370	-1.90474	-2.99906
C	2.77961	4.00138	0.56102	H	4.21772	-1.69128	-4.67503
H	2.93204	5.04704	0.81787	H	6.64387	-2.04095	-1.14465
C	-3.81598	1.67505	-0.02155	H	6.39178	-2.23920	-3.60615
H	-4.59759	0.93833	0.15647	C	2.05256	-1.26242	1.08884
C	-3.13620	3.97843	-0.36505	C	2.36513	-2.62792	1.15211
H	-3.39872	5.03090	-0.44265	C	1.67281	-0.61143	2.27157
C	-4.15312	3.04362	-0.09344	C	2.32537	-3.31169	2.36338
Ni	-0.00833	-0.26679	-1.45794	H	2.64296	-3.15669	0.24220
P	1.94563	-0.38987	-0.52111	C	1.62985	-1.29717	3.47862
P	-1.88007	-0.42570	-0.36045	H	1.39991	0.44208	2.23827
B	-0.04313	1.57188	-0.69024	C	1.96197	-2.64951	3.53339
H	-0.12261	-0.34668	-2.97337	H	2.57820	-4.36944	2.39071
				H	1.32601	-0.77338	4.38190

H	1.92152	-3.18583	4.47869	C	-2.11271	-1.29809	0.95843
C	1.29953	2.19277	-0.16789	C	-1.89295	-0.78056	2.24421
C	-1.45086	2.20641	-0.45733	C	-2.32744	-2.68120	0.83536
C	-5.49345	3.47300	0.08873	C	-1.90486	-1.61120	3.36074
C	5.16002	3.59573	0.99130	H	-1.70325	0.28381	2.36881
N	-6.59838	3.83130	0.24825	C	-2.35630	-3.50648	1.95250
N	6.21896	3.99059	1.30204	H	-2.47282	-3.10763	-0.15633
B-TS-NH₂				C	-2.14670	-2.97530	3.22598
C	-2.32072	1.40343	0.09123	H	-1.71544	-1.18629	4.34456
C	-1.21661	2.28524	0.05412	H	-2.53708	-4.57289	1.82922
C	1.52093	2.33923	-0.33269	H	-2.15335	-3.62225	4.10050
C	1.92959	3.68313	-0.24905	C	3.34404	-1.24725	-1.06045
H	1.19619	4.47972	-0.36968	C	3.41621	-1.42949	-2.44659
C	2.54686	1.37211	-0.19853	C	4.37581	-1.75728	-0.26226
C	4.25501	3.06326	0.06703	C	4.49777	-2.08817	-3.02300
C	3.87388	1.71443	0.02881	H	2.58977	-1.05752	-3.05292
H	4.63325	0.93793	0.13527	C	5.45298	-2.42946	-0.83696
C	-1.43111	3.56113	0.60786	H	4.32678	-1.63266	0.81856
H	-0.60339	4.26710	0.66201	C	5.51879	-2.59321	-2.21879
C	3.26469	4.04128	-0.08362	H	4.53904	-2.22118	-4.10210
H	3.55321	5.09285	-0.06639	H	6.24395	-2.82690	-0.20333
C	-3.55710	1.77767	0.60102	H	6.35860	-3.12026	-2.66700
H	-4.38504	1.06677	0.61865	C	1.80102	-0.97295	1.29940
C	-2.67225	3.96385	1.08898	C	1.46479	-2.32405	1.48302
H	-2.81137	4.96956	1.48725	C	1.95705	-0.16970	2.43598
C	-3.75814	3.07915	1.08225	C	1.32333	-2.85923	2.75562
Ni	0.03224	-0.04257	-1.50920	H	1.29144	-2.94885	0.60764
P	1.87330	-0.32524	-0.42272	C	1.80004	-0.70499	3.71407
P	-1.88853	-0.27372	-0.55307	H	2.20486	0.88316	2.31809
B	0.10070	1.73129	-0.60617	C	1.49215	-2.05117	3.88068
H	0.11779	0.24029	-3.00383	H	1.04876	-3.90558	2.87266
H	0.03470	-1.00096	-2.73496	H	1.92275	-0.06209	4.58381
C	-3.39426	-0.72510	-1.52127	H	1.36050	-2.46667	4.87758
C	-3.30645	-0.58177	-2.91172	N	5.59488	3.42362	0.29824
C	-4.60096	-1.17423	-0.96887	H	6.24068	2.70821	-0.00556
C	-4.39908	-0.86276	-3.72622	H	5.83949	4.30348	-0.13426
H	-2.35248	-0.25791	-3.32896	N	-5.00008	3.46243	1.61074
C	-5.69192	-1.46717	-1.78473	H	-5.18167	4.45105	1.51378
H	-4.67667	-1.31220	0.10871	H	-5.76742	2.93116	1.22455
C	-5.59560	-1.30780	-3.16524	B-TS-NO₂			
H	-4.31381	-0.74713	-4.80466	C	-2.16204	1.10486	-0.11713
H	-6.62050	-1.82227	-1.34135	C	-1.05091	1.95705	-0.37161
H	-6.44733	-1.53851	-3.80178	C	1.65672	1.93859	-0.82553

C	2.11309	3.26350	-1.04178
H	1.41231	4.03199	-1.36227
C	2.63981	0.98327	-0.43971
C	4.37386	2.62237	-0.49650
C	3.97143	1.30063	-0.26188
H	4.71706	0.56776	0.03213
C	-1.22674	3.32926	-0.05478
H	-0.39725	4.01798	-0.20019
C	3.44516	3.59684	-0.89719
H	3.80553	4.60388	-1.07648
C	-3.34976	1.57066	0.41731
H	-4.19924	0.92068	0.60741
C	-2.41242	3.81690	0.45789
H	-2.54535	4.86453	0.70596
C	-3.47715	2.93734	0.69975
Ni	0.12668	-0.56276	-1.67538
P	1.80331	-0.61603	-0.25766
P	-1.84131	-0.59829	-0.68881
B	0.24259	1.34718	-0.96122
H	1.05378	-0.67978	-2.82982
H	-0.10958	-1.78533	-2.58650
C	-3.31228	-0.99334	-1.70835
C	-3.18181	-0.92109	-3.09874
C	-4.55579	-1.31826	-1.15384
C	-4.28230	-1.14828	-3.92039
H	-2.19965	-0.70105	-3.51640
C	-5.65293	-1.55206	-1.97705
H	-4.65995	-1.39967	-0.07326
C	-5.51853	-1.46213	-3.36114
H	-4.17185	-1.08841	-5.00024
H	-6.61510	-1.80278	-1.53715
H	-6.37707	-1.64504	-4.00296
C	-2.08592	-1.67814	0.76851
C	-2.29027	-1.18718	2.06168
C	-1.99028	-3.06534	0.57956
C	-2.40692	-2.06337	3.13863
H	-2.34447	-0.11498	2.23131
C	-2.12003	-3.93648	1.65386
H	-1.80725	-3.45403	-0.42091
C	-2.33015	-3.43721	2.93921
H	-2.55363	-1.66262	4.13866
H	-2.04940	-5.00917	1.48987
H	-2.42170	-4.11861	3.78171
C	3.09636	-1.89642	-0.49176

C	3.06142	-2.70518	-1.63091
C	4.13765	-2.06202	0.43230
C	4.05453	-3.65856	-1.84627
H	2.24005	-2.57621	-2.33390
C	5.13063	-3.01067	0.21220
H	4.16085	-1.45173	1.33286
C	5.08985	-3.81072	-0.92831
H	4.01688	-4.28499	-2.73397
H	5.93718	-3.12573	0.93192
H	5.86457	-4.55457	-1.09789
C	1.44400	-0.76723	1.53388
C	1.39296	-2.02564	2.14943
C	1.10690	0.36326	2.29023
C	1.04882	-2.14470	3.49198
H	1.62795	-2.91702	1.57138
C	0.77119	0.24149	3.63406
H	1.11575	1.34512	1.81898
C	0.74591	-1.01227	4.24280
H	1.00852	-3.13061	3.94964
H	0.52730	1.13196	4.20800
H	0.47641	-1.10646	5.29202
N	-4.70437	3.43809	1.24561
N	5.74979	2.98311	-0.32101
O	-4.78866	4.65692	1.48689
O	-5.62504	2.62795	1.45931
O	6.54250	2.10774	0.07087
O	6.08806	4.15670	-0.56217

B-TS-OCH₃

C	-2.35499	1.18099	-0.20820
C	-1.23899	2.04508	-0.33320
C	1.51575	2.02541	-0.61260
C	1.92264	3.36746	-0.68747
H	1.19518	4.14202	-0.92633
C	2.53756	1.08260	-0.32841
C	4.22245	2.79807	-0.21995
C	3.85608	1.45136	-0.10851
H	4.62648	0.71486	0.11422
C	-1.46012	3.38911	0.00705
H	-0.62688	4.08996	-0.00893
C	3.25500	3.75624	-0.52331
H	3.52424	4.80343	-0.63068
C	-3.60388	1.63246	0.18937
H	-4.45279	0.95820	0.28576

C	-2.71703	3.87521	0.37201
H	-2.84289	4.93084	0.59658
C	-3.79511	2.99326	0.45592
Ni	0.04299	-0.48590	-1.49550
P	1.86850	-0.63031	-0.34835
P	-1.90819	-0.57520	-0.56787
B	0.09814	1.39160	-0.85248
H	0.17004	-0.46622	-3.01152
H	0.06426	-1.66056	-2.51370
C	-3.38899	-1.18608	-1.47972
C	-3.26279	-1.29458	-2.87011
C	-4.61814	-1.50801	-0.88978
C	-4.34226	-1.69351	-3.65245
H	-2.29265	-1.06512	-3.31156
C	-5.69590	-1.91748	-1.67135
H	-4.72483	-1.44980	0.19210
C	-5.56234	-2.00609	-3.05524
H	-4.22898	-1.77048	-4.73164
H	-6.64424	-2.16565	-1.19847
H	-6.40527	-2.32389	-3.66523
C	-2.14528	-1.33524	1.09063
C	-1.85993	-0.61466	2.26083
C	-2.43917	-2.70275	1.21722
C	-1.88600	-1.23217	3.50613
H	-1.60871	0.44204	2.18962
C	-2.47975	-3.31541	2.46440
H	-2.64234	-3.28818	0.32167
C	-2.20503	-2.58306	3.61908
H	-1.64568	-0.65302	4.39530
H	-2.72312	-4.37406	2.53491
H	-2.22388	-3.06490	4.59439
C	3.32559	-1.62701	-0.88642
C	3.38604	-1.96135	-2.24469
C	4.35696	-2.05499	-0.04128
C	4.45876	-2.68838	-2.74997
H	2.55878	-1.65156	-2.88369
C	5.42463	-2.79565	-0.54429
H	4.31653	-1.81124	1.01936
C	5.48051	-3.11017	-1.90007
H	4.49231	-2.93993	-3.80782
H	6.21690	-3.12680	0.12442
H	6.31445	-3.68907	-2.29167
C	1.79870	-1.06275	1.43853
C	1.40978	-2.36728	1.78399

C	2.00327	-0.13732	2.46940
C	1.25860	-2.73965	3.11214
H	1.20233	-3.08312	0.98921
C	1.83589	-0.50835	3.80300
H	2.29582	0.88120	2.22373
C	1.47045	-1.80959	4.13090
H	0.94327	-3.75195	3.35582
H	1.99505	0.22758	4.58887
H	1.32906	-2.09573	5.17117
O	5.55563	3.07433	-0.02349
O	-5.07263	3.36122	0.80111
C	5.94197	4.41648	-0.15169
H	5.43694	5.06543	0.57962
H	7.01843	4.44925	0.02867
H	5.73396	4.81317	-1.15660
C	-5.28253	4.72143	1.07631
H	-6.34203	4.82963	1.31697
H	-4.68399	5.06784	1.93178
H	-5.04331	5.35967	0.21309

B-PC-H

C	-2.65795	1.58587	-0.48031
C	-1.56124	2.47545	-0.46728
C	1.11802	2.31537	0.25353
C	1.17574	3.50934	1.00267
H	0.28541	4.13168	1.07769
C	2.29287	1.52339	0.27166
C	3.49624	3.14572	1.59598
C	3.46542	1.93803	0.90022
H	4.34710	1.29616	0.87947
C	-1.87698	3.84713	-0.43247
H	-1.07474	4.58381	-0.44717
C	2.33377	3.91519	1.65961
H	2.33355	4.84335	2.23035
C	-3.98209	2.01945	-0.49817
H	-4.79796	1.29863	-0.53047
C	-3.19690	4.29345	-0.43904
H	-3.40546	5.36274	-0.43271
C	-4.25558	3.38585	-0.47620
Ni	-0.04084	-0.25091	-1.13831
P	2.00717	-0.13522	-0.44134
P	-2.02689	-0.12545	-0.43006
B	-0.12441	1.79099	-0.57626
H	0.14117	1.52899	-1.77244

H	-0.01605	-1.59640	-1.97135
C	-3.40066	-1.13927	-1.13445
C	-3.18684	-1.73247	-2.38198
C	-4.64163	-1.31461	-0.50715
C	-4.19817	-2.46272	-3.00180
H	-2.19667	-1.62500	-2.82782
C	-5.65062	-2.05064	-1.12244
H	-4.80985	-0.88275	0.47859
C	-5.43186	-2.62184	-2.37518
H	-4.01907	-2.91848	-3.97324
H	-6.60868	-2.18189	-0.62339
H	-6.22011	-3.19754	-2.85588
C	-2.13996	-0.55756	1.35331
C	-1.81298	0.39167	2.33275
C	-2.38522	-1.87710	1.75872
C	-1.74815	0.03432	3.67399
H	-1.59164	1.41362	2.02833
C	-2.31439	-2.23447	3.10354
H	-2.62089	-2.63083	1.01007
C	-1.99749	-1.28138	4.06770
H	-1.49289	0.78593	4.41752
H	-2.50256	-3.26572	3.39609
H	-1.93755	-1.56091	5.11703
C	3.46921	-0.43585	-1.50942
C	4.23683	0.60992	-2.03500
C	3.76465	-1.74679	-1.91491
C	5.28287	0.35273	-2.91896
H	4.01340	1.63316	-1.74171
C	4.81337	-2.00372	-2.78904
H	3.15776	-2.56746	-1.53654
C	5.58076	-0.95386	-3.29405
H	5.86990	1.18005	-3.31245
H	5.03134	-3.02818	-3.08307
H	6.39964	-1.15472	-3.98114
C	2.38294	-1.23008	0.99081
C	1.30772	-1.68375	1.76215
C	3.68295	-1.58347	1.37477
C	1.52415	-2.45594	2.89969
H	0.29815	-1.42408	1.44870
C	3.89942	-2.36797	2.50401
H	4.53011	-1.24848	0.77881
C	2.82076	-2.80239	3.27241
H	0.67167	-2.78904	3.48774
H	4.91475	-2.63809	2.78728

H	2.99241	-3.41349	4.15615
H	-5.28420	3.74052	-0.49025
H	4.39966	3.46294	2.11251

B-PC-CH₃

C	-2.68031	1.26980	-0.62379
C	-1.60381	2.16546	-0.79172
C	1.10225	2.15029	-0.16619
C	1.17465	3.44071	0.39690
H	0.28322	4.06584	0.41057
C	2.29073	1.38582	-0.07875
C	3.53236	3.19599	0.95962
C	3.47697	1.90022	0.43722
H	4.37014	1.27241	0.47239
C	-1.95194	3.52165	-0.93676
H	-1.17010	4.26589	-1.08337
C	2.35078	3.94593	0.94214
H	2.36099	4.95131	1.36670
C	-4.01211	1.67861	-0.64775
H	-4.81558	0.95008	-0.53450
C	-3.27978	3.93874	-0.95021
H	-3.51212	4.99654	-1.08397
C	-4.33442	3.02760	-0.81608
Ni	-0.05951	-0.61378	-1.11546
P	2.01170	-0.36181	-0.53773
P	-2.00824	-0.40180	-0.32945
B	-0.15929	1.49548	-0.86395
H	0.06131	1.06150	-2.01843
H	-0.04367	-2.06322	-1.75291
C	-3.39446	-1.54006	-0.77547
C	-3.22776	-2.35490	-1.89872
C	-4.60157	-1.60600	-0.06609
C	-4.25340	-3.19828	-2.31993
H	-2.26151	-2.32322	-2.40536
C	-5.62558	-2.45134	-0.48378
H	-4.73047	-0.99927	0.82924
C	-5.45438	-3.24620	-1.61615
H	-4.11083	-3.82811	-3.19556
H	-6.55727	-2.49420	0.07678
H	-6.25390	-3.90852	-1.94193
C	-2.02583	-0.53400	1.50538
C	-1.69068	0.57103	2.30050
C	-2.21648	-1.77368	2.13298
C	-1.56831	0.44373	3.67898

H	-1.51457	1.53388	1.82409	C	2.30748	1.21553	-0.25662
C	-2.08587	-1.90088	3.51420	C	3.54013	3.05905	0.64545
H	-2.46186	-2.64483	1.52896	C	3.51850	1.75014	0.17773
C	-1.76418	-0.79335	4.29440	H	4.42510	1.14870	0.19482
H	-1.31047	1.31456	4.27698	C	-1.96832	3.30152	-0.99954
H	-2.23298	-2.87312	3.98059	H	-1.19385	4.03919	-1.20372
H	-1.65940	-0.89298	5.37226	C	2.37440	3.81873	0.69682
C	3.43081	-0.78213	-1.62428	H	2.40689	4.82645	1.10189
C	4.14471	0.19233	-2.33186	C	-4.02299	1.45188	-0.57940
C	3.73673	-2.13185	-1.85806	H	-4.82883	0.74004	-0.41977
C	5.14722	-0.16961	-3.22937	C	-3.29363	3.72905	-0.99132
H	3.91306	1.24283	-2.17014	H	-3.54920	4.77150	-1.16113
C	4.74250	-2.49203	-2.74555	C	-4.30674	2.79611	-0.78778
H	3.17127	-2.90067	-1.33477	Ni	-0.07328	-0.83757	-1.08679
C	5.45463	-1.51095	-3.43628	P	2.02155	-0.55478	-0.62296
H	5.69241	0.60365	-3.76652	P	-2.00170	-0.60536	-0.25691
H	4.96900	-3.54394	-2.90629	B	-0.17691	1.27959	-0.91954
H	6.23942	-1.79290	-4.13468	H	-0.00298	0.81095	-2.06507
C	2.47964	-1.24519	1.00846	H	-0.06751	-2.32715	-1.60951
C	1.44951	-1.63965	1.86850	C	-3.40788	-1.74824	-0.60395
C	3.80429	-1.51048	1.37865	C	-3.30500	-2.60092	-1.70619
C	1.73338	-2.26531	3.07882	C	-4.57473	-1.78143	0.17192
H	0.42116	-1.45738	1.56197	C	-4.35605	-3.45193	-2.04095
C	4.08875	-2.14928	2.58226	H	-2.36992	-2.59411	-2.26782
H	4.61635	-1.22545	0.71167	C	-5.62317	-2.63433	-0.15932
C	3.05423	-2.52476	3.43757	H	-4.65110	-1.14485	1.05236
H	0.91475	-2.55634	3.73362	C	-5.51646	-3.46869	-1.27061
H	5.12225	-2.35425	2.85427	H	-4.26488	-4.11189	-2.90080
H	3.27857	-3.02407	4.37795	H	-6.52295	-2.65136	0.45156
C	-5.76209	3.48293	-0.87537	H	-6.33488	-4.13702	-1.52955
H	-6.08179	3.69870	-1.90333	C	-1.93889	-0.67693	1.57889
H	-6.44239	2.72029	-0.48365	C	-1.57681	0.45039	2.32865
H	-5.92431	4.40126	-0.29926	C	-2.09488	-1.90131	2.24394
C	4.78785	3.73203	1.57942	C	-1.39436	0.35874	3.70352
H	4.83944	4.82397	1.50996	H	-1.42631	1.40151	1.82044
H	4.86278	3.47980	2.64576	C	-1.90383	-1.99246	3.62057
H	5.68372	3.32466	1.09832	H	-2.35953	-2.78868	1.67278
B-PC-Cl				C	-1.55520	-0.86341	4.35698
C	-2.68575	1.05804	-0.58080	H	-1.11678	1.24539	4.26813
C	-1.61787	1.95086	-0.81500	H	-2.02479	-2.95305	4.11728
C	1.10778	1.96741	-0.30690	H	-1.40312	-0.93468	5.43136
C	1.18615	3.27308	0.22185	C	3.40182	-1.02195	-1.73781
H	0.28706	3.88458	0.27139	C	4.08285	-0.08250	-2.52032
				C	3.71427	-2.37999	-1.90207

C	5.06373	-0.48618	-3.42401	B	-0.16058	1.38338	-0.83557
H	3.84500	0.97365	-2.41477	H	-0.00808	0.82538	-1.94250
C	4.69724	-2.78106	-2.79771	H	-0.06598	-2.30122	-1.23437
H	3.17430	-3.12207	-1.31692	C	-3.43263	-1.64327	-0.71999
C	5.37889	-1.83423	-3.56244	C	-3.24916	-2.48990	-1.81700
H	5.58612	0.25997	-4.01868	C	-4.65226	-1.67856	-0.03054
H	4.93088	-3.83810	-2.90414	C	-4.27377	-3.33517	-2.23527
H	6.14685	-2.14860	-4.26537	H	-2.27674	-2.48440	-2.30932
C	2.54364	-1.35703	0.94807	C	-5.67490	-2.52567	-0.44677
C	1.54292	-1.73073	1.85022	H	-4.79393	-1.04749	0.84546
C	3.88269	-1.57209	1.29755	C	-5.48811	-3.35168	-1.55367
C	1.86985	-2.28623	3.08387	H	-4.12026	-3.98943	-3.09017
H	0.50396	-1.58602	1.56030	H	-6.61761	-2.54415	0.09503
C	4.20994	-2.13957	2.52548	H	-6.28744	-4.01400	-1.87803
H	4.67257	-1.30448	0.59774	C	-2.04725	-0.62295	1.56276
C	3.20437	-2.49371	3.42338	C	-1.70750	0.48630	2.34785
H	1.07392	-2.56065	3.77292	C	-2.22859	-1.86292	2.19051
H	5.25396	-2.30373	2.78357	C	-1.57133	0.36203	3.72542
H	3.46272	-2.93527	4.38354	H	-1.53702	1.44807	1.86758
Cl	5.04728	3.74348	1.25198	C	-2.08420	-1.98578	3.57067
Cl	-5.98367	3.34017	-0.79139	H	-2.47704	-2.73506	1.58938
B-PC-CN				C	-1.75733	-0.87488	4.34333
C	-2.68601	1.16673	-0.59920	H	-1.31011	1.23397	4.31936
C	-1.58806	2.05272	-0.75571	H	-2.22528	-2.95633	4.04121
C	1.14100	2.04365	-0.27573	H	-1.64173	-0.97148	5.42005
C	1.25064	3.34548	0.27529	C	3.40288	-1.03544	-1.66164
H	0.35362	3.94987	0.39164	C	3.99252	-0.15414	-2.57541
C	2.34837	1.28580	-0.28089	C	3.78654	-2.38408	-1.68728
C	3.65479	3.14831	0.54665	C	4.95292	-0.60451	-3.47795
C	3.57465	1.82575	0.06951	H	3.69986	0.89329	-2.57227
H	4.47999	1.22208	0.02087	C	4.74838	-2.83127	-2.58530
C	-1.91570	3.42196	-0.88147	H	3.32420	-3.08272	-0.99283
H	-1.12208	4.15284	-1.02039	C	5.33662	-1.94241	-3.48407
C	2.45827	3.88521	0.67530	H	5.40451	0.09592	-4.17626
H	2.50365	4.89094	1.08664	H	5.03884	-3.87909	-2.58631
C	-4.00709	1.58427	-0.64050	H	6.08781	-2.29344	-4.18734
H	-4.82561	0.87415	-0.54552	C	2.51899	-1.24407	1.04438
C	-3.22716	3.86574	-0.90302	C	1.49795	-1.65953	1.90479
H	-3.45064	4.92267	-1.02792	C	3.85090	-1.38096	1.45468
C	-4.29486	2.95300	-0.79247	C	1.80055	-2.18463	3.15858
Ni	-0.06765	-0.75644	-0.95957	H	0.46484	-1.57377	1.57012
P	2.04428	-0.49135	-0.56126	C	4.15322	-1.91545	2.70270
P	-2.05740	-0.51207	-0.26798	H	4.65519	-1.07839	0.78628
				C	3.12755	-2.31435	3.55867

H	0.99246	-2.49560	3.81677	C	-2.04334	-0.56761	1.50699
H	5.19148	-2.01718	3.00993	C	-1.71299	0.52177	2.32603
H	3.36561	-2.72984	4.53534	C	-2.25087	-1.81598	2.11217
C	4.89817	3.71073	0.93100	C	-1.61352	0.37179	3.70379
C	-5.63870	3.41166	-0.82762	H	-1.52307	1.49082	1.86817
N	5.92743	4.18160	1.23909	C	-2.14489	-1.96576	3.49329
N	-6.74605	3.79453	-0.85786	H	-2.49177	-2.67659	1.49129
B-PC-NH₂				C	-1.82919	-0.87300	4.29661
C	-2.66293	1.28615	-0.57544	H	-1.35901	1.23134	4.31935
C	-1.59023	2.18610	-0.73772	H	-2.30659	-2.94420	3.94170
C	1.12152	2.15722	-0.13183	H	-1.74379	-0.99007	5.37447
C	1.21137	3.44836	0.42287	C	3.43703	-0.77381	-1.59351
H	0.32792	4.08500	0.43520	C	4.13646	0.20450	-2.31113
C	2.29854	1.37980	-0.03805	C	3.76132	-2.12065	-1.82035
C	3.55929	3.17820	0.98136	C	5.14117	-0.14985	-3.20892
C	3.49278	1.87474	0.47817	H	3.88994	1.25284	-2.15679
H	4.37564	1.23440	0.52965	C	4.76950	-2.47362	-2.70799
C	-1.94764	3.53948	-0.86705	H	3.20845	-2.89386	-1.29012
H	-1.17283	4.29073	-1.01665	C	5.46702	-1.48832	-3.40760
C	2.39092	3.94995	0.96409	H	5.67381	0.62698	-3.75387
H	2.41621	4.95537	1.38655	H	5.00944	-3.52368	-2.86181
C	-3.99717	1.68183	-0.58084	H	6.25353	-1.76453	-4.10641
H	-4.79644	0.94850	-0.46998	C	2.45402	-1.26459	1.02161
C	-3.27629	3.95720	-0.86935	C	1.41272	-1.66255	1.86653
H	-3.51812	5.01367	-0.99274	C	3.77287	-1.54307	1.40318
C	-4.32043	3.03413	-0.73572	C	1.67937	-2.30498	3.07188
Ni	-0.05697	-0.57306	-1.15355	H	0.38923	-1.46868	1.55125
P	2.00387	-0.36256	-0.52014	C	4.04042	-2.19918	2.60128
P	-1.99136	-0.39569	-0.32421	H	4.59405	-1.25563	0.74855
B	-0.14589	1.51649	-0.83565	C	2.99459	-2.57840	3.44103
H	0.06898	1.08820	-2.00085	H	0.85172	-2.59745	3.71463
H	-0.04947	-1.96971	-1.90715	H	5.06972	-2.41408	2.88171
C	-3.38055	-1.51096	-0.82546	H	3.20589	-3.09064	4.37747
C	-3.21213	-2.24509	-2.00309	N	-5.66164	3.46462	-0.69627
C	-4.58780	-1.62895	-0.12306	H	-5.81156	4.29816	-1.24794
C	-4.23429	-3.06107	-2.48170	H	-6.29907	2.74344	-1.00463
H	-2.24506	-2.17326	-2.50491	N	4.73927	3.66552	1.57737
C	-5.60784	-2.44999	-0.59714	H	5.56735	3.23320	1.19160
H	-4.72032	-1.08230	0.81003	H	4.82025	4.66978	1.50102
C	-5.43415	-3.16399	-1.78199	B-PC-NO₂			
H	-4.08976	-3.62762	-3.39941	C	-2.68087	0.95741	-0.57958
H	-6.53914	-2.53584	-0.04047	C	-1.58039	1.84974	-0.73286
H	-6.23056	-3.80716	-2.15138	C	1.16574	1.85048	-0.33697

C	1.30152	3.16107	0.19759
H	0.40923	3.76378	0.34976
C	2.37561	1.08820	-0.38454
C	3.69542	2.95573	0.34761
C	3.61478	1.62994	-0.09337
H	4.53107	1.04899	-0.15659
C	-1.91520	3.22396	-0.82636
H	-1.12367	3.95685	-0.96283
C	2.52369	3.70783	0.52778
H	2.61633	4.71590	0.91742
C	-4.00145	1.37311	-0.59544
H	-4.83360	0.68250	-0.50152
C	-3.22515	3.66586	-0.82688
H	-3.47727	4.71570	-0.93071
C	-4.27014	2.73912	-0.71795
Ni	-0.06198	-0.95622	-0.89386
P	2.07580	-0.69459	-0.59255
P	-2.07688	-0.72112	-0.22828
B	-0.15560	1.20889	-0.82833
H	-0.04182	0.53283	-1.87718
H	0.00524	-2.51094	-0.94093
C	-3.44134	-1.86919	-0.63812
C	-3.25920	-2.77190	-1.68991
C	-4.65629	-1.87027	0.06002
C	-4.28267	-3.64239	-2.05554
H	-2.29337	-2.78991	-2.19336
C	-5.67795	-2.73997	-0.30628
H	-4.79440	-1.19308	0.90101
C	-5.49318	-3.62446	-1.36729
H	-4.13159	-4.34192	-2.87396
H	-6.61862	-2.72955	0.23848
H	-6.29207	-4.30529	-1.65152
C	-2.01673	-0.80756	1.60187
C	-1.68030	0.31440	2.36925
C	-2.16279	-2.04601	2.24088
C	-1.51041	0.20184	3.74452
H	-1.53969	1.27619	1.87969
C	-1.98582	-2.15603	3.61785
H	-2.40990	-2.92663	1.65169
C	-1.66004	-1.03349	4.37420
H	-1.25156	1.08245	4.32620
H	-2.10106	-3.12479	4.09867
H	-1.51853	-1.12007	5.44865
C	3.37876	-1.29515	-1.72304

C	3.95162	-0.44698	-2.67735
C	3.74199	-2.64914	-1.71852
C	4.87732	-0.93738	-3.59487
H	3.67658	0.60487	-2.69184
C	4.66828	-3.13573	-2.63355
H	3.29351	-3.32007	-0.98857
C	5.23995	-2.28090	-3.57472
H	5.31968	-0.26318	-4.32380
H	4.94466	-4.18703	-2.61325
H	5.96442	-2.66248	-4.28969
C	2.57456	-1.40269	1.02237
C	1.57059	-1.79844	1.91145
C	3.91498	-1.51727	1.41084
C	1.89962	-2.28595	3.17368
H	0.53040	-1.72879	1.59555
C	4.24241	-2.01401	2.66779
H	4.70468	-1.22239	0.72225
C	3.23450	-2.39585	3.55229
H	1.10587	-2.58250	3.85554
H	5.28629	-2.09769	2.95989
H	3.49302	-2.78108	4.53605
N	4.96852	3.52552	0.66147
N	-5.63252	3.19894	-0.72297
O	5.00497	4.70365	1.06369
O	5.98539	2.82323	0.50686
O	-5.83992	4.41816	-0.85224
O	-6.53853	2.35668	-0.60000

B-PC-OCH₃

C	-2.69766	0.95146	-0.60261
C	-1.65122	1.85072	-0.90629
C	1.07217	1.92907	-0.39984
C	1.13458	3.25460	0.06194
H	0.23461	3.86709	0.04590
C	2.27292	1.18738	-0.27317
C	3.47872	3.07645	0.61371
C	3.45604	1.74308	0.19700
H	4.36409	1.14956	0.29499
C	-2.03640	3.17837	-1.14156
H	-1.28371	3.92088	-1.40428
C	2.30517	3.82891	0.56267
H	2.29059	4.85820	0.91084
C	-4.03475	1.32788	-0.57012
H	-4.83108	0.61942	-0.35352

C	-3.37215	3.58804	-1.10717	C	3.91737	-1.61864	1.26292
H	-3.61857	4.62485	-1.31866	C	1.94640	-2.23154	3.13144
C	-4.37429	2.65853	-0.82574	H	0.55103	-1.52413	1.63993
Ni	-0.06630	-0.91223	-1.12214	C	4.26903	-2.16926	2.49241
P	2.01393	-0.59323	-0.61990	H	4.69036	-1.38781	0.53183
P	-1.97200	-0.68726	-0.23817	C	3.28516	-2.47291	3.43162
B	-0.19802	1.20092	-1.00802	H	1.16609	-2.46530	3.85271
H	-0.01340	0.68829	-2.13872	H	5.31609	-2.36008	2.71901
H	-0.04654	-2.38628	-1.70494	H	3.56282	-2.90204	4.39224
C	-3.36139	-1.87521	-0.51313	O	4.68562	3.54069	1.08757
C	-3.23973	-2.78667	-1.56530	O	-5.71797	2.95590	-0.77342
C	-4.52331	-1.89781	0.27043	C	4.69838	4.85373	1.57873
C	-4.26458	-3.68972	-1.84033	H	3.99908	4.98945	2.41740
H	-2.30697	-2.78028	-2.13241	H	5.71494	5.04617	1.92845
C	-5.54570	-2.80236	-0.00060	H	4.44284	5.59140	0.80288
H	-4.61540	-1.21205	1.11169	C	-6.07402	4.28861	-1.02480
C	-5.41840	-3.69928	-1.06013	H	-7.16080	4.34308	-0.93361
H	-4.15678	-4.39702	-2.66000	H	-5.61948	4.98392	-0.30287
H	-6.44093	-2.81172	0.61760	H	-5.78436	4.61327	-2.03554
H	-6.21518	-4.41005	-1.26999				
C	-1.88427	-0.68952	1.60056				
C	-1.47921	0.46232	2.29094				
C	-2.04764	-1.87762	2.32703				
C	-1.26311	0.42928	3.66325				
H	-1.31640	1.38422	1.73459				
C	-1.82338	-1.91049	3.70151				
H	-2.34386	-2.78547	1.80557				
C	-1.43249	-0.75762	4.37732				
H	-0.95066	1.33451	4.17891				
H	-1.95044	-2.84545	4.24417				
H	-1.25256	-0.78367	5.44965				
C	3.39395	-1.04924	-1.74315				
C	4.12352	-0.10701	-2.47698				
C	3.65319	-2.41107	-1.96403				
C	5.09764	-0.51249	-3.38784				
H	3.92868	0.95252	-2.32798				
C	4.63166	-2.81425	-2.86328				
H	3.06909	-3.15427	-1.42426				
C	5.36088	-1.86494	-3.58032				
H	5.65567	0.23633	-3.94616				
H	4.82202	-3.87480	-3.01374				
H	6.12315	-2.18065	-4.28913				
C	2.57425	-1.37123	0.95204				
C	1.59474	-1.69451	1.89676				

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