

Supporting Information

The Critical Role of Boron Hybridization (sp³ vs. sp² vs. sp) in Hydrogenation Mechanisms by Boron-Based Ru Catalysts

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1. Absolute energies of all optimized structures

Table S1. The absolute energies of all optimized structures in hydrogen activation

Species	ZPE	Hc	Gc	E/(hartree)	H/(hartree)	G/(hartree)	Solvation Energy/(hartree)
H_2	0.010027	0.013332	-0.001464	-1.160237	-1.156932	-1.171728	-1.171140115 (THF) -1.17117827 (toluene)
sp^3 -Cat	0.534187	0.574333	0.45951	-3205.515595	-3205.47545	-3205.590273	-3207.582716
sp^3 -RC	0.551151	0.592224	0.475675	-3206.643963	-3206.602889	-3206.719438	-3208.728744
sp^3 -TS	0.547849	0.588802	0.471366	-3206.637701	-3206.596749	-3206.714184	-3208.717505
sp^3 -PC	0.553305	0.594311	0.476174	-3206.667414	-3206.626408	-3206.744545	-3208.749569
sp^2 -Cat	0.659684	0.700284	0.591504	-2424.983956	-2424.943357	-2425.052136	-2427.05703
sp^2 -RC	0.676621	0.717973	0.609228	-2426.137857	-2426.096506	-2426.205251	-2428.234652
sp^2 -TS	0.673911	0.714681	0.607646	-2426.124525	-2426.083754	-2426.190789	-2428.221439
sp^2 -PC	0.67665	0.717589	0.610028	-2426.133022	-2426.092083	-2426.199645	-2428.229653
sp -Cat	1.16011	1.215653	1.070473	-3022.291594	-3022.236051	-3022.381231	-3024.978023
sp -RC	1.176541	1.233143	1.08797	-3023.443256	-3023.386654	-3023.531827	-3026.146699
sp -TS	1.174127	1.2297	1.087385	-3023.426521	-3023.370948	-3023.513263	-3026.134365
sp -PC	1.179196	1.235637	1.089089	-3023.459285	-3023.402844	-3023.549391	-3026.168097

Table S2. The absolute energies of all optimized structures in hydrogenation

Species	ZPE	Hc	Gc	E/(hartree)	H/(hartree)	G/(hartree)	Solvation Energy/(hartree)
C_2H_4	0.050943	0.054941	0.029415	-78.522385	-78.518387	-78.543913	-78.59469505 (THF) -78.59486731 (toluene)
C_2H_6	0.074998	0.07942	0.053593	-79.742543	-79.738121	-79.763949	-79.8371441

							(THF) -79.83786979 (toluene)
sp^3 -hy-Cat	0.544039	0.582713	0.471408	-3093.291473	-3093.2528	-3093.364105	-3095.337153
sp^3 -hy-RC	0.59981	0.640853	0.527158	-3171.86508	-3171.824037	-3171.937732	-3173.977538
sp^3 -a- TS_1	0.598473	0.63847	0.527323	-3171.850011	-3171.810014	-3171.921161	-3173.960986
sp^3 -a- IM	0.599845	0.640063	0.52991	-3171.863895	-3171.823677	-3171.933831	-3173.978869
sp^3 -a- TS_2	0.599235	0.64001	0.52804	-3171.861945	-3171.821169	-3171.93314	-3173.975165
sp^3 -b- TS_1	0.59518	0.635736	0.524327	-3171.825302	-3171.784747	-3171.896155	-3173.942205
sp^3 -b- IM	0.59835	0.639221	0.526878	-3171.841665	-3171.800794	-3171.913137	-3173.957051
sp^3 -b- TS_2	0.597733	0.638138	0.527302	-3171.842171	-3171.801767	-3171.912603	-3173.956154
sp^3 -hy-PC	0.524124	0.562188	0.453334	-3092.122996	-3092.084932	-3092.193786	-3094.143029
sp^2 -hy-Cat	0.668208	0.706783	0.60376	-2312.750171	-2312.711596	-2312.814619	-2314.808378
sp^2 -hy-RC	0.724906	0.766225	0.657779	-2391.316318	-2391.274999	-2391.383446	-2393.436131
sp^2 -a- TS_1	0.723083	0.764092	0.657199	-2391.31126	-2391.270251	-2391.377143	-2393.430582
sp^2 -a- IM	0.725087	0.766957	0.656857	-2391.334195	-2391.292325	-2391.402425	-2393.456156
sp^2 -a- TS_2	0.723568	0.76567	0.654538	-2391.322033	-2391.279931	-2391.391063	-2393.441901
sp^2 -b- TS_1	0.722378	0.762648	0.658356	-2391.285367	-2391.245097	-2391.349389	-2393.408825
sp^2 -b- IM	0.724466	0.765502	0.658746	-2391.285917	-2391.244881	-2391.351638	-2393.409846
sp^2 -b- TS_2	0.723158	0.764019	0.657831	-2391.286833	-2391.245971	-2391.352159	-2393.408855
sp^2 -hy-PC	0.650122	0.688378	0.585593	-2311.592419	-2311.554163	-2311.656949	-2313.623748
sp -hy-Cat	1.176596	1.230785	1.088063	-2563.049481	-2562.995293	-2563.138014	-2565.754935
sp -hy-RC	1.235948	1.293095	1.14737	-2641.600662	-2641.543514	-2641.68924	-2644.378508
sp -a- TS_1	1.23601	1.292469	1.147547	-2641.589291	-2641.532832	-2641.677754	-2644.365903
sp -a- IM	1.238368	1.294186	1.151837	-2641.594319	-2641.538501	-2641.68085	-2644.372149

sp_a-TS_2	1.235236	1.292601	1.14502	-2641.583239	-2641.525873	-2641.673454	-2644.358662
sp_b-TS_1	1.232177	1.288114	1.145053	-2641.576533	-2641.520596	-2641.663658	-2644.35473
sp_b-IM	1.236314	1.29397	1.14607	-2641.585268	-2641.527612	-2641.675512	-2644.362122
sp_b-TS_2	1.234077	1.290039	1.147033	-2641.561204	-2641.505243	-2641.648249	-2644.337195
sp_hy-PC	1.158319	1.212235	1.070257	-2561.872528	-2561.818612	-2561.960591	-2564.554195

2. The calculated results of orbital occupancy for nickel-hydride insertion and silicon-hydride migration mechanisms in Si/Ni catalyzed hydrogenation

Table S3. Bond orbital occupancy for sp^3 -B-Ru catalyzes hydrogen activation

	B-Ru	Ru-H ^b	B-H ^b -Ru	Ru-H ^a	H-H	H ^b
sp^3 -RC	1. 62055	0	0	0	1. 66727	0
2	1. 61648	0	0	0	1. 67722	0
3	1. 61633	0	0	0	1. 67677	0
4	1. 61629	0	0	0	1. 67701	0
5	1. 61607	0	0	0	1. 67633	0
6	1. 61602	0	0	0	1. 67679	0
7	1. 61569	0	0	0	1. 67567	0
8	1. 61564	0	0	0	1. 67633	0
9	1. 61515	0	0	0	1. 67448	0
10	1. 61512	0	0	0	1. 67489	0
11	1. 61463	0	0	0	1. 67251	0
12	1. 61463	0	0	0	1. 67234	0
13	1. 61424	0	0	0	1. 66995	0
14	1. 61422	0	0	0	1. 66967	0
15	1. 61373	0	0	0	1. 66711	0
16	1. 61329	0	0	0	1. 66397	0
17	1. 61201	0	0	0	1. 65348	0
18	1. 60926	0	0	0	1. 63794	0
19	1. 48882	0	0	1. 34547	0	0. 81238
20	1. 49437	0	0	1. 38258	0	0. 80504
21	1. 49595	0	0	1. 41369	0	0. 79892
22	1. 49482	0	0	1. 4381	0	0. 79411
23	1. 49158	0	0	1. 46278	0	0. 78931
24	1. 4862	0	0	1. 485	0	0. 78542
25	1. 47835	0	0	1. 50636	0	0. 78232
26	1. 46799	0	0	1. 52789	0	0. 7799
27	1. 45532	0	0	1. 54826	0	0. 77827
28	1. 44083	0	0	1. 56669	0	0. 77738
29	1. 42527	0	0	1. 58245	0	0. 77715
30	1. 40933	0	0	1. 5954	0	0. 77744
31	1. 39354	0	0	1. 60576	0	0. 77808
32	1. 37815	0	0	1. 61392	0	0. 77897
33	1. 36314	0	0	1. 62026	0	0. 7802
34	1. 34837	0	0	1. 62502	0	0. 78187
35	0	1. 40272	0	1. 78509	0	0
36	0	1. 39796	0	1. 78499	0	0

37	0	1.37963	0	1.68827	0	0
38	0	1.3626	0	1.68907	0	0
39	0	1.3527	0	1.68808	0	0
40	0	0	1.53299	1.72666	0	0
41	0	0	1.5406	1.72882	0	0
42	0	0	1.54975	1.73048	0	0
43	0	0	1.55995	1.73198	0	0
44	0	0	1.57022	1.73312	0	0
45	0	0	1.57876	1.73388	0	0
46	0	0	1.58509	1.73427	0	0
47	0	0	1.59024	1.73444	0	0
48	0	0	1.59484	1.73452	0	0
49	0	0	1.60334	1.73452	0	0
50	0	0	1.61129	1.73436	0	0
51	0	0	1.63868	1.73242	0	0
52	0	0	1.60391	1.7318	0	0
53	0	0	1.61237	1.73124	0	0
54	0	0	1.62032	1.73068	0	0
sp^3 -PC	0	0	1.63173	1.72988	0	0

Table S4. Bond orbital occupancy for sp^2 -B-Ru catalyzes hydrogen activation

	B-Ru	B-H ^b	Ru-H ^a	H-H	H ^b
1	1.70331	0	0	1.69081	0
2	1.71399	0	0	1.65843	0
3	1.71416	0	0	1.65385	0
4	1.71423	0	0	1.65264	0
5	1.71438	0	0	1.64793	0
6	1.71448	0	0	1.64598	0
7	1.71462	0	0	1.64059	0
8	1.71471	0	0	1.63812	0
9	1.71481	0	0	1.63213	0
10	1.71487	0	0	1.62424	0
11	1.71486	0	0	1.62417	0
12	1.71477	0	0	1.61449	0
13	1.7147	0	0	1.60766	0
14	1.43079	0	1.42373	0	0.77942
15	1.42761	0	1.46134	0	0.76897
16	1.42115	0	1.49212	0	0.76029
17	1.41175	0	1.51724	0	0.75364
18	0	1.47327	1.72046	0	0
19	0	1.48476	1.7273	0	0
20	0	1.49766	1.73234	0	0

21	0	1.50678	1.73508	0	0
22	0	1.50958	1.73595	0	0
23	0	1.51287	1.73682	0	0
24	0	1.51365	1.73709	0	0
25	0	1.51657	1.73778	0	0
26	0	1.51608	1.73779	0	0
27	0	1.51895	1.73843	0	0
28	0	1.51792	1.73838	0	0
29	0	1.52	1.73888	0	0
30	0	1.51925	1.73892	0	0
31	0	1.53929	1.74607	0	0

Table S5. Bond orbital occupancy for sp-B-Ru catalyzes hydrogen activation

	B-Ru	B-H ^b	Ru-H ^a	H-H	H ^b
<i>sp</i> -RC	1.78962	0	0	1.76553	0
2	1.78951	0	0	1.72714	0
3	1.78896	0	0	1.7266	0
4	1.78839	0	0	1.73015	0
5	1.78771	0	0	1.7249	0
6	1.78712	0	0	1.72433	0
7	1.78619	0	0	1.72004	0
8	1.78496	0	0	1.71204	0
9	1.78351	0	0	1.70204	0
10	1.78163	0	0	1.68673	0
11	1.77976	0	0	1.67147	0
12	1.77737	0	0	1.65189	0
13	1.77437	0	0	1.62935	0
14	1.57089	0	1.4205	0	0.81417
15	1.5583	0	1.46447	0	0.80401
16	1.54137	0	1.50318	0	0.79525
17	1.52168	0	1.53459	0	0.7881
18	0	1.38394	1.63636	0	0
19	0	1.38376	1.64081	0	0
20	0	1.39673	1.65893	0	0
21	0	1.40685	1.67459	0	0
22	0	1.38975	1.67797	0	0
23	0	1.39375	1.68453	0	0
24	0	1.39418	1.68728	0	0
25	0	1.38653	1.68311	0	0
<i>sp</i> -PC	0	1.40828	1.78432	0	0

Table S6. Bond orbital occupancy for terminal pathway in *sp*³-B-Ru catalyzed ethylene hydrogenation

Ru-H ^a	C ² -H ^a
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sp^3 -hy-RC	1. 72733	0
2	1. 72513	0
3	1. 72286	0
4	1. 72052	0
5	1. 71785	0
6	1. 71441	0
7	1. 70951	0
8	1. 69372	0
11	1. 68278	0
12	0	1. 60434
13	0	1. 62551
14	0	1. 64322
15	0	1. 65194
16	0	1. 65996
17	0	1. 66201
18	0	1. 66524
19	0	1. 66632
20	0	1. 66797
21	0	1. 66769
22	0	1. 66975
23	0	1. 66919
sp^3 -a-IM	0	1. 67154

Table S7. Bond orbital occupancy for terminal pathway in sp^2 -B-Ru catalyzed ethylene hydrogenation

	Ru-H ^a	C ² -H ^a
sp^2 -hy-RC	1. 55646	0
2	1. 52153	0
3	1. 51972	0
4	1. 51785	0
5	1. 51595	0
6	1. 51399	0
7	1. 51198	0
8	1. 50991	0
9	1. 50778	0
10	1. 50555	0
11	1. 50321	0
12	1. 50066	0
13	1. 49776	0
14	1. 49419	0
15	1. 48954	0

16	1.48309	0
17	1.47438	0
18	1.4633	0
19	1.45002	0
20	1.43455	0
21	1.41629	0
22	1.39649	0
23	1.37489	0
24	1.35047	0
25	0	1.61504
26	0	1.64851
27	0	1.67778
28	0	1.70025
29	0	1.71605
30	0	1.72799
31	0	1.73787
32	0	1.74657
33	0	1.75439
34	0	1.76169
35	0	1.76838
36	0	1.77496
37	0	1.78066
38	0	1.78741
39	0	1.791
sp^2 -a-IM	0	1.85527

Table S8. Bond orbital occupancy for terminal pathway in sp -B-Ru catalyzed ethylene hydrogenation

	Ru-H ^a	C ² -H ^a
sp -hy-RC	1.77098	0
4	1.74893	0
7	1.72504	0
10	1.699	0
13	1.67206	0
16	1.64367	0
19	1.61548	0
20	0	1.51589
21	0	1.55145
22	0	1.6213
23	0	1.64946
24	0	1.66987
25	0	1.68383
26	0	1.69517
27	0	1.70442

28	0	1. 71378
29	0	1. 71979
30	0	1. 7299
31	0	1. 73281
32	0	1. 73941
33	0	1. 74271
34	0	1. 74768
35	0	1. 74934
36	0	1. 75128
37	0	1. 75241
<i>sp</i> -a-IM	0	1. 77366

Table S9. Bond orbital occupancy for bridging pathway in sp^3 -B-Ru catalyzed ethylene hydrogenation

	B-H ^b -Ru	C ¹ -H ^b	B-Ru	H ^b
<i>sp</i> ³ -hy-RC	1. 63622	0	0	0
2	1. 63442	0	0	0
3	1. 6294	0	0	0
4	1. 62589	0	0	0
5	1. 62083	0	0	0
6	1. 61623	0	0	0
7	1. 61053	0	0	0
8	1. 60465	0	0	0
9	0	0	0	0. 89712
10	0	0	0	0. 88883
11	0	0	0	0. 8761
12	0	0	0	0. 85884
13	0	0	0	0. 84073
14	0	0	0	0. 82369
15	0	0	0	0. 80801
16	0	0	0	0. 79358
17	0	0	0	0. 77982
18	0	0	1. 56716	0. 76687
19	0	0	1. 58969	0. 75521
20	0	0	1. 61201	0. 74427
21	0	0	1. 63216	0. 73431
22	0	0	1. 65135	0. 72533
23	0	0	1. 66773	0. 71843
24	0	1. 59718	1. 67941	0
25	0	1. 62001	1. 68779	0
26	0	1. 62941	1. 69106	0
27	0	1. 64072	1. 69479	0
28	0	1. 64841	1. 6973	0

29	0	1.65791	1.7002	0
30	0	1.66328	1.70187	0
31	0	1.66808	1.70324	0
32	0	1.66976	1.70379	0
33	0	1.67384	1.70474	0
34	0	1.6774	1.70552	0
35	0	1.68219	1.70644	0
36	0	1.68314	1.7066	0
37	0	1.68682	1.70716	0
38	0	1.68916	1.70745	0
39	0	1.6938	1.70805	0
40	0	1.69395	1.70791	0
41	0	1.69736	1.70819	0
sp^3 -b-IM	0	1.7136	1.67416	0

Table S10. Bond orbital occupancy for bridging pathway in sp^2 -B-Ru catalyzed ethylene hydrogenation

	B-H ^b	C ¹ -H ^b	B-Ru	H ^b
sp^2 -hy-RC	1.70622	0	0	0
2	1.62368	0	0	0
3	1.62004	0	0	0
4	1.61593	0	0	0
5	1.61154	0	0	0
6	1.60656	0	0	0
7	1.60104	0	0	0
8	0	0	0	0.88024
9	0	0	0	0.87354
10	0	0	0	0.86101
11	0	0	0	0.84718
12	0	0	0	0.83432
13	0	0	0	0.82271
14	0	0	0	0.81183
15	0	0	0	0.80126
16	0	0	0	0.79072
17	0	0	0	0.78013
18	0	0	1.55134	0.76958
19	0	0	1.57004	0.75923
20	0	0	1.58823	0.74907
21	0	0	1.60607	0.73926
22	0	0	1.62319	0.73
23	0	0	1.6373	0.72266
24	0	1.59024	1.65023	0

25	0	1.61891	1.65906	0
26	0	1.63853	1.66386	0
27	0	1.65168	1.66627	0
28	0	1.66225	1.66764	0
29	0	1.66919	1.66791	0
30	0	1.67848	1.66871	0
31	0	1.68306	1.66856	0
32	0	1.68476	1.66787	0
33	0	1.69117	1.66827	0
34	0	1.69363	1.66816	0
35	0	1.69344	1.66767	0
36	0	1.69695	1.66795	0
37	0	1.69815	1.66799	0
38	0	1.69929	1.66806	0
39	0	1.69859	1.66791	0
40	0	1.70113	1.66832	0
41	0	1.70121	1.66844	0
42	0	1.70173	1.66862	0
sp^2 -b-IM	0	1.69387	1.66719	0

Table S11. Bond orbital occupancy for bridging pathway in sp -B-Ru catalyzed ethylene hydrogenation

	B-H ^b	C ^l -H ^b	B-Ru	H ^b
sp -hy-RC	1.69451	0	0	0
2	1.59357	0	0	0
3	1.59237	0	0	0
4	1.58777	0	0	0
5	1.5846	0	0	0
6	1.57974	0	0	0
7	1.57492	0	0	0
8	1.56865	0	0	0
9	1.56157	0	0	0
10	1.55237	0	0	0
11	1.54053	0	0	0
12	1.52213	0	0	0
13	0	0	0	0.84171
14	0	0	0	0.83141
15	0	0	0	0.82144
16	0	0	1.56716	0.81179
17	0	0	1.58969	0.80208
18	0	0	1.61201	0.7921
19	0	0	1.63216	0.78219
20	0	0	1.65135	0.77253
21	0	0	1.66773	0.76334

22	0	0	1.67941	0.75433
23	0	1.59621	1.68779	0
24	0	1.62776	1.69106	0
25	0	1.65138	1.69479	0
26	0	1.66801	1.6973	0
27	0	1.68217	1.7002	0
28	0	1.69384	1.70187	0
29	0	1.70555	1.70324	0
30	0	1.71401	1.70379	0
31	0	1.72394	1.70474	0
32	0	1.73203	1.70552	0
33	0	1.74384	1.70644	0
34	0	1.7501	1.7066	0
35	0	1.75605	1.70716	0
36	0	1.76549	1.70745	0
37	0	1.76994	1.70805	0
38	0	1.77801	1.70791	0
39	0	1.78365	1.70819	0
<i>sp</i> -b-IM	0	1.84376	1.67416	0

3.The Cartesian coordinates (xyz) for all structures

(1) For structures in hydrogen activation

<i>sp</i> ³ -Cat				H	3.810712	0.852778	−4.56966
				C	3.239068	0.479713	−2.534306
Ru	−0.200921	0.069966	−0.153045	H	3.068711	1.532308	−2.315369
S	−0.555497	0.813461	2.222805	C	3.166321	1.573244	0.45932
S	−0.731385	−2.287153	0.441955	C	4.523724	1.764153	0.167649
S	−0.449024	2.335559	−0.915226	H	5.075455	0.990692	−0.362314
P	2.273298	0.015374	0.05519	C	5.165571	2.943298	0.528129
B	−2.303873	0.054319	−0.128924	H	6.217737	3.079816	0.291484
N	−2.911402	−0.118339	1.364485	C	4.461177	3.948916	1.188587
N	−2.818546	−1.248355	−0.879593	H	4.964525	4.870615	1.468951
N	−2.967328	1.385071	−0.69685	C	3.112577	3.77218	1.479106
O	−0.168786	−0.838691	−3.033071	H	2.555028	4.555041	1.985788
C	3.032074	−0.478287	−1.532925	C	2.467363	2.592979	1.112961
C	3.224265	−1.830032	−1.844324	H	1.407151	2.463384	1.324052
H	3.044482	−2.587859	−1.08476	C	3.016844	−1.167071	1.252007
C	3.63795	−2.210218	−3.117312	C	4.360163	−1.562817	1.192871
H	3.786876	−3.263312	−3.341384	H	4.997902	−1.194416	0.391692
C	3.856199	−1.249129	−4.100662	C	4.880199	−2.440381	2.137443
H	4.176796	−1.547964	−5.094983	H	5.922223	−2.743652	2.077329
C	3.65192	0.096552	−3.805632	C	4.0671	−2.930867	3.15837

H	4.474995	-3.618097	3.894942
C	2.733397	-2.542562	3.227729
H	2.092645	-2.923626	4.01841
C	2.210166	-1.667448	2.27825
H	1.166412	-1.36224	2.327964
C	-2.179434	0.356014	2.42855
C	-2.799926	0.405185	3.702507
H	-2.220234	0.815807	4.521742
C	-4.064617	-0.089273	3.896198
H	-4.516772	-0.063177	4.883733
C	-4.75469	-0.660125	2.81082
H	-5.734571	-1.107658	2.925123
C	-4.146625	-0.647023	1.58289
H	-4.626579	-1.088054	0.713496
C	-2.190889	-2.405155	-0.450455
C	-2.750789	-3.642637	-0.829326
H	-2.290789	-4.543367	-0.437489
C	-3.78265	-3.70049	-1.739577
H	-4.168984	-4.66246	-2.063787
C	-4.294489	-2.51098	-2.282079
H	-5.060317	-2.513847	-3.048402
C	-3.801104	-1.316607	-1.81204
H	-4.171294	-0.364684	-2.176384
C	-2.144299	2.431526	-1.066432
C	-2.74709	3.624223	-1.546916
H	-2.08196	4.422979	-1.856641
C	-4.107774	3.767899	-1.596639
H	-4.547788	4.691908	-1.960262
C	-4.928892	2.709265	-1.154853
H	-6.009558	2.784772	-1.149183
C	-4.321954	1.564684	-0.718934
H	-4.907216	0.726654	-0.356143
C	-0.150769	-0.477399	-1.921225

*sp*³-RC

Ru	0.028557	-0.085563	-0.531476
S	0.297491	-1.964798	1.087333
S	0.320064	1.738385	1.084127
S	5.44102	-0.99375	0.101764
P	-2.458761	-0.127886	-0.130078
B	2.224712	0.020513	-0.260447
N	2.523506	-0.473805	1.248892
N	2.634083	1.554824	-0.231172

N	3.134162	-0.737622	-1.337402
O	0.156795	2.081889	-2.636111
C	-3.457398	0.702026	-1.417284
C	-3.12539	2.02563	-1.744227
H	-2.318483	2.523913	-1.208866
C	-3.819189	2.703245	-2.739165
H	-3.552606	3.72895	-2.977873
C	-4.84483	2.064062	-3.4345
H	-5.380962	2.590058	-4.219449
C	-5.175384	0.749259	-3.123003
H	-5.97338	0.245747	-3.661887
C	-4.490223	0.070532	-2.116908
H	-4.761728	-0.954273	-1.877171
C	-3.282659	-1.752841	0.076743
C	-4.509253	-1.865191	0.745439
H	-4.97098	-0.97748	1.173375
C	-5.135638	-3.100437	0.867836
H	-6.085698	-3.174038	1.390161
C	-4.545382	-4.240671	0.325729
H	-5.032766	-5.206466	0.427106
C	-3.325945	-4.14138	-0.336458
H	-2.854951	-5.028126	-0.751294
C	-2.697472	-2.904618	-0.457766
H	-1.733727	-2.835358	-0.95821
C	-2.953923	0.730907	1.412337
C	-3.964701	1.695697	1.476815
H	-4.504135	1.981048	0.576976
C	-4.287761	2.294323	2.692786
H	-5.07333	3.044508	2.729824
C	-3.612266	1.932932	3.854246
H	-3.865676	2.402781	4.800876
C	-2.606781	0.969931	3.798114
H	-2.069826	0.687152	4.699389
C	-2.275208	0.375522	2.586727
H	-1.474387	-0.362675	2.538638
C	1.767951	-1.46904	1.812385
C	2.154585	-2.00846	3.056374
H	1.570009	-2.833611	3.44693
C	3.167976	-1.430313	3.78696
H	3.422925	-1.818566	4.769273
C	3.828308	-0.314175	3.267186
H	4.608896	0.200383	3.813521
C	3.510075	0.099175	1.996204
H	4.030325	0.92901	1.541688

C	1.827436	2.360041	0.533949
C	2.268571	3.658402	0.844456
H	1.635852	4.276732	1.471123
C	3.452435	4.134666	0.320283
H	3.772887	5.148968	0.540772
C	4.227343	3.313054	-0.51003
H	5.15656	3.656678	-0.94755
C	3.796882	2.027267	-0.74486
H	4.373966	1.311769	-1.32006
C	4.346783	-1.403526	-1.111147
C	4.710739	-2.412793	-2.056118
H	5.55719	-3.033471	-1.78486
C	4.112464	-2.51094	-3.281004
H	4.454261	-3.244261	-4.006312
C	3.075997	-1.608465	-3.597365
H	2.618982	-1.570306	-4.57903
C	2.614046	-0.788755	-2.608907
H	1.780723	-0.121865	-2.781697
C	0.061171	1.24074	-1.828129
H	0.456767	-1.37372	-1.626418
H	-0.399349	-1.324116	-1.711715

sp^3 -TS

Ru	0.011868	0.011772	-0.718272
S	0.370084	-2.276858	0.26398
S	0.304353	1.39966	1.42684
S	5.4902	0.269702	0.143802
P	-2.446706	-0.113692	-0.198942
B	2.21398	0.009212	-0.282705
N	2.365058	-0.733733	1.143305
N	2.513465	1.537489	-0.072742
N	3.304433	-0.739634	-1.199549
O	0.01097	2.738887	-2.026779
C	-3.424224	1.191146	-1.021078
C	-3.052559	2.520752	-0.770444
H	-2.227875	2.725417	-0.087333
C	-3.724334	3.568187	-1.387146
H	-3.428227	4.592932	-1.181203
C	-4.766214	3.303411	-2.275291
H	-5.286436	4.122232	-2.764178
C	-5.132633	1.987629	-2.538595
H	-5.941262	1.775648	-3.232916
C	-4.469694	0.933495	-1.912222

H	-4.76864	-0.090906	-2.119805
C	-3.345722	-1.66012	-0.590028
C	-4.60769	-1.905859	-0.032512
H	-5.037023	-1.185728	0.661098
C	-5.309944	-3.059497	-0.360111
H	-6.288551	-3.238509	0.076753
C	-4.7581	-3.984946	-1.244552
H	-5.306321	-4.888232	-1.497984
C	-3.501736	-3.754373	-1.796086
H	-3.0636	-4.477379	-2.47817
C	-2.797566	-2.597827	-1.468973
H	-1.809902	-2.419342	-1.889515
C	-2.853572	0.121392	1.57444
C	-3.897887	0.941253	2.016944
H	-4.496226	1.494991	1.297501
C	-4.173889	1.055585	3.377235
H	-4.986222	1.697398	3.707771
C	-3.414301	0.353294	4.307937
H	-3.629831	0.446572	5.368932
C	-2.373151	-0.464433	3.874976
H	-1.770003	-1.009174	4.596187
C	-2.090639	-0.578994	2.518933
H	-1.264608	-1.203923	2.181313
C	1.660416	-1.891361	1.334756
C	1.948259	-2.687876	2.457138
H	1.406644	-3.620566	2.568409
C	2.836386	-2.246676	3.416514
H	3.030376	-2.852052	4.297689
C	3.442269	-0.996856	3.266224
H	4.106776	-0.586109	4.016246
C	3.193483	-0.280436	2.117578
H	3.643226	0.684739	1.936372
C	1.736112	2.182414	0.863798
C	2.086456	3.486644	1.241072
H	1.508406	3.961326	2.025849
C	3.054151	4.177925	0.535626
H	3.275456	5.210418	0.790087
C	3.695042	3.561874	-0.542249
H	4.417248	4.08513	-1.156258
C	3.427152	2.234289	-0.791749
H	3.912831	1.68851	-1.589136
C	4.701562	-0.662474	-1.026854
C	5.509376	-1.432553	-1.916185
H	6.579446	-1.303152	-1.803521

C	4.991011	-2.307844	-2.829966
H	5.647376	-2.88619	-3.474485
C	3.596483	-2.456243	-2.893143
H	3.116424	-3.16546	-3.556465
C	2.822614	-1.674138	-2.082667
H	1.750297	-1.784563	-2.081649
C	-0.036092	1.683788	-1.532645
H	0.66068	-0.475287	-2.107204
H	-0.469521	-0.760789	-2.083633

sp^3 -PC

Ru	0.278707	0.033167	0.646164
S	-0.358904	-2.114137	-0.493835
S	-0.502479	1.715968	-1.260789
S	-5.781857	-0.146007	-0.166512
P	2.495857	-0.121697	0.173051
B	-2.556768	0.059666	0.291573
N	-2.514495	-0.578335	-1.153651
N	-2.810472	1.587516	0.18594
N	-3.520624	-0.771663	1.222748
O	0.615147	2.401121	2.48802
C	3.586113	0.989919	1.128665
C	3.430548	2.372258	0.951324
H	2.699032	2.74437	0.235246
C	4.197887	3.266405	1.685578
H	4.069439	4.334858	1.537508
C	5.122493	2.793261	2.615835
H	5.719148	3.493125	3.194366
C	5.274585	1.42379	2.806195
H	5.989925	1.04995	3.533385
C	4.512126	0.5231	2.065051
H	4.638717	-0.545688	2.216921
C	3.281433	-1.768714	0.351558
C	4.548427	-1.998649	-0.202938
H	5.04722	-1.206651	-0.757718
C	5.170971	-3.231464	-0.048313
H	6.154354	-3.396931	-0.479689
C	4.532301	-4.253116	0.652876
H	5.017151	-5.218794	0.767724
C	3.272607	-4.03508	1.201036
H	2.767794	-4.829256	1.743481
C	2.649395	-2.79792	1.053592
H	1.665665	-2.620856	1.48148

C	2.890568	0.312891	-1.568292
C	4.043947	1.025001	-1.921873
H	4.727662	1.370976	-1.150659
C	4.32099	1.299685	-3.258351
H	5.216822	1.857404	-3.517613
C	3.452698	0.867224	-4.256029
H	3.667018	1.088302	-5.298049
C	2.306744	0.153513	-3.913604
H	1.622342	-0.185751	-4.686259
C	2.025571	-0.122579	-2.579941
H	1.127519	-0.676306	-2.311979
C	-1.687951	-1.632297	-1.477564
C	-1.90124	-2.292138	-2.703496
H	-1.265582	-3.141678	-2.925013
C	-2.825293	-1.82866	-3.615088
H	-2.949719	-2.333338	-4.569188
C	-3.556849	-0.677043	-3.316861
H	-4.25966	-0.24152	-4.015782
C	-3.382756	-0.093884	-2.085547
H	-3.934054	0.787271	-1.792686
C	-1.943622	2.35103	-0.587232
C	-2.286363	3.709124	-0.783427
H	-1.633853	4.292709	-1.422554
C	-3.359616	4.279339	-0.140977
H	-3.582639	5.332545	-0.28754
C	-4.139099	3.503644	0.731767
H	-4.968985	3.921392	1.287834
C	-3.842746	2.172159	0.856542
H	-4.420309	1.50967	1.486541
C	-4.89021	-0.976289	1.001413
C	-5.541551	-1.920172	1.847553
H	-6.598059	-2.072249	1.659496
C	-4.889911	-2.593205	2.844928
H	-5.427733	-3.301188	3.469829
C	-3.518446	-2.354505	3.048188
H	-2.952172	-2.859078	3.821237
C	-2.886089	-1.464891	2.22859
H	-1.82365	-1.26672	2.324737
C	0.533796	1.496756	1.754206
H	-1.527343	-0.06129	0.91773
H	0.57788	-0.913244	1.908945

sp^2 -Cat

Ru	-0.047539	-0.917722	-0.364905
Cl	-0.249662	-3.14702	0.663135
C	0.009337	0.042051	-1.906461
O	0.039808	0.646281	-2.914713
P	-2.367055	-0.378478	-0.051536
P	2.339288	-0.542151	-0.03615
B	0.023152	1.058233	0.051163
N	-1.098783	1.955546	0.11663
N	1.202102	1.876484	0.087319
C	-0.613024	3.262208	0.11974
C	-1.275748	4.481058	0.129984
H	-2.361993	4.521849	0.128674
C	-0.511678	5.652134	0.125463
H	-1.014917	6.61475	0.125296
C	0.881117	5.602719	0.115734
H	1.451635	6.526822	0.108539
C	1.558897	4.380237	0.108393
H	2.645079	4.341465	0.088718
C	0.80959	3.212418	0.106489
C	-2.420668	1.495206	-0.235207
H	-2.65999	1.753915	-1.277085
H	-3.203047	1.937006	0.391796
C	-3.649262	-1.02711	-1.280726
C	-5.08228	-0.610997	-0.95494
H	-5.191865	0.477217	-0.883544
H	-5.443267	-1.053777	-0.022562
H	-5.752014	-0.952002	-1.754017
C	-3.524556	-2.554011	-1.334408
H	-3.863143	-3.042201	-0.419476
H	-2.488411	-2.865219	-1.505313
H	-4.138583	-2.933732	-2.15966
C	-3.276923	-0.491552	-2.667867
H	-3.952499	-0.939049	-3.405738
H	-2.256438	-0.761072	-2.953003
H	-3.379344	0.59388	-2.756239
C	-2.947095	-0.634399	1.745583
C	-1.722598	-0.417141	2.642754
H	-2.033136	-0.492654	3.692311
H	-1.276668	0.573086	2.496415
H	-0.958738	-1.180384	2.461114
C	-4.034573	0.352103	2.183085
H	-4.898959	0.380681	1.514385

H	-3.649064	1.37021	2.291143
H	-4.399313	0.047162	3.170997
C	-3.443393	-2.066501	1.949707
H	-2.719266	-2.802055	1.586948
H	-4.410914	-2.244761	1.470483
H	-3.582254	-2.236379	3.024188
C	2.491341	1.324742	-0.23593
H	3.292431	1.717484	0.406601
H	2.76993	1.556483	-1.276332
C	3.607492	-1.199247	-1.280386
C	2.909298	-1.172751	-2.644145
H	3.600173	-1.544055	-3.410241
H	2.603818	-0.163394	-2.939261
H	2.018018	-1.808076	-2.652134
C	3.942946	-2.650337	-0.9349
H	4.495574	-3.102062	-1.76725
H	3.041156	-3.250223	-0.768702
H	4.576182	-2.729216	-0.045933
C	4.888611	-0.368599	-1.377682
H	5.460592	-0.348405	-0.448653
H	4.69221	0.665051	-1.678773
H	5.535923	-0.804994	-2.148223
C	2.955701	-0.775177	1.746631
C	2.724894	-2.210993	2.219663
H	3.304467	-2.942426	1.652137
H	1.674471	-2.502734	2.152511
H	3.039593	-2.286544	3.267786
C	4.431129	-0.420522	1.932094
H	4.664576	-0.437151	3.003626
H	4.688268	0.578435	1.563219
H	5.093109	-1.145871	1.450065
C	2.108158	0.155086	2.622432
H	1.03665	-0.022743	2.481852
H	2.29942	1.214984	2.429971
H	2.34531	-0.040112	3.674836

sp^2 -RC

Ru	0.000004	-0.887939	-0.131455
Cl	0.0002	-3.440301	-0.638968
C	-0.000064	-0.086303	-1.792712
O	-0.000135	0.507315	-2.798868
P	-2.343996	-0.425176	0.090119

P	2.344095	-0.424939	0.090109
B	-0.000097	1.115494	0.252366
N	-1.15313	1.97571	0.182743
N	1.152853	1.975809	0.183025
C	-0.711376	3.285782	-0.00502
C	-1.417877	4.465469	-0.19067
H	-2.504942	4.464462	-0.202769
C	-0.69707	5.648105	-0.380304
H	-1.233968	6.579479	-0.535566
C	0.696678	5.648162	-0.38012
H	1.233542	6.579581	-0.53523
C	1.417509	4.465571	-0.190293
H	2.504578	4.464611	-0.202105
C	0.711025	3.285853	-0.004818
C	-2.447121	1.438074	-0.157586
H	-2.687466	1.638699	-1.214152
H	-3.262735	1.867795	0.442834
C	-3.567165	-1.11946	-1.180156
C	-4.834331	-0.28003	-1.360295
H	-4.613238	0.742878	-1.681941
H	-5.455194	-0.22661	-0.464804
H	-5.444849	-0.734098	-2.150085
C	-3.919587	-2.557645	-0.797452
H	-4.580708	-2.609595	0.073054
H	-3.019457	-3.153159	-0.6023
H	-4.451809	-3.027556	-1.632754
C	-2.822326	-1.160386	-2.517683
H	-3.494855	-1.56496	-3.283114
H	-1.94059	-1.807556	-2.463759
H	-2.509632	-0.166241	-2.852862
C	-3.035528	-0.626809	1.853089
C	-2.247879	0.323538	2.763257
H	-2.582545	0.18042	3.797423
H	-2.400554	1.375731	2.506805
H	-1.169534	0.13598	2.732458
C	-4.518715	-0.264547	1.956046
H	-5.157691	-0.993125	1.449789
H	-4.745353	0.7297	1.556614
H	-4.810409	-0.260596	3.01311
C	-2.852295	-2.059717	2.360464
H	-1.812782	-2.389569	2.33563
H	-3.435438	-2.787146	1.793795
H	-3.18801	-2.109083	3.403222
C	2.447004	1.438358	-0.156997

H	3.26241	1.868142	0.443644
H	2.687561	1.639201	-1.213492
C	3.567381	-1.118712	-1.180303
C	2.822852	-1.158898	-2.518034
H	3.495514	-1.563254	-3.283465
H	2.510351	-0.164561	-2.852815
H	1.941047	-1.805992	-2.464646
C	3.919272	-2.557147	-0.798118
H	4.451466	-3.027016	-1.633467
H	3.018924	-3.152439	-0.603247
H	4.580265	-2.609521	0.072458
C	4.834774	-0.279494	-1.359851
H	5.455641	-0.226839	-0.464326
H	4.613912	0.743681	-1.68082
H	5.445213	-0.733163	-2.149931
C	3.035477	-0.627298	1.853148
C	2.852454	-2.060537	2.359744
H	3.437496	-2.787092	1.7939
H	1.813378	-2.391616	2.332713
H	3.186301	-2.109975	3.403089
C	4.518578	-0.264788	1.956528
H	4.810153	-0.261488	3.013631
H	4.744966	0.729803	1.557815
H	5.157771	-0.992864	1.449818
C	2.247744	0.322751	2.763574
H	1.169247	0.136155	2.732147
H	2.401331	1.374996	2.50786
H	2.581832	0.178814	3.797796
H	0.002147	-1.321591	1.728041
H	-0.001299	-2.043225	1.36917

*sp*²-TS

Ru	-0.000003	-0.874599	-0.054854
Cl	-0.00011	-3.265281	-0.951248
C	0	-0.080223	-1.8286
O	0.0000001	0.587276	-2.77904
P	-2.355492	-0.446344	0.127077
P	2.355492	-0.44638	0.127063
B	0.000012	1.137784	0.294558
N	-1.158849	1.977977	0.220303
N	1.158887	1.977958	0.220283
C	-0.711668	3.28324	-0.005534
C	-1.417671	4.456189	-0.229495

H	2.505353	4.426598	-0.057136
C	0.712575	3.262919	0.213057
C	-2.459841	1.408276	0.138241
H	-2.736776	1.707876	-0.883987
H	-3.257182	1.767252	0.805586
C	-3.551306	-0.968992	-1.244037
C	-4.846279	-0.15304	-1.284896
H	-4.661582	0.921035	-1.38976
H	-5.48614	-0.304071	-0.414423
H	-5.422164	-0.459812	-2.166305
C	-3.861255	-2.461084	-1.114974
H	-4.514566	-2.675169	-0.263719
H	-2.943584	-3.053688	-1.023375
H	-4.384905	-2.796558	-2.017713
C	-2.8034	-0.750389	-2.562509
H	-3.456461	-1.058769	-3.387484
H	-1.888392	-1.350349	-2.608755
H	-2.549853	0.301806	-2.730301
C	-3.077443	-0.95755	1.84132
C	-2.290552	-0.171536	2.897166
H	-2.732378	-0.364438	3.881466
H	-2.307988	0.911324	2.734518
H	-1.248226	-0.498742	2.939645
C	-4.562219	-0.625282	1.985998
H	-5.187624	-1.268193	1.361065
H	-4.791382	0.418919	1.744662
H	-4.868071	-0.79266	3.025636
C	-2.854569	-2.449721	2.103403
H	-1.81499	-2.735075	1.915843
H	-3.494987	-3.086748	1.490255
H	-3.086592	-2.665328	3.153234
C	2.459815	1.408238	0.138154
H	3.257208	1.767309	0.805381
H	2.736641	1.707766	-0.884129
C	3.551293	-0.969018	-1.244064
C	2.803402	-0.750365	-2.562545
H	3.456508	-1.058659	-3.387518
H	2.549819	0.30183	-2.730271
H	1.888433	-1.350374	-2.608841
C	3.861229	-2.461112	-1.115055
H	4.384911	-2.79655	-2.01779
H	2.943553	-3.053716	-1.023525
H	4.514512	-2.675246	-0.263791
C	4.84626	-0.153058	-1.284913

H	5.48607	-0.303982	-0.414388
H	4.661548	0.920999	-1.389911
H	5.422205	-0.459913	-2.166254
C	3.077456	-0.95754	1.841333
C	2.854638	-2.449716	2.103426
H	3.495047	-3.086721	1.490241
H	1.815059	-2.735104	1.915921
H	3.086723	-2.665322	3.153244
C	4.562222	-0.625245	1.986069
H	4.868029	-0.792647	3.025718
H	4.791395	0.418961	1.744775
H	5.187662	-1.26814	1.361154
C	2.290544	-0.171561	2.89719
H	1.248212	-0.498754	2.939627
H	2.308003	0.911303	2.734592
H	2.732339	-0.364518	3.881494
H	-0.000061	0.079293	1.326741
H	0.000045	-1.885318	1.238054

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C	0.274919	2.964614	-0.021927
C	0.380036	3.681439	-1.238423
C	0.305583	2.998446	-2.574495
H	-0.55198	3.36461	-3.152562
H	0.206606	1.91077	-2.484544
H	1.198213	3.206634	-3.176282
C	0.550864	5.065459	-1.207881
H	0.633609	5.608466	-2.149448
C	0.622074	5.771581	-0.008285
C	0.811184	7.256834	0.007113
H	-0.029171	7.762954	0.494383
H	0.904278	7.664462	-1.002541
H	1.709797	7.539965	0.565474
C	0.51214	5.056191	1.186383
H	0.563566	5.592828	2.13393
C	0.336717	3.675094	1.205122
C	0.206195	2.981129	2.529493
H	1.040283	3.233931	3.193322
H	0.173223	1.891754	2.434629
H	-0.710707	3.291528	3.044288
C	-2.738233	-2.30913	-0.337699
H	-2.076373	-2.545625	-1.189565
C	-2.332754	-3.233307	0.816449
H	-1.329901	-2.993252	1.188694

H	-3.005989	-3.060096	1.66941	C	-4.819423	0.272936	1.26042
C	-2.433862	-4.694746	0.393265	H	-4.892307	1.17934	0.640656
H	-1.717876	-4.877704	-0.42256	H	-5.322143	-0.521658	0.697287
H	-2.132212	-5.349211	1.219207	C	3.561466	-0.135395	1.25388
C	-3.837792	-5.040756	-0.087381	H	4.515032	0.025837	0.719771
H	-4.536922	-4.958423	0.757745	C	3.83293	-1.06731	2.441445
H	-3.887257	-6.081652	-0.426906	H	2.879058	-1.280185	2.942975
C	-4.286556	-4.095275	-1.195152	H	4.23558	-2.029794	2.105484
H	-5.31416	-4.32026	-1.5036	C	4.813151	-0.430169	3.42342
H	-3.656765	-4.249618	-2.084329	H	4.986144	-1.109849	4.265616
C	-4.174963	-2.635126	-0.763218	H	5.787405	-0.299724	2.927378
H	-4.520834	-1.979454	-1.571223	C	4.322901	0.924179	3.918067
H	-4.847936	-2.463443	0.089352	H	3.395704	0.784213	4.492398
C	-3.180169	0.350042	-1.410751	H	5.051843	1.370932	4.604194
H	-4.255392	0.136475	-1.299063	C	4.041133	1.853354	2.744817
C	-2.739635	-0.168228	-2.782393	H	4.982188	2.075835	2.218049
H	-1.665267	0.032542	-2.90618	H	3.651003	2.817351	3.094275
H	-2.85625	-1.256909	-2.84948	C	3.055398	1.213069	1.777549
C	-3.527807	0.512833	-3.896726	H	2.82221	1.899332	0.953063
H	-3.204544	0.134251	-4.873242	H	2.10535	1.019464	2.293089
H	-4.591559	0.246493	-3.800422	C	3.28207	-0.365972	-1.59604
C	-3.377475	2.02761	-3.835313	H	4.288644	-0.806632	-1.491998
H	-2.327616	2.285424	-4.039234	C	2.629901	-0.94406	-2.852831
H	-3.970828	2.508467	-4.621385	H	2.569434	-2.036624	-2.782315
C	-3.763934	2.569183	-2.463939	H	1.592218	-0.583325	-2.90867
H	-4.843006	2.42238	-2.304946	C	3.383567	-0.544674	-4.116805
H	-3.589229	3.650781	-2.414008	H	4.393703	-0.980972	-4.092657
C	-2.993579	1.866653	-1.351316	H	2.887421	-0.967951	-4.997739
H	-1.922793	2.084699	-1.453162	C	3.493211	0.969191	-4.235796
H	-3.289399	2.263201	-0.371764	H	2.483363	1.393432	-4.341647
C	-3.343259	-0.062179	1.503565	H	4.042986	1.249552	-5.141531
H	-3.295681	-0.971254	2.125185	C	4.160861	1.558368	-3.000365
C	-2.662163	1.048627	2.308829	H	4.210257	2.651744	-3.068016
H	-1.629512	0.751072	2.510536	H	5.202159	1.206452	-2.953898
H	-2.615408	1.969641	1.704136	C	3.439913	1.152537	-1.719261
C	-3.402625	1.322512	3.611557	H	2.438161	1.607171	-1.695503
H	-3.320856	0.432895	4.253164	H	3.977978	1.552021	-0.851557
H	-2.914024	2.137361	4.15913	C	2.499918	-2.644894	0.12026
C	-4.873641	1.638954	3.37389	H	2.390968	-2.792558	1.206293
H	-5.395105	1.801404	4.324313	C	1.319169	-3.389785	-0.517177
H	-4.955752	2.581254	2.811246	H	0.367702	-2.959228	-0.167926
C	-5.546293	0.527212	2.578259	H	1.327293	-3.264565	-1.609169
H	-6.598165	0.768944	2.385499	C	1.375438	-4.872957	-0.163651
H	-5.545858	-0.397456	3.174052	H	1.22842	-4.979546	0.921588

H	0.547619	-5.410459	-0.640503
C	2.710251	-5.492851	-0.564752
H	2.798262	-5.473715	-1.661471
H	2.744346	-6.548581	-0.273511
C	3.887283	-4.733545	0.037609
H	3.862515	-4.829817	1.133049
H	4.836582	-5.172211	-0.29083
C	3.828571	-3.254197	-0.328416
H	4.674705	-2.7107	0.110988
H	3.931486	-3.147811	-1.419272
P	-2.330813	-0.516727	-0.0011
P	2.366921	-0.799674	-0.033341
B	0.131156	1.439993	-0.018684
Ru	0.042963	-0.362836	0.114166
Cl	0.175697	-1.218345	2.510629
H	-0.009259	-0.335828	-1.501563

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C	-0.002569	2.953821	-0.209932
C	0.014256	3.696335	0.997379
C	0.078712	3.032131	2.343598
H	0.935936	3.39592	2.922017
H	0.155674	1.942084	2.273843
H	-0.816595	3.260488	2.933682
C	-0.07863	5.086932	0.953806
H	-0.071542	5.644716	1.890372
C	-0.205094	5.781132	-0.249286
C	-0.287203	7.275433	-0.272235
H	0.70742	7.724453	-0.37674
H	-0.720085	7.671363	0.65031
H	-0.887167	7.635114	-1.112695
C	-0.247191	5.041666	-1.432812
H	-0.371487	5.56386	-2.381486
C	-0.143252	3.65289	-1.436916
C	-0.205165	2.934323	-2.754189
H	-0.987901	3.354377	-3.394663
H	-0.409289	1.865272	-2.63424
H	0.738682	3.025559	-3.304879
C	2.826177	-2.470548	0.216641
H	1.944281	-2.881806	0.73079
C	2.880238	-3.172365	-1.146248
H	2.006496	-2.897769	-1.748183
H	3.778994	-2.842287	-1.692828
C	2.931108	-4.684262	-0.968971

H	1.996505	-5.004108	-0.48844
H	2.963854	-5.177201	-1.947526
C	4.127089	-5.095921	-0.120858
H	5.055489	-4.85171	-0.660059
H	4.139044	-6.180915	0.034308
C	4.123768	-4.368943	1.217981
H	5.006274	-4.639903	1.809691
H	3.248245	-4.690813	1.800063
C	4.060616	-2.851588	1.044295
H	4.047807	-2.378371	2.032339
H	4.982072	-2.507738	0.551959
C	3.152852	0.099983	1.525953
H	4.176172	-0.308737	1.551643
C	2.433987	-0.341058	2.805879
H	1.415306	0.071999	2.793216
H	2.304282	-1.430376	2.830342
C	3.173674	0.148055	4.044608
H	2.656356	-0.184051	4.951722
H	4.175086	-0.308014	4.075182
C	3.303928	1.665521	4.028495
H	2.299203	2.104939	4.109862
H	3.864177	2.017966	4.902068
C	3.966262	2.15218	2.744853
H	5.014298	1.816795	2.735311
H	3.997489	3.248142	2.718935
C	3.275253	1.623067	1.489118
H	2.276317	2.067143	1.386641
H	3.838331	1.945261	0.606472
C	3.383592	-0.086554	-1.41985
H	3.150922	-0.845717	-2.183689
C	2.94103	1.254033	-2.016125
H	1.864807	1.222504	-2.216239
H	3.086507	2.068331	-1.29191
C	3.712248	1.569688	-3.293481
H	3.453052	0.825397	-4.06129
H	3.400317	2.543039	-3.691143
C	5.218007	1.543028	-3.061333
H	5.756045	1.756877	-3.991782
H	5.488347	2.343812	-2.356673
C	5.653787	0.202485	-2.483834
H	6.734363	0.190809	-2.300882
H	5.456353	-0.590933	-3.22016
C	4.899434	-0.118463	-1.197833
H	5.179277	0.612876	-0.425349

H	5.208683	-1.098072	-0.817765
C	-3.363205	-1.448378	-1.535154
H	-4.302661	-0.869717	-1.587002
C	-3.745752	-2.928654	-1.415268
H	-2.827894	-3.527845	-1.350429
H	-4.311116	-3.121906	-0.497911
C	-4.588437	-3.363809	-2.612571
H	-4.851371	-4.423434	-2.514367
H	-5.539384	-2.808961	-2.602635
C	-3.87974	-3.109181	-3.936122
H	-2.984169	-3.744054	-3.992315
H	-4.519098	-3.397193	-4.778675
C	-3.458471	-1.649981	-4.051216
H	-4.354021	-1.01131	-4.101045
H	-2.905615	-1.478426	-4.98235
C	-2.612088	-1.237815	-2.853455
H	-2.273971	-0.197259	-2.953859
H	-1.705138	-1.857815	-2.819819
C	-3.460006	0.864417	0.128177
H	-4.504394	0.528263	0.233206
C	-3.068344	1.637213	1.385738
H	-3.189969	1.008602	2.276389
H	-1.998174	1.866707	1.324284
C	-3.856277	2.933568	1.540832
H	-4.918071	2.695359	1.706728
H	-3.520249	3.471021	2.436471
C	-3.722984	3.814909	0.305696
H	-2.674406	4.127124	0.194633
H	-4.310248	4.733257	0.422058
C	-4.154174	3.060859	-0.944744
H	-4.021392	3.68676	-1.836088
H	-5.229274	2.835051	-0.88196
C	-3.375426	1.759551	-1.111621
H	-2.319079	1.995643	-1.300683
H	-3.73506	1.221475	-1.997707
C	-2.963452	-1.762422	1.35112
H	-2.81447	-2.7696	0.93844
C	-2.065849	-1.699874	2.589825
H	-1.029808	-1.882891	2.287688
H	-2.093398	-0.694928	3.039065
C	-2.498739	-2.740925	3.618017
H	-2.321045	-3.740312	3.194334
H	-1.86763	-2.670021	4.511559
C	-3.970526	-2.608457	3.988795

H	-4.132579	-1.644232	4.494446
H	-4.260525	-3.384455	4.706703
C	-4.851489	-2.671175	2.747929
H	-4.757641	-3.66441	2.284216
H	-5.908529	-2.55166	3.013961
C	-4.440547	-1.608429	1.733849
H	-5.086114	-1.657754	0.846783
H	-4.610323	-0.615042	2.175743
P	2.357317	-0.663329	0.031015
P	-2.436107	-0.680997	-0.079633
B	0.043108	1.419456	-0.208883
Ru	-0.013014	-0.430346	-0.221965
Cl	-0.380806	-3.085287	-0.300079
H	-0.112884	-0.258353	1.358343
H	0.09259	-1.105257	-2.087911
H	0.202869	-0.326808	-2.18216

sp-TS

C	-0.208669	2.997214	-0.247193
C	-0.456631	3.740618	0.938726
C	-0.468217	3.104418	2.299404
H	0.460957	3.318078	2.841546
H	-0.577352	2.01624	2.261773
H	-1.286273	3.506817	2.905941
C	-0.721118	5.106163	0.85349
H	-0.926047	5.657935	1.770611
C	-0.75018	5.779865	-0.366674
C	-1.09701	7.233458	-0.438396
H	-0.82777	7.761755	0.479999
H	-2.175633	7.369565	-0.581631
H	-0.600515	7.729188	-1.276912
C	-0.501225	5.044651	-1.525972
H	-0.53392	5.549588	-2.491201
C	-0.238215	3.677304	-1.495554
C	-0.013744	2.995057	-2.815577
H	1.010283	3.150319	-3.175179
H	-0.681245	3.408212	-3.578089
H	-0.18087	1.915775	-2.78842
C	3.088909	-2.262899	-0.184534
H	2.558392	-2.871491	0.559111
C	2.638413	-2.771425	-1.556987
H	1.557221	-2.639787	-1.658567
H	3.117105	-2.174394	-2.351233
C	3.002285	-4.240142	-1.735033

H	2.423484	-4.827652	-1.008404	H	5.460354	0.028349	0.136623
H	2.693187	-4.586208	-2.728258	C	-2.903174	-1.948831	-1.591241
C	4.490262	-4.487232	-1.521018	H	-3.9053	-1.554384	-1.838402
H	5.060582	-3.977068	-2.312259	C	-3.059699	-3.439723	-1.266054
H	4.724856	-5.554052	-1.613199	H	-2.074356	-3.849128	-1.00544
C	4.942796	-3.957607	-0.165929	H	-3.701047	-3.596308	-0.393079
H	6.020602	-4.106934	-0.030567	C	-3.659539	-4.192581	-2.452303
H	4.446632	-4.527293	0.632936	H	-3.75562	-5.255892	-2.204074
C	4.595127	-2.479299	-0.008282	H	-4.682908	-3.824993	-2.626013
H	4.935558	-2.109485	0.967749	C	-2.843868	-4.0113	-3.72506
H	5.144147	-1.906966	-0.772548	H	-1.859105	-4.481529	-3.592019
C	3.029236	-0.178088	1.883583	H	-3.3226	-4.525366	-4.566643
H	4.128217	-0.249504	1.906375	C	-2.645202	-2.533181	-4.032807
C	2.457398	-1.193914	2.878247	H	-3.61616	-2.073134	-4.274093
H	1.363147	-1.212329	2.77233	H	-2.014232	-2.403929	-4.919948
H	2.799427	-2.206046	2.631655	C	-2.025057	-1.814702	-2.840793
C	2.84242	-0.848401	4.313178	H	-1.821257	-0.763113	-3.076944
H	2.394362	-1.573675	5.001461	H	-1.045822	-2.257031	-2.613246
H	3.932593	-0.943692	4.43249	C	-3.47297	0.600869	-0.40569
C	2.4279	0.570509	4.682075	H	-4.48664	0.169134	-0.448526
H	1.330436	0.64925	4.638994	C	-3.406678	1.56658	0.77849
H	2.717453	0.803334	5.71329	H	-3.671643	1.049296	1.707587
C	3.032732	1.575441	3.709944	H	-2.367666	1.894019	0.902507
H	4.129773	1.555688	3.797564	C	-4.294888	2.792111	0.59064
H	2.723943	2.597463	3.962873	H	-5.350697	2.481377	0.593193
C	2.625712	1.244527	2.279729	H	-4.171093	3.471413	1.443572
H	1.535493	1.312077	2.189828	C	-3.982475	3.509847	-0.714223
H	3.037236	1.983279	1.578324	H	-2.954816	3.898648	-0.676012
C	3.613457	0.48892	-0.936127	H	-4.638782	4.378436	-0.844293
H	3.845683	-0.197507	-1.768339	C	-4.114389	2.559052	-1.895379
C	2.933476	1.712429	-1.548286	H	-3.86453	3.070444	-2.83345
H	2.012281	1.398249	-2.048356	H	-5.162706	2.238234	-1.988845
H	2.629148	2.405567	-0.747372	C	-3.224282	1.330295	-1.728477
C	3.841832	2.439039	-2.534683	H	-2.171848	1.64654	-1.765015
H	4.022628	1.784095	-3.399981	H	-3.372276	0.647045	-2.573562
H	3.336651	3.332001	-2.924486	C	-3.001008	-1.719012	1.321003
C	5.176359	2.813402	-1.904202	H	-2.655066	-2.74882	1.158913
H	5.827866	3.299671	-2.63896	C	-2.406043	-1.315116	2.671992
H	5.00519	3.550459	-1.105836	H	-1.31499	-1.357345	2.60613
C	5.85434	1.586488	-1.309742	H	-2.67046	-0.276986	2.922561
H	6.804886	1.86009	-0.837499	C	-2.911277	-2.253276	3.76416
H	6.102036	0.878353	-2.114886	H	-2.521438	-3.261709	3.561745
C	4.949149	0.893943	-0.295209	H	-2.500513	-1.954717	4.735698
H	4.762765	1.586213	0.537797	C	-4.433666	-2.303425	3.820147

H	-4.81881	-1.314506	4.112576	H	-2.874997	-4.594788	-0.870734
H	-4.770322	-3.004595	4.592695	H	-3.000107	-5.103694	0.807175
C	-5.020978	-2.680621	2.465961	C	-4.854129	-4.368932	-0.039623
H	-4.716575	-3.70629	2.209159	H	-5.307309	-4.219502	0.95209
H	-6.116794	-2.683224	2.504249	H	-5.195936	-5.35046	-0.38792
C	-4.533449	-1.731273	1.375648	C	-5.344095	-3.270805	-0.975764
H	-4.964217	-2.01228	0.404955	H	-6.439051	-3.269237	-1.032227
H	-4.908811	-0.720305	1.593881	H	-4.979437	-3.468436	-1.994225
P	2.472245	-0.540592	0.149671	C	-4.837942	-1.900727	-0.529861
P	-2.313276	-0.848694	-0.177186	H	-5.216271	-1.121856	-1.204595
B	-0.029054	1.481368	-0.173925	H	-5.249653	-1.68358	0.467866
Ru	0.05696	-0.388751	-0.111247	C	-3.225358	0.826745	-1.512937
Cl	-0.009506	-2.882511	0.646065	H	-4.319356	0.813159	-1.382858
H	-0.148937	-0.032131	1.527698	C	-2.896929	0.266494	-2.901455
H	0.316272	-0.911701	-1.704465	H	-1.802999	0.219214	-3.015276
H	0.063993	0.420586	-1.515968	H	-3.246555	-0.767405	-2.99852

sp-PC

C	0.74096	3.021037	-0.014329	H	-3.507904	1.126634	-4.001744
C	0.981145	3.845731	-1.152252	H	-3.250613	0.715264	-4.984136
C	0.852454	3.330666	-2.557563	H	-4.605174	1.082316	-3.927292
H	1.065955	4.122476	-3.280303	C	-3.058547	2.577093	-3.894106
H	-0.149488	2.94417	-2.775548	H	-1.973766	2.628794	-4.071759
H	1.542581	2.502574	-2.755658	H	-3.526197	3.188264	-4.674529
C	1.382809	5.169186	-0.983876	C	-3.364687	3.146405	-2.513588
H	1.564393	5.780103	-1.867714	H	-4.454959	3.20249	-2.37586
C	1.573714	5.73007	0.279015	H	-2.989029	4.173209	-2.426468
C	1.982828	7.16089	0.434455	C	-2.760652	2.281647	-1.411589
H	1.106813	7.815514	0.51258	H	-1.666818	2.304772	-1.499872
H	2.565802	7.510668	-0.421894	H	-2.988307	2.706292	-0.425354
H	2.576802	7.317019	1.339265	C	-3.325741	0.315822	1.403328
C	1.358005	4.91767	1.391333	H	-3.515253	-0.633271	1.933226
H	1.519443	5.32954	2.387205	C	-2.415614	1.152628	2.301744
C	0.946072	3.591105	1.271543	H	-1.463064	0.631595	2.448843
C	0.741594	2.813953	2.539376	H	-2.171131	2.094768	1.782874
H	1.164458	3.348482	3.394176	C	-3.067985	1.45962	3.645061
H	1.200386	1.820925	2.506022	H	-3.192663	0.517725	4.199712
H	-0.320533	2.652215	2.750137	H	-2.402577	2.085241	4.252627
C	-3.307634	-1.89778	-0.469182	C	-4.428724	2.123086	3.478529
H	-2.921513	-2.195931	-1.45216	H	-4.897333	2.292883	4.45446
C	-2.828837	-2.967657	0.516874	H	-4.295401	3.115594	3.02307
H	-1.736403	-2.96657	0.562648	C	-5.3328	1.284272	2.585035
H	-3.200511	-2.735227	1.528436	H	-6.302449	1.775458	2.444054
C	-3.336364	-4.341859	0.09427	H	-5.542498	0.32241	3.076904
				C	-4.679754	1.019809	1.231714
				H	-4.529917	1.980841	0.72028

H	-5.35316	0.437931	0.595341	H	5.443941	2.267485	1.893813
C	2.350192	-1.88765	1.852778	H	6.090041	1.035144	0.820993
H	3.432087	-2.026309	2.023203	C	3.9866	0.824468	1.214319
C	1.664744	-3.259217	1.953728	H	3.132178	1.472517	1.467978
H	0.587466	-3.119408	1.782491	H	4.153548	0.165228	2.073709
H	2.006844	-3.942833	1.170542	C	2.741852	-2.565587	-0.937922
C	1.895135	-3.890903	3.322573	H	1.895715	-3.265076	-0.900495
H	1.400881	-4.867987	3.370008	C	2.905316	-2.166799	-2.408867
H	2.97133	-4.084209	3.451586	H	2.040349	-1.585731	-2.744298
C	1.408322	-2.987511	4.447532	H	3.801123	-1.534392	-2.513403
H	0.315549	-2.885706	4.377388	C	3.083204	-3.41285	-3.26927
H	1.615811	-3.438215	5.424922	H	2.1708	-4.020601	-3.192554
C	2.041171	-1.606413	4.343765	H	3.182414	-3.134348	-4.324765
H	3.124745	-1.687602	4.520208	C	4.292551	-4.221819	-2.816352
H	1.652294	-0.942715	5.124918	H	5.204833	-3.635608	-3.004228
C	1.800935	-0.98941	2.9696	H	4.391024	-5.13949	-3.407793
H	2.239234	0.012237	2.93041	C	4.218744	-4.552926	-1.330362
H	0.72239	-0.857037	2.802897	H	3.379664	-5.241424	-1.151211
C	3.636956	0.012688	-0.033731	H	5.124378	-5.080161	-1.007375
H	4.493986	-0.646983	-0.248321	C	4.010003	-3.299261	-0.482279
C	3.462041	0.965561	-1.22147	H	3.974676	-3.573574	0.577669
H	3.17337	0.426389	-2.129146	H	4.883601	-2.639688	-0.599185
H	2.630268	1.639944	-0.992045	P	-2.494491	-0.249316	-0.180555
C	4.702942	1.817332	-1.459784	P	2.174536	-1.154934	0.140929
H	5.549414	1.171268	-1.737563	B	0.343634	1.547213	-0.232059
H	4.533234	2.488544	-2.310754	Ru	-0.084939	-0.373559	-0.196543
C	5.055048	2.61505	-0.210867	Cl	-0.395147	-2.291426	-1.79108
H	4.245696	3.331187	-0.003373	H	0.276821	1.074575	-1.407248
H	5.962788	3.208415	-0.369251	H	-0.378567	-1.384305	1.007114
C	5.222709	1.691264	0.988015	H	0.099719	0.844132	0.94512

(2) For structures in hydrogenation

*sp*³-*hy*-Cat

Ru	-0.499679	0.039402	-1.586257
S	1.278699	0.640689	-3.18012
S	-0.066892	-2.143383	-0.998482
S	4.853621	0.131365	1.435205
P	-2.206444	0.098113	-0.1291
B	1.895525	0.066946	-0.034857
N	2.773725	-0.532889	-1.20986
N	1.544793	-1.08413	0.950364
N	2.558588	1.354407	0.609167

C	-1.668675	0.169494	1.620805
C	-1.633457	-0.97738	2.424208
H	-2.051598	-1.909382	2.0493
C	-1.070346	-0.931092	3.697167
H	-1.05078	-1.829956	4.308131
C	-0.526027	0.254689	4.18358
H	-0.085934	0.286364	5.176837
C	-0.536977	1.397264	3.385344
H	-0.106294	2.325867	3.751573
C	-1.100608	1.35261	2.114945
H	-1.111537	2.250551	1.499289
C	-3.121109	1.674334	-0.358179

C	-3.812673	2.328052	0.669358
H	-3.827593	1.899259	1.669439
C	-4.463247	3.533397	0.424477
H	-4.995028	4.03249	1.230037
C	-4.431032	4.101253	-0.847587
H	-4.936855	5.0447	-1.034257
C	-3.750202	3.45822	-1.877872
H	-3.723863	3.89539	-2.872178
C	-3.100032	2.251704	-1.634643
H	-2.576907	1.735536	-2.440926
C	-3.537513	-1.164198	-0.104098
C	-4.504112	-1.191191	0.910374
H	-4.445249	-0.480703	1.733202
C	-5.532393	-2.125932	0.880416
H	-6.276611	-2.137932	1.672358
C	-5.607914	-3.044916	-0.16511
H	-6.412417	-3.775214	-0.189025
C	-4.652858	-3.025644	-1.176904
H	-4.707935	-3.741247	-1.992638
C	-3.621084	-2.090244	-1.147464
H	-2.871077	-2.063581	-1.934989
C	2.68048	-0.098187	-2.521677
C	3.742277	-0.413316	-3.396953
H	3.689559	-0.006533	-4.400345
C	4.738817	-1.287981	-3.029642
H	5.521627	-1.5499	-3.73615
C	4.691608	-1.879996	-1.762938
H	5.409617	-2.625526	-1.444787
C	3.720433	-1.463846	-0.887895
H	3.662316	-1.85841	0.11584
C	0.853472	-2.180843	0.45917
C	0.875357	-3.372643	1.216251
H	0.375335	-4.240027	0.797715
C	1.44863	-3.406404	2.465382
H	1.438769	-4.326365	3.0428
C	1.988075	-2.227433	3.00974
H	2.380249	-2.186221	4.018581
C	2.021149	-1.10278	2.228401
H	2.430898	-0.167341	2.583895
C	3.836303	1.451102	1.179356
C	4.261877	2.751261	1.585908
H	5.255281	2.807904	2.01577
C	3.475884	3.862934	1.462419
H	3.839116	4.831351	1.795504

C	2.195105	3.731164	0.893764
H	1.530202	4.575995	0.759656
C	1.797298	2.492532	0.480863
H	0.831595	2.3423	0.010522
H	0.865958	0.545702	-0.423727
H	-1.571553	-0.391534	-2.694435

*sp*³-hy-RC

Ru	0.441375	0.317957	-1.559765
S	-1.491438	0.596261	-3.101533
S	-0.211121	2.405043	-0.262289
S	-5.081202	-0.616475	1.302284
P	2.15775	-0.112128	-0.109749
B	-2.082976	0.026761	0.047405
N	-2.955688	1.007335	-0.815649
N	-1.659966	0.759401	1.356348
N	-2.694241	-1.413011	0.270716
C	1.651228	-1.45849	1.029375
C	0.864418	-1.159235	2.151516
H	0.708084	-0.119256	2.432274
C	0.294066	-2.171793	2.916799
H	-0.306904	-1.91226	3.784773
C	0.493168	-3.507179	2.57426
H	0.042716	-4.297685	3.167787
C	1.2715	-3.820982	1.462934
H	1.43826	-4.859695	1.189284
C	1.843462	-2.808825	0.697444
H	2.457712	-3.069726	-0.161088
C	3.793545	-0.667404	-0.754163
C	4.636979	-1.5172	-0.026921
H	4.30085	-1.934266	0.919219
C	5.908705	-1.826965	-0.497139
H	6.547353	-2.492707	0.077197
C	6.366037	-1.278703	-1.692995
H	7.359196	-1.522337	-2.060288
C	5.549527	-0.407958	-2.408771
H	5.90411	0.035816	-3.334968
C	4.274073	-0.10304	-1.94204
H	3.638871	0.587689	-2.493547
C	2.784223	1.215872	1.004067
C	3.222838	0.985399	2.312153
H	3.141544	-0.008219	2.746453
C	3.771465	2.020515	3.065732

H	4.102845	1.828092	4.082849
C	3.903997	3.292456	2.515013
H	4.334159	4.098611	3.103491
C	3.493512	3.525308	1.204498
H	3.601103	4.513002	0.765008
C	2.934867	2.495447	0.455378
H	2.600091	2.67887	-0.56334
C	-2.83021	1.145449	-2.187619
C	-3.835978	1.866828	-2.87125
H	-3.754558	1.917261	-3.950774
C	-4.812632	2.557841	-2.195523
H	-5.548302	3.138856	-2.744668
C	-4.805139	2.551707	-0.79528
H	-5.510025	3.128784	-0.209784
C	-3.884825	1.764503	-0.155923
H	-3.847821	1.704191	0.921292
C	-0.830937	1.865719	1.241229
C	-0.49281	2.551394	2.431174
H	0.164516	3.409253	2.338137
C	-0.930287	2.11205	3.660122
H	-0.633481	2.640294	4.561916
C	-1.735262	0.964104	3.739884
H	-2.093257	0.577468	4.68634
C	-2.076994	0.324049	2.575104
H	-2.713652	-0.552284	2.56101
C	-4.012871	-1.728974	0.621243
C	-4.41334	-3.086056	0.441858
H	-5.457042	-3.301681	0.639697
C	-3.532426	-4.075765	0.09989
H	-3.874063	-5.10263	0.000434
C	-2.177757	-3.746136	-0.094513
H	-1.422236	-4.489283	-0.321977
C	-1.817846	-2.432152	-0.017887
H	-0.793396	-2.120423	-0.18864
H	-1.065857	-0.252869	-0.523126
H	1.476211	1.224543	-2.349736
C	1.241212	-0.855621	-3.215944
H	0.779566	-0.504271	-4.136456
H	2.325138	-0.897577	-3.244572
C	0.533365	-1.705508	-2.351324
H	1.066063	-2.407087	-1.710392
H	-0.487442	-1.997745	-2.594509

sp^3 -a- TS_1

Ru	0.413585	-0.845366	-1.36019
S	-1.55434	-1.810236	-2.52033
S	-0.231856	1.625838	-1.894343
S	-4.88651	0.676813	1.431225
P	2.102448	-0.156151	0.026415
B	-1.997942	0.105616	0.001034
N	-2.886409	0.219866	-1.294202
N	-1.580214	1.524084	0.463596
N	-2.64663	-0.840056	1.084285
C	1.538328	-0.495838	1.739841
C	0.791754	0.471967	2.426471
H	0.693134	1.470725	2.007022
C	0.177924	0.177624	3.64037
H	-0.393213	0.949364	4.151124
C	0.296781	-1.093056	4.196503
H	-0.184561	-1.324811	5.142468
C	1.032757	-2.067025	3.525794
H	1.132419	-3.063004	3.949584
C	1.640798	-1.775551	2.308915
H	2.20706	-2.550552	1.799344
C	3.753346	-0.967376	-0.103089
C	4.522112	-1.373148	0.99382
H	4.12697	-1.274399	2.001262
C	5.804033	-1.88597	0.810592
H	6.38462	-2.198883	1.674195
C	6.346102	-1.98406	-0.467358
H	7.346498	-2.383915	-0.607331
C	5.603873	-1.554273	-1.564429
H	6.024949	-1.609402	-2.564614
C	4.320196	-1.050903	-1.382105
H	3.750027	-0.69604	-2.239719
C	2.706127	1.586432	0.090785
C	3.122034	2.21509	1.270681
H	3.053066	1.691151	2.22072
C	3.631022	3.510427	1.24207
H	3.940896	3.987161	2.168448
C	3.753975	4.18684	0.031217
H	4.150775	5.198464	0.009382
C	3.380666	3.556129	-1.153196
H	3.486379	4.070894	-2.104379
C	2.85809	2.266999	-1.123387
H	2.54933	1.78073	-2.045143
C	-2.839946	-0.697328	-2.323695
C	-3.863583	-0.656957	-3.294808

H	-3.837166	-1.413157	-4.070877	N	1.50771	1.478156	0.641915
C	-4.798906	0.352056	-3.30673	C	-2.026717	-0.53476	1.713044
H	-5.554491	0.384851	-4.086737	C	-2.280479	-1.885006	1.993605
C	-4.726285	1.360927	-2.340014	H	-2.406907	-2.594428	1.185332
H	-5.401128	2.207656	-2.335736	C	-2.36246	-2.34688	3.303229
C	-3.778197	1.250399	-1.355782	H	-2.559012	-3.400273	3.484775
H	-3.689192	1.985975	-0.570646	C	-2.187923	-1.47206	4.371157
C	-0.765102	2.254419	-0.397606	H	-2.244262	-1.834296	5.394059
C	-0.356618	3.538447	0.036598	C	-1.952605	-0.125391	4.113727
H	0.294732	4.09675	-0.627104	H	-1.832258	0.577553	4.934557
C	-0.715337	4.028329	1.270312	C	-1.88081	0.337257	2.801958
H	-0.360873	5.004804	1.58923	H	-1.707225	1.394337	2.626083
C	-1.507605	3.244042	2.126066	C	-2.090525	1.813799	0.053273
H	-1.798846	3.583838	3.112809	C	-3.172258	2.328855	0.786661
C	-1.911538	2.007759	1.691385	H	-3.832885	1.649612	1.322457
H	-2.516599	1.351649	2.303105	C	-3.402968	3.698466	0.840673
C	-3.926086	-0.695758	1.639063	H	-4.241066	4.081438	1.417153
C	-4.397734	-1.768831	2.449971	C	-2.564195	4.577486	0.155038
H	-5.397467	-1.652042	2.851816	H	-2.744511	5.648314	0.201927
C	-3.640267	-2.873342	2.730728	C	-1.50454	4.077515	-0.593009
H	-4.036543	-3.662883	3.363932	H	-0.842965	4.748173	-1.135656
C	-2.344475	-2.96623	2.192193	C	-1.270911	2.705105	-0.644499
H	-1.69158	-3.808457	2.388445	H	-0.436809	2.325881	-1.228963
C	-1.904085	-1.957477	1.384334	C	-3.256457	-0.639686	-0.895176
H	-0.920556	-1.995057	0.925628	C	-4.256554	0.18629	-1.420557
H	-0.944634	-0.462467	-0.176428	H	-4.205512	1.261311	-1.274738
C	1.510071	-2.531638	-2.27077	C	-5.317149	-0.353976	-2.146243
H	1.473415	-1.210018	-2.603002	H	-6.078264	0.307382	-2.551709
H	2.597286	-2.581611	-2.360253	C	-5.401533	-1.726111	-2.355006
C	0.949253	-2.870986	-0.97789	H	-6.230261	-2.144399	-2.919608
H	1.658293	-3.065285	-0.17201	C	-4.404888	-2.559427	-1.850905
H	0.078754	-3.526935	-0.95585	H	-4.447528	-3.631131	-2.025249
H	1.008704	-2.933535	-3.153381	C	-3.337993	-2.019517	-1.143337

sp³-a-IM

Ru	0.099	-0.743959	-1.239299
S	1.971168	-1.497619	-2.588782
S	0.29337	-2.82428	0.104847
S	2.419583	2.529373	-1.707036
P	-1.752962	0.010268	-0.038455
B	1.619842	-0.017921	0.088022
N	3.087947	-0.180428	-0.542397
N	1.725358	-0.978107	1.430261

N	1.50771	1.478156	0.641915
C	-2.026717	-0.53476	1.713044
C	-2.280479	-1.885006	1.993605
H	-2.406907	-2.594428	1.185332
C	-2.36246	-2.34688	3.303229
H	-2.559012	-3.400273	3.484775
C	-2.187923	-1.47206	4.371157
H	-2.244262	-1.834296	5.394059
C	-1.952605	-0.125391	4.113727
H	-1.832258	0.577553	4.934557
C	-1.88081	0.337257	2.801958
H	-1.707225	1.394337	2.626083
C	-2.090525	1.813799	0.053273
C	-3.172258	2.328855	0.786661
H	-3.832885	1.649612	1.322457
C	-3.402968	3.698466	0.840673
H	-4.241066	4.081438	1.417153
C	-2.564195	4.577486	0.155038
H	-2.744511	5.648314	0.201927
C	-1.50454	4.077515	-0.593009
H	-0.842965	4.748173	-1.135656
C	-1.270911	2.705105	-0.644499
H	-0.436809	2.325881	-1.228963
C	-3.256457	-0.639686	-0.895176
C	-4.256554	0.18629	-1.420557
H	-4.205512	1.261311	-1.274738
C	-5.317149	-0.353976	-2.146243
H	-6.078264	0.307382	-2.551709
C	-5.401533	-1.726111	-2.355006
H	-6.230261	-2.144399	-2.919608
C	-4.404888	-2.559427	-1.850905
H	-4.447528	-3.631131	-2.025249
C	-3.337993	-2.019517	-1.143337
H	-2.53103	-2.673029	-0.814365
C	3.284272	-0.894133	-1.696046
C	4.610396	-1.095409	-2.15326
H	4.740055	-1.679151	-3.0578
C	5.680318	-0.555354	-1.488905
H	6.689981	-0.71203	-1.857643
C	5.449946	0.225551	-0.341516
H	6.255757	0.714171	0.192241
C	4.158749	0.388565	0.077753
H	3.91973	1.026404	0.920043
C	1.19044	-2.247024	1.422129

C	1.415553	-3.09264	2.540144
H	0.967743	-4.079861	2.507724
C	2.158484	-2.679082	3.613933
H	2.31305	-3.338822	4.462795
C	2.710241	-1.384841	3.598568
H	3.302189	-1.002021	4.421394
C	2.474611	-0.593805	2.507397
H	2.856116	0.418636	2.471001
C	1.913724	2.600677	-0.101066
C	1.806156	3.865401	0.55407
H	2.200835	4.712295	0.003556
C	1.180614	4.029509	1.759929
H	1.082472	5.01819	2.200024
C	0.634085	2.899035	2.394885
H	0.077022	2.963724	3.323344
C	0.827986	1.677725	1.811829
H	0.430476	0.782016	2.269892
H	0.726894	0.694001	-1.418657
C	-1.152122	-1.049631	-3.442964
H	-1.071216	-1.854444	-2.65491
H	-2.227431	-1.024271	-3.648586
C	-0.595251	0.265439	-2.981412
H	-1.349625	1.036153	-2.805195
H	0.217795	0.657416	-3.592538
H	-0.608583	-1.467674	-4.294372

sp^3 -a- TS_2

Ru	0.127315	-0.346698	-1.389757
S	2.012924	-0.725933	-2.872267
S	0.28139	-2.676636	-0.693058
S	2.48749	2.787397	-1.067574
P	-1.738701	0.023501	-0.048923
B	1.613463	-0.066198	0.111164
N	3.102785	-0.128532	-0.500676
N	1.625853	-1.318984	1.179814
N	1.529966	1.264557	0.981952
C	-2.023423	-1.024968	1.451683
C	-2.301618	-2.393132	1.318241
H	-2.458405	-2.823406	0.336199
C	-2.370075	-3.224964	2.431491
H	-2.586828	-4.281266	2.294
C	-2.158313	-2.714161	3.708851
H	-2.202404	-3.36681	4.576407

C	-1.901918	-1.355757	3.862942
H	-1.759331	-0.933136	4.854347
C	-1.847832	-0.521609	2.749068
H	-1.677474	0.540937	2.89473
C	-2.110505	1.708678	0.588739
C	-3.216917	1.950331	1.419787
H	-3.86324	1.12325	1.70779
C	-3.491643	3.231784	1.882313
H	-4.349021	3.399558	2.528922
C	-2.673673	4.299318	1.511797
H	-2.89081	5.301294	1.872594
C	-1.584018	4.07588	0.678013
H	-0.936433	4.897489	0.383081
C	-1.303198	2.789536	0.223236
H	-0.434455	2.626367	-0.408966
C	-3.221131	-0.344016	-1.091254
C	-4.233816	0.588388	-1.341539
H	-4.208655	1.562221	-0.861524
C	-5.276666	0.289352	-2.21676
H	-6.04913	1.031218	-2.400809
C	-5.329691	-0.945709	-2.85314
H	-6.14455	-1.177131	-3.53358
C	-4.319425	-1.878376	-2.626421
H	-4.337902	-2.839379	-3.133569
C	-3.270086	-1.574683	-1.767196
H	-2.452744	-2.285441	-1.646419
C	3.315002	-0.467226	-1.812231
C	4.648273	-0.560054	-2.281873
H	4.791015	-0.844289	-3.3185
C	5.710821	-0.274122	-1.464538
H	6.726557	-0.337175	-1.844407
C	5.46707	0.122867	-0.137445
H	6.26944	0.395209	0.537588
C	4.16792	0.182736	0.287151
H	3.920332	0.526215	1.284569
C	1.07218	-2.520974	0.800077
C	1.171018	-3.633078	1.673055
H	0.706923	-4.558174	1.348637
C	1.808577	-3.535004	2.88191
H	1.85852	-4.390992	3.548567
C	2.391483	-2.307104	3.244724
H	2.912313	-2.17408	4.185526
C	2.288304	-1.256668	2.373189
H	2.706817	-0.290349	2.625625

C	1.985491	2.509566	0.516684
C	1.932555	3.592221	1.446779
H	2.366655	4.525242	1.104333
C	1.309684	3.499999	2.662203
H	1.255876	4.362709	3.320856
C	0.704847	2.280184	3.018388
H	0.137267	2.156605	3.934525
C	0.847964	1.220609	2.167397
H	0.402049	0.263422	2.399618
H	0.553965	1.210488	-1.434535
C	-1.045293	0.175304	-3.607705
H	-1.071455	-0.837278	-3.124631
H	-2.099066	0.371461	-3.833046
C	-0.429079	1.252197	-2.738479
H	-1.164996	1.964548	-2.356898
H	0.379606	1.791059	-3.236146
H	-0.48539	0.022165	-4.53363

$sp^3\text{-b-}TS_1$

Ru	-0.083988	-1.198728	-0.660865
S	1.608231	-2.896791	-1.034249
S	0.03206	-1.686516	1.724663
S	4.045276	-0.037364	-2.373225
P	-2.045871	-0.008704	-0.206559
B	1.803675	0.030454	0.07081
N	2.991816	-1.001003	0.265491
N	1.541393	0.512354	1.598733
N	2.3553	1.318672	-0.700959
C	-1.781951	1.747656	0.23333
C	-1.448648	2.073829	1.557988
H	-1.477175	1.299648	2.322979
C	-1.082512	3.370496	1.903367
H	-0.826525	3.598608	2.934886
C	-1.051866	4.372514	0.933698
H	-0.77898	5.388696	1.205094
C	-1.366151	4.05972	-0.386447
H	-1.33165	4.829938	-1.152835
C	-1.70859	2.756508	-0.737889
H	-1.921706	2.522983	-1.778258
C	-3.394125	0.012219	-1.47054
C	-4.216064	1.112378	-1.742202
H	-4.041595	2.063144	-1.246637
C	-5.283114	0.998081	-2.630113

H	-5.904942	1.865837	-2.833825
C	-5.560628	-0.219268	-3.243618
H	-6.392856	-0.304645	-3.936824
C	-4.775636	-1.331306	-2.949148
H	-4.995799	-2.29268	-3.405102
C	-3.704472	-1.216568	-2.070669
H	-3.096562	-2.087656	-1.830988
C	-3.11808	-0.60378	1.177338
C	-4.019175	0.264121	1.806314
H	-4.021087	1.321587	1.55206
C	-4.921047	-0.212762	2.752709
H	-5.610112	0.476215	3.234001
C	-4.946591	-1.56758	3.072904
H	-5.652183	-1.941304	3.809982
C	-4.070069	-2.441773	2.436869
H	-4.086534	-3.501673	2.675109
C	-3.162667	-1.964302	1.495764
H	-2.481544	-2.64728	0.993956
C	2.961426	-2.286309	-0.215512
C	4.106986	-3.10056	-0.0348
H	4.053933	-4.116846	-0.408503
C	5.234962	-2.619336	0.57507
H	6.105913	-3.256833	0.697275
C	5.252898	-1.288676	1.032408
H	6.12575	-0.854164	1.504203
C	4.130728	-0.531834	0.850749
H	4.098366	0.508212	1.155959
C	0.875054	-0.380318	2.405633
C	0.886806	-0.186423	3.80871
H	0.365105	-0.918336	4.415627
C	1.498065	0.907774	4.365959
H	1.472386	1.062439	5.440795
C	2.153589	1.824623	3.52409
H	2.656036	2.702632	3.912233
C	2.170337	1.578251	2.176148
H	2.699353	2.23884	1.500528
C	3.400297	1.331839	-1.644323
C	3.856222	2.628328	-2.043366
H	4.743323	2.641574	-2.666163
C	3.168153	3.775248	-1.759265
H	3.518071	4.733724	-2.133105
C	1.974624	3.68478	-1.013169
H	1.343962	4.542796	-0.813116
C	1.622651	2.465044	-0.511149

H	0.73782	2.341823	0.104036
H	0.858283	0.026568	-1.404375
H	-1.135733	-2.479104	-0.595326
C	-0.485663	-1.396092	-2.764534
H	-0.054242	-2.308666	-3.166963
H	-1.522433	-1.226368	-3.031928
C	0.372001	-0.245336	-2.654517
H	-0.06944	0.735473	-2.84503
H	1.392805	-0.349402	-3.031982

sp^3 -b- IM

Ru	-0.160446	-0.905072	-1.012362
S	-2.240772	-1.841426	-2.028243
S	-0.364692	1.143968	-2.254299
S	-0.81922	-1.128945	2.853209
P	1.857757	-0.140255	-0.163348
B	-1.873796	0.106775	0.111987
N	-2.95591	-1.012143	0.407785
N	-2.669951	1.030339	-0.955585
N	-1.649414	1.018429	1.38806
C	1.90941	1.178044	1.122299
C	1.425836	2.435818	0.735313
H	0.951913	2.54653	-0.239406
C	1.57791	3.540302	1.563475
H	1.208937	4.509917	1.238209
C	2.190052	3.403922	2.807454
H	2.310417	4.268079	3.456035
C	2.642172	2.153595	3.215921
H	3.116239	2.03458	4.18677
C	2.509661	1.047315	2.379298
H	2.901538	0.088122	2.702123
C	2.928349	-1.470049	0.515177
C	2.575849	-2.122475	1.706739
H	1.694263	-1.794117	2.259062
C	3.339903	-3.183743	2.184801
H	3.057664	-3.66818	3.11596
C	4.451512	-3.626953	1.472178
H	5.042626	-4.459482	1.844208
C	4.796106	-3.001382	0.278165
H	5.657937	-3.343153	-0.288728
C	4.043589	-1.930879	-0.196684
H	4.329435	-1.452195	-1.129496
C	3.009946	0.646725	-1.380102

C	4.101662	1.398665	-0.919773
H	4.235349	1.560087	0.147706
C	5.020828	1.937515	-1.812116
H	5.86111	2.5151	-1.43582
C	4.86556	1.738863	-3.182814
H	5.582118	2.163498	-3.880749
C	3.788923	0.994404	-3.651196
H	3.657317	0.834445	-4.717915
C	2.869281	0.44974	-2.756313
H	2.033026	-0.138806	-3.12525
C	-3.230706	-1.875481	-0.629575
C	-4.318865	-2.761712	-0.5001
H	-4.525509	-3.427441	-1.330565
C	-5.068099	-2.794512	0.656073
H	-5.890637	-3.497793	0.752518
C	-4.753638	-1.92221	1.706575
H	-5.31014	-1.920264	2.635999
C	-3.705376	-1.047299	1.541239
H	-3.4357	-0.326134	2.302242
C	-1.977177	1.611876	-1.97983
C	-2.625833	2.572981	-2.790302
H	-2.053372	3.028718	-3.590599
C	-3.948264	2.88036	-2.5855
H	-4.44576	3.602982	-3.226095
C	-4.655871	2.237151	-1.552413
H	-5.705126	2.434402	-1.369115
C	-3.9808	1.340318	-0.766125
H	-4.465774	0.832818	0.061933
C	-1.087676	0.518582	2.575361
C	-0.784382	1.452652	3.603512
H	-0.327739	1.035236	4.493867
C	-1.073581	2.787343	3.50969
H	-0.843736	3.462946	4.329059
C	-1.649902	3.259121	2.319793
H	-1.883589	4.306528	2.165705
C	-1.8905	2.370571	1.309676
H	-2.291968	2.732538	0.375403
H	-0.469592	-1.964803	0.523729
H	0.625008	-1.23669	-2.412208
C	0.570422	-2.907221	-1.241787
H	0.091524	-3.428108	-2.067022
H	1.649693	-3.046717	-1.214338
C	-0.121882	-2.986879	0.062582
H	0.520913	-3.29761	0.88996

H	-1.060765	-3.54628	0.0444
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sp³-b-TS₂

Ru	-0.171279	-0.925349	-0.979058
S	-2.239615	-1.888497	-1.974738
S	-0.368746	1.057528	-2.30493
S	-0.823033	-1.097237	2.854032
P	1.846601	-0.132993	-0.150501
B	-1.86695	0.112278	0.112137
N	-2.963092	-0.994095	0.432963
N	-2.65949	1.021457	-0.971038
N	-1.642476	1.041503	1.375023
C	1.913307	1.223619	1.093311
C	1.421641	2.468628	0.676645
H	0.939894	2.551762	-0.297248
C	1.573792	3.594829	1.475217
H	1.197494	4.553904	1.128063
C	2.196078	3.493822	2.717561
H	2.316294	4.375012	3.342815
C	2.658825	2.256981	3.154383
H	3.141819	2.165698	4.1239
C	2.525039	1.128775	2.347988
H	2.92417	0.180001	2.691866
C	2.919814	-1.443903	0.562574
C	2.566079	-2.055618	1.775183
H	1.680464	-1.713182	2.311978
C	3.331876	-3.096003	2.293646
H	3.04802	-3.547091	3.240899
C	4.446545	-3.561464	1.600401
H	5.039581	-4.378001	2.003569
C	4.791934	-2.978474	0.385175
H	5.655921	-3.338154	-0.167321
C	4.038335	-1.926901	-0.129679
H	4.327142	-1.479713	-1.077281
C	2.992401	0.607619	-1.403184
C	4.085849	1.379254	-0.981475
H	4.227584	1.582188	0.07783
C	4.996398	1.886145	-1.901261
H	5.83746	2.480576	-1.554255
C	4.831214	1.634554	-3.261882
H	5.540151	2.035264	-3.981364
C	3.753744	0.868574	-3.692353
H	3.613878	0.667116	-4.751015

C	2.843035	0.356315	-2.769848
H	2.006125	-0.247096	-3.111982
C	-3.236387	-1.883715	-0.580354
C	-4.326853	-2.764111	-0.433639
H	-4.5306	-3.451502	-1.247038
C	-5.08105	-2.765016	0.719692
H	-5.904901	-3.464463	0.831753
C	-4.768816	-1.865557	1.747581
H	-5.327833	-1.838869	2.675103
C	-3.717064	-0.998391	1.563421
H	-3.446431	-0.260813	2.308462
C	-1.969425	1.560357	-2.020144
C	-2.612005	2.508593	-2.851122
H	-2.040566	2.932687	-3.669475
C	-3.92753	2.841456	-2.643153
H	-4.420527	3.553154	-3.299235
C	-4.634794	2.237644	-1.585918
H	-5.679478	2.454772	-1.398902
C	-3.964499	1.354757	-0.780202
H	-4.448094	0.877746	0.066855
C	-1.080168	0.550182	2.564679
C	-0.765688	1.492822	3.581303
H	-0.305206	1.082724	4.473148
C	-1.050137	2.827905	3.475306
H	-0.81241	3.510857	4.286329
C	-1.633242	3.290065	2.284884
H	-1.86435	4.336778	2.122448
C	-1.88094	2.392513	1.284212
H	-2.284555	2.745657	0.347207
H	-0.420491	-2.025792	0.543221
H	0.643714	-1.400165	-2.332365
C	0.618239	-2.916072	-1.258516
H	0.142895	-3.467088	-2.066936
H	1.699614	-3.044491	-1.240197
C	-0.055896	-3.026089	0.061756
H	0.610999	-3.340669	0.868878
H	-0.975922	-3.615274	0.044084

sp³-hy - PC

Ru	0.006777	0.183087	-1.453291
S	1.792569	0.605274	-2.991128
S	0.127692	-2.13034	-1.497828
S	3.943745	0.444037	2.152213

P	-1.826462	0.168024	-0.056855
B	1.537245	-0.093264	-0.094241
N	2.859761	-0.612099	-0.862614
N	1.100178	-1.287641	0.842152
N	1.899551	1.314261	0.568317
C	-1.851253	1.560453	1.142408
C	-0.931219	1.564699	2.202807
H	-0.299853	0.69421	2.366295
C	-0.786891	2.674565	3.026301
H	-0.056423	2.654567	3.831388
C	-1.551009	3.816413	2.794475
H	-1.432234	4.691366	3.427501
C	-2.459708	3.832475	1.740355
H	-3.056948	4.720404	1.550136
C	-2.610026	2.716435	0.919986
H	-3.318832	2.748988	0.09625
C	-3.314021	0.468408	-1.088942
C	-4.616339	0.394616	-0.580176
H	-4.768864	0.149264	0.469359
C	-5.708981	0.631855	-1.406866
H	-6.716102	0.57432	-1.002631
C	-5.513783	0.938627	-2.752849
H	-6.369016	1.120991	-3.397859
C	-4.22368	1.007843	-3.272043
H	-4.067766	1.239357	-4.321922
C	-3.13049	0.773593	-2.441737
H	-2.116282	0.823457	-2.846649
C	-2.388027	-1.292894	0.911312
C	-2.397561	-1.37059	2.307329
H	-2.121982	-0.506726	2.905006
C	-2.781144	-2.546927	2.949733
H	-2.786244	-2.586521	4.036024
C	-3.160224	-3.660626	2.207919
H	-3.458944	-4.576573	2.711086
C	-3.166016	-3.591709	0.815325
H	-3.468827	-4.453378	0.226412
C	-2.781178	-2.421641	0.173476
H	-2.780319	-2.374769	-0.912993
C	3.074148	-0.159573	-2.140083
C	4.313904	-0.415331	-2.756732
H	4.478308	-0.00713	-3.747477
C	5.24394	-1.224677	-2.143168
H	6.184451	-1.447613	-2.639806
C	4.948488	-1.789281	-0.896584

H	5.63268	-2.462599	-0.394926
C	3.765175	-1.445505	-0.285569
H	3.496903	-1.817861	0.694124
C	0.603133	-2.371354	0.142442
C	0.430727	-3.593818	0.812418
H	0.071444	-4.441874	0.238922
C	0.626651	-3.674533	2.174279
H	0.440984	-4.609701	2.695261
C	1.010588	-2.527701	2.88708
H	1.130758	-2.538934	3.963745
C	1.258854	-1.368504	2.190641
H	1.633317	-0.470709	2.667502
C	2.996618	1.614167	1.387246
C	3.303224	2.9953	1.579666
H	4.167771	3.205461	2.198756
C	2.563676	4.003829	1.025836
H	2.833202	5.042087	1.20083
C	1.443919	3.67628	0.239311
H	0.792817	4.426781	-0.192029
C	1.166657	2.353612	0.049981
H	0.259073	2.077044	-0.494001

sp²-hy-Cat

Ru	0.000012	-1.020562	-0.284971
Cl	-0.000137	0.801728	-1.910076
P	-2.330082	-0.629943	-0.047025
P	2.330106	-0.629815	-0.047042
B	-0.000032	0.861509	0.871829
N	-1.172959	1.694441	0.853133
N	1.172856	1.6945	0.853129
C	-0.709475	2.999103	0.654965
C	-1.415966	4.173632	0.442812
H	-2.503017	4.170099	0.427572
C	-0.696777	5.353752	0.232409
H	-1.234456	6.281934	0.060841
C	0.696487	5.353786	0.232408
H	1.234119	6.281995	0.060837
C	1.415735	4.173703	0.442808
H	2.502786	4.170225	0.427567
C	0.709304	2.999138	0.654964
C	-2.427564	1.215561	0.301521
H	-2.590825	1.693185	-0.676403
H	-3.294326	1.456522	0.936422

C	-3.591791	-0.85452	-1.445889
C	-4.872313	-0.03281	-1.278185
H	-4.660989	1.038872	-1.205915
H	-5.474419	-0.319043	-0.415264
H	-5.496825	-0.170107	-2.169461
C	-3.914629	-2.343032	-1.588395
H	-4.495627	-2.741824	-0.751845
H	-3.000313	-2.938671	-1.689674
H	-4.508747	-2.496864	-2.496916
C	-2.911701	-0.402379	-2.741278
H	-3.601137	-0.582676	-3.575607
H	-1.980412	-0.944502	-2.92639
H	-2.662265	0.661967	-2.731548
C	-3.01263	-1.42043	1.551194
C	-2.372088	-0.736737	2.765668
H	-2.803849	-1.16613	3.677778
H	-2.549811	0.342433	2.792526
H	-1.292625	-0.899295	2.811229
C	-4.52744	-1.320178	1.724654
H	-5.084636	-1.867052	0.960782
H	-4.870274	-0.279944	1.719826
H	-4.806463	-1.747847	2.695697
C	-2.576561	-2.888972	1.555391
H	-1.483606	-2.974825	1.478612
H	-3.010385	-3.465494	0.7339
H	-2.876505	-3.368471	2.495402
C	2.427488	1.215693	0.301511
H	3.294242	1.456696	0.936407
H	2.590719	1.69333	-0.676412
C	3.591873	-0.854387	-1.445869
C	2.911817	-0.402503	-2.74136
H	3.60131	-0.582893	-3.575623
H	2.662319	0.661829	-2.731818
H	1.980571	-0.94471	-2.926437
C	3.914895	-2.342877	-1.588158
H	4.509111	-2.496758	-2.496606
H	3.000655	-2.938632	-1.68944
H	4.495858	-2.741494	-0.751499
C	4.872299	-0.032513	-1.278231
H	5.474414	-0.31855	-0.415252
H	4.660853	1.039156	-1.206127
H	5.496853	-0.169872	-2.169468
C	3.012714	-1.420307	1.551157
C	2.576717	-2.888869	1.555321

H	3.010549	-3.465334	0.733795
H	1.483764	-2.974777	1.478572
H	2.876717	-3.368389	2.495304
C	4.527524	-1.320014	1.724575
H	4.806583	-1.74766	2.695618
H	4.870331	-0.279771	1.719723
H	5.084709	-1.866896	0.960697
C	2.3722	-0.736689	2.765688
H	1.292758	-0.899343	2.811327
H	2.549836	0.342494	2.792552
H	2.804064	-1.166063	3.677759
H	-0.000007	-0.287577	1.386414
H	0.000024	-1.860629	-1.669488

sp²-hy-RC

Ru	-0.002945	-1.002781	0.219272
Cl	0.004328	0.981269	1.809047
P	2.389083	-0.529551	0.066309
P	-2.389264	-0.523467	0.067453
B	-0.001121	0.966814	-1.040431
N	1.175369	1.779458	-0.942887
N	-1.174766	1.78338	-0.939163
C	0.709957	3.079855	-0.715002
C	1.421345	4.245485	-0.467194
H	2.508174	4.239157	-0.451114
C	0.705089	5.418876	-0.224561
H	1.243961	6.341392	-0.028562
C	-0.689744	5.421269	-0.222326
H	-1.224824	6.345647	-0.024714
C	-1.410855	4.250347	-0.462659
H	-2.497637	4.247853	-0.443087
C	-0.704328	3.082214	-0.712669
C	2.397126	1.317513	-0.299446
H	2.456023	1.804732	0.682486
H	3.296653	1.595427	-0.867235
C	3.54338	-0.654261	1.58115
C	4.665039	0.38862	1.595673
H	4.273222	1.405029	1.693788
H	5.312818	0.358282	0.718496
H	5.29575	0.209814	2.475048
C	4.137918	-2.06378	1.623655
H	4.878109	-2.240069	0.839505
H	3.36319	-2.835097	1.544598

H	4.643707	-2.207981	2.585398
C	2.715064	-0.461119	2.852266
H	3.362862	-0.648476	3.71814
H	1.862	-1.144398	2.895662
H	2.312328	0.549477	2.93267
C	3.366185	-1.181709	-1.447641
C	2.623894	-0.675126	-2.693763
H	3.139561	-1.043651	-3.588702
H	2.612226	0.418029	-2.747819
H	1.587739	-1.013493	-2.746312
C	4.804227	-0.666241	-1.561059
H	5.455783	-1.052506	-0.773498
H	4.870352	0.426594	-1.558176
H	5.222327	-1.007512	-2.516423
C	3.417578	-2.721869	-1.451437
H	2.568814	-3.193463	-0.95146
H	4.319101	-3.095126	-0.96001
H	3.43997	-3.092715	-2.482982
C	-2.39533	1.324484	-0.291041
H	-3.296397	1.606928	-0.854116
H	-2.448136	1.808908	0.692754
C	-3.538144	-0.655576	1.584868
C	-2.706618	-0.458078	2.853266
H	-3.351702	-0.646042	3.721017
H	-2.306838	0.553944	2.931218
H	-1.851432	-1.138644	2.895583
C	-4.122388	-2.069445	1.627378
H	-4.615727	-2.222597	2.594171
H	-3.342792	-2.834678	1.534503
H	-4.870777	-2.246518	0.85116
C	-4.666131	0.380306	1.6057
H	-5.322493	0.342009	0.735371
H	-4.279761	1.399633	1.695606
H	-5.286949	0.20136	2.492042
C	-3.369661	-1.166933	-1.448974
C	-3.420169	-2.705969	-1.466666
H	-4.297953	-3.085961	-0.939184
H	-2.548736	-3.182105	-1.012609
H	-3.49014	-3.063715	-2.500811
C	-4.808946	-0.653395	-1.55366
H	-5.228228	-0.985562	-2.511719
H	-4.87798	0.439132	-1.538729
H	-5.457599	-1.050228	-0.768937
C	-2.631947	-0.651103	-2.693789

H	-1.594422	-0.984697	-2.749824
H	-2.624909	0.442253	-2.743273
H	-3.14752	-1.01802	-3.589432
H	-0.001289	-0.186174	-1.48014
H	-0.000169	-1.719539	1.644956
C	-0.03187	-3.164726	-0.005368
H	0.864569	-3.59801	0.432317
H	-0.957422	-3.568692	0.399694
C	0.00081	-2.614098	-1.294764
H	-0.892605	-2.604877	-1.907563
H	0.916425	-2.63615	-1.873078

sp^2 -a- TS_1

Ru	-0.002566	-0.98049	0.17619
Cl	0.002135	0.933174	1.921014
P	2.380811	-0.513448	0.038014
P	-2.380332	-0.507007	0.038268
B	0.00064	1.00287	-0.875605
N	1.173417	1.824766	-0.838805
N	-1.169896	1.828152	-0.838012
C	0.711984	3.129257	-0.633835
C	1.42209	4.300277	-0.410751
H	2.508887	4.294629	-0.391822
C	0.704684	5.478131	-0.19086
H	1.242996	6.404103	-0.009854
C	-0.689806	5.48024	-0.190496
H	-1.225221	6.407849	-0.009281
C	-1.41094	4.30455	-0.409958
H	-2.497738	4.302264	-0.390439
C	-0.704545	3.131334	-0.633372
C	2.403407	1.348041	-0.233867
H	2.475726	1.782632	0.772398
H	3.294577	1.654092	-0.799156
C	3.571217	-0.705487	1.516489
C	4.693635	0.337272	1.543253
H	4.310041	1.348321	1.704741
H	5.308594	0.347766	0.641164
H	5.356451	0.113732	2.388086
C	4.182498	-2.107639	1.498523
H	4.906879	-2.246542	0.691886
H	3.419355	-2.88943	1.413492
H	4.714021	-2.273751	2.442872
C	2.763852	-0.562211	2.807206

H	3.424493	-0.772051	3.658041
H	1.917723	-1.255492	2.838965
H	2.347565	0.439263	2.926618
C	3.292246	-1.145816	-1.51889
C	2.429716	-0.713455	-2.713151
H	2.932111	-1.007879	-3.642549
H	2.27696	0.370776	-2.745864
H	1.44501	-1.188682	-2.701119
C	4.693261	-0.56492	-1.725716
H	5.404074	-0.910908	-0.970645
H	4.708572	0.529475	-1.738288
H	5.075313	-0.89991	-2.698222
C	3.40876	-2.684354	-1.506698
H	2.681526	-3.170803	-0.852492
H	4.39795	-3.013449	-1.179581
H	3.257277	-3.081527	-2.516989
C	-2.400508	1.354554	-0.231767
H	-3.291572	1.662575	-0.796172
H	-2.471037	1.788895	0.774779
C	-3.567418	-0.702064	1.518415
C	-2.75867	-0.558753	2.808277
H	-3.417914	-0.771319	3.659512
H	-2.344644	0.443538	2.928652
H	-1.910785	-1.249955	2.838124
C	-4.175199	-2.105751	1.499296
H	-4.706318	-2.274228	2.443454
H	-3.40959	-2.885255	1.413618
H	-4.898968	-2.245948	0.692335
C	-4.691593	0.338685	1.54827
H	-5.309918	0.347406	0.648539
H	-4.308995	1.350513	1.707429
H	-5.350839	0.114816	2.395794
C	-3.295034	-1.135869	-1.518358
C	-3.41313	-2.674571	-1.509795
H	-4.404506	-3.00287	-1.18834
H	-2.69018	-3.163812	-0.852947
H	-3.257121	-3.070131	-2.520011
C	-4.696214	-0.553715	-1.720968
H	-5.079656	-0.885297	-2.694083
H	-4.71149	0.540726	-1.729605
H	-5.405822	-0.90252	-0.966077
C	-2.435042	-0.7006	-2.713458
H	-1.449738	-1.174623	-2.704508
H	-2.283363	0.383793	-2.744567

H	-2.938946	-0.993823	-3.64241
H	0.000926	-0.147118	-1.397456
H	-0.003849	-1.96819	1.489305
C	-0.020231	-3.181028	0.375394
H	0.877374	-3.62384	0.807093
H	-0.932805	-3.603187	0.796802
C	-0.007608	-2.787677	-0.996974
H	-0.907251	-2.924307	-1.589106
H	0.896995	-2.941231	-1.577434

sp²-a-IM

Ru	-0.000420	-0.930665	0.129123
Cl	-0.000075	0.41979	2.303712
P	2.3959	-0.488873	0.012422
P	-2.395867	-0.48864	0.012397
B	-0.000205	1.029816	-0.424504
N	1.161272	1.877763	-0.458761
N	-1.161543	1.87795	-0.458592
C	0.709535	3.193012	-0.327353
C	1.416839	4.378603	-0.193349
H	2.503774	4.376642	-0.174543
C	0.696893	5.569765	-0.059657
H	1.2343	6.506928	0.05457
C	-0.696472	5.569885	-0.059532
H	-1.233693	6.507144	0.054783
C	-1.416667	4.378863	-0.193087
H	-2.503599	4.377122	-0.174093
C	-0.709612	3.193125	-0.327217
C	2.413627	1.387341	0.065218
H	2.50118	1.667761	1.125077
H	3.284967	1.796409	-0.464069
C	3.642648	-0.936382	1.392613
C	4.731134	0.125723	1.584424
H	4.324001	1.069084	1.95688
H	5.304103	0.336667	0.67841
H	5.439553	-0.233034	2.341221
C	4.305886	-2.281319	1.094117
H	4.999069	-2.236777	0.25103
H	3.573213	-3.070593	0.894703
H	4.883143	-2.589931	1.973475
C	2.879932	-1.07789	2.709847
H	3.584629	-1.391832	3.490416
H	2.085154	-1.828142	2.642426

H	2.403613	-0.14673	3.020409
C	3.247838	-0.858882	-1.662204
C	2.322142	-0.299223	-2.750816
H	2.813099	-0.408427	-3.725413
H	2.093808	0.761583	-2.605715
H	1.374942	-0.844038	-2.792044
C	4.619012	-0.198094	-1.82619
H	5.360456	-0.598586	-1.129986
H	4.589472	0.88976	-1.711216
H	4.989204	-0.401523	-2.838667
C	3.42025	-2.375453	-1.894778
H	2.743223	-2.991964	-1.299855
H	4.435558	-2.710017	-1.669521
H	3.232578	-2.611991	-2.948295
C	-2.413927	1.387562	0.065435
H	-3.285226	1.796632	-0.463908
H	-2.501501	1.667945	1.125297
C	-3.642192	-0.936915	1.392733
C	-2.879509	-1.078365	2.709984
H	-3.584152	-1.392996	3.490315
H	-2.403813	-0.147015	3.020868
H	-2.084268	-1.828104	2.6424
C	-4.304889	-2.282071	1.093941
H	-4.882239	-2.590959	1.973137
H	-3.57187	-3.071063	0.894688
H	-4.997885	-2.237734	0.250683
C	-4.730976	0.12484	1.584724
H	-5.304153	0.335635	0.678804
H	-4.324061	1.068326	1.957126
H	-5.439211	-0.234099	2.341612
C	-3.248019	-0.858523	-1.66219
C	-3.420053	-2.37508	-1.895062
H	-4.435469	-2.709851	-1.670578
H	-2.743346	-2.991519	-1.299701
H	-3.231596	-2.611545	-2.94846
C	-4.619309	-0.197889	-1.825708
H	-4.989653	-0.400872	-2.838219
H	-4.589966	0.889912	-1.710191
H	-5.360557	-0.598875	-1.129575
C	-2.32253	-0.298436	-2.750757
H	-1.375305	-0.843194	-2.79221
H	-2.094243	0.762352	-2.605457
H	-2.813592	-0.407451	-3.725321
H	-0.000286	-0.198649	-1.309918

H	-0.000021	-2.781185	1.10457
C	0.000825	-3.444136	0.183091
H	0.893076	-4.063376	0.322853
H	-0.890145	-4.065274	0.322643
C	0.000175	-2.640458	-1.087428
H	-0.883159	-2.777441	-1.709464
H	0.88357	-2.77628	-1.70961

sp^2 -a- TS_2

Ru	-0.007494	-0.945671	-0.144581
Cl	0.006184	0.306805	-2.30557
P	-2.377016	-0.455488	-0.027937
P	2.378776	-0.487242	-0.02614
B	0.006816	1.020959	0.342568
N	-1.143617	1.889432	0.36481
N	1.16855	1.873355	0.375556
C	-0.687378	3.20455	0.255862
C	-1.385655	4.397726	0.14162
H	-2.472648	4.404405	0.118189
C	-0.656689	5.58659	0.034574
H	-1.187085	6.529622	-0.063857
C	0.736518	5.576744	0.041419
H	1.281206	6.512154	-0.051454
C	1.447209	4.377608	0.155507
H	2.534374	4.368532	0.142882
C	0.730844	3.194628	0.262763
C	-2.39793	1.412056	-0.158954
H	-2.481832	1.667696	-1.226163
H	-3.268749	1.838749	0.358442
C	-3.630944	-0.980959	-1.37474
C	-4.733776	0.056298	-1.61064
H	-4.33384	0.995179	-2.002435
H	-5.323297	0.284717	-0.72038
H	-5.426144	-0.33233	-2.367967
C	-4.265377	-2.32428	-1.011165
H	-4.931882	-2.266091	-0.147588
H	-3.512407	-3.093925	-0.808318
H	-4.863357	-2.673651	-1.861191
C	-2.875564	-1.17033	-2.690955
H	-3.577238	-1.543959	-3.447604
H	-2.056629	-1.890471	-2.59324
H	-2.43306	-0.241811	-3.054596
C	-3.237645	-0.733989	1.662341

C	-2.363751	-0.053247	2.724514
H	-2.851315	-0.152794	3.702034
H	-2.217542	1.012583	2.526054
H	-1.372864	-0.508046	2.802763
C	-4.635449	-0.116498	1.764483
H	-5.358334	-0.603941	1.105904
H	-4.646656	0.95727	1.553078
H	-5.002822	-0.243182	2.79054
C	-3.353338	-2.241122	1.985052
H	-2.724895	-2.872995	1.353218
H	-4.377938	-2.602406	1.864042
H	-3.068202	-2.431035	3.02595
C	2.420837	1.381759	-0.139534
H	3.292358	1.79281	0.389164
H	2.519431	1.645703	-1.203331
C	3.63129	-1.006559	-1.377727
C	2.880915	-1.16552	-2.700757
H	3.580803	-1.542807	-3.457291
H	2.459102	-0.224304	-3.056277
H	2.047567	-1.870487	-2.617734
C	4.245872	-2.363542	-1.031541
H	4.847993	-2.705621	-1.881572
H	3.480624	-3.126723	-0.850413
H	4.904243	-2.329026	-0.160256
C	4.748707	0.019463	-1.5943
H	5.338056	0.227692	-0.699307
H	4.362396	0.968843	-1.974211
H	5.438464	-0.367379	-2.354898
C	3.238491	-0.788722	1.661821
C	3.348507	-2.300071	1.972334
H	4.38039	-2.652644	1.892403
H	2.753744	-2.929576	1.307001
H	3.019339	-2.504611	2.997248
C	4.640157	-0.180691	1.77073
H	5.003811	-0.317007	2.796851
H	4.660646	0.894284	1.566427
H	5.360591	-0.670136	1.110977
C	2.36784	-0.112978	2.729678
H	1.375723	-0.565725	2.804157
H	2.225513	0.955038	2.53966
H	2.854737	-0.221931	3.706508
H	-0.012296	-1.148629	1.459132
H	0.008596	-2.99348	-0.893772
C	-0.146918	-3.509864	0.085773

H	-1.135363	-3.973545	0.01641
H	0.609028	-4.302507	0.095643
C	-0.024218	-2.588636	1.291567
H	0.889358	-2.767385	1.857937
H	-0.857407	-2.717114	1.984885

sp^2 -**b**- TS_1

Ru	-0.000001	-1.051629	0.075421
Cl	0.000015	0.525522	2.040068
P	2.397658	-0.535045	0.070336
P	-2.39766	-0.535061	0.070352
B	-0.000021	0.978575	-0.536162
N	1.170033	1.819485	-0.531169
N	-1.170082	1.819476	-0.531114
C	0.708584	3.132184	-0.368169
C	1.415643	4.313522	-0.195891
H	2.50262	4.310672	-0.175931
C	0.696833	5.49981	-0.025153
H	1.234226	6.432983	0.118433
C	-0.696883	5.499805	-0.025116
H	-1.234276	6.432975	0.118497
C	-1.415694	4.313512	-0.195818
H	-2.50267	4.310655	-0.175801
C	-0.708635	3.132179	-0.368133
C	2.384204	1.341925	0.101819
H	2.387175	1.649357	1.158019
H	3.293829	1.741325	-0.369552
C	3.504222	-1.013197	1.553459
C	4.648758	-0.02888	1.812725
H	4.279279	0.981541	2.012314
H	5.380172	0.027579	1.006022
H	5.185673	-0.350109	2.713891
C	4.055235	-2.420927	1.313286
H	4.820342	-2.455391	0.533526
H	3.259089	-3.128356	1.052183
H	4.521669	-2.783032	2.236781
C	2.649361	-1.066951	2.821233
H	3.263222	-1.487768	3.627718
H	1.759908	-1.689713	2.691672
H	2.308725	-0.078073	3.130643
C	3.422894	-0.819881	-1.530321
C	2.791436	0.039374	-2.637735
H	3.252047	-0.225972	-3.597094

H	2.971292	1.105078	-2.471799
H	1.712449	-0.078769	-2.738721
C	4.885281	-0.373874	-1.438073
H	5.480601	-1.004889	-0.774225
H	4.991661	0.666753	-1.115146
H	5.335319	-0.446377	-2.436469
C	3.41898	-2.298819	-1.937136
H	2.43724	-2.768674	-1.876649
H	4.092033	-2.893304	-1.316462
H	3.76998	-2.392848	-2.972285
C	-2.384222	1.341902	0.101923
H	-3.293875	1.74132	-0.369381
H	-2.38713	1.649289	1.158134
C	-3.504213	-1.013287	1.553445
C	-2.64933	-1.067129	2.821202
H	-3.263189	-1.487965	3.627679
H	-2.308643	-0.078282	3.130653
H	-1.759908	-1.689924	2.691587
C	-4.055229	-2.420999	1.313183
H	-4.52167	-2.783163	2.236651
H	-3.259078	-3.128408	1.052041
H	-4.820324	-2.455417	0.53341
C	-4.648736	-0.028976	1.812788
H	-5.380132	0.027582	1.006076
H	-4.279246	0.98142	2.012485
H	-5.185676	-0.350282	2.713911
C	-3.422885	-0.819835	-1.530325
C	-3.418953	-2.298762	-1.937202
H	-4.092179	-2.893243	-1.316709
H	-2.437246	-2.76866	-1.876499
H	-3.769714	-2.392742	-2.972435
C	-4.885273	-0.37383	-1.43806
H	-5.335334	-0.446374	-2.436443
H	-4.991651	0.66681	-1.115173
H	-5.480573	-1.004822	-0.774175
C	-2.791433	0.039458	-2.63771
H	-1.7125	-0.078967	-2.738948
H	-2.970962	1.105182	-2.471561
H	-3.252311	-0.225611	-3.597018
H	-0.00003	-0.631075	-1.616166
H	0.000031	-2.141972	1.328753
C	0.000045	-2.933076	-0.926565
H	0.909753	-3.500486	-0.748945
H	-0.909621	-3.500544	-0.74892

C	-0.000005	-1.956735	-1.9934
H	-0.898547	-1.888339	-2.601637
H	0.898508	-1.888264	-2.601675

sp^2 -b-IM

Ru	0.000222	-1.057815	0.080875
Cl	0.000139	0.443622	2.087558
P	2.392639	-0.521987	0.072963
P	-2.392621	-0.522453	0.072908
B	0.000012	0.99924	-0.396883
N	1.165804	1.843932	-0.416208
N	-1.165959	1.843673	-0.4161
C	0.709523	3.160547	-0.289921
C	1.415864	4.349227	-0.171158
H	2.502961	4.348177	-0.155732
C	0.696481	5.541501	-0.051654
H	1.233611	6.480356	0.049603
C	-0.697426	5.541344	-0.051584
H	-1.234759	6.480077	0.049725
C	-1.416547	4.348906	-0.171018
H	-2.503643	4.347608	-0.155484
C	-0.709945	3.16039	-0.289848
C	2.391114	1.355064	0.176611
H	2.421047	1.627707	1.242227
H	3.291581	1.766331	-0.302002
C	3.532356	-1.046414	1.511302
C	4.674803	-0.063035	1.782865
H	4.301895	0.930822	2.047907
H	5.37626	0.046203	0.954605
H	5.247587	-0.423899	2.646238
C	4.090231	-2.438023	1.205231
H	4.835062	-2.43292	0.40534
H	3.295435	-3.142713	0.93338
H	4.582361	-2.831222	2.102419
C	2.70066	-1.153975	2.790802
H	3.3346	-1.582829	3.577253
H	1.825152	-1.795162	2.655556
H	2.341165	-0.182431	3.133236
C	3.376394	-0.767296	-1.556339
C	2.683626	0.086217	-2.62993
H	3.150342	-0.118617	-3.601077
H	2.794338	1.15545	-2.429024
H	1.613831	-0.101993	-2.724735

C	4.829393	-0.286576	-1.508119
H	5.45614	-0.899136	-0.856327
H	4.921169	0.75865	-1.195567
H	5.254756	-0.356164	-2.517505
C	3.387723	-2.248953	-1.970316
H	2.4872	-2.793038	-1.680938
H	4.230321	-2.784018	-1.526828
H	3.495545	-2.331784	-3.058608
C	-2.391104	1.35458	0.176867
H	-3.291676	1.765915	-0.301484
H	-2.420813	1.627014	1.242545
C	-3.532215	-1.046945	1.511399
C	-2.700139	-1.154761	2.790637
H	-3.33395	-1.583446	3.577283
H	-2.340312	-0.183303	3.132977
H	-1.824821	-1.796157	2.65515
C	-4.090483	-2.438429	1.205396
H	-4.58148	-2.832019	2.103032
H	-3.296123	-3.143073	0.932166
H	-4.836429	-2.432916	0.406528
C	-4.674452	-0.063461	1.783443
H	-5.376073	0.046042	0.955356
H	-4.301371	0.930285	2.048646
H	-5.247104	-0.42445	2.646853
C	-3.376563	-0.767254	-1.556398
C	-3.388388	-2.248632	-1.970915
H	-4.228581	-2.784645	-1.524097
H	-2.486132	-2.792013	-1.685765
H	-3.500779	-2.330881	-3.058802
C	-4.82949	-0.286344	-1.507823
H	-5.254955	-0.355442	-2.517198
H	-4.921132	0.758744	-1.194784
H	-5.456232	-0.899139	-0.856241
C	-2.683685	0.086331	-2.629821
H	-1.613939	-0.102171	-2.724708
H	-2.794088	1.155549	-2.42866
H	-3.150497	-0.11818	-3.600991
H	0.000177	-0.901223	-1.754272
H	0.000495	-2.160002	1.315453
C	-0.00004	-2.971074	-0.849199
H	0.902541	-3.555009	-0.68389
H	-0.903068	-3.55441	-0.68424
C	0.000518	-2.070436	-2.019805
H	-0.893364	-2.117997	-2.642146

H	0.895121	-2.118042	-2.641074
sp^2 - b - TS_2			
Ru	-0.000007	-1.025551	0.12449
Cl	-0.000058	0.453548	2.121243
P	2.3745	-0.488479	0.062266
P	-2.374499	-0.488538	0.062229
B	-0.000004	1.011297	-0.433297
N	1.160075	1.867666	-0.454003
N	-1.160102	1.867637	-0.45412
C	0.709404	3.184839	-0.337008
C	1.416294	4.373343	-0.219073
H	2.503427	4.372177	-0.202279
C	0.696866	5.566042	-0.101534
H	1.23405	6.504999	-0.001024
C	-0.697022	5.566025	-0.101613
H	-1.234241	6.504969	-0.001164
C	-1.416406	4.373308	-0.21923
H	-2.503541	4.372113	-0.202559
C	-0.709473	3.184822	-0.337084
C	2.40052	1.388286	0.106523
H	2.477927	1.698113	1.159473
H	3.286387	1.774861	-0.418467
C	3.55714	-0.972882	1.481805
C	4.695888	0.02896	1.697409
H	4.321937	1.013313	1.993226
H	5.343921	0.159237	0.82903
H	5.325882	-0.328385	2.52171
C	4.131355	-2.362673	1.20054
H	4.842067	-2.372822	0.370766
H	3.343415	-3.09445	0.98852
H	4.667921	-2.712586	2.09023
C	2.759022	-1.060562	2.783596
H	3.417375	-1.457185	3.567068
H	1.892054	-1.720435	2.685043
H	2.387405	-0.08735	3.107864
C	3.306193	-0.822591	-1.580416
C	2.537917	-0.081583	-2.684131
H	3.025671	-0.275943	-3.64726
H	2.53326	1.000575	-2.524439
H	1.495854	-0.395969	-2.770492
C	4.743086	-0.295772	-1.622206
H	5.407584	-0.834524	-0.943205

H	4.814743	0.773578	-1.399298
H	5.139663	-0.437182	-2.635636
C	3.3452	-2.334853	-1.886289
H	2.573439	-2.905885	-1.364177
H	4.303616	-2.77843	-1.605782
H	3.218549	-2.507617	-2.961664
C	-2.400602	1.388241	0.106276
H	-3.286419	1.774711	-0.418879
H	-2.478191	1.698199	1.15917
C	-3.557235	-0.972787	1.481757
C	-2.759194	-1.060261	2.783609
H	-3.417604	-1.456715	3.567118
H	-2.387567	-0.086999	3.107716
H	-1.892237	-1.720175	2.685228
C	-4.131435	-2.362621	1.200672
H	-4.668047	-2.712391	2.09039
H	-3.343497	-3.094437	0.98881
H	-4.842109	-2.372902	0.370867
C	-4.69602	0.029062	1.697164
H	-5.344027	0.159179	0.828743
H	-4.322119	1.013475	1.992839
H	-5.326029	-0.328173	2.521501
C	-3.30611	-0.822876	-1.580448
C	-3.34501	-2.33518	-1.886113
H	-4.303399	-2.77878	-1.605552
H	-2.573209	-2.906076	-1.363904
H	-3.218327	-2.508094	-2.96146
C	-4.743033	-0.296145	-1.622374
H	-5.139547	-0.437721	-2.635805
H	-4.814764	0.773234	-1.399623
H	-5.407544	-0.834835	-0.943337
C	-2.537831	-0.081971	-2.684229
H	-1.495792	-0.39643	-2.770603
H	-2.533105	1.000195	-2.524604
H	-3.025618	-0.276365	-3.647334
H	-0.000047	-1.240639	-1.699133
H	-0.000071	-2.235878	1.272669
C	0.000427	-3.112761	-0.433491
H	0.901194	-3.677685	-0.202088
H	-0.899969	-3.678278	-0.202119
C	0.000193	-2.423796	-1.748733
H	-0.893463	-2.589056	-2.350495
H	0.893834	-2.588648	-2.35063

sp²_hy - PC

Ru	-0.115822	-1.038927	0.299783
Cl	-0.123774	-0.576894	2.638373
P	2.250568	-0.622956	0.033132
P	-2.359077	-0.53887	-0.014295
B	-0.078667	0.91771	-0.000011
N	1.085693	1.766288	0.038482
N	-1.207179	1.818875	-0.068295
C	0.677368	3.094162	0.057329
C	1.409345	4.27102	0.127194
H	2.49419	4.244177	0.193837
C	0.716925	5.48638	0.127382
H	1.275041	6.416398	0.188388
C	-0.674153	5.520106	0.057321
H	-1.189828	6.476314	0.064363
C	-1.421976	4.339557	-0.014241
H	-2.507974	4.367362	-0.058223
C	-0.744917	3.128493	-0.013085
C	2.387716	1.229171	0.316202
H	2.677824	1.402004	1.363872
H	3.174702	1.667486	-0.317845
C	3.657265	-1.281079	1.141011
C	4.897989	-0.385723	1.195058
H	4.668937	0.613985	1.575991
H	5.40376	-0.27552	0.234925
H	5.619974	-0.829175	1.892381
C	4.053021	-2.689884	0.698621
H	4.607841	-2.700419	-0.24431
H	3.178873	-3.342025	0.589772
H	4.70234	-3.139287	1.459688
C	3.083462	-1.377962	2.556439
H	3.867807	-1.739743	3.233399
H	2.235284	-2.064672	2.607491
H	2.725288	-0.416329	2.934796
C	2.812758	-0.767548	-1.792522
C	1.967862	0.211269	-2.617105
H	2.191487	0.066427	-3.68143
H	2.183734	1.255501	-2.372274
H	0.893477	0.062838	-2.474462
C	4.280044	-0.423881	-2.044215
H	4.965221	-1.155329	-1.608612
H	4.547337	0.567435	-1.662649
H	4.466333	-0.413295	-3.125649

C	2.542757	-2.189743	-2.29275
H	1.514677	-2.507687	-2.094346
H	3.205599	-2.927097	-1.83378
H	2.702595	-2.236318	-3.377245
C	-2.550587	1.327755	0.062239
H	-3.226171	1.704036	-0.720571
H	-2.989539	1.600397	1.032426
C	-3.85865	-1.179061	0.93601
C	-3.716524	-0.663121	2.374444
H	-4.472449	-1.155363	2.998396
H	-3.892112	0.414096	2.45006
H	-2.728193	-0.873866	2.794362
C	-3.768595	-2.705824	0.981117
H	-4.579154	-3.105806	1.601716
H	-2.819452	-3.026256	1.424285
H	-3.856693	-3.171222	-0.005414
C	-5.204314	-0.720869	0.374744
H	-5.450157	-1.191289	-0.579149
H	-5.244236	0.366027	0.240878
H	-6.001343	-0.985026	1.081113
C	-2.419988	-0.978021	-1.882325
C	-1.225791	-1.936572	-2.00777
H	-1.366917	-2.874977	-1.463172
H	-0.265824	-1.445021	-1.706326
H	-1.02802	-2.187634	-3.060775
C	-3.674873	-1.645283	-2.435594
H	-3.487772	-1.950995	-3.473207
H	-4.522975	-0.955346	-2.454607
H	-3.974155	-2.54092	-1.88515
C	-2.132693	0.259553	-2.73433
H	-1.248241	0.805549	-2.394505
H	-2.976512	0.955882	-2.738907
H	-1.963594	-0.050007	-3.773168

sp-hy-Cat

C	1.994758	2.416017	-0.040849
C	2.514382	3.083719	-1.187935
C	2.061509	2.747002	-2.579196
H	2.475557	3.450371	-3.304767
H	0.969236	2.775937	-2.676276
H	2.37372	1.74188	-2.888575
C	3.472624	4.079856	-1.026522
H	3.868946	4.57639	-1.91096
C	3.937906	4.462821	0.233327

C	4.953337	5.549134	0.381237
H	4.465805	6.519253	0.530138
H	5.582595	5.641192	-0.507018
H	5.599331	5.384187	1.247119
C	3.401776	3.825249	1.355601
H	3.742899	4.121564	2.346236
C	2.443127	2.824674	1.24562
C	1.899615	2.205328	2.497232
H	2.402693	2.59637	3.384329
H	2.015133	1.116362	2.50179
H	0.826998	2.402718	2.615418
C	-3.481084	-0.6655	-0.76046
H	-3.101798	-0.829168	-1.784134
C	-3.381901	-2.006869	-0.022422
H	-2.336281	-2.337101	0.048167
H	-3.723091	-1.878627	1.016018
C	-4.235023	-3.071782	-0.706049
H	-3.826657	-3.265264	-1.708972
H	-4.162852	-4.016611	-0.156316
C	-5.687162	-2.632609	-0.839765
H	-6.130598	-2.533655	0.161189
H	-6.271327	-3.398355	-1.35976
C	-5.785956	-1.297359	-1.565267
H	-6.827482	-0.966875	-1.631847
H	-5.431589	-1.41289	-2.600064
C	-4.947626	-0.231684	-0.866182
H	-5.036888	0.729191	-1.388054
H	-5.345203	-0.078948	0.147329
C	-2.62861	2.11987	-1.118907
H	-3.67556	2.411272	-0.941771
C	-2.463445	1.834882	-2.61457
H	-1.428367	1.504056	-2.803102
H	-3.116223	1.012157	-2.931528
C	-2.767447	3.080496	-3.442901
H	-2.624877	2.864098	-4.50682
H	-3.830391	3.334174	-3.321492
C	-1.914538	4.268048	-3.015522
H	-0.858893	4.054493	-3.241715
H	-2.176935	5.156852	-3.597954
C	-2.056497	4.542239	-1.523586
H	-3.084804	4.863609	-1.303861
H	-1.404044	5.366597	-1.217246
C	-1.735959	3.295142	-0.707393
H	-0.684837	3.01766	-0.879071

H	-1.821823	3.50193	0.36717	H	4.901331	1.073445	-1.63349
C	-3.032289	1.046493	1.611576	H	6.389954	0.287824	-2.143817
H	-3.479448	0.094152	1.943878	C	5.536906	-0.510753	-0.321814
C	-1.956074	1.420964	2.637928	H	6.112258	0.146066	0.338682
H	-1.183829	0.644349	2.670386	H	6.10219	-1.451258	-0.389775
H	-1.454301	2.344818	2.306227	C	4.172273	-0.789228	0.300032
C	-2.552834	1.634261	4.024625	H	3.654422	0.16783	0.476001
H	-2.948696	0.675391	4.389286	H	4.301831	-1.261527	1.280532
H	-1.763533	1.925917	4.726518	C	0.753851	-3.200614	-0.879246
C	-3.673288	2.665262	4.010231	H	0.045464	-3.65567	-0.17159
H	-4.109869	2.771718	5.008302	C	-0.114755	-2.537925	-1.960335
H	-3.259236	3.649779	3.748302	H	-0.819707	-1.794925	-1.509163
C	-4.741874	2.287537	2.994275	H	0.503071	-1.973742	-2.670642
H	-5.532343	3.044406	2.961116	C	-0.951099	-3.580054	-2.697772
H	-5.225699	1.348789	3.301038	H	-1.6632	-4.027894	-1.989211
C	-4.140718	2.111383	1.603173	H	-1.548091	-3.103574	-3.483257
H	-3.716423	3.072927	1.28051	C	-0.059782	-4.675997	-3.276202
H	-4.925717	1.866671	0.880278	H	0.605985	-4.239006	-4.034127
C	1.937665	-2.665847	1.799307	H	-0.672791	-5.417465	-3.79765
H	2.939832	-3.120992	1.726021	C	0.779821	-5.341475	-2.191249
C	0.939029	-3.766405	2.176068	H	0.116074	-5.846086	-1.474418
H	-0.078717	-3.343808	2.156466	H	1.417365	-6.120219	-2.621303
H	0.957991	-4.578111	1.43958	C	1.628844	-4.315715	-1.44904
C	1.229152	-4.340736	3.560166	H	2.200179	-4.793163	-0.642515
H	0.483586	-5.105475	3.801381	H	2.37081	-3.891071	-2.140254
H	2.199727	-4.856412	3.533922	P	-2.328282	0.624828	-0.066185
C	1.2643	-3.259664	4.630086	P	1.607108	-1.900495	0.131571
H	0.266201	-2.808173	4.725726	B	1.031682	1.26567	-0.254041
H	1.500443	-3.694706	5.60638	Ru	-0.108896	-0.284458	-0.088917
C	2.271419	-2.178646	4.265491	H	0.582502	0.877075	-1.388136
H	3.284019	-2.607424	4.263126	H	-0.665112	-1.122118	1.180612
H	2.278173	-1.381196	5.016166	H	0.331909	0.728785	1.064057
C	1.970032	-1.58928	2.892894				
H	2.704884	-0.815244	2.644961	<i>sp_hy</i> - RC			
H	0.988627	-1.089851	2.910405	C	0.926718	2.974983	-0.053948
C	3.298093	-1.671389	-0.601039	C	1.312075	3.724603	-1.206399
H	3.750038	-2.676378	-0.645127	C	1.147006	3.186541	-2.598832
C	3.21666	-1.103506	-2.019461	H	1.459242	3.924041	-3.341178
H	2.653221	-1.780767	-2.673319	H	0.104536	2.92342	-2.8171
H	2.643107	-0.165398	-1.982852	H	1.73838	2.279188	-2.771884
C	4.591426	-0.821127	-2.61492	C	1.8588	4.993498	-1.051649
H	5.131788	-1.768536	-2.753287	H	2.154658	5.552915	-1.937547
H	4.475982	-0.386147	-3.613805	C	2.044969	5.570804	0.208867
C	5.40312	0.096183	-1.710925	C	2.630342	6.938465	0.344552

H	1.870553	7.706542	0.161151	C	-3.025946	-0.306149	1.51275
H	3.429794	7.109505	-0.380989	H	-2.845325	-1.376461	1.704877
H	3.029741	7.112663	1.346022	C	-2.144974	0.457608	2.506198
C	1.639947	4.84636	1.332867	H	-1.0884	0.244887	2.322031
H	1.761704	5.290492	2.319288	H	-2.272999	1.537971	2.362131
C	1.074114	3.579937	1.226946	C	-2.505059	0.100822	3.942915
C	0.596186	2.905986	2.478398	H	-2.288462	-0.965149	4.111925
H	0.915251	3.452938	3.368047	H	-1.863634	0.659316	4.634894
H	0.954863	1.875049	2.577466	C	-3.977018	0.370045	4.227404
H	-0.499019	2.85439	2.502199	H	-4.231756	0.082668	5.252358
C	-3.534299	-1.427761	-1.168513	H	-4.166154	1.450913	4.154554
H	-2.945645	-1.636856	-2.075627	C	-4.866786	-0.362635	3.2318
C	-3.615242	-2.737197	-0.369167	H	-5.922263	-0.136676	3.415319
H	-2.631869	-3.014189	0.034997	H	-4.755389	-1.447778	3.372815
H	-4.269132	-2.583634	0.501772	C	-4.506884	-0.017277	1.78879
C	-4.189208	-3.860063	-1.225493	H	-4.711705	1.047575	1.602624
H	-3.509012	-4.054971	-2.068215	H	-5.148542	-0.579001	1.101563
H	-4.236082	-4.787797	-0.645898	C	2.098704	-2.096695	1.746815
C	-5.566053	-3.48467	-1.758296	H	3.14692	-2.109731	2.090468
H	-6.264672	-3.394478	-0.914336	C	1.565001	-3.536743	1.77182
H	-5.960919	-4.279356	-2.399157	H	0.518901	-3.527402	1.42592
C	-5.521282	-2.164214	-2.515915	H	2.112806	-4.188204	1.084556
H	-6.520964	-1.88218	-2.862219	C	1.645089	-4.123807	3.178937
H	-4.906076	-2.283999	-3.419652	H	1.256167	-5.147506	3.174064
C	-4.93369	-1.036324	-1.669172	H	2.703717	-4.2005	3.466999
H	-4.902182	-0.117417	-2.263852	C	0.906128	-3.272122	4.201487
H	-5.599001	-0.831976	-0.819741	H	-0.17113	-3.296693	3.979098
C	-3.204871	1.467644	-0.905781	H	1.022678	-3.691281	5.205996
H	-4.300089	1.359716	-0.870429	C	1.388146	-1.828483	4.157498
C	-2.774307	1.65829	-2.365258	H	2.435499	-1.77553	4.488985
H	-1.673768	1.682426	-2.396221	H	0.814616	-1.205098	4.852856
H	-3.074646	0.794944	-2.974995	C	1.275467	-1.268606	2.744051
C	-3.323038	2.947878	-2.963694	H	1.554065	-0.20865	2.723649
H	-2.971922	3.056833	-3.995587	H	0.223159	-1.315592	2.428571
H	-4.419484	2.886195	-3.015915	C	3.582975	-0.150987	0.098804
C	-2.922514	4.153388	-2.123439	H	4.483489	-0.784303	0.111355
H	-1.827585	4.266376	-2.143673	C	3.625868	0.735702	-1.149701
H	-3.333351	5.073914	-2.55004	H	3.622279	0.134398	-2.065301
C	-3.379421	3.981421	-0.682433	H	2.703352	1.327076	-1.172802
H	-4.478029	3.959104	-0.649934	C	4.808191	1.698066	-1.140936
H	-3.072318	4.836874	-0.071732	H	5.747024	1.129132	-1.201193
C	-2.837775	2.693787	-0.06701	H	4.771816	2.329211	-2.036725
H	-1.742084	2.770615	0.017692	C	4.806542	2.553513	0.11843
H	-3.22112	2.585485	0.953423	H	3.914145	3.197117	0.117891

H	5.672075	3.223829	0.130036
C	4.791134	1.6807	1.364735
H	4.753889	2.297694	2.269512
H	5.726213	1.105293	1.421946
C	3.610519	0.714054	1.361118
H	2.677852	1.295244	1.413913
H	3.644134	0.085625	2.257806
C	2.858483	-2.757512	-0.966886
H	2.092588	-3.542777	-0.878418
C	3.030726	-2.472232	-2.462762
H	2.14594	-1.976939	-2.877235
H	3.870046	-1.777769	-2.603718
C	3.328976	-3.764799	-3.215594
H	2.466955	-4.441573	-3.11802
H	3.440428	-3.561237	-4.285734
C	4.578674	-4.44358	-2.666207
H	5.452264	-3.812817	-2.883721
H	4.754744	-5.39562	-3.176937
C	4.484195	-4.657657	-1.160036
H	3.695114	-5.391979	-0.940331
H	5.415263	-5.084895	-0.773525
C	4.16535	-3.356326	-0.425179
H	4.120112	-3.534339	0.655466
H	4.986077	-2.643772	-0.587266
P	-2.515256	-0.138391	-0.270162
P	2.147107	-1.348813	0.031833
B	0.435212	1.546917	-0.212574
Ru	-0.123833	-0.490421	-0.477464
H	0.337234	1.075261	-1.361571
H	-0.539091	-1.719978	0.462784
H	0.108339	0.860997	0.790629
C	-0.386577	-1.103743	-2.542703
H	-1.311673	-0.690287	-2.939682
H	0.506556	-0.804362	-3.089272
C	-0.396522	-2.268813	-1.764683
H	0.470669	-2.917379	-1.739857
H	-1.328694	-2.781895	-1.559185

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C	0.525029	2.918983	0.046838
C	0.693043	3.697848	-1.143551
C	0.520778	3.110396	-2.513936
H	0.577369	3.886926	-3.279996

H	-0.439427	2.597932	-2.635183
H	1.293701	2.368047	-2.745911
C	1.056484	5.034374	-1.051894
H	1.182414	5.610264	-1.967479
C	1.277159	5.660888	0.180427
C	1.705941	7.090253	0.241696
H	1.074025	7.725462	-0.385795
H	2.729563	7.206295	-0.131501
H	1.679886	7.481597	1.260665
C	1.104807	4.905168	1.338575
H	1.268426	5.377263	2.305954
C	0.730998	3.562724	1.300177
C	0.552235	2.872015	2.620588
H	1.239867	3.280183	3.366262
H	0.712122	1.792716	2.57767
H	-0.461233	3.027391	3.009873
C	-3.414994	-2.028513	-0.585044
H	-2.756763	-2.519404	-1.316707
C	-3.507399	-2.953837	0.637426
H	-2.561466	-2.975945	1.196543
H	-4.258227	-2.549281	1.332026
C	-3.931001	-4.358925	0.225233
H	-3.163636	-4.791427	-0.435016
H	-3.982947	-5.009432	1.104448
C	-5.26891	-4.324893	-0.5017
H	-6.049272	-4.002545	0.202249
H	-5.552071	-5.328598	-0.834055
C	-5.231971	-3.363935	-1.683066
H	-6.211815	-3.312805	-2.168975
H	-4.532969	-3.745254	-2.441901
C	-4.789654	-1.960505	-1.269783
H	-4.769598	-1.313605	-2.152186
H	-5.53496	-1.532187	-0.587154
C	-3.254585	0.766203	-1.387379
H	-4.342453	0.607204	-1.323086
C	-2.803173	0.440842	-2.816173
H	-1.715743	0.606603	-2.884567
H	-2.958273	-0.621143	-3.048778
C	-3.53263	1.317891	-3.828057
H	-3.202478	1.077198	-4.843948
H	-4.606816	1.084717	-3.790355
C	-3.32271	2.797701	-3.531304
H	-2.267257	3.0521	-3.703556
H	-3.898541	3.413197	-4.229927

C	-3.696436	3.140256	-2.094439	H	2.39883	1.698933	-1.109325
H	-4.782572	3.027602	-1.964822	C	4.427063	2.307937	-1.366622
H	-3.470176	4.189744	-1.877597	H	5.406456	1.854118	-1.576965
C	-2.990013	2.240475	-1.082744	H	4.193342	2.948515	-2.225232
H	-1.907653	2.42947	-1.107298	C	4.504175	3.128013	-0.086749
H	-3.317101	2.499163	-0.069621	H	3.547553	3.652412	0.062719
C	-3.199022	0.031816	1.495248	H	5.275653	3.90075	-0.166622
H	-3.127651	-0.908724	2.061617	C	4.772543	2.224384	1.108027
C	-2.362672	1.050193	2.276727	H	4.802355	2.8048	2.036846
H	-1.348081	0.660872	2.405346	H	5.76475	1.762805	1.002012
H	-2.260573	1.987921	1.708422	C	3.722352	1.125473	1.232166
C	-2.965338	1.342849	3.648492	H	2.747167	1.588833	1.446787
H	-2.896136	0.435639	4.266092	H	3.96405	0.485666	2.087995
H	-2.365359	2.104448	4.160578	C	3.13612	-2.368683	-1.064309
C	-4.422821	1.769128	3.557286	H	2.411428	-3.196686	-1.094544
H	-4.829742	1.962825	4.554694	C	3.342639	-1.901492	-2.512555
H	-4.494569	2.716955	3.003868	H	2.464921	-1.368928	-2.89962
C	-5.238841	0.703344	2.841283	H	4.172854	-1.181289	-2.534694
H	-6.290601	0.998202	2.766084	C	3.70437	-3.087387	-3.39987
H	-5.219891	-0.226153	3.428906	H	2.871052	-3.805642	-3.396442
C	-4.682098	0.429439	1.448147	H	3.825067	-2.75991	-4.437779
H	-4.807911	1.331324	0.833479	C	4.975342	-3.766824	-2.902319
H	-5.269159	-0.35577	0.959751	H	5.821944	-3.079071	-3.038941
C	2.556909	-1.806192	1.74595	H	5.201098	-4.651567	-3.505927
H	3.639618	-1.745845	1.950007	C	4.873005	-4.142037	-1.42872
C	2.139531	-3.2796	1.87016	H	4.124478	-4.93824	-1.302272
H	1.044901	-3.342048	1.788288	H	5.821412	-4.556299	-1.071374
H	2.5499	-3.901541	1.066626	C	4.468017	-2.950641	-0.561874
C	2.555674	-3.833736	3.230332	H	4.42137	-3.253316	0.488639
H	2.280513	-4.891013	3.304054	H	5.244839	-2.174907	-0.622595
H	3.651574	-3.794143	3.312321	P	-2.510035	-0.429347	-0.180797
C	1.924564	-3.035543	4.364353	P	2.339539	-1.085621	0.035834
H	0.836279	-3.19272	4.347029	B	0.225707	1.428072	-0.052649
H	2.271545	-3.405492	5.334438	Ru	-0.066953	-0.637281	-0.274809
C	2.211511	-1.545652	4.225189	H	0.112773	0.915472	-1.205647
H	3.284202	-1.359882	4.382908	H	-0.263486	-1.994321	0.647821
H	1.686847	-0.979188	5.002038	H	0.104548	0.720789	0.977369
C	1.81767	-1.026898	2.845178	C	-0.216103	-2.09025	-1.842441
H	2.00213	0.048771	2.775267	H	-1.120467	-1.97152	-2.437652
H	0.735802	-1.158097	2.688735	H	0.691119	-2.141979	-2.437654
C	3.607232	0.294405	-0.050024	C	-0.272294	-2.839783	-0.627654
H	4.566842	-0.228781	-0.194915	H	0.591074	-3.440498	-0.350231
C	3.369509	1.216485	-1.250033	H	-1.202124	-3.326459	-0.34464
H	3.294159	0.650101	-2.182204				

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C	0.354784	2.881681	0.063258
C	0.486555	3.599869	-1.168356
C	0.417392	2.920667	-2.505627
H	0.492241	3.649794	-3.315492
H	-0.52169	2.373907	-2.646187
H	1.220242	2.187956	-2.650509
C	0.702649	4.97098	-1.151225
H	0.807593	5.498855	-2.097837
C	0.796024	5.694232	0.043566
C	1.023417	7.170459	0.02473
H	0.141707	7.698475	-0.354538
H	1.853031	7.438639	-0.636131
H	1.23942	7.563022	1.020483
C	0.669263	4.994685	1.24105
H	0.74939	5.538755	2.180971
C	0.451012	3.617177	1.279504
C	0.321074	2.995024	2.640365
H	0.965244	3.508707	3.359693
H	0.575592	1.933289	2.667535
H	-0.704743	3.085892	3.017425
C	-3.272391	-2.189801	-0.570414
H	-2.574928	-2.652313	-1.283453
C	-3.344958	-3.114063	0.65354
H	-2.407129	-3.093003	1.225921
H	-4.124989	-2.744391	1.335013
C	-3.696618	-4.538829	0.238657
H	-2.896843	-4.938753	-0.404175
H	-3.736207	-5.188158	1.119402
C	-5.018511	-4.570755	-0.517616
H	-5.828381	-4.28183	0.167227
H	-5.246999	-5.588241	-0.850119
C	-4.999654	-3.613848	-1.701983
H	-5.969213	-3.611179	-2.21085
H	-4.265468	-3.96319	-2.442867
C	-4.634874	-2.190639	-1.28295
H	-4.630686	-1.544934	-2.165925
H	-5.413531	-1.798835	-0.615501
C	-3.252301	0.606701	-1.38524
H	-4.330726	0.390425	-1.331104
C	-2.771585	0.300178	-2.808906
H	-1.69341	0.517404	-2.86758
H	-2.87051	-0.768144	-3.041759
C	-3.533713	1.139117	-3.829643

H	-3.180558	0.914368	-4.84146
H	-4.595203	0.852481	-3.803682
C	-3.403437	2.628278	-3.533556
H	-2.359692	2.936397	-3.689208
H	-3.999427	3.212581	-4.242039
C	-3.814883	2.951794	-2.102706
H	-4.894476	2.777594	-1.98591
H	-3.650405	4.012586	-1.884813
C	-3.068002	2.094387	-1.083827
H	-1.998201	2.341672	-1.104661
H	-3.413075	2.339611	-0.073247
C	-3.208742	-0.1117	1.500605
H	-3.103097	-1.046812	2.070778
C	-2.442679	0.947136	2.298511
H	-1.410359	0.613069	2.441303
H	-2.383631	1.890449	1.733726
C	-3.083992	1.199844	3.660444
H	-2.976815	0.29417	4.274912
H	-2.534703	1.989518	4.186451
C	-4.560628	1.547663	3.545403
H	-4.994563	1.712583	4.53658
H	-4.673631	2.494126	2.996601
C	-5.305737	0.44508	2.808509
H	-6.370162	0.684165	2.71508
H	-5.247954	-0.486103	3.390973
C	-4.709325	0.210091	1.424388
H	-4.867253	1.109373	0.813456
H	-5.247053	-0.599367	0.919308
C	2.706905	-1.757946	1.695983
H	3.752385	-1.512678	1.952075
C	2.576526	-3.288116	1.735488
H	1.51932	-3.562703	1.615361
H	3.121306	-3.777298	0.921392
C	3.059726	-3.815295	3.085076
H	2.992461	-4.907987	3.105336
H	4.125227	-3.57028	3.202407
C	2.260664	-3.209782	4.232668
H	1.224245	-3.572662	4.173818
H	2.650422	-3.554271	5.195733
C	2.254252	-1.686913	4.170526
H	3.265767	-1.303861	4.370283
H	1.610196	-1.272988	4.953739
C	1.801112	-1.189549	2.802131
H	1.76194	-0.095169	2.779672

H	0.768233	-1.521557	2.607697
C	3.601286	0.527253	0.132702
H	4.60491	0.071086	0.113199
C	3.448662	1.448679	-1.080125
H	3.565254	0.897159	-2.016459
H	2.424201	1.83175	-1.07645
C	4.401626	2.637075	-1.047989
H	5.438668	2.281946	-1.133618
H	4.218086	3.269936	-1.924214
C	4.236068	3.434318	0.23696
H	3.225983	3.870665	0.262476
H	4.938889	4.273348	0.267229
C	4.428517	2.533731	1.448728
H	4.278047	3.094567	2.378353
H	5.466561	2.172094	1.473385
C	3.483345	1.335977	1.428529
H	2.449849	1.697335	1.528498
H	3.683904	0.702884	2.299452
C	3.288787	-2.071226	-1.156631
H	2.664404	-2.978962	-1.117912
C	3.308216	-1.61067	-2.621253
H	2.357096	-1.155124	-2.921568
H	4.07201	-0.830917	-2.735748
C	3.686227	-2.783609	-3.520329
H	2.925176	-3.572218	-3.42278
H	3.678171	-2.475516	-4.570895
C	5.05719	-3.334006	-3.138096
H	5.819354	-2.579132	-3.377824
H	5.300396	-4.214109	-3.741727
C	5.146098	-3.670351	-1.652764
H	4.496322	-4.529654	-1.429363
H	6.163289	-3.981183	-1.392492
C	4.716996	-2.494017	-0.777415
H	4.8086	-2.752638	0.28316
H	5.396228	-1.646884	-0.948008
P	-2.462177	-0.539801	-0.162665
P	2.430054	-0.930444	0.036379
B	0.174972	1.365805	0.071824
Ru	0.000641	-0.619396	-0.22453
H	0.098776	0.804477	-1.143737
H	0.122397	0.685867	1.132271
C	-0.091246	-2.10566	-1.709552
H	-0.997286	-2.093612	-2.315633
H	0.790622	-2.189719	-2.340363

C	-0.104784	-3.00392	-0.526005
H	0.788946	-3.62064	-0.412614
H	-0.992359	-3.630682	-0.411857
H	-0.125819	-2.415513	0.48375

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C	0.35451	2.803364	0.139908
C	0.579659	3.394459	-1.141501
C	0.695444	2.556169	-2.380447
H	0.870524	3.177465	-3.262099
H	-0.20882	1.96195	-2.56259
H	1.516857	1.83207	-2.308555
C	0.720469	4.770075	-1.248903
H	0.89635	5.207374	-2.230605
C	0.650105	5.61185	-0.130389
C	0.790272	7.091917	-0.284127
H	-0.077204	7.517015	-0.800559
H	1.666426	7.350879	-0.885905
H	0.878993	7.5956	0.680647
C	0.444864	5.02874	1.116621
H	0.404164	5.666374	1.998661
C	0.298798	3.648352	1.276351
C	0.115448	3.137958	2.676661
H	0.95821	3.440892	3.308482
H	0.030417	2.051339	2.740727
H	-0.783231	3.564338	3.136189
C	-3.222434	-2.156243	-0.619299
H	-2.605724	-2.498563	-1.464743
C	-3.072529	-3.198182	0.498369
H	-2.064368	-3.178193	0.934644
H	-3.76323	-2.947423	1.315781
C	-3.420387	-4.594037	-0.011246
H	-2.703278	-4.884485	-0.79448
H	-3.307164	-5.327092	0.79433
C	-4.832737	-4.632508	-0.581767
H	-5.552063	-4.466545	0.232601
H	-5.054758	-5.624181	-0.988434
C	-5.029335	-3.561389	-1.646612
H	-6.061305	-3.566975	-2.01242
H	-4.394299	-3.785876	-2.516483
C	-4.673555	-2.171937	-1.121733
H	-4.839561	-1.425692	-1.906113
H	-5.352352	-1.917481	-0.296676

C	-3.238052	0.664678	-1.390334	H	2.318532	-4.804846	4.375932
H	-4.327091	0.545569	-1.284412	C	1.833559	-2.770167	3.814723
C	-2.855007	0.320221	-2.832688	H	2.743468	-2.363708	4.280174
H	-1.76357	0.424603	-2.937016	H	1.032917	-2.652383	4.552582
H	-3.088776	-0.727225	-3.067426	C	1.518689	-1.95826	2.564074
C	-3.552535	1.253189	-3.818313	H	1.345069	-0.905343	2.817607
H	-3.263078	0.999352	-4.843403	H	0.570319	-2.313573	2.12572
H	-4.638316	1.090036	-3.756019	C	3.545491	0.476295	0.714379
C	-3.240561	2.714479	-3.516257	H	4.511249	-0.040662	0.845098
H	-2.168108	2.895669	-3.684081	C	3.738057	1.599621	-0.306855
H	-3.773957	3.37091	-4.211253	H	4.124904	1.19501	-1.246987
C	-3.582162	3.067978	-2.074437	H	2.762049	2.045504	-0.53348
H	-4.670252	3.007193	-1.926669	C	4.673273	2.69256	0.200292
H	-3.297147	4.102484	-1.853583	H	5.68602	2.27991	0.317695
C	-2.8862	2.124818	-1.100205	H	4.749095	3.484459	-0.552626
H	-1.802217	2.242878	-1.199253	C	4.20021	3.251675	1.533238
H	-3.122456	2.39728	-0.064156	H	3.219213	3.732629	1.397974
C	-3.308925	-0.094657	1.468452	H	4.88217	4.030079	1.890279
H	-3.382693	-1.075241	1.962164	C	4.082326	2.13353	2.55753
C	-2.47166	0.788605	2.395288	H	3.736352	2.517812	3.523421
H	-1.490663	0.326402	2.550954	H	5.076912	1.701797	2.739172
H	-2.282591	1.760785	1.911676	C	3.137447	1.033076	2.081896
C	-3.153139	1.004677	3.742671	H	2.119336	1.441919	2.015466
H	-3.199627	0.041965	4.272478	H	3.106969	0.232869	2.829745
H	-2.539651	1.664875	4.3661	C	3.345902	-1.631387	-1.317399
C	-4.562977	1.554653	3.587408	H	2.864722	-2.619397	-1.422275
H	-5.037415	1.677678	4.566092	C	3.192188	-0.925997	-2.673135
H	-4.517525	2.557271	3.137325	H	2.155999	-0.623615	-2.857484
C	-5.393578	0.641458	2.697655	H	3.776623	0.002291	-2.674716
H	-6.405903	1.03771	2.567002	C	3.722912	-1.831798	-3.781043
H	-5.505999	-0.338787	3.183203	H	3.121243	-2.753001	-3.812139
C	-4.736434	0.458154	1.332692	H	3.600243	-1.350325	-4.756786
H	-4.71006	1.431878	0.825214	C	5.188327	-2.181523	-3.539904
H	-5.350319	-0.1943	0.704045	H	5.791058	-1.267746	-3.63929
C	2.633713	-2.110617	1.51492	H	5.54996	-2.870468	-4.309756
H	3.582056	-1.805154	1.989071	C	5.413089	-2.773364	-2.152415
C	2.773775	-3.593977	1.151432	H	4.929109	-3.759287	-2.088644
H	1.828754	-3.960861	0.731059	H	6.480315	-2.944795	-1.977655
H	3.538675	-3.754025	0.38418	C	4.839267	-1.874889	-1.059399
C	3.105752	-4.413043	2.39746	H	5.01878	-2.309282	-0.068103
H	3.214905	-5.468957	2.128951	H	5.361256	-0.906521	-1.069328
H	4.08258	-4.091673	2.78609	P	-2.473889	-0.498587	-0.166596
C	2.046234	-4.240735	3.478394	P	2.412612	-0.883981	0.103028
H	1.097045	-4.668581	3.123405	B	0.176733	1.294258	0.223572

Ru	0.009373	-0.552521	-0.18107
H	0.120727	-0.342906	-1.761595
H	0.103063	0.542571	1.286934
C	-0.102815	-1.879541	-1.945432
H	-1.053129	-1.813622	-2.477708
H	0.695882	-1.906282	-2.686965
C	-0.02537	-3.077515	-1.015996
H	0.904743	-3.634105	-1.150737
H	-0.862065	-3.769385	-1.154082
H	-0.057529	-2.814705	0.067697

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C	0.418921	2.967921	-0.014021
C	0.583432	3.75837	-1.188002
C	0.532181	3.177425	-2.571388
H	0.726405	3.946538	-3.32199
H	-0.449993	2.747171	-2.801329
H	1.267994	2.381268	-2.726537
C	0.780453	5.131988	-1.070005
H	0.90829	5.723028	-1.975245
C	0.812388	5.776143	0.167657
C	1.025158	7.251291	0.269494
H	1.150208	7.714249	-0.71119
H	1.912472	7.483092	0.867146
H	0.181466	7.73986	0.767349
C	0.636188	4.99916	1.316727
H	0.655601	5.483427	2.291885
C	0.444888	3.624612	1.255069
C	0.274022	2.873612	2.544422
H	0.32221	3.551743	3.398774
H	1.050218	2.113001	2.685663
H	-0.686149	2.346037	2.59939
C	-3.306331	-1.538506	-1.548024
H	-2.699317	-1.339217	-2.447063
C	-3.177737	-3.034762	-1.228061
H	-2.161689	-3.277286	-0.888507
H	-3.845078	-3.273007	-0.386265
C	-3.574966	-3.883984	-2.429486
H	-2.87343	-3.691409	-3.255258
H	-3.479694	-4.947321	-2.186359
C	-4.993467	-3.557436	-2.87936
H	-5.69787	-3.858059	-2.090587
H	-5.260373	-4.140358	-3.766466

C	-5.156353	-2.067925	-3.154225
H	-6.188337	-1.838304	-3.438847
H	-4.531441	-1.785568	-4.014421
C	-4.752664	-1.215671	-1.952203
H	-4.874789	-0.155279	-2.198048
H	-5.435171	-1.419843	-1.117103
C	-3.360689	1.132313	-0.381393
H	-4.435044	0.891684	-0.402237
C	-2.981023	1.811853	-1.701015
H	-1.893381	1.972105	-1.688729
H	-3.185834	1.151313	-2.554632
C	-3.671541	3.158149	-1.880727
H	-3.355179	3.613339	-2.825967
H	-4.757178	3.0038	-1.960608
C	-3.369948	4.080554	-0.706771
H	-2.290539	4.296858	-0.685106
H	-3.876332	5.042891	-0.832717
C	-3.77938	3.430278	0.607779
H	-4.871199	3.303816	0.626758
H	-3.530163	4.078827	1.455081
C	-3.115694	2.070615	0.800285
H	-2.033386	2.217005	0.921174
H	-3.47563	1.614004	1.728192
C	-2.989619	-1.252157	1.380449
H	-2.698762	-2.305732	1.24018
C	-2.198081	-0.760395	2.597024
H	-1.126448	-0.818302	2.384389
H	-2.421308	0.295498	2.799999
C	-2.539575	-1.588027	3.831231
H	-2.219304	-2.627457	3.662512
H	-1.966518	-1.225571	4.692677
C	-4.034894	-1.558204	4.122447
H	-4.270469	-2.173868	4.996242
H	-4.331315	-0.531079	4.380589
C	-4.834711	-2.021967	2.912636
H	-5.909824	-1.964508	3.111989
H	-4.614264	-3.081116	2.714148
C	-4.494731	-1.208355	1.666136
H	-4.810881	-0.165014	1.813609
H	-5.065343	-1.585578	0.810779
C	2.479625	-1.634572	1.815399
H	3.564316	-1.656955	2.014605
C	1.915111	-3.048578	2.026627
H	0.827405	-3.011007	1.86671

H	2.304786	-3.762394	1.293772
C	2.205169	-3.54276	3.441486
H	1.805258	-4.554174	3.569047
H	3.293396	-3.623579	3.580322
C	1.625394	-2.600784	4.488099
H	0.527726	-2.622347	4.418948
H	1.876756	-2.94209	5.497491
C	2.10884	-1.173313	4.268107
H	3.190489	-1.11636	4.459523
H	1.635248	-0.489882	4.982027
C	1.827711	-0.704944	2.844425
H	2.152334	0.33044	2.716142
H	0.743941	-0.710645	2.670587
C	3.630123	0.282026	-0.171163
H	4.572177	-0.26744	-0.332339
C	3.338905	1.129038	-1.413486
H	3.178023	0.503617	-2.299352
H	2.395706	1.657574	-1.231731
C	4.423586	2.16522	-1.681002
H	5.369483	1.656696	-1.917403
H	4.160266	2.75246	-2.568493
C	4.613432	3.071189	-0.472337
H	3.691281	3.650624	-0.308763
H	5.409948	3.799565	-0.65483
C	4.915946	2.246237	0.770175
H	5.025851	2.890131	1.64906
H	5.880577	1.734661	0.642123
C	3.832567	1.203977	1.034158
H	2.883554	1.722382	1.250612
H	4.08906	0.623036	1.926764
C	3.094674	-2.464388	-0.899587
H	2.321954	-3.24949	-0.889735
C	3.407015	-2.121252	-2.364398
H	2.562768	-1.62629	-2.857855
H	4.238015	-1.400549	-2.387137
C	3.817565	-3.37169	-3.136792
H	2.975497	-4.079275	-3.143889
H	4.015323	-3.117245	-4.183207
C	5.036656	-4.028931	-2.503741
H	5.902514	-3.361162	-2.617353
H	5.292786	-4.953162	-3.031342
C	4.809134	-4.304717	-1.023593
H	4.032046	-5.074286	-0.90758
H	5.714916	-4.713516	-0.563647

C	4.370783	-3.049524	-0.27137
H	4.239718	-3.288327	0.787477
H	5.173489	-2.299124	-0.320834
P	-2.474582	-0.496588	-0.238852
P	2.325708	-1.051709	0.049257
B	0.217473	1.463768	-0.03287
Ru	-0.016798	-0.459665	-0.401806
H	-0.220445	-1.786406	0.568562
H	0.0295	0.739439	1.012555
C	0.079755	-0.365485	-2.620608
H	-0.780279	0.072116	-3.131427
H	1.033172	-0.074656	-3.066466
C	-0.048941	-1.718052	-2.122492
H	0.807095	-2.379179	-2.206273
H	-0.990605	-2.226994	-2.289579
H	0.150925	0.724444	-1.630141

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C	0.37915	2.93777	0.021872
C	0.536417	3.729029	-1.153112
C	0.514918	3.147893	-2.536079
H	0.666054	3.927744	-3.285594
H	-0.440316	2.663278	-2.766424
H	1.29288	2.394267	-2.693149
C	0.702974	5.105648	-1.03581
H	0.827348	5.695519	-1.94245
C	0.709367	5.755449	0.200939
C	0.855841	7.239502	0.287806
H	-0.115626	7.731949	0.166112
H	1.507645	7.629582	-0.497952
H	1.254844	7.55349	1.254939
C	0.548146	4.97748	1.34876
H	0.555949	5.46269	2.32352
C	0.386094	3.597238	1.289781
C	0.227856	2.848061	2.582561
H	0.268734	3.530525	3.433831
H	1.013816	2.097785	2.725543
H	-0.726393	2.309947	2.640869
C	-3.267785	-1.569666	-1.561994
H	-2.637336	-1.379087	-2.445874
C	-3.136784	-3.062196	-1.225766
H	-2.123154	-3.29781	-0.87387
H	-3.81291	-3.300703	-0.391113
C	-3.507352	-3.925146	-2.426167

H	-2.789683	-3.737264	-3.238865	H	-5.034712	-1.65934	0.72229
H	-3.412585	-4.985536	-2.170168	C	2.495948	-1.598607	1.842573
C	-4.917306	-3.609193	-2.908787	H	3.577139	-1.66841	2.045638
H	-5.637323	-3.901051	-2.130787	C	1.875857	-2.996198	2.008981
H	-5.164218	-4.204796	-3.793263	H	0.792117	-2.916604	1.828453
C	-5.077027	-2.123893	-3.206638	H	2.255592	-3.703228	1.264014
H	-6.102401	-1.900143	-3.518762	C	2.110577	-3.544466	3.413148
H	-4.431853	-1.851241	-4.054881	H	1.662429	-4.53968	3.501538
C	-4.704305	-1.256407	-2.005646	H	3.190719	-3.678893	3.571374
H	-4.82048	-0.199452	-2.268473	C	1.552853	-2.604883	4.472729
H	-5.409106	-1.450013	-1.186843	H	0.45767	-2.563545	4.375348
C	-3.371113	1.110396	-0.410145	H	1.758529	-2.988279	5.477241
H	-4.44109	0.855009	-0.458912	C	2.119443	-1.201772	4.307062
C	-2.962981	1.794938	-1.717999	H	3.199566	-1.214155	4.513018
H	-1.875808	1.952576	-1.678057	H	1.676321	-0.516268	5.038006
H	-3.144404	1.135408	-2.577226	C	1.883761	-0.667309	2.89639
C	-3.65088	3.14004	-1.912479	H	2.276739	0.348927	2.811304
H	-3.307132	3.599472	-2.846083	H	0.802081	-0.59605	2.718031
H	-4.733212	2.983075	-2.026345	C	3.64763	0.33701	-0.155042
C	-3.389101	4.059389	-0.726799	H	4.593694	-0.199337	-0.335365
H	-2.31195	4.279919	-0.671398	C	3.313965	1.177106	-1.390852
H	-3.895763	5.019981	-0.864885	H	3.125918	0.547344	-2.268254
C	-3.836227	3.402365	0.571672	H	2.372209	1.696482	-1.178559
H	-4.927146	3.267728	0.553905	C	4.379543	2.223954	-1.688355
H	-3.620364	4.049678	1.428905	H	5.326011	1.725555	-1.943893
C	-3.1704	2.046431	0.78198	H	4.090548	2.805635	-2.571539
H	-2.093817	2.197958	0.944628	C	4.583022	3.135259	-0.485602
H	-3.562988	1.584529	1.693652	H	3.656484	3.702387	-0.304488
C	-2.992239	-1.259918	1.369619	H	5.365293	3.874221	-0.686062
H	-2.660922	-2.305058	1.251704	C	4.923735	2.31932	0.753092
C	-2.278261	-0.732466	2.621988	H	5.043843	2.968336	1.62682
H	-1.194222	-0.724057	2.470316	H	5.892596	1.821144	0.605589
H	-2.570275	0.306729	2.819705	C	3.862252	1.26111	1.045615
C	-2.631465	-1.584049	3.837332	H	2.911337	1.765235	1.286518
H	-2.258862	-2.607281	3.676714	H	4.150938	0.683586	1.930477
H	-2.109365	-1.202534	4.722456	C	3.154757	-2.421661	-0.860085
C	-4.136425	-1.621278	4.070632	H	2.386576	-3.210635	-0.873965
H	-4.378239	-2.255202	4.929535	C	3.491389	-2.068685	-2.316191
H	-4.48599	-0.610373	4.326132	H	2.643172	-1.594499	-2.822428
C	-4.868854	-2.105015	2.826966	H	4.304007	-1.326912	-2.321039
H	-5.952518	-2.087348	2.982787	C	3.948069	-3.306148	-3.084136
H	-4.602968	-3.154278	2.631098	H	3.122382	-4.032111	-3.114853
C	-4.508197	-1.271207	1.600097	H	4.164626	-3.041249	-4.124208
H	-4.862923	-0.239275	1.741441	C	5.164982	-3.940256	-2.425026

H	6.016756	-3.249916	-2.505167
H	5.458808	-4.851513	-2.955432
C	4.899135	-4.239284	-0.956451
H	4.131792	-5.022883	-0.874616
H	5.797066	-4.63909	-0.473687
C	4.416909	-3.00196	-0.201677
H	4.25136	-3.26171	0.847592
H	5.210574	-2.239973	-0.209585
P	-2.462899	-0.505038	-0.252511
P	2.360387	-1.008415	0.07462
B	0.201378	1.429247	0.064145
Ru	0.010181	-0.462508	-0.396986
H	-0.163881	-1.362719	0.906541
H	0.010958	0.695689	1.070591
C	0.115783	-0.414826	-2.892588
H	-0.773664	-0.189392	-3.488953
H	1.005044	-0.359168	-3.529316
C	0.007893	-1.68996	-2.09791
H	0.862982	-2.358663	-2.19026
H	-0.907384	-2.250641	-2.274701
H	0.235287	0.49625	-2.236992

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C	0.543677	2.824118	-0.053383
C	0.851115	3.550326	-1.240263
C	0.771596	2.940407	-2.6112
H	1.704094	3.081758	-3.168499
H	-0.017708	3.425963	-3.196917
H	0.553355	1.869641	-2.590982
C	1.183331	4.899188	-1.156526
H	1.425379	5.438225	-2.071833
C	1.193711	5.585836	0.059039
C	1.523109	7.04247	0.115077
H	0.640545	7.649639	-0.115614
H	2.290269	7.311869	-0.615275
H	1.869684	7.343556	1.106224
C	0.840497	4.882057	1.211979
H	0.814059	5.408359	2.165321
C	0.514457	3.530173	1.183052
C	0.113362	2.886544	2.478969
H	-0.646682	3.491832	2.98482
H	0.961082	2.808276	3.168956
H	-0.30134	1.883602	2.358093

C	-3.452871	-1.609089	-1.345926
H	-2.795761	-1.743078	-2.219185
C	-3.63126	-2.994004	-0.702664
H	-2.70143	-3.345293	-0.238552
H	-4.36347	-2.917324	0.113747
C	-4.1407	-4.004974	-1.724243
H	-3.390988	-4.123639	-2.521442
H	-4.249069	-4.988225	-1.255013
C	-5.460468	-3.545822	-2.329592
H	-6.230607	-3.536909	-1.545191
H	-5.804634	-4.255526	-3.088471
C	-5.333511	-2.14997	-2.924057
H	-6.296349	-1.80683	-3.316364
H	-4.647034	-2.181575	-3.783112
C	-4.802606	-1.138544	-1.909734
H	-4.717099	-0.157838	-2.387938
H	-5.529087	-1.022204	-1.093505
C	-3.254399	1.239217	-0.631054
H	-4.342764	1.078732	-0.6739
C	-2.765186	1.711454	-2.005384
H	-1.669445	1.797112	-1.962279
H	-2.976545	0.957183	-2.77567
C	-3.357294	3.060616	-2.392648
H	-2.980674	3.365925	-3.375232
H	-4.447738	2.96555	-2.498471
C	-3.036836	4.110993	-1.336742
H	-1.947415	4.263213	-1.292024
H	-3.473536	5.077485	-1.608267
C	-3.536342	3.669825	0.031967
H	-4.634591	3.621492	0.0191
H	-3.270203	4.408255	0.79722
C	-2.983739	2.304441	0.434938
H	-1.902041	2.389681	0.598257
H	-3.416582	2.006192	1.395526
C	-3.047625	-0.875068	1.469053
H	-2.893981	-1.965036	1.485349
C	-2.181459	-0.321401	2.604871
H	-1.132851	-0.584729	2.422979
H	-2.232332	0.775818	2.624331
C	-2.629573	-0.873548	3.954873
H	-2.439183	-1.957216	3.975425
H	-2.017167	-0.439785	4.75348
C	-4.108796	-0.615548	4.210774
H	-4.411973	-1.041162	5.172563

H	-4.279887	0.468336	4.285622	H	2.337094	-2.402041	-2.565376
C	-4.961957	-1.179448	3.083135	H	4.037969	-2.10378	-2.25911
H	-6.023041	-0.972164	3.256535	C	3.553033	-4.190465	-2.459958
H	-4.861262	-2.274566	3.060627	H	2.697095	-4.851588	-2.258137
C	-4.537228	-0.613535	1.731287	H	3.70971	-4.211331	-3.543575
H	-4.733491	0.467701	1.714963	C	4.782603	-4.70874	-1.7264
H	-5.152644	-1.044324	0.933204	H	5.656513	-4.112855	-2.025615
C	2.467423	-1.213788	1.915268	H	5.000269	-5.740456	-2.019969
H	3.554577	-1.290865	2.082883	C	4.60054	-4.609666	-0.218203
C	1.798545	-2.480687	2.471737	H	3.803519	-5.297495	0.100521
H	0.708672	-2.372693	2.352342	H	5.507867	-4.931836	0.303146
H	2.07836	-3.378274	1.910205	C	4.231039	-3.194064	0.222239
C	2.146735	-2.667391	3.945954	H	4.117466	-3.171335	1.310069
H	1.663531	-3.571382	4.331658	H	5.060766	-2.512045	-0.015641
H	3.229966	-2.837099	4.035225	P	-2.494181	-0.4152	-0.251043
C	1.753731	-1.453075	4.777303	P	2.284009	-1.064728	0.063407
H	0.656923	-1.36516	4.783278	B	0.258432	1.334703	-0.139243
H	2.058263	-1.585916	5.820442	Ru	-0.054925	-0.549569	-0.480269
C	2.344175	-0.172716	4.199695	H	-0.308552	-2.132244	0.118271
H	3.439836	-0.190893	4.291804	H	-0.006042	0.470632	0.899811
H	2.002314	0.69929	4.768919	C	-0.170274	-1.48079	-2.659188
C	1.958862	-0.021714	2.732147	H	-1.088195	-1.425905	-3.248493
H	2.30729	0.934112	2.329272	H	0.688564	-1.649282	-3.31147
H	0.863361	-0.001971	2.667407	C	-0.257979	-2.473353	-1.529595
C	3.657401	0.072498	-0.504104	H	0.58398	-3.158341	-1.483581
H	4.542253	-0.57715	-0.601048	H	-1.191986	-3.026747	-1.518462
C	3.327737	0.647554	-1.884751	H	-0.010219	-0.366881	-2.366958
H	3.029432	-0.142708	-2.584703				
H	2.448782	1.29194	-1.766994	<i>sp_hy - PC</i>			
C	4.48066	1.468803	-2.448458	C	0.964517	2.794345	-0.136464
H	5.349075	0.814228	-2.612858	C	0.978706	3.399344	-1.42239
H	4.209439	1.868251	-3.432425	C	0.62827	2.622353	-2.659394
C	4.860494	2.591487	-1.492205	H	-0.039132	3.194737	-3.311631
H	4.01661	3.293714	-1.407397	H	0.132306	1.671431	-2.426056
H	5.705281	3.166534	-1.884859	H	1.520017	2.382316	-3.250462
C	5.186065	2.036605	-0.111786	C	1.305899	4.744201	-1.538924
H	5.432781	2.845469	0.583968	H	1.305429	5.206022	-2.52564
H	6.082012	1.40272	-0.176689	C	1.63365	5.521909	-0.422397
C	4.031352	1.210348	0.449361	C	1.975518	6.969069	-0.580208
H	3.159262	1.867983	0.591382	H	1.11379	7.541732	-0.938661
H	4.299652	0.818776	1.437616	H	2.77207	7.113215	-1.316301
C	2.957547	-2.720958	-0.497209	H	2.30149	7.415218	0.361422
H	2.159119	-3.439815	-0.256581	C	1.613862	4.917341	0.834327
C	3.203416	-2.776119	-2.009825	H	1.854133	5.514606	1.71268

C	1.279226	3.574176	1.002347	C	-3.900359	-2.623344	2.588602
C	1.230766	3.012253	2.392713	H	-3.696127	-3.494149	1.945951
H	0.512265	3.562403	3.011528	H	-3.582631	-2.904061	3.598739
H	2.202749	3.10373	2.890625	C	-5.392784	-2.314632	2.558112
H	0.942941	1.956768	2.413154	H	-5.971019	-3.185141	2.883261
C	-2.453839	-0.125169	-1.937577	H	-5.609079	-1.515251	3.28084
H	-2.103367	0.809425	-2.401867	C	-5.838688	-1.867716	1.171157
C	-1.377616	-1.190469	-2.219299	H	-6.899949	-1.599137	1.174734
H	-0.372524	-0.840815	-1.878788	H	-5.735089	-2.70369	0.463711
H	-1.61319	-2.115032	-1.665245	C	-5.005971	-0.690782	0.670302
C	-1.24326	-1.504246	-3.70639	H	-5.158663	0.16953	1.338911
H	-0.852123	-0.612267	-4.217642	H	-5.343413	-0.374652	-0.323102
H	-0.503166	-2.298176	-3.858279	C	1.50329	-3.231387	0.575208
C	-2.590656	-1.887256	-4.306983	H	2.266793	-3.705727	1.213057
H	-2.932967	-2.8308	-3.85816	C	1.357703	-4.059107	-0.705138
H	-2.482699	-2.079585	-5.378917	H	0.659297	-3.543384	-1.386145
C	-3.633174	-0.802953	-4.059922	H	2.313019	-4.127619	-1.237343
H	-4.597792	-1.093489	-4.487816	C	0.828922	-5.46141	-0.415796
H	-3.33118	0.117958	-4.578742	H	0.72031	-6.014767	-1.354322
C	-3.791042	-0.51034	-2.570083	H	1.575582	-6.008073	0.176834
H	-4.528718	0.285661	-2.4096	C	-0.488648	-5.4278	0.347125
H	-4.186894	-1.406558	-2.068401	H	-1.265327	-4.965279	-0.282944
C	-3.100712	1.88412	0.224183	H	-0.834372	-6.443705	0.562019
H	-4.197285	1.79791	0.190883	C	-0.349726	-4.622189	1.631174
C	-2.664583	2.90487	-0.832625	H	0.359298	-5.120264	2.307635
H	-1.571067	2.870874	-0.930037	H	-1.301776	-4.566599	2.170578
H	-3.076091	2.635616	-1.813042	C	0.163415	-3.220559	1.330899
C	-3.081793	4.327161	-0.471833	H	0.227576	-2.612912	2.240979
H	-2.692957	5.019186	-1.227283	H	-0.59101	-2.723948	0.681248
H	-4.177337	4.406619	-0.514556	C	3.203422	-1.09571	1.651391
C	-2.602733	4.720957	0.918627	H	4.032559	-1.81128	1.526649
H	-1.501497	4.724413	0.93588	C	3.75904	0.32685	1.536409
H	-2.92073	5.74101	1.157151	H	4.272459	0.458712	0.576517
C	-3.121917	3.738631	1.960365	H	2.91432	1.03298	1.530303
H	-4.219914	3.784294	1.99112	C	4.705955	0.667449	2.682083
H	-2.775641	4.011326	2.963326	H	5.60714	0.04297	2.60145
C	-2.676535	2.318652	1.634491	H	5.043927	1.705201	2.58443
H	-1.578436	2.260583	1.699537	C	4.055024	0.433648	4.038706
H	-3.060362	1.610139	2.380123	H	3.210348	1.127148	4.163973
C	-3.515488	-1.047828	0.668625	H	4.759869	0.658814	4.845434
H	-3.376958	-1.938079	0.0271	C	3.547242	-0.996787	4.154718
C	-3.077714	-1.442149	2.086075	H	3.062601	-1.160642	5.122732
H	-2.004327	-1.667794	2.114682	H	4.399727	-1.689929	4.116373
H	-3.217102	-0.582749	2.758631	C	2.575132	-1.332886	3.028719

H	1.673531	-0.706593	3.119577	H	5.61204	-1.055496	-4.19552
H	2.241944	-2.374182	3.122399	C	5.048307	-2.272771	-2.496039
C	2.996641	-1.471245	-1.283912	H	4.461336	-2.972148	-3.109594
H	2.393806	-2.112892	-1.946305	H	6.038845	-2.723719	-2.377755
C	3.091271	-0.117689	-1.995739	C	4.376067	-2.118691	-1.136011
H	2.084584	0.303473	-2.117786	H	4.297829	-3.089574	-0.628777
H	3.649604	0.602286	-1.380628	H	5.005055	-1.485461	-0.493091
C	3.779801	-0.273726	-3.349043	P	-2.386913	0.209114	-0.107834
H	3.144524	-0.891512	-4.001524	P	2.002626	-1.447861	0.285567
H	3.868448	0.701553	-3.840415	B	0.515229	1.349661	-0.004485
C	5.148472	-0.931399	-3.211811	Ru	-0.098805	-0.357098	0.196944
H	5.812543	-0.267255	-2.640217	H	0.014067	-0.002752	1.73705
