Supporting Information

Understanding the Reactivity of Carbene-Analogous Phosphane Complexes with Group 13 Elements as a Central Atom: A Theoretical Investigation

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IRC path animations

The six IRC path animations created in this work are included in this Supporting Information. The animation files are viewable by VLC.

1. The reaction of **0B** with methane:
   See file `carb-B-cat-CH4-IRC.mp4`

2. The reaction of **0Tl** with methane:
   See file `carb-Tl-cat-CH4-IRC.mp4`

3. The reaction of **0B** with ethene:
   See file `carb-B-cat-C2H4-IRC.mp4`

4. The reaction of **0Al** with ethene:
   See file `carb-Al-cat-C2H4-IRC.mp4`

5. The reaction of **0In** with ethene:
   See file `carb-In-cat-C2H4-IRC.mp4`

6. The reaction of **0Tl** with ethene:
   See file `carb-Tl-cat-C2H4-IRC.mp4`

Table S1: The activation energies and reaction enthalpies of the transition states and products of the reactions with methane and ethene are shown in parts (a) and (b), respectively. ΔE and ΔG are the total and free energies at 298.15 K, respectively.

(a) Reaction with CH_4 : $0M + CH_4 \rightarrow TS1M \rightarrow 1M$									
	Transition State **TS1M**					Product **1M**			
Energy	TS1B	TS1Al	TS1Ga	TS1In	TS1Tl	1B	1Al	1Ga	1In	1Tl
ΔE	28.37	44.62	58.75	72.26	90.11	−47.45	−20.25	1.68	20.74	44.54
ΔG	44.32	56.35	71.27	83.09	99.19	−29.71	−6.12	13.00	29.77	53.56

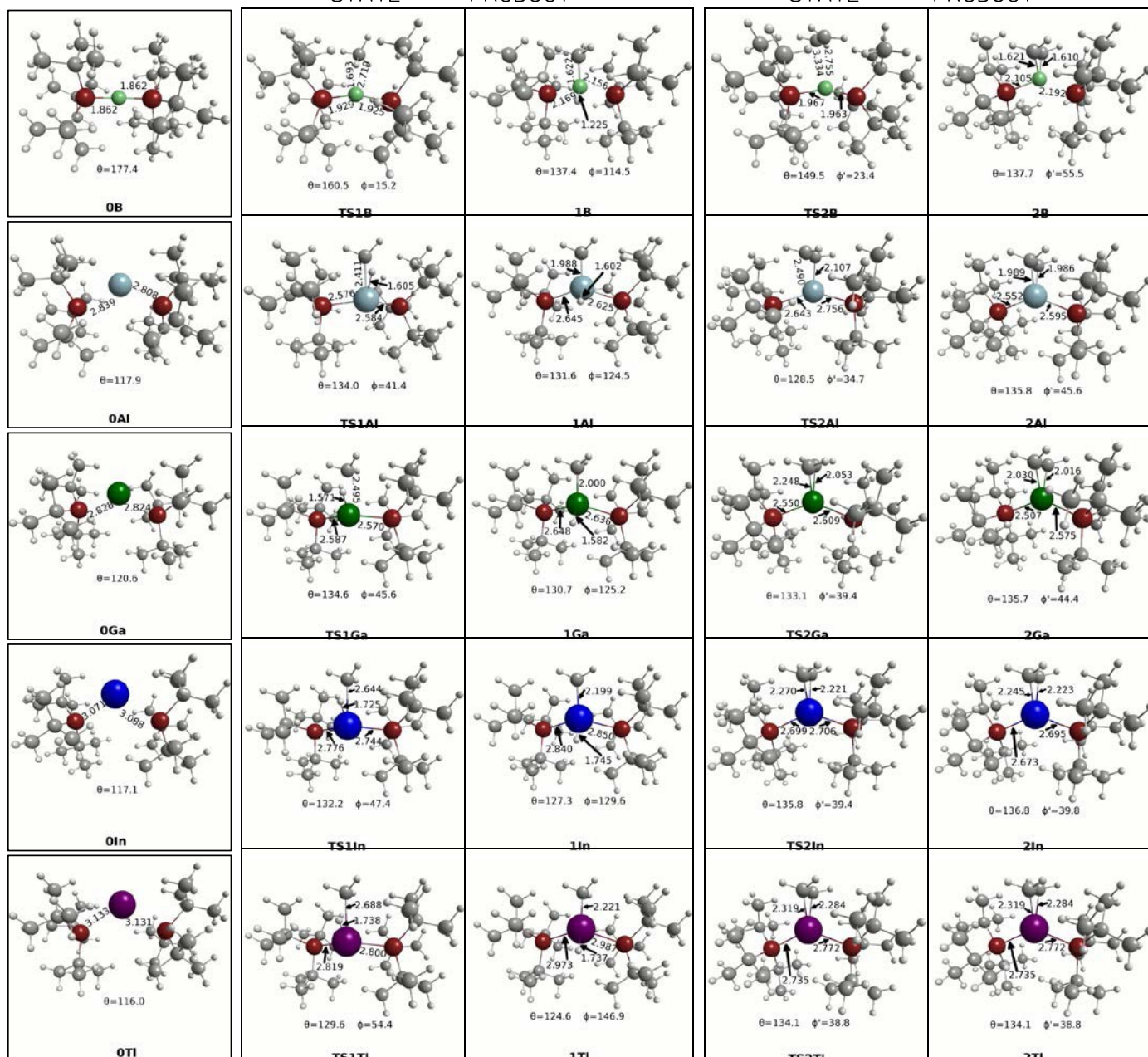| (b) Reaction with C_2H_4 : $0M + C_2H_4 \rightarrow TS2M \rightarrow 2M$									
	Transition State **TS2M**					Product **2M**			
Energy	TS2B	TS2Al	TS2Ga	TS2In	TS2Tl	2B	2Al	2Ga	2In	2Tl
ΔE	33.81	3.01	19.23	37.52	65.57	−39.01	−8.74	16.72	37.06	65.57
ΔG	50.62	19.15	36.39	52.74	81.05	−19.26	8.87	34.65	52.69	81.05

Figure S1: The geometric structures of the reactants, transition states, and products of the reactions with methane and ethene are plotted. The structures of the reactants **0M** are shown in the first column, where **M** = **B**, **Al**, **Ga**, **In**, and **Tl**. The structures of the transition states **TS1M** and products **1M** of the methane reactions are depicted in the second and third columns, respectively. The structures of the transition states **TS2M** and products **2M** of the ethene reactions are illustrated in the fourth and fifth columns, respectively. Some bond lengths and bond angles of importance are labeled, including the lengths of the M−P$_1$ and M−P$_2$ bonds and the bond angles θ in between, the lengths of the M−C and M−H bonds and the bond angles φ in between for **TS1M** and **1M**, and the lengths of the M−C$_1$ and M−C$_2$ bonds and the bind angles φ' in between for **TS2M** and **2M**.

(a) NRT of reactant 0B
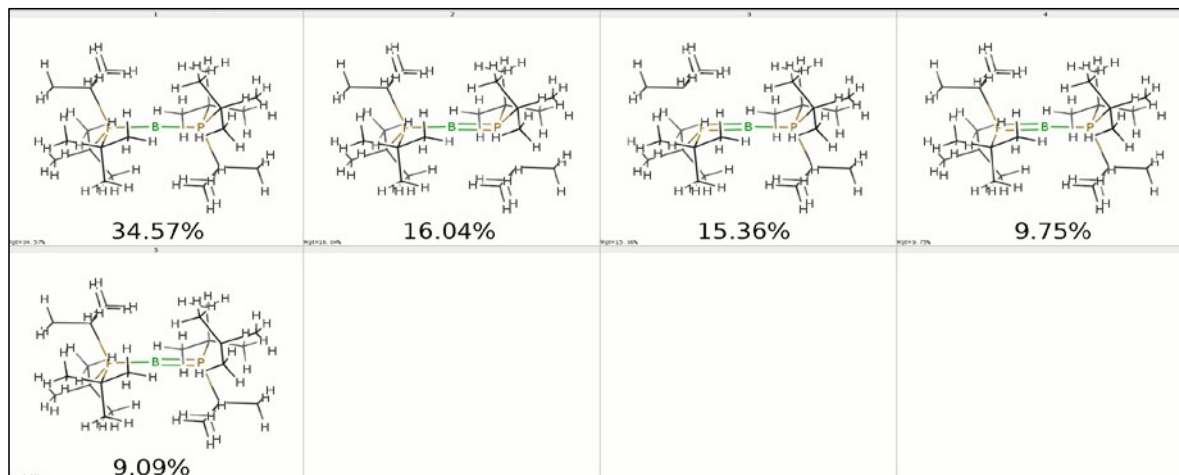
34.57%   16.04%   15.36%   9.75%

9.09%

(b) NRT of reactant 0Al

17.12%   1.58%   1.48%   1.18%

1.01%

(c) NRT of reactant 0Ga

18.84%   1.36%   1.20%   1.12%

(d) NRT of reactant 0In

22.28%

(e) NRT of reactant 0Tl

22.55%
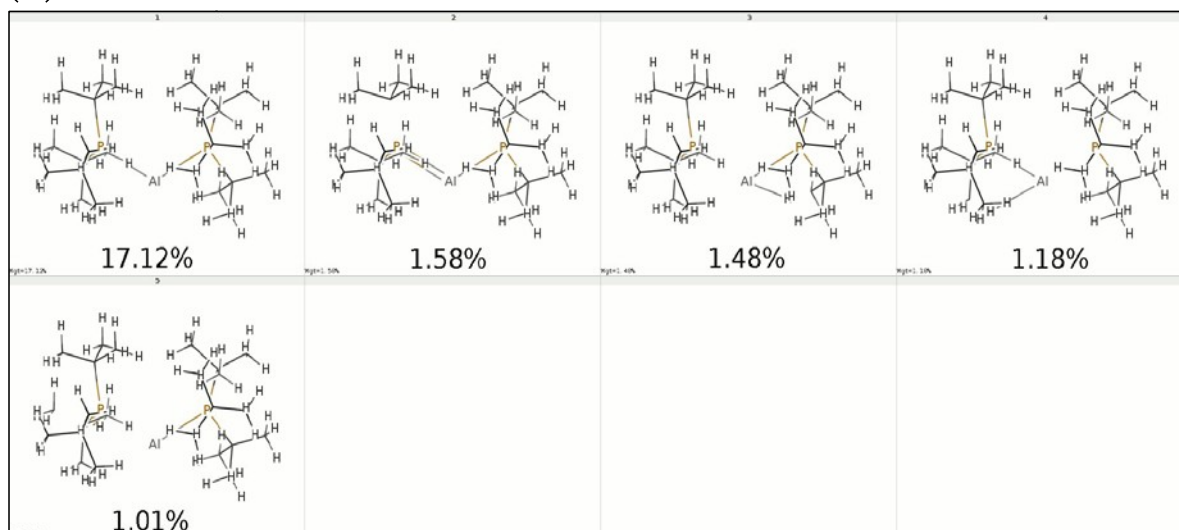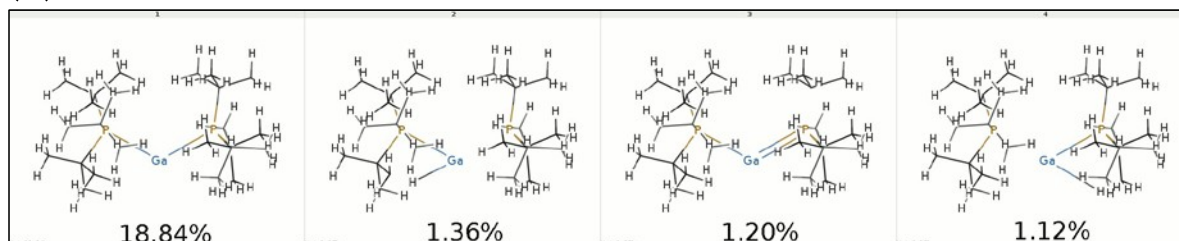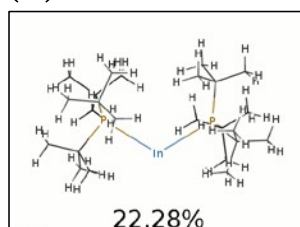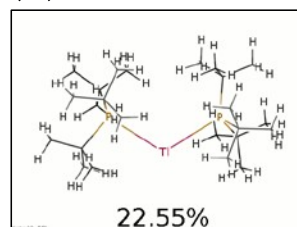
Figure S2: The NRT contributions of the resonance structures of reactants (a) **0B**, (b) **0Al**, (c) **0Ga**, (d) **0In**, and (e) **0Tl** are depicted. In all subplots, only the structures with resonance contributions over 1% are shown. The most probable resonance structures of each reactants are employed for the subsequent computations.
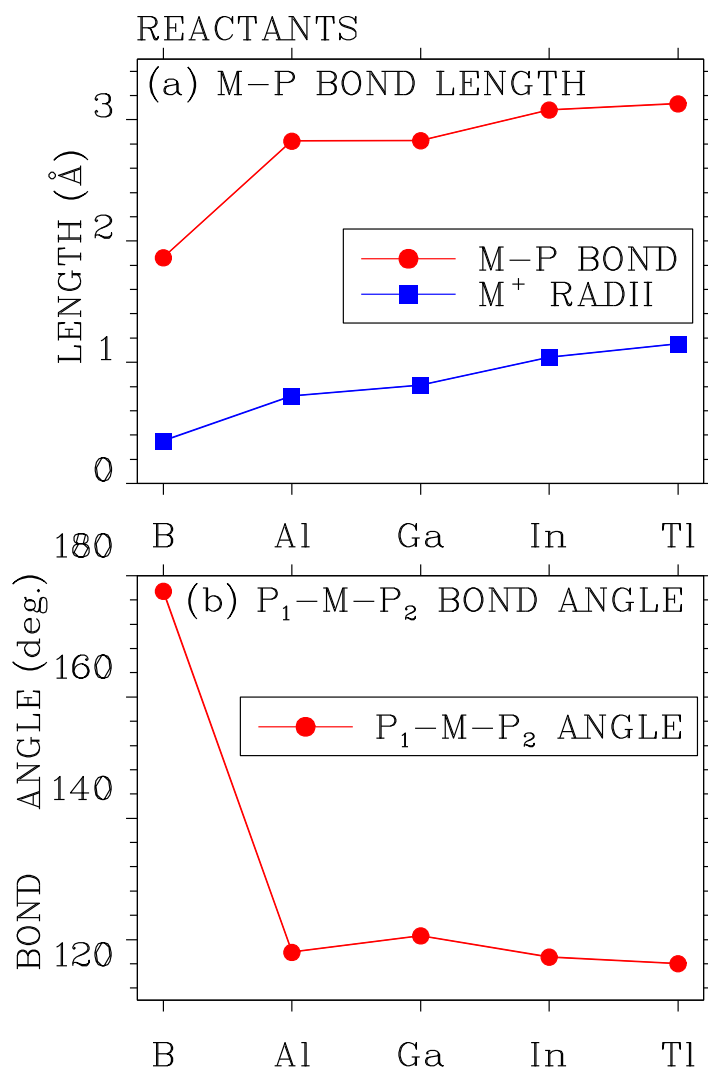
Figure S3: The M−P bond lengths and the bond angles between M−P$_1$ and M−P$_2$ bonds are shown in subplots (a) and (b), respectively. The M−P bond lengths depicted in subplot (a) are the length average of bonds M−P$_1$ and M−P$_2$. The radii of the M$^+$ ions are also plotted for comparison. It can be seen that the difference between the B−P and Al−P bond lengths is much larger than the difference between the radii of the B$^+$ and Al$^+$ ions.

(a) CH₄ REACTION

(b) C₂H₄ REACTION
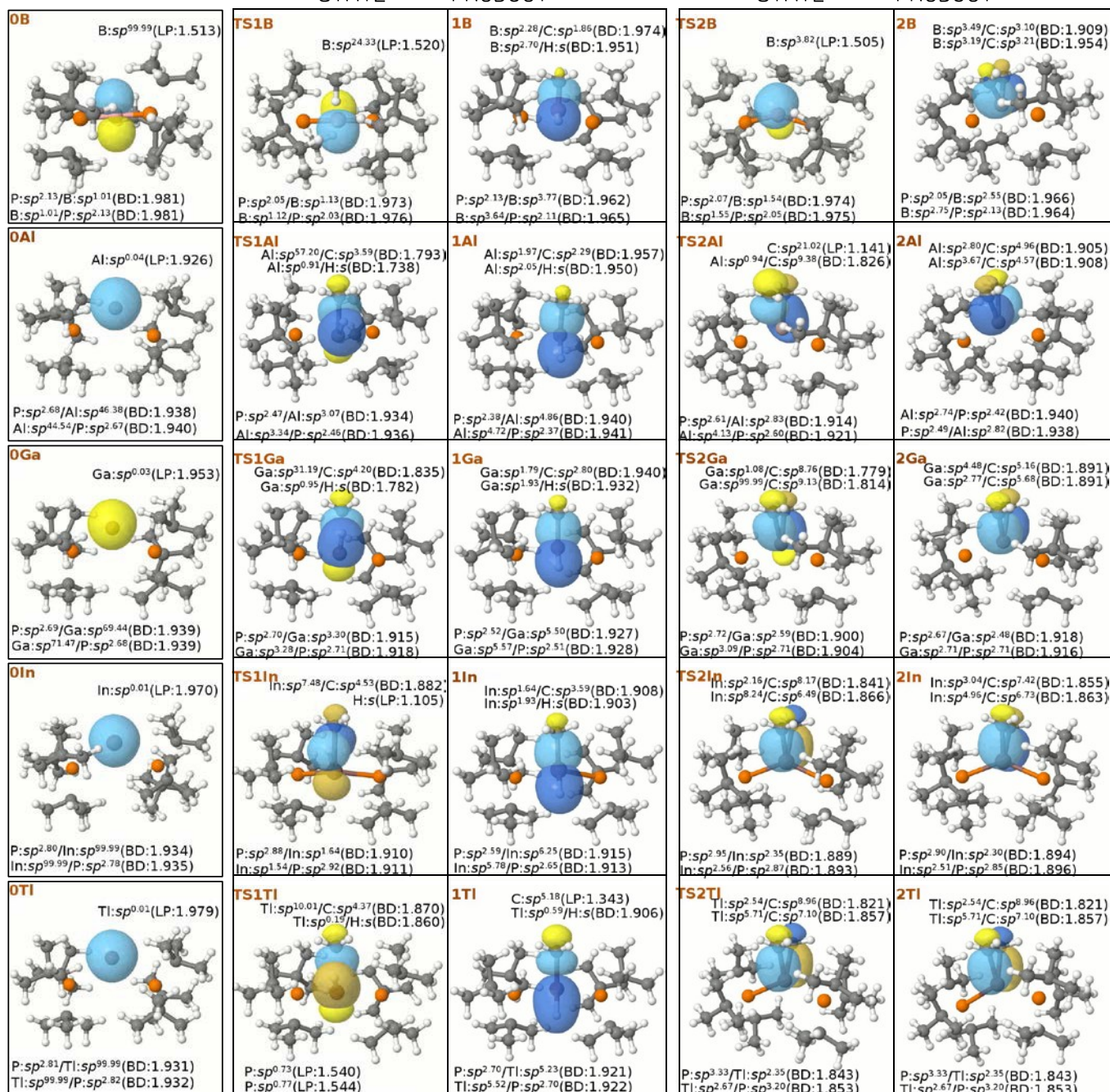
Figure S4: The NBO of the lone pairs of the electrons of atoms M in the reactants **0M** are depicted in the first column of subplots. The NBO of the forming or established bonds between the two molecular fragments of the reactions are shown, including (1) the NBO of the M−C and M−H bonds for transition states **TS1M** and products **1M** of the reactions with methane in the second and third columns, and (2) the NBO of the M−C₁ and M−C₂ bonds for transition states **TS2M** and products **2M** of the reactions with ethene in the fourth and fifth columns, respectively. In each subplot, the orbital contributions of atoms to the NBO of lone pairs and bonds are annotated by LP and BD, respectively. The numbers following LP and BD are the occupation numbers of the NBO. For instance, in subplot **0B**, "B:$sp^{99.99}$(LP:1.513)" means the B atom contributes $sp^{99.99}$ orbitals to the LP and the LP has the occupation number of 1.513; "P:$sp^{2.13}$/B:$sp^{1.01}$(BD:1.938)" stands for a P−B bond with the occupation number of 1.938, and the P and B atoms contribute $sp^{2.13}$ and $sp^{1.01}$ orbitals to the NBO, respectively.

Structure data

The Cartesian coordinates of the atomic positions of the structures of the reactants (**0B**, **0Al**, **0Ga**, **0In**, and **0Tl**), the transition states (**TS1B**, **TS1Al**, **TS1Ga**, **TS1In**, and **TS1Tl**) and products (**1B**, **1Al**, **1Ga**, **1In**, and **1Tl**) of the reactions with methane, and the transition states (**TS2B**, **TS2Al**, **TS2Ga**, **TS2In**, and **TS2Tl**) and products (**2B**, **2Al**, **2Ga**, **2In**, and **2Tl**) of the reactions with ethene are listed in the following subsections. The first and second columns of the list are the atomic symbols and atomic numbers, respectively. The last three columns are the (x, y, z) coordinates of the atomic positions in the unit of Å. All structure data are obtained from the output files of the quantum chemistry simulation package GAMESS-US.

Reactants

Reactant **0B**:

ATOM	CHARGE	X	Y	Z
P	15.0	1.8614238580	0.0122284832	0.0185438442
B	5.0	0.0001424401	0.0454629858	0.0105598564
P	15.0	-1.8615054568	-0.0024068318	-0.0170750164
C	6.0	2.2137276439	1.0240914985	-1.6126549333
C	6.0	3.6019199507	0.7507229860	-2.2253038745
H	1.0	4.4304190943	1.0466036743	-1.5528284219
H	1.0	3.6997401354	1.3635988734	-3.1483164186
H	1.0	3.7499319381	-0.3030450700	-2.5252447287
C	6.0	1.0958796306	0.6102299679	-2.5979684006
H	1.0	0.0932092209	0.7742747204	-2.1336886364
H	1.0	1.1680389054	-0.4404714698	-2.9315585952
H	1.0	1.1326979184	1.2622512875	-3.4982832679
C	6.0	2.0784063772	2.5434000585	-1.3664285533
H	1.0	2.8812051729	2.9541923630	-0.7259445205
H	1.0	1.1000679592	2.8139901496	-0.9244785870
H	1.0	2.1594237319	3.0567921917	-2.3490580348
C	6.0	2.6447151789	-1.8055528647	-0.1340225593
C	6.0	4.1791906455	-1.8707727061	0.0140302823
H	1.0	4.5302834974	-1.5801196233	1.0230850892
H	1.0	4.7168165635	-1.2569922569	-0.7342749247
H	1.0	4.5039861627	-2.9232924000	-0.1407886789
C	6.0	2.2329853283	-2.4038100818	-1.4965323860
H	1.0	1.1351945065	-2.3584684998	-1.6444702120
H	1.0	2.5198363826	-3.4775281362	-1.5073172726
H	1.0	2.7347521808	-1.9306027965	-2.3622061174
C	6.0	1.9716410134	-2.6825802911	0.9449213675
H	1.0	2.2758791018	-2.4396653049	1.9786920979
H	1.0	2.2458055123	-3.7441819594	0.7633796202
H	1.0	0.8661564299	-2.6130047509	0.8730157881
C	6.0	-2.6597941026	1.8092793596	0.0094846387
C	6.0	-2.6825949053	-1.0040182836	-1.5151822487
C	6.0	-2.2475862111	2.5006536782	1.3269369104
H	1.0	-2.7504669470	2.0890995333	2.2233122008
H	1.0	-2.5314777496	3.5733096526	1.2644234800
H	1.0	-1.1490247201	2.4574755340	1.4754668116
C	6.0	-2.0012826600	2.6191681351	-1.1291033883
H	1.0	-2.2846392335	2.2795835466	-2.1412525166
H	1.0	-0.8959330170	2.5965503795	-1.0380236602
H	1.0	-2.3165995927	3.6809307034	-1.0373098291
C	6.0	-4.1944918734	1.8416352747	-0.1442174969
H	1.0	-4.5347586788	1.4667167284	-1.1289755560
H	1.0	-4.5373899762	2.8972538220	-0.0728398038
H	1.0	-4.7247695645	1.2772344519	0.6465949184
C	6.0	-2.7568185479	-0.1490333709	-2.8010972020
H	1.0	-3.1158800074	-0.8049790166	-3.6234800695
H	1.0	-1.7698289079	0.2455301317	-3.1151152913
H	1.0	-3.4697173306	0.6941349375	-2.7293940985
C	6.0	-4.1109323419	-1.4757578284	-1.1610537916
H	1.0	-4.5272569393	-2.0070105870	-2.0447884750
H	1.0	-4.8007108787	-0.6424902488	-0.9310655395
H	1.0	-4.1365052525	-2.1944323972	-0.3198257450
C	6.0	-1.7874261095	-2.2196461479	-1.8269670921
H	1.0	-2.2472607191	-2.7946104580	-2.6599493167
H	1.0	-1.6622737528	-2.9117212261	-0.9747071218
H	1.0	-0.7784774886	-1.9003444197	-2.1518964864
C	6.0	2.6941595801	0.8955548508	1.5782573454
C	6.0	1.8215353120	2.0996694601	1.9876355866
H	1.0	2.3098412741	2.6104815056	2.8457097360
H	1.0	0.8136644373	1.7772290989	2.3113724832
H	1.0	1.6949703015	2.8445466139	1.1819730205
C	6.0	2.7793188016	-0.0580471003	2.7922841255
H	1.0	3.1624911895	0.5248037778	3.6575060352
H	1.0	3.4823185894	-0.8972778019	2.6349103244
H	1.0	1.7951791748	-0.4688443492	3.0929606316

Reactant **0Al**:

ATOM	CHARGE	X	Y	Z
		4.1260443221	1.3733060687	1.2406602973
C	6.0	4.5656069625	1.8182210778	2.1599527416
H	1.0	4.1516971519	2.1608186392	0.4637677443
H	1.0	4.7958970734	0.5508744675	0.9278061160
H	1.0	-2.2131859985	-0.9119130088	1.6767794561
C	6.0	-2.0692540420	-2.4447243579	1.5360450387
C	6.0	-2.8688203872	-2.9068676896	0.9274384969
H	1.0	-2.1456819495	-2.8833209570	2.5540575825
H	1.0	-1.0879520136	-2.7393964576	1.1172870467
H	1.0	-3.6088211051	-0.6069986867	2.2581414456
C	6.0	-3.7136210902	-1.1735668127	3.2093399850
H	1.0	-4.4298045997	-0.9375457333	1.5929553028
H	1.0	-3.7597259114	0.4606313249	2.5029263915
H	1.0	-1.1092107915	-0.4351097879	2.6480725911
C	6.0	-1.1736992199	0.6391835756	2.8969959931
H	1.0	-0.1009406891	-0.6450635685	2.2190013848
H	1.0	-1.1753819090	-1.0124499523	3.5965119131

Reactant **0Al**:

ATOM	CHARGE	X	Y	Z
P	15.0	-2.4086983307		-0.0238054782
AL	13.0	0.0183267801	-1.4599990110	-0.3948273579
P	15.0	2.4284993006	-0.0645174511	-0.0355261722
C	6.0	-3.1721539377	-0.6432378628	-1.7162235974
C	6.0	-4.5493623702	-0.0473420656	-2.0781652934
H	1.0	-5.3245253152	-0.2872093413	-1.3247005178
H	1.0	-4.8829323683	-0.4866590020	-3.0438410121
H	1.0	-4.5272873688	1.0510084005	-2.2160295026
C	6.0	-2.1362924081	-0.2805125770	-2.8104897731
H	1.0	-1.1297330499	-0.7078466684	-2.5741744163
H	1.0	-2.0172725238	0.8055758530	-2.9731907907
H	1.0	-2.4452614548	-0.7342201846	-3.7768725053
C	6.0	-3.2907310251	-2.1878717125	-1.7221330324
H	1.0	-4.0704100629	-2.5703161412	-1.0360059867
H	1.0	-2.3280885630	-2.6862198939	-1.4777209293
H	1.0	-3.5731478247	-2.5102100380	-2.7476034380
C	6.0	-2.7071018437	1.8884584864	0.1610465046
C	6.0	-4.1519998297	2.2794742375	0.5420333278
H	1.0	-4.4463597524	1.9092922938	1.5430525437
H	1.0	-4.8997689102	1.9276087495	-0.1941045679
H	1.0	-4.2214030103	3.3891521880	0.5774490647
C	6.0	-2.3317630325	2.5953723538	-1.1621325232
H	1.0	-1.3116515998	2.3301928500	-1.5071146543
H	1.0	-2.3415822418	3.6928651915	-0.9868347600
H	1.0	-3.0481793809	2.3937931200	-1.9808920912
C	6.0	-1.7267350297	2.4108715730	1.2393441791
H	1.0	-1.9594337823	2.0517333294	2.2577035181
H	1.0	-1.7811525054	3.5210359824	1.2641558784
H	1.0	-0.6794503179	2.1357810817	1.0027137371
C	6.0	3.5662811551	-1.4838051381	-0.7545479732
C	6.0	2.8964563281	1.6233606853	-0.8953221197
C	6.0	3.4522644638	-2.7491278116	0.1317309080
H	1.0	3.9148313957	-2.6298621245	1.1299780008
H	1.0	3.9904331238	-3.5771939781	-0.3781826315
H	1.0	2.4010061479	-3.0862832634	0.2632136549
C	6.0	2.9902979352	-1.8697577942	-2.1413089889
H	1.0	3.3011101703	-1.0808128314	-2.9056631323
H	1.0	1.9116260789	-2.1425859388	-2.0727590705
H	1.0	3.5217290696	-2.7713110565	-2.5161621932
C	6.0	5.0560808669	-1.1079438475	-0.9021955133
H	1.0	5.2202109796	-0.2985563055	-1.6397969612
H	1.0	5.6119119741	-1.9968105957	-1.2738498296
H	1.0	5.5231792901	-0.8073767858	0.0554531365
C	6.0	2.9921993758	1.4173383617	-2.4254631160
H	1.0	3.0933453708	2.4149497934	-2.9049791552
H	1.0	2.0817800095	0.9423494059	-2.8467641164
H	1.0	3.8748818887	0.8243783829	-2.7314243557
C	6.0	4.2113367278	2.2562475123	-0.3883603860
H	1.0	4.3844314622	3.2017743509	-0.9475468796
H	1.0	5.0927605186	1.6088606336	-0.5568682907
H	1.0	4.1744218463	2.5204383238	0.6863552194
C	6.0	1.7222772634	2.6020824985	-0.6599781486
H	1.0	9.1846464584	3.5420086364	-1.2203130904
H	1.0	1.5814204100	2.8769080894	0.4003887447
H	1.0	0.7673060471	2.1843648215	-1.0398739746
C	6.0	-3.2794124461	-0.9577688439	1.4587798100
C	6.0	-2.6539607681	-2.3710088966	1.5696722307
H	1.0	-3.1196274331	-2.9027867713	2.4284691903
H	1.0	-1.5621561101	-2.3249465191	1.7804831424
H	1.0	-2.8026144709	-3.0038680892	0.6758025557
C	6.0	-2.9556598943	-0.2387447084	2.7894549487
H	1.0	-3.3130630084	-0.8798721662	3.6240885893
H	1.0	-3.4650767676	0.7380394118	2.8958922234
H	1.0	-1.8658349471	-0.0891897008	2.9381461489
C	6.0	-4.8122436764	-1.0864260510	1.3172382819
H	1.0	-5.2147226043	-1.5839534173	2.2272018464
H	1.0	-5.1070570567	-1.7134494016	0.4536660316
H	1.0	-5.3225495727	-0.1084549994	1.2262324696
C	6.0	2.6915106425	0.0656283911	1.8894905195
C	6.0	2.1327461263	1.4055558263	2.4207820409
H	1.0	2.7348730354	2.2824479134	2.1153089108
H	1.0	2.1505096195	1.3733900903	3.5317772901
H	1.0	1.0794320200	1.5738547675	2.1171405227

C	6.0	4.1599241765	-0.0667564990	2.3520310533
H	1.0	4.1970926312	0.0438594572	3.4580708631
H	1.0	4.8091319561	0.7211093074	1.9227261795
C	6.0	4.6058720753	-1.0512272375	2.1133357850
C	6.0	1.8271581843	-1.0492306282	2.5320025010
H	1.0	2.0883458264	-2.0695159227	2.1979479826
H	1.0	0.7423963743	-0.8821362685	2.3376632571
H	1.0	1.9541415689	-0.0204109590	3.6364666955

Reactant 0Ga:

ATOM	CHARGE	X	Y	Z
P	15.0	2.4466987548	0.0616614295	0.0219105739
GA	31.0	-0.0041883155	-1.3333194328	0.2348868065
P	15.0	-2.4612949493	0.0379249369	0.0000602476
C	6.0	3.2275284901	-0.7207579082	1.6331816424
C	6.0	4.6026749606	-0.1475501361	2.0367663278
H	1.0	5.3680336200	-0.2968722796	1.2504764355
H	1.0	4.9609149156	-0.6757398288	2.9479482983
H	1.0	4.5683523877	0.9304487701	2.2868247406
C	6.0	2.2035402303	-0.4920715521	2.7745857166
H	1.0	1.2117347617	-0.9411617395	2.5278311759
H	1.0	2.0437058164	0.5714408519	3.0265442229
H	1.0	2.5571591898	-1.0056001778	3.6949883451
C	6.0	3.3659079550	-2.2540164585	1.4698947456
H	1.0	4.1366452539	-2.5448856864	0.7310807587
H	1.0	2.4087941848	-2.7463481712	1.1945526491
H	1.0	3.6770253928	-2.6802616295	2.4481869926
C	6.0	2.7311623905	1.9925931706	0.0375639438
C	6.0	4.1673135960	2.4362612364	-0.3169466117
H	1.0	4.4506178413	2.1670869228	-1.3528797573
H	1.0	4.9282368407	2.0227860294	0.3721701654
H	1.0	4.2242748285	3.5447806702	-0.2454132626
C	6.0	2.3564929042	2.5488039224	1.4312073451
H	1.0	1.3283129091	2.2612612138	1.7335789813
H	1.0	2.3830738078	3.6590484171	1.3835019197
H	1.0	3.0600718099	2.2445593784	2.2292763046
C	6.0	1.7334040180	2.6202784285	-0.9672039289
H	1.0	1.9476556603	2.3668304649	-2.0205966413
H	1.0	1.7889506528	3.7271753591	-0.8787442252
H	1.0	0.6897101738	2.3219051050	-0.7412997032
C	6.0	-3.5773958230	-1.4614656732	0.5717911836
C	6.0	-2.9725301864	1.6419525407	0.9892702485
C	6.0	-3.4255011852	-2.6404262334	-0.4189257753
H	1.0	-3.8764270805	-2.4450239211	-1.4107615733
H	1.0	-3.9515081236	-3.5219152017	0.0075784058
H	1.0	-2.3655922547	-2.9412218512	-0.5636357693
C	6.0	-3.0164228486	-1.9626743542	1.9288764570
H	1.0	-3.0589213631	-1.2097848498	2.7352476080
H	1.0	-1.9657331743	-2.3197691159	1.8386094529
H	1.0	-3.6165480169	-2.8369129306	2.2634562805
C	6.0	-5.0760984423	-1.1250180486	0.7256457733
H	1.0	-5.2650140680	-0.3632314868	1.5066436103
H	1.0	-5.6182656295	-2.0449780639	1.0376824815
H	1.0	-5.5383223009	-0.7771108206	-0.2181549999
C	6.0	-3.0910015828	1.3052468856	2.4946153001
H	1.0	-3.2248754979	2.2564326325	3.0531670734
H	1.0	-2.1735940365	0.8212266601	2.8899447837
H	1.0	-3.9615359945	0.6649563120	2.7331775494
C	6.0	-4.2879691787	2.2982205456	0.5141583870
H	1.0	-4.4949751730	3.1807619729	1.1588874367
H	1.0	-5.1598398240	1.6214937741	0.5943410955
H	1.0	-4.2302746061	2.6709162801	-0.5270263060
C	6.0	-1.8096009403	2.6555143334	0.8614816707
H	1.0	-2.0261974480	3.5313342552	1.5108045673
H	1.0	-1.6667086590	3.0383637239	-0.1647020909
H	1.0	-0.8506149004	2.2160161262	1.2058197172
C	6.0	3.2935864312	-0.7109758229	-1.5553684396
C	6.0	2.6915324234	-2.1210460494	-1.7898668226
H	1.0	3.1477285805	-2.5474401332	-2.7098946213
H	1.0	1.5941159627	-2.0836258843	-1.9701487907
H	1.0	2.8796591567	-2.8382790885	-0.9709077591
C	6.0	2.9157602518	0.1288255192	-2.7980051455
H	1.0	3.2551854076	-0.4153494738	-3.7058155998
H	1.0	3.4022677416	1.1227913285	-2.8183755596
H	1.0	1.8188332191	0.2705230158	-2.8945791839
C	6.0	4.8329347643	-0.8181834282	-1.4726758387
H	1.0	5.2146313865	-1.2293102175	-2.4333941933
H	1.0	5.1741627978	-1.5058382939	-0.6745392556
H	1.0	5.3229115133	0.1618954451	-1.3176045389
C	6.0	-2.7010603467	0.3312256248	-1.9114020175
C	6.0	-2.1441660698	1.7182329279	-2.3068850613
H	1.0	-2.7646081960	2.5582173382	-1.9401674647
H	1.0	-2.1315308243	1.7848090775	-3.4163548315
H	1.0	-1.1017969600	1.8660596028	-1.9582413812
C	6.0	-4.1599666149	0.2255588528	-2.4071666233
H	1.0	-4.1856300798	0.4571446150	-3.4947920657
H	1.0	-4.8300769482	0.9488774390	-1.9032165790
H	1.0	-4.5866015112	-0.7883743417	-2.2840549126
C	6.0	-1.8168897463	-0.7133884903	-2.6413816818
H	1.0	-2.0791401553	-1.7624262481	-2.4145591046
H	1.0	-0.7364213820	-0.5615471076	-2.4149048078
H	1.0	-1.9271838341	-0.5775789400	-3.7397822569

Reactant 0In:

ATOM	CHARGE	X	Y	Z
P	15.0	2.6285135588	0.0995332154	0.0018768651
IN	49.0	-0.0019764293	-1.4779368720	-0.1424885944
P	15.0	-2.6268841457	0.1402092124	0.0304455712
C	6.0	3.1144608115	-0.2412764335	1.8607900671
C	6.0	4.3695811638	0.5056237887	2.3620480267
H	1.0	5.2739701501	0.2534417461	1.7758224329
H	1.0	4.5693105971	0.2140998673	3.4168553611
H	1.0	4.2452493951	1.6059455456	2.3515773577
C	6.0	1.8936845106	0.1573613372	2.7292161860
H	1.0	0.9687776928	-0.3840838144	2.4239930918
H	1.0	1.6717880618	1.2395916050	2.7122947964
H	1.0	2.0915052538	-0.1248248869	3.7864033953
C	6.0	3.3201097525	-1.7607874087	2.0706435505
H	1.0	4.2251789407	-2.1529139290	1.5687387514
H	1.0	2.4465841989	-2.3599016114	1.7336785307
H	1.0	3.4424910979	-1.9529013994	3.1586925482
C	6.0	2.7949191583	2.0035146395	-0.3854091803
C	6.0	4.2432525818	2.4995905404	-0.5885970751
H	1.0	4.7334221709	2.0441528430	-1.4705149744
H	1.0	4.8834220503	2.3191862645	0.2966629714
H	1.0	4.2255035265	3.5982846410	-0.7621913411
C	6.0	2.1459560353	2.8226324688	0.7532489350
H	1.0	1.1016403610	2.5097477558	0.9566694700
H	1.0	2.1123369604	3.8888558258	0.4402754820
H	1.0	2.7214086923	2.7841003379	1.6980421710
C	6.0	1.9583789951	2.2848989798	-1.6590988678
H	1.0	2.3464086310	1.7891359356	-2.5665150085
H	1.0	1.9628141569	3.3790727358	-1.8569163041
H	1.0	0.9006518092	1.9777607080	-1.5225375051
C	6.0	-3.8473860169	-1.3829219443	0.1470588236
C	6.0	-3.0196268824	1.3880913885	1.4758819888
C	6.0	-3.7609938858	-2.2139443503	-1.1558479798
H	1.0	-4.1863353225	-1.6984216570	-2.0379328212
H	1.0	-4.3450331157	-3.1491872304	-1.0159844551
H	1.0	-2.7195820320	-2.5204359046	-1.3941211083
C	6.0	-3.3302758302	-2.3069667794	1.2801472442
H	1.0	-3.4090657681	-1.8652258051	2.2892066225
H	1.0	-2.2710891349	-2.6057275237	1.1157964252
H	1.0	-3.9298682237	-3.2430889439	1.2821993809
C	6.0	-5.3242133720	-1.0231890267	0.4187892300
H	1.0	-5.4672223829	-0.5400258788	1.4049467346
H	1.0	-5.9266564151	-1.9583444705	0.4264799396
H	1.0	-5.7560108115	-0.3624108182	-0.3569890740
C	6.0	-3.1660065237	0.6134364444	2.8063882121
H	1.0	-3.2146116369	1.3522605380	3.6356625022
H	1.0	-2.2981494064	-0.0475880181	3.0115374844
H	1.0	-4.0929668676	0.0111980041	2.8584941120
C	6.0	-4.2824306322	2.2514760670	1.2587585723
H	1.0	-4.4267418246	2.9077263477	2.1453072167
H	1.0	-5.2011922062	1.6443355068	1.1469162408
H	1.0	-4.1975530155	2.9177969530	0.3787240953
C	6.0	-1.7809484018	2.3036141281	1.6378002520
H	1.0	-1.9361584059	2.9656926869	2.5174521728
H	1.0	-1.5995663975	2.9583880625	0.7662736091
P	15.0	-0.8629012361	1.7090993452	1.8272172179
C	6.0	3.8252343542	-0.8977003678	-1.1792017785
C	6.0	3.3519836498	-2.3735365152	-1.2113555969
H	1.0	4.0091811932	-2.9423648010	-1.9049097302
H	1.0	2.3179584908	-2.4637163614	-1.6094086464
H	1.0	3.3954020312	-2.8840146329	-0.2321077170
C	6.0	3.6832908621	-0.3725984523	-2.6275421996
H	1.0	4.2467035782	-1.0543226668	-3.3009876830
H	1.0	4.1058402287	0.6399440429	-2.7686924734
H	1.0	2.6298104405	-0.3709432898	-2.9784689951
C	6.0	5.3154233466	-0.8449729791	-0.7726590757
H	1.0	5.9141978666	-1.4090038567	-1.5215323534
H	1.0	5.5070550648	-1.3173363614	0.2103061063
H	1.0	5.7129987605	0.1875026443	-0.7452776501
C	6.0	-2.8741707192	1.0250543419	-1.6892828157
C	6.0	-2.2515226339	2.4393221047	-1.6595154099
H	1.0	-2.8148550561	3.1509175966	-1.0261366679
H	1.0	-2.2648058432	2.8464693984	-2.6939047153
H	1.0	-1.1932838145	2.4319204738	-1.3264443009
C	6.0	-4.3426159204	1.1487550094	-2.1532545261
H	1.0	-4.3728939605	1.6981977366	-3.1200790713
H	1.0	-4.9649655426	1.7169654869	-1.4348058559
H	1.0	-4.8260324772	0.1683026170	-2.3283101163
C	6.0	-2.0602789558	0.2110424447	-2.7287772422
H	1.0	-2.3809269383	-0.8430393699	-2.8175599022
H	1.0	-0.9706990824	0.2285878507	-2.4987571353
H	1.0	-2.1773550466	0.6761441345	-3.7320997253

Reactant 0Tl:

ATOM	CHARGE	X	Y	Z
P	15.0	2.6482156335	0.2891097204	0.0440507865
TL	81.0	-0.0138775107	-1.3611086317	-0.0332003923
P	15.0	-2.6637695057	0.3063169582	0.0147962625
C	6.0	3.4941091689	-0.6108596597	1.5587178420
C	6.0	4.8488928655	-0.0191443759	2.0045609980

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H      1.0   5.6106219888   -0.0481666990    1.2018811605
H      1.0   5.2454393119   -0.6177083277    2.8546121911
H      1.0   4.7620626869    1.0246339969    2.3631705233
C      6.0   2.4917499773   -0.5482882737    2.7406703253
H      1.0   1.5032672865   -0.9883991190    2.4773072517
H      1.0   2.3133524246    0.4755562890    3.1143531430
H      1.0   2.8916679716   -1.1457281691    3.5887583998
C      6.0   3.6925637831   -2.1095858002    1.2317459935
H      1.0   4.4628183515   -2.2912078709    0.4579580297
H      1.0   2.7491855421   -2.6024661818    0.9132493161
H      1.0   4.0311779099   -2.6297469909    2.1540752941
C      6.0   2.8168461239    2.2204708145    0.2812058106
C      6.0   4.2138438588    2.7957616745   -0.0441028036
H      1.0   4.4897882757    2.6764649681   -1.1096099980
H      1.0   5.0148302799    2.3492439514    0.5757866700
H      1.0   4.2079916728    3.8884747736    0.1642196856
C      6.0   2.4477929068    2.6082622994    1.7320916221
H      1.0   1.4602798385    2.2058870783    2.0384807464
H      1.0   2.3775674996    3.7162640900    1.7872319196
H      1.0   3.2066971990    2.2983661090    2.4760712561
C      6.0   1.7533714240    2.8824638186   -0.6288711345
H      1.0   1.9134721221    2.6962057297   -1.7060012443
H      1.0   1.7846709568    3.9836243545   -0.4771798998
H      1.0   0.7323811660    2.5392676788   -0.3637098921
C      6.0  -3.9203866619   -1.1847255727    0.1546276664
C      6.0  -3.0489281707    1.6015878069    1.4195677569
C      6.0  -3.8190739635   -2.0559470448   -1.1207852511
H      1.0  -4.2056248489   -1.5563982947   -2.0295707337
H      1.0  -4.4306201433   -2.9724590810   -0.9731995897
H      1.0  -2.7796247781   -2.3947268759   -1.3204924916
C      6.0  -3.4546811338   -2.0843609430    1.3296306553
H      1.0  -3.5901954623   -1.6231530565    2.3237073109
H      1.0  -2.3870904866   -2.3814009857    1.2324789949
H      1.0  -4.0498125556   -3.0233626220    1.3190516910
C      6.0  -5.3960134959   -0.7889648145    0.3806333980
H      1.0  -5.5489894072   -0.2730616888    1.3487662838
H      1.0  -6.0171824943   -1.7113950865    0.4034486277
H      1.0  -5.7975897149   -0.1430827001   -0.4232359390
C      6.0  -3.2210718035    0.8633496952    2.7675104703
H      1.0  -3.2530399232    1.6214785196    3.5799639545
H      1.0  -2.3720351314    0.1839302409    2.9903219658
H      1.0  -4.1645798759    0.2880569413    2.8304725619
C      6.0  -4.2936108314    2.4822036732    1.1698474779
H      1.0  -4.4353445320    3.1603874748    2.0401572647
H      1.0  -5.2220416634    1.8891752470    1.0615191563
H      1.0  -4.1887471485    3.1280704394    0.2764850237
C      6.0  -1.7963777855    2.5003615168    1.5700633987
H      1.0  -1.9410027945    3.1726257971    2.4436151460
H      1.0  -1.6087288051    3.1441264476    0.6918174972
H      1.0  -0.8833630738    1.8979965331    1.7605559403
C      6.0   3.5566738082   -0.2321640457   -1.6057744023
C      6.0   3.0320808034   -1.6333503383   -2.0116667255
H      1.0   3.5261746259   -1.9471872974   -2.9572942655
H      1.0   1.9388068044   -1.6270236334   -2.2195161503
H      1.0   3.2309488387   -2.4202289691   -1.2618910350
C      6.0   3.1488023915    0.7271809493   -2.7486311092
H      1.0   3.5420361296    0.3196237271   -3.7053537220
H      1.0   3.5696135548    1.7444427434   -2.6359617955
H      1.0   2.0469876013    0.8106000555   -2.8585814515
C      6.0   5.0982371042   -0.2738505749   -1.5151327720
H      1.0   5.5124048682   -0.5372172440   -2.5134608139
H      1.0   5.4642231735   -1.0410160066   -0.8051613445
H      1.0   5.5347112680    0.7017200804   -1.2277078731
C      6.0  -2.8687710071    1.1507885425   -1.7312604381
C      6.0  -2.2191305968    2.5530344845   -1.7308462249
H      1.0  -2.7734455861    3.2916125239   -1.1208411575
H      1.0  -2.2166427528    2.9350944848   -2.7750398583
H      1.0  -1.1641252460    2.5316335542   -1.3897283929
C      6.0  -4.3269659765    1.2892124646   -2.2216496524
H      1.0  -4.3311157179    1.8117473705   -3.2036991647
H      1.0  -4.9478273288    1.8903942002   -1.5289996632
H      1.0  -4.8274001174    0.3138976952   -2.3765729731
C      6.0  -2.0509741408    0.2947278584   -2.7331195832
H      1.0  -2.3803352441   -0.7589469156   -2.7889898211
H      1.0  -0.9649714058    0.3112319932   -2.4877902697
H      1.0  -2.1513909024    0.7258678786   -3.7531473327
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H      1.0  -1.8773410035    2.7636327582    1.8223134092
H      1.0  -1.1938882730    3.7197660676    0.4890815576
C      6.0  -1.8578288326    2.3580866590   -1.6370353019
H      1.0  -2.6214345736    2.0433007760   -2.3730963320
H      1.0  -0.8813248737    1.9715741242   -1.9819510227
H      1.0  -1.8218918186    3.4689896798   -1.6698635974
C      6.0  -2.8155084534   -0.5815203394    1.6777618626
C      6.0  -4.3560029878   -0.6149430095    1.5699910946
H      1.0  -4.7228617869   -1.3981431452    0.8793637696
H      1.0  -4.8026214585    0.3505294206    1.2723313448
H      1.0  -4.7647249097   -0.8621169465    2.5745953052
C      6.0  -2.3981152985    0.3888208860    2.8027125750
H      1.0  -1.2991959835    0.5371824121    2.8383558137
H      1.0  -2.7031003082   -0.0514713358    3.7765563155
H      1.0  -2.8928934656    1.3747686992    2.7299205258
C      6.0  -2.3327336821   -1.9793051744    2.1084376615
H      1.0  -2.6331563288   -2.7824345529    1.4102615134
H      1.0  -2.7972563283   -2.2199374123    3.0893362049
H      1.0  -1.2360467594   -2.0092617337    2.2536374767
C      6.0   2.4140182759    1.6795622184   -0.9226887564
C      6.0   2.5434391502    0.0955211260    1.8875958122
C      6.0   2.2502496371    1.4728147275   -2.4465881386
H      1.0   3.0074712606    0.7999054212   -2.8883955642
H      1.0   2.3682475843    2.4585893437   -2.9458512088
H      1.0   1.2437785244    1.0803553740   -2.6960293986
C      6.0   1.5132336541    2.8690054839   -0.5455844370
H      1.0   1.5200690601    3.1077921106    0.5322536204
H      1.0   0.4753996804    2.7262666817   -0.8789244995
H      1.0   1.9020746362    3.7632586360   -1.0791255318
C      6.0   3.8580841941    2.1188639634   -0.5807617371
H      1.0   3.9384607976    2.5072595901    0.4531808064
H      1.0   4.1081752067    2.9654607755   -1.2565379232
H      1.0   4.6313894180    1.3487916343   -0.7289628961
C      6.0   2.0155950434    1.4065514682    2.5061568962
H      1.0   2.1927519107    1.3797500574    3.6031661714
H      1.0   0.9216920831    1.5207512477    2.3590940244
H      1.0   2.5281907534    2.3093332094    2.1209312740
C      6.0   4.0735496879    0.0330630563    2.0815200166
H      1.0   4.2878866650    0.1336359989    3.1681257414
H      1.0   4.6123892849    0.8516986986    1.5708729134
H      1.0   4.5162749440   -0.9300515326    1.7633344289
C      6.0   1.8800465522   -1.0658103540    2.6582368324
H      1.0   2.0760869783   -0.9337309993    3.7441622112
H      1.0   2.2753159391   -2.0591297285    2.3752388033
H      1.0   0.7787580361   -1.0599398816    2.5144525889
C      6.0  -2.8549107260   -0.9213499356   -1.5479436504
C      6.0  -1.9410706679   -0.8546637829   -2.7887187450
H      1.0  -2.4479493885   -1.3849457809   -3.6240527411
H      1.0  -0.9601472297   -1.3371094252   -2.6126138117
H      1.0  -1.7407506762    0.1794469731   -3.1242468173
C      6.0  -3.1494491534   -2.4143732540   -1.2684255010
H      1.0  -3.7040279379   -2.8165504018   -2.1435059652
H      1.0  -3.7905417677   -2.5883678298   -0.3834300923
H      1.0  -2.2348537040   -3.0249119950   -1.1780210467
C      6.0  -4.2077814729   -0.2523805860   -1.8873662714
H      1.0  -4.6787276230   -0.8421098047   -2.7033785438
H      1.0  -4.1000122545    0.7787085116   -2.2718512224
H      1.0  -4.9222626120   -0.2465798936   -1.0431133158
C      6.0   2.9543957002   -1.4589593303   -0.9026676491
C      6.0   3.1816957424   -2.6886055752    0.0125844802
H      1.0   3.8901352386   -2.4740441943    0.8342828331
H      1.0   3.6522302023   -3.4817949660   -0.6078874395
H      1.0   2.2701331357   -3.1236158883    0.4466254008
C      6.0   4.3782839428   -0.9917828200   -1.2944228260
H      1.0   4.9011317984   -1.8748556667   -1.7207216727
H      1.0   4.9811646885   -0.6560458351   -0.4296784341
H      1.0   4.4009933718   -0.2092317547   -2.0738772131
C      6.0   2.2297460217   -1.8941070213   -2.1956751640
H      1.0   2.1570687654   -1.0807134191   -2.9392549396
H      1.0   1.2062736329   -2.2670698708   -2.0229633204
H      1.0   2.8169066310   -2.7166808865   -2.6586621560
C      6.0  -0.0652827982   -2.9804380136    0.1165109548
C      6.0   0.4756479791   -2.9190006577    1.0718209681
H      1.0  -1.0961624641   -3.3165325295    0.2862150643
H      1.0   0.4500977123   -3.6459704361   -0.5996995730
H      1.0  -0.1011583275   -1.9580131960   -0.4373970770
```

Transition states of the reactions with methane

Transition state **TS1B**:

```
ATOM   CHARGE       X             Y             Z
-------------------------------------------------------------
P      15.0  -1.9055942070   -0.0169347418   -0.0200431551
B       5.0  -0.0026280998   -0.2873351694   -0.1785038234
P      15.0   1.8925026686   -0.0051285137    0.0070546506
C       6.0  -2.2239852411    1.9217594908   -0.1951568972
C       6.0  -3.6865067200    2.3584994509    0.0656170139
H       1.0  -4.4278238652    1.9072245444   -0.6151776398
H       1.0  -3.7232565791    3.4583651633   -0.0951121054
H       1.0  -4.0045868199    2.1843777531    1.1102288264
C       6.0  -1.3630106041    2.6828964325    0.8488758197
H       1.0  -0.3798078960    2.2216198934    1.0338929322
```

Transition state **TS1Al**:

```
ATOM   CHARGE       X             Y             Z
-------------------------------------------------------------
P      15.0  -0.0001368007   -0.0103155236    0.0108881333
AL     13.0  -0.0197619161    0.0487582250    2.5859032146
P      15.0   1.8233338921    0.0019426406    4.3961352218
C       6.0   0.4341848486   -1.8694047154   -0.4063984536
C       6.0   0.6167834659   -2.1658678789   -1.9123308162
H       1.0  -0.2795081368   -1.9412296347   -2.5180561226
H       1.0   0.8253508139   -3.2518451482   -2.0268748987
H       1.0   1.4809714857   -1.6290130151   -2.3494009059
C       6.0   1.7501502855   -2.2234977517    0.3193063186
H       1.0   1.6977637660   -1.9950484680    1.4014525210
H       1.0   2.6360381330   -1.7213706420   -0.1071537172
H       1.0   1.9216030389   -3.3187865893    0.2356123318
C       6.0  -0.6672997460   -2.7915926216    0.1680985644
H       1.0  -1.6258437642   -2.7146537158   -0.3794652758
```

```
H       1.0   -0.8618691559  -2.5971850018   1.2448706076        H       1.0   -4.9438753602  -1.0040579932   1.6308928567
H       1.0   -0.3227927207  -3.8439565755   0.0738419273        H       1.0   -4.8926701444   0.7857613175   1.7713049519
C       6.0    1.1706931744   1.1672303469  -1.0385623156        H       1.0   -4.6068492223  -0.2400364687   3.2032428981
C       6.0    0.7942709319   1.2548393902  -2.5353117967        C       6.0   -2.2509238415   0.9361177986   2.7345608772
H       1.0   -0.1998063116   1.7104430755  -2.7021505203        H       1.0   -1.1571243861   1.0222706557   2.5745901576
H       1.0    0.8247284075   0.2770200850  -3.0521026280        H       1.0   -2.4036875797   0.6832221777   3.8060545803
H       1.0    1.5357377731   1.9128195259  -3.0395456930        H       1.0   -2.7148931840   1.9274764247   2.5710162991
C       6.0    2.6338471900   0.6838447811  -0.9285969171        C       6.0   -2.3190958904  -1.5258117007   2.3925013446
H       1.0    2.9578506534   0.5314422077   0.1208786751        H       1.0   -2.7468211262  -2.4091814842   1.8861582305
H       1.0    3.2904206992   1.4691871611  -1.3615192913        H       1.0   -2.5523710690  -1.6200717614   3.4750095245
H       1.0    2.8257664237  -0.2447021073  -1.4996630602        H       1.0   -1.2188565300  -1.5676895622   2.2812402707
C       6.0    1.1080803201   2.5815576841  -0.4170282163        C       6.0    2.9704865847   1.4312231889  -1.2106006359
H       1.0    0.1066264334   3.0426591497  -0.4799984128        C       6.0    2.5181827062   0.6266542260   1.8563352173
H       1.0    1.8084421941   3.2415032459  -0.9733290226        C       6.0    3.1912352773   0.8502526161  -2.6278876974
H       1.0    1.4218598914   2.5825404594   0.6447604809        H       1.0    4.0815266880   0.1985637385  -2.7034338192
C       6.0    1.8383453395  -1.8528992732   5.0350099730        H       1.0    3.3584547314   1.7020515377  -3.3222955410
C       6.0    3.6212102208   0.5162715857   3.8248284358        H       1.0    2.3036953047   0.2963945618  -2.9994931872
C       6.0    0.5246011950  -2.1463828980   5.7985055382        C       6.0    1.8413503487   2.4750741730  -1.3478766612
H       1.0    0.4635667086  -1.6512406886   6.7857570849        H       1.0    1.6058287944   3.0033429639  -0.4068730569
H       1.0    0.4735567167  -3.2407070330   5.9853474393        H       1.0    0.9126720940   2.0072479439  -1.7382180931
H       1.0   -0.3707677009  -1.8713479356   5.2016619314        H       1.0    2.1567067272   3.2431222631  -2.0864792260
C       6.0    1.8491108868  -2.8188009591   3.8316413516        C       6.0    4.2565386455   2.1468727907  -0.7397873074
H       1.0    2.7466379577  -2.7281922599   3.1937971593        H       1.0    4.1150185312   2.6940833466   0.2125452789
H       1.0    0.9408987749  -2.6967404503   3.2029071862        H       1.0    4.5344210933   2.9043350320  -1.5047616677
H       1.0    1.8295372797  -3.8590105528   4.2224708785        H       1.0    5.1204010511   1.4666877162  -0.6264984884
C       6.0    3.0524359558  -2.1808060614   5.9348528368        C       6.0    1.9101524355   2.0411802455   1.9903463697
H       1.0    4.0118243366  -2.1453706657   5.3822955524        H       1.0    1.8333866527   2.2820305722   3.0726855730
H       1.0    2.9373276109  -3.2216815797   6.3080514297        H       1.0    0.8879071446   2.1090747255   1.5684574063
H       1.0    3.1359907665  -1.5253394023   6.8204412637        H       1.0    2.5357625350   2.8299446564   1.5296709819
C       6.0    4.2078073052  -0.5886163196   2.9188830799        C       6.0    3.9609463020   0.6574486824   2.4121835398
H       1.0    5.1497047932  -0.2088256315   2.4666782759        H       1.0    3.9261501630   1.0496330227   3.4522712894
H       1.0    3.5277982160  -0.8539827778   2.0846603225        H       1.0    4.6321122870   1.3222946990   1.8364214689
H       1.0    4.4663167023  -1.5120964293   3.4716982101        H       1.0    4.4246473089  -0.3459245775   2.4673229217
C       6.0    4.6114147948   0.7944398707   4.9780165518        C       6.0    1.6543664100  -0.3260858466   2.7156365088
H       1.0    5.6024370892   1.0357604241   4.5348026766        H       1.0    1.6747863796   0.0262527838   3.7695352683
H       1.0    4.7587613398  -0.0740468064   5.6473834446        H       1.0    2.0130745507  -1.3708371763   2.7102519257
H       1.0    4.3167547619   1.6664170547   5.5920026411        H       1.0    0.5962910176  -0.3251875547   2.3826851255
C       6.0    3.4782973656   1.7892913472   2.9568983994        C       6.0   -3.5451713676  -1.0987231473  -1.1156518998
H       1.0    4.4789961945   2.0665120610   2.5602193121        C       6.0   -2.8741284851  -1.3351201269  -2.4917405480
H       1.0    3.0930890026   2.6623267729   3.5139021949        H       1.0   -3.6027345418  -1.8731295010  -3.1365900393
H       1.0    2.8150636089   1.6162362395   2.0840321537        H       1.0   -1.9702155939  -1.9701898191  -2.4165853566
C       6.0   -1.8762232284   0.3246328142  -0.5139576578        H       1.0   -2.5929236778  -0.4060302362  -3.0195029858
C       6.0   -2.8243229289  -0.2136662548   0.5857007881        C       6.0   -3.7744750122  -2.4906965119  -0.4808601111
H       1.0   -3.8700427810  -0.0437301572   0.2483741059        H       1.0   -4.3455581404  -3.1023542394  -1.2119100648
H       1.0   -2.6908262173   0.3140783379   1.5504866462        H       1.0   -4.3745407123  -2.4596442445   0.4477771337
H       1.0   -2.7124664584  -1.2950309230   0.7826568883        H       1.0   -2.8307060096  -3.0308949796  -0.2799227442
C       6.0   -2.1550292000   1.8402902705  -0.6458600434        C       6.0   -4.9315188634  -0.4475025216  -1.3355806847
H       1.0   -3.2440200583   1.9714218153  -0.8232573558        H       1.0   -5.5594496319  -1.1706745173  -1.9001406755
H       1.0   -1.6325989573   2.3119338106  -1.4991903218        H       1.0   -4.8860535481   0.4754469364  -1.9437551512
H       1.0   -1.9125337947   2.4016977123   0.2760640111        H       1.0   -5.4627259844  -0.2256636603  -0.3907258581
C       6.0   -2.2406758235  -0.3426900045  -1.8607365865        C       6.0    3.5606177268  -1.5409806681  -0.2563302566
H       1.0   -3.2817262156  -0.0450946216  -2.1125915795        C       6.0    3.4180301278  -2.5361185321   0.9200713448
H       1.0   -2.2299349320  -1.4480174164  -1.8131923762        H       1.0    3.8223429256  -2.1439078320   1.8726301650
H       1.0   -1.5979300529  -0.0185659546  -2.7010678962        H       1.0    4.0130682121  -3.4403865322   0.6688587835
C       6.0    1.2729678386   1.1474424944   5.9016394745        H       1.0    2.3756543920  -2.8671892017   1.0794358758
C       6.0    1.6319871264   2.6266782978   5.6209283507        C       6.0    5.0538385723  -1.1579797671  -0.3769178748
H       1.0    2.7216413893   2.8198907850   5.6336953104        H       1.0    5.6353195839  -2.1002251651  -0.4763938939
H       1.0    1.1950681387   3.2405566354   6.4380447356        H       1.0    5.4422411377  -0.6303113792   0.5149094503
H       1.0    1.2110795233   3.0073893284   4.6726598247        H       1.0    5.2762950992  -0.5504686475  -1.2741518245
C       6.0    1.9419965199   0.7455478494   7.2374505896        C       6.0    3.1227011652  -2.2774278081  -1.5457673536
H       1.0    1.6211034073   1.4774765487   8.0105967903        H       1.0    3.2687786512  -1.6808340845  -2.4626677484
H       1.0    3.0475271575   0.7766195304   7.2015512586        H       1.0    2.0643933234  -2.5926539464  -1.5034802343
H       1.0    1.6251185275  -0.2522331842   7.5936328356        H       1.0    3.7397709374  -3.1962157222  -1.6493503674
C       6.0   -0.2635727296   1.0639546124   6.0768492553        C       6.0   -0.0370246588  -2.8263894586   0.1463025284
H       1.0   -0.6193572905   0.0615198213   6.3709023554        H       1.0    0.2861887586  -2.6472803311   1.1892634622
H       1.0   -0.8125053387   1.3656648293   5.1658654190        H       1.0   -1.0754278699  -3.1966553053   0.1233920941
H       1.0   -0.5537212338   1.7664196105   6.8881149719        H       1.0    0.6317756214  -3.5632499569  -0.3366318413
C       6.0   -0.3913773651   2.4282149077   7.2092597231        H       1.0    0.0042116571  -1.9770635660  -1.4302514760
H       1.0    0.6531085846   2.7946060513   2.6619011330
H       1.0   -0.9404167326   2.7379287997   1.8034548340
H       1.0   -0.8825745254   2.8671690005   3.5993247556
H       1.0   -1.1460886121   1.0668748507   3.1071091439
```

Transition state **TS1Ga**:

```
ATOM    CHARGE       X              Y              Z
-------------------------------------------------------------
P       15.0   -2.3713550016   0.0237130382   0.0044937055
GA      31.0    0.0163267222  -0.5278349509  -0.8231740215
P       15.0    2.3865835133   0.0124935255   0.0107592490
C        6.0   -2.6120458864   1.8907079566  -0.5198225205
C        6.0   -3.9488761201   2.5277344520  -0.0766594467
H        1.0   -4.8404965745   2.0140374989  -0.4786760845
H        1.0   -3.9736145252   3.5716390608  -0.4582613491
H        1.0   -4.0444220173   2.5905961622   1.0247311175
C        6.0   -1.4596041605   2.7117636286   0.1014722891
H        1.0   -0.4734250517   2.2611983601  -0.1177202264
H        1.0   -1.5530938995   2.8405344868   1.1938950232
H        1.0   -1.4609811796   3.7265997899  -0.3513705898
C        6.0   -2.4694249119   2.0032686933  -2.0564421798
H        1.0   -3.3203150670   1.5624630673  -2.6100135100
H        1.0   -1.5305111828   1.5350656721  -2.4212558981
H        1.0   -2.4313438373   3.0809134962  -2.3252148839
C        6.0   -2.8918791010  -0.1835898238   1.8830213649
C        6.0   -4.4202703897  -0.1555172796   2.1101383471
```

Transition state **TS1In**:

```
ATOM    CHARGE       X              Y              Z
-------------------------------------------------------------
P       15.0   -2.5193109259   0.1034595342   0.0249289100
IN      49.0    0.0222870689  -0.7678527052  -0.6744438085
P       15.0    2.5281682620   0.0900030969   0.0416570313
C        6.0   -2.7349188186   1.8748063036  -0.7691797006
C        6.0   -4.0519041912   2.5831796851  -0.3781767554
H        1.0   -4.9556625348   2.0117640005  -0.6601494995
H        1.0   -4.0988534486   3.5547926741  -0.9172048087
H        1.0   -4.1084370868   2.8174801868   0.7024093659
C        6.0   -1.5413874312   2.7518130092  -0.3263614367
H        1.0   -0.5765818124   2.2745508288  -0.5868617117
H        1.0   -1.5398683676   2.9888963719   0.7521815926
H        1.0   -1.5886841287   3.7173487052  -0.8749205793
C        6.0   -2.6576362979   1.7671146301  -2.3106855819
H        1.0   -3.5359450055   1.3625408983  -2.7553348646
H        1.0   -1.7382394990   1.2455637299  -2.6511032237
H        1.0   -2.6285580057   2.7972618155  -2.7259658014
C        6.0   -3.0271668337   0.1843619071   1.9181411289
C        6.0   -4.5539702491   0.2352897473   2.1514273663
H        1.0   -5.0659357167  -0.6914841609   1.8284608371
H        1.0   -5.0419783788   1.0970559251   1.6588809977
H        1.0   -4.7337987013   0.3356269779   3.2442257851
C        6.0   -2.3776730176   1.4237317164   2.5746298673
```

```
H        1.0    -1.2809505289     1.4614056666     2.4121664692
H        1.0    -2.5408114702     1.3579827195     3.6719842953
H        1.0    -2.8217861481     2.3810106489     2.2414721172
C        6.0    -2.4395568073    -1.0548843437     2.6293566707
H        1.0    -2.8520943122    -2.0123936241     2.2654419780
H        1.0    -2.6761051371    -0.9822893889     3.7129430797
H        1.0    -1.3385314327    -1.0981748458     2.5267579900
C        6.0     3.0592900568     1.2546843875    -1.4381784487
C        6.0     2.6374656726     1.0550762683     1.7303536103
C        6.0     3.2630987969     0.3947997370    -2.7066938768
H        1.0     4.1534868770    -0.2591542711    -2.6543472183
H        1.0     3.4130512297     1.0790257943    -3.5690951850
H        1.0     2.3697297649    -0.2252008294    -2.9311620115
C        6.0     1.9119354050     2.2395433044    -1.7656768863
H        1.0     1.6771444815     2.9382046822    -0.9432709977
H        1.0     0.9821200982     1.7125271554    -2.0708870836
H        1.0     2.2277878808     2.8535550411    -2.6367868814
C        6.0     4.3436332745     2.0653940026    -1.1463409938
H        1.0     4.2047687945     2.8038382940    -0.3328268200
H        1.0     4.6075269259     2.6406773388    -2.0602721358
H        1.0     5.2142052690     1.4299156854    -0.8989035603
C        6.0     2.0017382719     2.4539507680     1.5667995258
H        1.0     1.9364474020     2.9270877477     2.5705398970
H        1.0     0.9705273882     2.4052698655     1.1619970457
H        1.0     2.6010038687     3.1319357766     0.9295395942
C        6.0     4.0772886184     1.2195430788     2.2665239004
H        1.0     4.0340332507     1.8167195628     3.2031899466
H        1.0     4.7393987906     1.7600098805     1.5636454552
H        1.0     4.5517417188     0.2528872433     2.5217784823
C        6.0     1.7785593340     0.2856134470     2.7618751918
H        1.0     1.7570189761     0.8656611743     3.7095658531
H        1.0     2.1678460832    -0.7206901240     2.9999703131
H        1.0     0.7308251292     0.1744359025     2.4131934393
C        6.0    -3.6801410069    -1.1700466638    -0.9148141944
C        6.0    -3.0523169456    -1.5509024045    -2.2786789412
H        1.0    -3.7330400881    -2.2747678590    -2.7770137208
H        1.0    -2.0666105912    -2.0455123686    -2.1718761697
H        1.0    -2.9257765282    -0.6957878618    -2.9662841298
C        6.0    -3.7903226085    -2.4752402399    -0.0944021520
H        1.0    -4.3559133346    -3.2141349018    -0.7021754390
H        1.0    -4.3441902598    -2.3536316343     0.8558752690
H        1.0    -2.8001972455    -2.9233255222     0.1217301563
C        6.0    -5.1001145495    -0.6117356978    -1.1638612310
H        1.0    -5.7088139449    -1.4167603498    -1.6304628018
H        1.0    -5.1059129042     0.2402828093    -1.8709404327
H        1.0    -5.6220019003    -0.3048771664    -0.2381576135
C        6.0     3.7100520222    -1.4746521287     0.0772711740
C        6.0     3.5674275617    -2.2080964405     1.4317276690
H        1.0     3.9931404552    -1.6413107334     2.2817157100
H        1.0     4.1409726340    -3.1570489067     1.3611304543
H        1.0     2.5200535208    -2.4772336859     1.6633676494
C        6.0     5.1987838242    -1.1121164997    -0.1272779841
H        1.0     5.7941934876    -2.0455207776    -0.0228302810
H        1.0     5.5819646167    -0.3963463797     0.6249942831
H        1.0     5.4144401377    -0.7130630034    -1.1370928562
C        6.0     3.2736380829    -2.4694994539    -1.0275339243
H        1.0     3.3688839309    -2.0691688990    -2.0520961720
H        1.0     2.2358144173    -2.8284267535    -0.8880308597
H        1.0     3.9367353676    -3.3594718020    -0.9628094546
C        6.0     0.0254171579    -2.8542521249     0.9499916494
H        1.0     0.2759244207    -2.3810006005     1.9203317098
H        1.0    -0.9840728610    -3.3030131819     0.9832809208
H        1.0     0.7776085789    -3.6212779889     0.6864295010
H        1.0     0.0053289284    -2.4689233299    -0.9603741458
```

Transition state TS1Tl:

```
 ATOM    CHARGE        X                Y                Z
 ----------------------------------------------------------------
P       15.0    -2.5390057920     0.1986320198     0.1016480873
TL      81.0     0.0095091933    -0.8291134800    -0.5279577476
P       15.0     2.5456366677     0.1923403827     0.0761562437
C        6.0    -2.7789709535     1.6533174259    -1.1753634364
C        6.0    -4.0734768610     2.4695690716    -0.9512733368
H        1.0    -4.9921303679     1.8570366269    -1.0054620326
H        1.0    -4.1408571003     3.2363090324    -1.7535513238
H        1.0    -4.0708560962     3.0156038492     0.0122382802
C        6.0    -1.5660946340     2.6073368837    -1.0758200236
H        1.0    -0.6076412894     2.0759581658    -1.2421620751
H        1.0    -1.5099139809     3.1459948920    -0.1137945660
H        1.0    -1.6561427828     3.3734478135    -1.8761636049
C        6.0    -2.7764245864     1.0741600112    -2.6087948573
H        1.0    -3.6737358669     0.4673219187    -2.8340555483
H        1.0    -1.8707975693     0.4625811377    -2.8063448097
H        1.0    -2.7663263533     1.9212747630    -3.3274240517
C        6.0    -2.8891096452     0.8358238921     1.9150062313
C        6.0    -4.3957017041     0.9833606967     2.2302244018
H        1.0    -4.9409878295     0.0208482141     2.2043830063
H        1.0    -4.9093733504     1.6959600958     1.5567745707
H        1.0    -4.4941519658     1.3810606126     3.2638928579
C        6.0    -2.2094724024     2.2055701633     2.1391626285
H        1.0    -1.1297270169     2.1937262157     1.8887574932
H        1.0    -2.2887823559     2.4537216018     3.2195302444
H        1.0    -2.6964188484     3.0299030300     1.5836241879
C        6.0    -2.2420293996    -0.1626014461     2.9039369918
```

Products of the reactions with methane

Product 1B:

```
H        1.0    -2.6813164223    -1.1746488139     2.8629610738
H        1.0    -2.3883535069     0.2214306938     3.9366588014
H        1.0    -1.1511461550    -0.2602581052     2.7346041347
C        6.0     3.1277287818     0.9025562846    -1.6510035702
C        6.0     2.5582905948     1.5930346696     1.4281616206
C        6.0     3.4178245180    -0.2657634176    -2.6243263194
H        1.0     4.3229466831    -0.8398054413    -2.3513094235
H        1.0     3.6010000090     0.1662402904    -3.6315485767
H        1.0     2.5634248468    -0.9683923242    -2.7223621697
C        6.0     1.9820597312     1.7312194732    -2.2761627466
H        1.0     1.7526821955     2.6552018527    -1.7160976009
H        1.0     1.0528568485     1.1314774520    -2.3721194622
H        1.0     2.2881555706     2.0333719181    -3.3007242457
C        6.0     4.3881199019     1.7924212515    -1.5423606279
H        1.0     4.2148671274     2.7133555854    -0.9521246004
H        1.0     4.6745709711     2.1186681261    -2.5659552734
H        1.0     5.2590487422     1.2617071363    -1.1141994569
C        6.0     1.9092372077     2.8731920444     0.8556212544
H        1.0     1.7796054369     3.5969013819     1.6891728194
H        1.0     0.9057017324     2.6829725277     0.4255122204
H        1.0     2.5331349422     3.3742289913     0.0905717406
C        6.0     3.9695883925     1.9425172437     1.9545960696
H        1.0     3.8729754686     2.7883510490     2.6695275440
H        1.0     4.6617680864     2.2684502339     1.1552774751
H        1.0     4.4384775796     1.1057189223     2.5073383836
C        6.0     1.6732976865     1.1215865175     2.6061835539
H        1.0     1.5891063707     1.9514618384     3.3410733764
H        1.0     2.0793951765     0.2466244474     3.1442126603
H        1.0     0.6461354402     0.8674255927     2.2741222743
C        6.0    -3.7664443596    -1.2690451972    -0.3305944926
C        6.0    -3.1851353049    -2.0753523172    -1.5179011637
H        1.0    -3.8891106021    -2.9032991670    -1.7504454750
H        1.0    -2.2102706546    -2.5363790485    -1.2672398982
H        1.0    -3.0606015482    -1.4834691237    -2.4425375544
C        6.0    -3.8695123050    -2.2448725274     0.8643617375
H        1.0    -4.4445891395    -3.1334146720     0.5253904675
H        1.0    -4.4144490059    -1.8253673509     1.7311847768
H        1.0    -2.8794454693    -2.6066639712     1.2030799070
C        6.0    -5.1857094453    -0.7779290015    -0.6950513172
H        1.0    -5.8286086707    -1.6716411753    -0.8532315842
H        1.0    -5.2138778944    -0.1991555727    -1.6383652955
H        1.0    -5.6588796280    -0.1762424551     0.1042354890
C        6.0     3.7285938174    -1.2730048580     0.6037007342
C        6.0     3.4892418986    -1.6136812254     2.0929596096
H        1.0     3.8510000649    -0.8280806020     2.7838204793
H        1.0     4.0664694699    -2.5341524426     2.3258398414
H        1.0     2.4251974652    -1.8316389258     2.3097314533
C        6.0     5.2249113090    -0.9433217975     0.3986165456
H        1.0     5.8217869054    -1.7953999662     0.7917021467
H        1.0     5.5511508570    -0.0376438957     0.9445839850
H        1.0     5.4993028058    -0.8298598544    -0.6679335339
C        6.0     3.3640964768    -2.5384068438    -0.2110042704
H        1.0     3.5019506554    -2.4233845532    -1.3001435218
H        1.0     2.3268125849    -2.8747884189    -0.0173384307
H        1.0     4.0381367322    -3.3594756674     0.1168583182
C        6.0    -0.0282914871    -2.7381181219     1.3645836922
H        1.0     0.1205692692    -2.1544802098     2.2954758718
H        1.0    -1.0234583179    -3.2199338616     1.3634314824
H        1.0     0.7623160187    -3.5039522649     1.2542824629
H        1.0     0.0421607367    -2.5429432645    -0.8179303106
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 ATOM    CHARGE        X                Y                Z
 ----------------------------------------------------------------
P       15.0    -2.0156900767    -0.0379868972    -0.0382516041
B        5.0     0.0094334317    -0.6684199894    -0.4939245294
P       15.0     2.0144570651    -0.0343909090    -0.0188884352
C        6.0    -2.3275604930     1.8713426206    -0.3166187111
C        6.0    -3.7480412890     2.4065811789    -0.0110058275
H        1.0    -4.5510391953     1.9404803423    -0.6057235097
H        1.0    -3.7495141201     3.4922365075    -0.2513250608
H        1.0    -4.0051008528     2.3236643288     1.0625288617
C        6.0    -1.3700409344     2.6556354565     0.6138505392
H        1.0    -0.3834487038     2.1769417045     0.7194204145
H        1.0    -1.7944249936     2.7907948186     1.6244652181
H        1.0    -1.2049948846     3.6699218888     0.1928734852
C        6.0    -1.9862223542     2.1889998384    -1.7954340732
H        1.0    -2.7636247789     1.8304780067    -2.4960939235
H        1.0    -1.0181288656     1.7594276946    -2.1191571792
H        1.0    -1.9244430806     3.2914781102    -1.9183061117
C        6.0    -2.7183685006    -0.5234047935     1.7218246969
C        6.0    -4.2643518664    -0.4778714009     1.7940768330
H        1.0    -4.7542825402    -1.2426204496     1.1633030887
H        1.0    -4.6871768363     0.5096985580     1.5346422216
H        1.0    -4.5610404174    -0.6946117499     2.8431507286
C        6.0    -2.1642251809     0.4434625103     2.7945885574
H        1.0    -1.0641363851     0.5637709893     2.7407781066
H        1.0    -2.3971134602     0.0204589418     3.7953834086
H        1.0    -2.6321539677     1.4445644795     2.7536508748
C        6.0    -2.2503675085    -1.9471501936     2.1072086215
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H      1.0    -2.5626591768   -2.7277813062    1.3913394343
H      1.0    -2.7020393886   -2.2039131181    3.0900423466
H      1.0    -1.1530720597   -2.0056983092    2.2291310326
C      6.0     2.5838744973    1.5759920864   -0.9941640532
C      6.0     2.3947608981    0.1819020271    1.8800283905
C      6.0     2.6505020374    1.2531119327   -2.5077773300
H      1.0     3.5105032995    0.6165797012   -2.7811787256
H      1.0     2.7700687793    2.2105540731   -3.0581343030
H      1.0     1.7232739319    0.7722189770   -2.8787692405
C      6.0     1.5565607894    2.7131675183   -0.8432389506
H      1.0     1.4354192415    3.0637308043    0.1968121092
H      1.0     0.5687765559    2.4344925424   -1.2467718105
H      1.0     1.9179505526    3.5804548725   -1.4372252222
C      6.0     3.9476322753    2.1376148715   -0.5216626520
H      1.0     3.8908646724    2.5833801111    0.4907688457
H      1.0     4.2291825799    2.9601539182   -1.2140569702
H      1.0     4.7729885900    1.4055172145   -0.5353507280
C      6.0     1.8496931410    1.5430443097    2.3684158197
H      1.0     1.9443164345    1.5781098222    3.4750794908
H      1.0     0.7774458707    1.6820042164    2.1311597450
H      1.0     2.4157298721    2.4065097107    1.9692935229
C      6.0     3.8939031484    0.1078040678    2.2524790200
H      1.0     3.9861771347    0.3054496502    3.3424829979
H      1.0     4.5086220990    0.8646687786    1.7317580479
H      1.0     4.3342368358   -0.8909576390    2.0735206947
C      6.0     1.6351497678   -0.9230083305    2.6509571923
H      1.0     1.8083583772   -0.7762232844    3.7390244502
H      1.0     1.9728765352   -1.9449789916    2.3998097784
H      1.0     0.5425714505   -0.8663617466    2.4817368409
C      6.0    -3.0911991471   -1.0236471263   -1.4121593642
C      6.0    -2.2888136724   -1.1358790303   -2.7313994282
H      1.0    -2.9586580106   -1.5827305634   -3.4973703641
H      1.0    -1.4060610391   -1.7959981054   -2.6399829653
H      1.0    -1.9495688983   -0.1589392127   -3.1224360050
C      6.0    -3.4963400402   -2.4609194492   -0.9901188313
H      1.0    -4.0572271325   -2.9016013630   -1.8420659553
H      1.0    -4.1763945911   -2.4884384985   -0.1189289426
H      1.0    -2.6484171673   -3.1428388991   -0.7939403219
C      6.0    -4.4232032228   -0.2942848134   -1.7200158546
H      1.0    -4.9853907104   -0.9220968439   -2.4442345567
H      1.0    -4.2873416760    0.6910289311   -2.2016253516
H      1.0    -5.0714690711   -0.1725344639   -0.8317421425
C      6.0     3.1714959573   -1.4918616984   -0.7217456720
C      6.0     3.1603821569   -2.7188619146    0.2286422516
H      1.0     3.6472162195   -2.5093016050    1.2004135240
H      1.0     3.7606062888   -3.5187458444   -0.2552269687
H      1.0     2.1579087375   -3.1364791641    0.4182890231
C      6.0     4.6599883126   -1.0852409031   -0.8657683381
H      1.0     5.2086951369   -1.9839636222   -1.2227574558
H      1.0     5.1336068716   -0.7786300150    0.0849781251
H      1.0     4.8277038915   -0.2966585794   -1.6213418375
C      6.0     2.6805022542   -1.9242725049   -2.1397625216
H      1.0     1.5975260060   -1.7923125839   -2.3134637253
H      1.0     2.9116774356   -3.0002285387   -2.2890701959
H      1.0     3.2081103386   -1.3736122796   -2.9404262191
C      6.0    -0.0416938411   -2.2741302336   -0.2685556134
H      1.0    -1.0386757389   -2.6863410547   -0.4997486686
H      1.0     0.6483215661   -2.8108200298   -0.9451803307
H      1.0     0.1829622922   -2.6063306091    0.7629368233
H      1.0     0.0172767220   -0.3204974757   -1.6684962208
```

Product 1Al:

```
 ATOM    CHARGE        X                Y                Z
----------------------------------------------------------------
P       15.0     2.3955103259    0.0085849381    0.0562398321
AL      13.0    -0.0171723272   -0.8131729621    0.7646344486
P       15.0    -2.4120888155   -0.0160571119    0.0453043741
C        6.0     2.6383517973    1.9013663213    0.4504306258
C        6.0     3.9807001949    2.5029388861   -0.0243103728
H        1.0     4.8660726967    2.0065177380    0.4117139303
H        1.0     4.0122562085    3.5679813993    0.2938038820
H        1.0     4.0816672414    2.4981232371   -1.1272227128
C        6.0     1.4939370151    2.6872898441   -0.2301060289
H        1.0     0.5032514668    2.2454348618   -0.0170384324
H        1.0     1.6121592252    2.7697496084   -1.3249307971
H        1.0     1.4823466955    3.7217718120    0.1757203516
C        6.0     2.4924522160    2.1115602586    1.9782196145
H        1.0     3.3349229266    1.6876640437    2.5570541842
H        1.0     1.5464413300    1.6935638653    2.3799644917
H        1.0     2.4849351787    3.2050415252    2.1761543059
C        6.0     2.8909791283   -0.3453423671   -1.7959369149
C        6.0     4.4162244066   -0.3236489200   -2.0490204120
H        1.0     4.9543503399   -1.1313041080   -1.5184152587
H        1.0     4.8842287954    0.6423072739   -1.7807110502
H        1.0     4.5936726858   -0.4806003011   -3.1356862571
C        6.0     2.2318884922    0.7031841154   -2.7212303214
H        1.0     1.1402847846    0.7986838732   -2.5502277603
H        1.0     2.3694505118    0.3719898896   -3.7731108890
H        1.0     2.6939087365    1.7047376882   -2.6341057535
C        6.0     2.3225587787   -1.7276848028   -2.1991711247
H        1.0     2.7529223917   -2.5686702128   -1.6271681663
H        1.0     2.5590948633   -1.9058258276   -3.2704743182
H        1.0     1.2201848429   -1.7709824450   -2.0945201737
C        6.0    -2.9796992179    1.5412187570    1.0854872376
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(right column, continuation of Product 1Al:)

```
C        6.0    -2.5415194126    0.3709058649   -1.8581234257
C        6.0    -3.2190614751    1.1186097744    2.5545669424
H        1.0    -4.1337313622    0.5114231941    2.6906414575
H        1.0    -3.3569285822    2.0425783926    3.1563354386
H        1.0    -2.3525213685    0.5743398760    2.9815675465
C        6.0    -1.8243344635    2.5659520250    1.1158414758
H        1.0    -1.5870100909    2.9932591643    0.1251740057
H        1.0    -0.9061068794    2.1228726832    1.5508129452
H        1.0    -2.1232818083    3.4106378365    1.7733107895
C        6.0    -4.2518235924    2.2301438707    0.5417503035
H        1.0    -4.1004750759    2.6957712681   -0.4517394231
H        1.0    -4.5244277862    3.0502556086    1.2408974379
H        1.0    -5.1238951144    1.5527163589    0.4805243996
C        6.0    -1.9186601376    1.7576621853   -2.1407231283
H        1.0    -1.8534564472    1.8935096212   -3.2420288784
H        1.0    -0.8895345330    1.8511102514   -1.7388016605
H        1.0    -2.5283143796    2.5939258436   -1.7490904553
C        6.0    -3.9785406038    0.3489325421   -2.4238253690
H        1.0    -3.9393809490    0.6270011958   -3.4997563478
H        1.0    -4.6474126677    1.0747928322   -1.9234960512
H        1.0    -4.4428566717   -0.6541391318   -2.3701598284
C        6.0    -1.6762241268   -0.6726312243   -2.6046343606
H        1.0    -1.6624380159   -0.4192749617   -3.6868033747
H        1.0    -2.0489563530   -1.7087048009   -2.5126666998
H        1.0    -0.6239092833   -0.6542739679   -2.2515504681
C        6.0     3.5804618503   -1.0349232352    1.2413670840
C        6.0     2.8841652269   -1.1907312732    2.6169300223
H        1.0     3.5689012058   -1.7514702769    3.2894720080
H        1.0     1.9452088732   -1.7772599684    2.5531762113
H        1.0     2.6532772592   -0.2299372520    3.1108312549
C        6.0     3.8170243648   -2.4613980572    0.6903281898
H        1.0     4.3753184357   -3.0327414140    1.4628794803
H        1.0     4.4325062724   -2.4797256524   -0.2281481207
H        1.0     2.8768003683   -3.0121788703    0.5003635682
C        6.0     4.9657520605   -0.3778960345    1.4431452945
H        1.0     5.5833139410   -1.0657828591    2.0608660775
H        1.0     4.9173841061    0.5821829407    1.9906326496
H        1.0     5.5090803230   -0.2181183767    0.4922953329
C        6.0    -3.5993012675   -1.5113224183    0.4934952263
C        6.0    -3.4124449427   -2.6479751877   -0.5399284954
H        1.0    -3.7897123516   -2.3816713887   -1.5457115958
H        1.0    -4.0071820652   -3.5224686748   -0.1980753778
H        1.0    -2.3629638649   -2.9856634221   -0.6304118741
C        6.0    -5.0958059458   -1.1221660373    0.5159141203
H        1.0    -5.6869192776   -2.0434677909    0.7096512489
H        1.0    -5.4529578840   -0.7018841437   -0.4430328343
H        1.0    -5.3409236063   -0.4106564271    1.3272528637
C        6.0    -3.2213587974   -2.0741926080    1.8899837722
H        1.0    -3.5063170248   -1.4066956485    2.7213449026
H        1.0    -2.1433024650   -2.3057421965    1.9933413272
H        1.0    -3.7740414175   -3.0274377161    2.0343027674
C        6.0     0.0503513333   -2.7625068183    0.3785310539
H        1.0     1.0466305499   -3.1786897013    0.6314775509
H        1.0    -0.6855170619   -3.3278299601    0.9874044452
H        1.0    -0.1394110433   -3.0193010176   -0.6847621958
H        1.0    -0.0387502543   -0.1783776661    2.2357542041
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Product 1Ga:

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 ATOM    CHARGE        X                Y                Z
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P       15.0     2.3946675543   -0.0490825866   -0.0009968205
GA      31.0    -0.0109158501    0.9237106463   -0.5269933774
P       15.0    -2.4074816327   -0.0515374752   -0.0222175563
C        6.0     2.6310098824   -1.8173500966   -0.7896874427
C        6.0     3.9735648303   -2.5053687963   -0.4540691815
H        1.0     4.8606887494   -1.9266536146   -0.7675909374
H        1.0     4.0104057795   -3.4777391920   -0.9928751509
H        1.0     4.0695482208   -2.7397959142    0.6242906626
C        6.0     1.4882739240   -2.7273907251   -0.2854038935
H        1.0     0.4970545344   -2.2635419584   -0.4370173107
H        1.0     1.5880560883   -3.0068998354    0.7778192685
H        1.0     1.5018363299   -3.6705413878   -0.8735380392
C        6.0     2.4734478181   -1.7041207118   -2.3261031091
H        1.0     3.3009247725   -1.1541259100   -2.8123025727
H        1.0     1.5151137874   -1.2273787671   -2.6181624360
H        1.0     2.4762527482   -2.7318111141   -2.7484430277
C        6.0     2.9032705175   -0.1052296799    1.8822464284
C        6.0     4.4297794252   -0.1940009303    2.1143976667
H        1.0     4.9770588426    0.6994636369    1.7592787134
H        1.0     4.8839217202   -1.0885623521    1.6490158808
H        1.0     4.6110196703   -0.2659085768    3.2090143890
C        6.0     2.2387484690   -1.3195259066    2.5708670433
H        1.0     1.1469306849   -1.3726820712    2.3853919656
H        1.0     2.3791100387   -1.2142618989    3.6683466075
H        1.0     2.6980303481   -2.2837961297    2.2803678522
C        6.0     2.3482344922    1.1642151438    2.5710673729
H        1.0     2.7610871252    2.1046070161    2.1658761530
H        1.0     2.6145602612    1.1240556850    3.6494704954
H        1.0     1.2436414678    1.2163132173    2.5060856123
C        6.0    -2.9513957680   -1.3105994472   -1.4169758917
C        6.0    -2.5561929940   -0.8828676205    1.7298362921
C        6.0    -3.1775532328   -0.5544442206   -2.7481106863
H        1.0    -4.0785602542    0.0862948511   -2.7357751677
H        1.0    -3.3281377583   -1.3101157762   -3.5488024970
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H	1.0	-2.2998691583	0.0586218215	-3.0362130820
C	6.0	-1.7909273018	-2.2973080909	-1.6722380887
H	1.0	-1.5652515167	-2.9414341462	-0.8038796453
H	1.0	-0.8668586357	-1.7708435095	-1.9838656980
H	1.0	-2.0781489207	-2.9704720887	-2.5093718526
C	6.0	-4.2245145420	-2.1145078620	-1.0659750578
H	1.0	-4.0791581881	-2.7916202971	-0.2017954615
H	1.0	-4.4790167171	-2.7581936407	-1.9362877481
H	1.0	-5.1042917898	-1.4752137701	-0.8659168377
C	6.0	-1.9143612656	-2.2883892096	1.6859415335
H	1.0	-1.8787945238	-2.6877579609	2.7227074360
H	1.0	-0.8725210678	-2.2667151452	1.3075569751
H	1.0	-2.4941254874	-3.0128958632	1.0824703055
C	6.0	-3.9998768602	-1.0161416756	2.2624302620
H	1.0	-3.9642506644	-1.5361458121	3.2443588811
H	1.0	-4.6484973467	-1.6171511249	1.5971529930
H	1.0	-4.4870929366	-0.0376403577	2.4361834459
C	6.0	-1.7163784976	-0.0352271998	2.7155777783
H	1.0	-1.6919987214	-0.5502581378	3.7002746941
H	1.0	-2.1219680973	0.9784614982	2.8835444726
H	1.0	-0.6665954811	0.0675081341	2.3710495530
C	6.0	3.5707613765	1.2237452328	-0.9412091722
C	6.0	2.8455491137	1.6995759940	-2.2253977831
H	1.0	3.5476645911	2.3367651677	-2.8057653506
H	1.0	1.9592542697	2.3253193191	-1.9978791030
H	1.0	2.5207803651	0.8750421565	-2.8853463555
C	6.0	3.8552114574	2.4854132722	-0.0923072238
H	1.0	4.4140765676	3.2014382888	-0.7329682634
H	1.0	4.4912881369	2.2863476465	0.7904344422
H	1.0	2.9380991793	3.0079050751	0.2411312339
C	6.0	4.9365755431	0.6077292087	-1.3230945302
H	1.0	5.5514111927	1.4027293208	-1.7985142355
H	1.0	4.8543416635	-0.2133877917	-2.0595276498
H	1.0	5.5048214974	0.2410515594	-0.4462851823
C	6.0	-3.6079164950	1.4994429069	-0.1029307670
C	6.0	-3.4624848505	2.3499903001	1.1818774352
H	1.0	-3.8790087460	1.8535458168	2.0793440764
H	1.0	-4.0426825856	3.2870431457	1.0398052915
H	1.0	-2.4165417727	2.6448428491	1.3894535226
C	6.0	-5.0987192417	1.1200430901	-0.2627645904
H	1.0	-5.6968367165	2.0565645246	-0.2162937588
H	1.0	-5.4707473968	0.4575151711	0.5413487215
H	1.0	-5.3240643655	0.6490895185	-1.2385320163
C	6.0	-3.1937102772	2.3952428515	-1.2984798195
H	1.0	-3.3324412342	1.9148453009	-2.2819350491
H	1.0	-2.1446294314	2.7393970428	-1.2280389695
H	1.0	-3.8340205480	3.3036176324	-1.2836612387
C	6.0	0.0541688524	2.7161601038	0.3573696695
H	1.0	1.0603931173	3.1601393157	0.2288648647
H	1.0	-0.6716625816	3.4130548554	-0.1066231061
H	1.0	-0.1542231415	2.6697685379	1.4442799195
H	1.0	-0.0722578406	0.6804565538	-2.0887927747

Product **1In**:

ATOM	CHARGE	X	Y	Z
P	15.0	-2.5432766020	0.1221816133	0.0195321854
IN	49.0	0.0023555299	-1.0072246905	-0.5371391410
P	15.0	2.5552613737	0.1292248612	0.0241849055
C	6.0	-2.7828436847	1.6953793020	-1.0992387068
C	6.0	-4.0612417503	2.5128486587	-0.8045776268
H	1.0	-4.9893596814	1.9228569995	-0.9213342318
H	1.0	-4.1113818659	3.3530726741	-1.5306339685
H	1.0	-4.0579074262	2.9640727879	0.2069648042
C	6.0	-1.5456235914	2.6019315907	-0.9010405145
H	1.0	-0.6027980808	2.0499177639	-1.0847601766
H	1.0	-1.4937180237	3.0643162330	0.1007587922
H	1.0	-1.5861569971	3.4297125868	-1.6417513240
C	6.0	-2.7824295274	1.2682085773	-2.5875193649
H	1.0	-3.6951842587	0.7175385614	-2.8846051445
H	1.0	-1.8944762645	0.6587082097	-2.8541885998
H	1.0	-2.7476944413	2.1896605789	-3.2080726026
C	6.0	-2.9143689643	0.5658103209	1.8809173778
C	6.0	-4.4197495008	0.7032062461	2.2042937236
H	1.0	-4.9802483346	-0.2440714478	2.0869407251
H	1.0	-4.9202771481	1.4819341834	1.5976399973
H	1.0	-4.5207097084	1.0049543954	3.2697113720
C	6.0	-2.2176760481	1.8952787213	2.2504719881
H	1.0	-1.1343183019	1.8926209857	2.0137159503
H	1.0	-2.3118706369	2.0430095210	3.3481771636
H	1.0	-2.6833669505	2.7750629337	1.7667364236
C	6.0	-2.2885261632	-0.5342551075	2.7720542303
H	1.0	-2.7293892140	-1.5348468121	2.6187415064
H	1.0	-2.4494806230	-0.2605072144	3.8372818237
H	1.0	-1.1938309590	-0.6116894664	2.6147469128
C	6.0	3.1524253780	1.2006442364	-1.4960073933
C	6.0	2.5943611749	1.2029082281	1.6453545678
C	6.0	3.4651191727	0.2681694875	-2.6911547663
H	1.0	4.3853508645	-0.3309836654	-2.5534653141
H	1.0	3.6283289551	0.9023093172	-3.5892412237
H	1.0	2.6216238232	-0.4138677328	-2.9216514441
C	6.0	1.9790754562	2.0983673984	-1.9506293332
H	1.0	1.6702788472	2.8469366295	-1.1985252349
H	1.0	1.0974087465	1.4915079178	-2.2391084261

H	1.0	2.2977026645	2.6583400984	-2.8565391640
C	6.0	4.3881395041	2.0796078121	-1.2000137249
H	1.0	4.1833013662	2.8684498568	-0.4500752010
H	1.0	4.6805570797	2.5991008163	-2.1387182974
H	1.0	5.2660719016	1.4970532604	-0.8625314060
C	6.0	1.9533148880	2.5819685149	1.3657820799
H	1.0	1.8229424453	3.1071417055	2.3363401409
H	1.0	0.9500296855	2.4931936182	0.9009185945
H	1.0	2.5799639321	3.2328162658	0.7267537796
C	6.0	4.0058894226	1.4190860050	2.2366756252
H	1.0	3.9221107935	2.0907730485	3.1193614929
H	1.0	4.7013754450	1.9016725760	1.5240829251
H	1.0	4.4693827809	0.4801290551	2.5957035930
C	6.0	1.6967630506	0.5006053567	2.6930613350
H	1.0	1.6638041982	1.1254780543	3.6116415826
H	1.0	2.0569420594	-0.5009532914	2.9878983530
H	1.0	0.6533115624	0.3969136593	2.3289432855
C	6.0	-3.7763606120	-1.2833514886	-0.5635830391
C	6.0	-3.1714088908	-1.9724662761	-1.8125369358
H	1.0	-3.8650862186	-2.7793905966	-2.1330822567
H	1.0	-2.1990645029	-2.4578623806	-1.5887519323
H	1.0	-3.0321988824	-1.2961763594	-2.6745138102
C	6.0	-3.9067008622	-2.3753214484	0.5251601310
H	1.0	-4.4855348546	-3.2207106112	0.0945075351
H	1.0	-4.4606693937	-2.0353855821	1.4209997421
H	1.0	-2.9281609110	-2.7835597830	0.8467359459
C	6.0	-5.1903992734	-0.7600919083	-0.9043961844
H	1.0	-5.8325004862	-1.6298194978	-1.1641002030
H	1.0	-5.1964100468	-0.0847823704	-1.7812738145
H	1.0	-5.6753191580	-0.2391471290	-0.0565216748
C	6.0	3.7552326231	-1.4022954031	0.2225836709
C	6.0	3.5008562814	-2.0694256098	1.5949216653
H	1.0	3.8374439612	-1.4472642078	2.4459472771
H	1.0	4.0831876787	-3.0153418407	1.6383680314
H	1.0	2.4362555079	-2.3366604460	1.7458448328
C	6.0	5.2555755285	-1.0498313936	0.1119408638
H	1.0	5.8421699056	-1.9836071064	0.2538662997
H	1.0	5.5930933778	-0.3312083602	0.8827386500
H	1.0	5.5311069757	-0.6507554841	-0.8833478425
C	6.0	3.4050607261	-2.4517569576	-0.8643586983
H	1.0	3.6750717766	-2.1378639513	-1.8876283165
H	1.0	2.3306354029	-2.7239860048	-0.8550595416
H	1.0	3.9750206509	-3.3811807034	-0.6482732354
C	6.0	-0.0796353636	-2.8644051735	0.6367502620
H	1.0	-0.9131594504	-3.4896567585	0.2591232150
H	1.0	0.8575570324	-3.4417225954	0.5238882800
H	1.0	-0.2487076942	-2.6526859677	1.7100495019
H	1.0	0.0581776139	-0.7855472325	-2.2666957962

Product **1Tl**:

ATOM	CHARGE	X	Y	Z
P	15.0	-2.6282410575	0.2555687480	0.0499585467
TL	81.0	-0.0012178206	-1.0600516482	-0.4040422701
P	15.0	2.6490048905	0.2406413099	0.0525819401
C	6.0	-2.8472212955	1.7362450052	-1.2001645002
C	6.0	-4.1137930162	2.5935173585	-0.9821673493
H	1.0	-5.0509694156	2.0113280332	-1.0617130272
H	1.0	-4.1463778082	3.3796838637	-1.7681459439
H	1.0	-4.1104912942	3.1189158109	-0.0070309250
C	6.0	-1.5975875525	2.6401105813	-1.0727988570
H	1.0	-0.6592188810	2.0682005578	-1.2176355464
H	1.0	-1.5379420067	3.1703643740	-0.1058006324
H	1.0	-1.6324810459	3.4165519519	-1.8680346629
C	6.0	-2.8471414036	1.1841922208	-2.6455577115
H	1.0	-3.7575257707	0.6051458065	-2.8905260071
H	1.0	-1.9578402062	0.5534442881	-2.8522027910
H	1.0	-2.8093062640	2.0441279682	-3.3484033628
C	6.0	-3.0225616718	0.8676421511	1.8599078744
C	6.0	-4.5266346018	1.0596546596	2.1563778057
H	1.0	-5.1036718319	0.1168260880	2.0947221254
H	1.0	-5.0027625062	1.8024446707	1.4881546833
H	1.0	-4.6360057624	1.4363020271	3.1969139811
C	6.0	-2.2954757381	2.2069452252	2.1246940862
H	1.0	-1.2123818427	2.1563919855	1.8896771362
H	1.0	-2.3832928457	2.4406467712	3.2077979374
H	1.0	-2.7398235826	3.0590178721	1.5752723835
C	6.0	-2.4253441111	-0.1609042981	2.8513367570
H	1.0	-2.8988590546	-1.1572455311	2.7968707589
H	1.0	-2.5723725660	0.2164127364	3.8864563498
H	1.0	-1.3350414368	-0.2876472579	2.6971133270
C	6.0	3.2170672516	1.1520554524	-1.5824900653
C	6.0	2.6570329191	1.4987618379	1.5402856005
C	6.0	3.5483494028	0.1044420554	-2.6725772817
H	1.0	4.4696569759	-0.4691610495	-2.4592620492
H	1.0	3.7199617978	0.6454625889	-3.6283785752
H	1.0	2.7128664323	-0.6048004903	-2.8462726187
C	6.0	2.0108556919	1.9617360920	-2.1141075343
H	1.0	1.7025099866	2.7829555636	-1.4434932425
H	1.0	1.1394276100	1.3015631485	-2.2968336791
H	1.0	2.2896415913	2.4198030795	-3.0880116720
C	6.0	4.4273992987	2.0954201449	-1.4036311229
H	1.0	4.2081618845	2.9453177366	-0.7286735607
H	1.0	4.6851261791	2.5309591384	-2.3939569528

H	1.0	5.3307456511	1.5769324722	-1.0299928278
C	6.0	1.9488246682	2.8025090281	1.1068788017
H	1.0	1.8022816954	3.4409219355	2.0053912286
H	1.0	0.9450549171	2.6145350327	0.6728107317
H	1.0	2.5409851475	3.3953461029	0.3838966257
C	6.0	4.0621253641	1.8518064221	2.0789684061
H	1.0	3.9525443818	2.5892465081	2.9042526492
H	1.0	4.7105834377	2.3140098277	1.3104662952
H	1.0	4.5918758961	0.9763224688	2.5016076946
C	6.0	1.8082357344	0.8879292838	2.6824409382
H	1.0	1.7524814650	1.6231189860	3.5142692089
H	1.0	2.2334942091	-0.0435676105	3.0961958224
H	1.0	0.7684459424	0.6817456326	2.3534757142
C	6.0	-3.8792461172	-1.1759548590	-0.4301832212
C	6.0	-3.2763149400	-1.9784849312	-1.6125963592
H	1.0	-4.0055739543	-2.7630470699	-1.9103810507
H	1.0	-2.3429223647	-2.5133292557	-1.3332180609
H	1.0	-3.0663897676	-1.3688470876	-2.5093520307
C	6.0	-4.0300813982	-2.1737173981	0.7416175000
H	1.0	-4.6047490141	-3.0526815524	0.3770756852
H	1.0	-4.5906169063	-1.7622501762	1.6026796508
H	1.0	-3.0542686719	-2.5530835965	1.1050601845
C	6.0	-5.2864311969	-0.6709440991	-0.8227162544
H	1.0	-5.9396144164	-1.5508264994	-1.0137965589
H	1.0	-5.2846951850	-0.0687010866	-1.7514258420
H	1.0	-5.7672167449	-0.0769474119	-0.0219208533
C	6.0	3.8979250083	-1.2166348385	0.4277904203
C	6.0	3.7112963297	-1.7170813125	1.8788097679
H	1.0	4.0711568886	-0.9968439450	2.6385740427
H	1.0	4.3104535303	-2.6446542419	2.0073684868
H	1.0	2.6585705137	-1.9785840876	2.1050356212
C	6.0	5.3832630958	-0.8397051042	0.2253857282
H	1.0	6.0125310943	-1.7077100184	0.5209981762
H	1.0	5.6961337856	0.0179016855	0.8508954974
H	1.0	5.6277054301	-0.6107262529	-0.8294924724
C	6.0	3.5425467484	-2.4072136236	-0.5003248221
H	1.0	3.6316129342	-2.1773272053	-1.5766680978
H	1.0	2.5194935972	-2.7953621225	-0.3137007386
H	1.0	4.2438062002	-3.2421532975	-0.2836285246
C	6.0	-0.0324970515	-2.5154784168	1.2738262760
H	1.0	-1.0570507139	-2.9175590283	1.3747078206
H	1.0	0.6738493649	-3.3323218829	1.0339861305
H	1.0	0.2695158229	-2.0007211626	2.2032482792
H	1.0	0.0448124463	-0.8219689398	-2.1237275153

H	1.0	2.2054709584	-1.3125151419	6.1962838287
C	6.0	3.6412903275	0.6785806606	2.9916442237
H	1.0	4.4460693827	1.4434237565	2.9424947132
H	1.0	3.3358936723	0.4635602002	1.9485485646
H	1.0	4.0875106327	-0.2346898818	3.4300581385
C	6.0	2.9994942241	1.5271350841	5.2588988666
H	1.0	3.8634329381	2.2234825031	5.1767787992
H	1.0	3.3682929532	0.6254273243	5.7815977496
H	1.0	2.2541383770	2.0305798973	5.9031198656
C	6.0	2.0320349034	2.5730185914	3.1901207589
H	1.0	2.9191782539	3.2291241802	3.0545296722
H	1.0	1.3051861984	3.1303635169	3.8104237182
H	1.0	1.5829670648	2.4077398304	2.1896251068
C	6.0	-1.8726688346	-0.2736652140	-0.6845691850
C	6.0	-2.6429455569	-1.1623730623	0.3176868742
H	1.0	-3.7137707579	-1.1810381186	0.0203183707
H	1.0	-2.5610279112	-0.8052371996	1.3604288817
H	1.0	-2.2831424354	-2.2083093625	0.3097601353
C	6.0	-2.6174552021	1.0730057765	-0.8680337778
H	1.0	-3.6846205087	0.8450861949	-1.0784083247
H	1.0	-2.2426801378	1.6495740300	-1.7350428256
H	1.0	-2.5956519783	1.7289682343	0.0153636354
C	6.0	-1.9248683881	-0.9711116959	-2.0654168586
H	1.0	-2.9889221316	-0.9837034516	-2.3866944581
H	1.0	-1.5995641535	-2.0278025120	-2.0362390311
H	1.0	-1.3587796798	-0.4409422325	-2.8536089362
C	6.0	-0.3183058156	0.4095214882	5.1994710522
C	6.0	-0.5309649372	1.9413584678	5.2983687441
H	1.0	0.3750420627	2.4603795238	5.6637661146
H	1.0	-1.3296969068	2.1286104062	6.0476244714
H	1.0	-0.8432497665	2.4279502087	4.3623086960
C	6.0	0.2246455312	-0.0057829285	6.5902800291
H	1.0	-0.5136120815	0.3609143074	7.3366117432
H	1.0	1.1949887326	0.4540767706	6.8523506126
H	1.0	0.2924140146	-1.0989696455	6.7352790786
C	6.0	-1.6673125866	-0.3400951349	4.9847774859
H	1.0	-1.7358842892	-1.2365644109	5.6295321034
H	1.0	-1.8140228197	-0.6766685440	3.9389069679
H	1.0	-2.5167582028	0.3162428135	5.2675443815
C	6.0	-1.7064123519	2.8554199442	2.1153865021
C	6.0	-2.1878565032	1.6274040036	2.4397811022
H	1.0	-1.9663878300	3.3508564059	1.1678965709
H	1.0	-1.0764807908	3.4483685195	2.7990766325
H	1.0	-2.9064524339	1.1063404830	1.7937507131
H	1.0	-2.0694931541	1.2048348195	3.4388253954

Transition states of the reactions with ethene

Transition state **TS2B**:

ATOM	CHARGE	X	Y	Z
P	15.0	-0.0054163221	0.0051974241	0.0009799846
B	5.0	-0.0353314805	-0.0261618043	1.9678927971
P	15.0	0.9329257323	-0.0117907719	3.6752985624
C	6.0	1.0371332137	-1.5803034423	-0.5621253719
C	6.0	1.2251853655	-1.7484449816	-2.0897112998
H	1.0	0.2933784142	-1.8593806763	-2.6671069859
H	1.0	1.8050979250	-2.6877212281	-2.2301841032
H	1.0	1.8337558637	-0.9403184104	-2.5366308272
C	6.0	2.4722365404	-1.4844810262	0.0112346241
H	1.0	2.5170977228	-1.0197992329	1.0076310367
H	1.0	3.1384915199	-0.9089520491	-0.6548912984
H	1.0	2.9013749670	-2.5056678828	0.0878293137
C	6.0	0.3045381536	-2.8405669472	-0.0352973119
H	1.0	-0.6120328794	-3.0495978281	-0.6186431484
H	1.0	0.0095526686	-2.7638633894	1.0291505411
H	1.0	0.9731852685	-3.7197842944	-0.1556027260
C	6.0	0.7590372572	1.5697043238	-1.0111075997
C	6.0	0.4502470237	1.5407572215	-2.5245729967
H	1.0	-0.6234908407	1.6828538665	-2.7493923031
H	1.0	0.7951531082	0.6237931585	-3.0344289568
H	1.0	0.9870979021	2.3934106388	-2.9958739251
C	6.0	2.2886462363	1.5844056299	-0.8092009436
H	1.0	2.5738712108	1.4616267855	0.2546102083
H	1.0	2.6770766988	2.5708824948	-1.1419864627
H	1.0	2.8118339480	0.8173999330	-1.4095672124
C	6.0	0.2139425906	2.8873768089	-0.4365137495
H	1.0	-0.8654657537	3.0260082081	-0.6232194173
H	1.0	0.7422411298	3.7277423212	-0.9365299337
H	1.0	0.4007843769	2.9813159671	0.6507864504
C	6.0	1.5589614501	-1.8598190801	4.1101632108
C	6.0	2.4787648009	1.2442151259	3.8329971054
C	6.0	0.3321835770	-2.7395950358	4.4444593571
H	1.0	-0.1486318252	-2.4823993097	5.4040321183
H	1.0	0.6806809197	-3.7912024002	4.5324633959
H	1.0	-0.4360100346	-2.7021289281	3.6467282628
C	6.0	2.2969722747	-2.5636628852	2.9601121640
H	1.0	3.2010800458	-2.0295595033	2.6188070680
H	1.0	1.6405287893	-2.7617105061	2.0988497377
H	1.0	2.6315401095	-3.5518035710	3.3433037882
C	6.0	2.5539087764	-1.8427874400	5.2964243034
H	1.0	3.5408281154	-1.4345318152	5.0056849360
H	1.0	2.7238172284	-2.9015524333	5.5902690751

Transition state **TS2Al**:

ATOM	CHARGE	X	Y	Z
P	15.0	0.0020923274	0.0014604179	-0.0064799610
AL	13.0	-0.0073438551	-0.0620280593	2.6357903016
P	15.0	2.1409420052	0.0046123842	4.3601143513
C	6.0	1.1637213141	-1.1947862269	-1.0557685037
C	6.0	1.4175307432	-0.7291770782	-2.5076120708
H	1.0	0.4902248855	-0.6617745150	-3.1073063186
H	1.0	2.0688141163	-1.4829699656	-3.0017748333
H	1.0	1.9488031998	0.2387759215	-2.5701708400
C	6.0	2.5073178059	-1.3010234548	-0.2993625602
H	1.0	2.3527838288	-1.6196080209	0.7523099640
H	1.0	3.0885947435	-0.3604242269	-0.3036896729
H	1.0	3.1363527279	-2.0743044789	-0.7912810625
C	6.0	0.5637031357	-2.6178667676	-1.1093531990
H	1.0	-0.3669434347	-2.6786903482	-1.7051036234
H	1.0	0.3777630515	-3.0358433143	-0.1017504183
H	1.0	1.3047284719	-3.2823293741	-1.6037723220
C	6.0	0.4812289839	1.8556129879	-0.4448573856
C	6.0	-0.0247235664	2.3300479879	-1.8278962635
H	1.0	-1.1277869210	2.4034727336	-1.8763902793
H	1.0	0.3233402079	1.6970210858	-2.6649096350
H	1.0	0.3690318847	3.3542900508	-2.0077761043
C	6.0	2.0200896047	2.0154800054	-0.4160542245
H	1.0	2.4780929680	1.6388340267	0.5179851080
H	1.0	2.2554351888	3.0996361073	-0.4789786551
H	1.0	2.5231051607	1.5265695778	-1.2710333656
C	6.0	-0.1080525198	2.7987191536	0.6312300532
H	1.0	-1.2117451571	2.8115977000	0.6452578396
H	1.0	0.2363176529	3.8342306027	0.4191382463
H	1.0	0.2258426117	2.5363664522	1.6563559522
C	6.0	3.0400865093	-1.6946232412	4.7976690120
C	6.0	3.4992078648	1.2947022924	3.7970125398
C	6.0	2.0524875932	-2.5900902825	5.5844107202
H	1.0	1.8540792205	-2.2172532994	6.6074700609
H	1.0	2.5059559632	-3.5989622573	5.6924339683
H	1.0	1.0820111287	-2.7252547601	5.0668472574
C	6.0	3.3862699788	-2.4231266113	3.4770641888
H	1.0	4.2391750805	-1.9682965023	2.9418573920
H	1.0	2.5274395240	-2.4599819019	2.7786005852
H	1.0	3.6722200277	-3.4713301865	3.7119313128
C	6.0	4.3394640607	-1.5519693542	5.6215340367
H	1.0	5.1391746438	-1.0205783679	5.0699182076
H	1.0	4.7244962960	-2.5738408538	5.8323081844
H	1.0	4.1941314477	-1.0521599155	6.5970910229
C	6.0	4.3760904814	0.6299919225	2.7096803160
H	1.0	5.0215313151	1.4109636079	2.2530216215

H	1.0	3.7747798150	0.1749301068	1.8964989095
H	1.0	5.0518022409	-0.1442210304	3.1197652970
C	6.0	4.4217182129	1.8175777120	4.9213511709
H	1.0	5.1801537625	2.4869925104	4.4590476611
H	1.0	4.9705588179	1.0153812446	5.4474893765
H	1.0	3.8813528400	2.4249535485	5.6728084496
C	6.0	2.7943228306	2.5075466743	3.1470665918
H	1.0	3.5509189219	3.1128613769	2.6027475438
H	1.0	2.3060994533	3.1757676811	3.8772662553
H	1.0	2.0275161025	2.1948066314	2.4139187620
C	6.0	-1.8671438100	-0.2641507240	-0.5519409592
C	6.0	-2.4166335575	-1.5610872027	0.0853034696
H	1.0	-3.4652597175	-1.6973654274	-0.2564779999
H	1.0	-2.4456690473	-1.4926840148	1.1877429708
H	1.0	-1.8593836528	-2.4699555923	-0.2034819549
C	6.0	-2.7478642406	0.8935337172	-0.0224299139
H	1.0	-3.8109639397	0.6257056917	-0.2059476676
H	1.0	-2.5672613324	1.8533265405	-0.5424473441
H	1.0	-2.6332631168	1.0533196180	1.0703604668
C	6.0	-2.0399122285	-0.3730299555	-2.0856282821
H	1.0	-3.1269852842	-0.4705508650	-2.2976457351
H	1.0	-1.5532115996	-1.2740369194	-2.5058497100
H	1.0	-1.6790870111	0.5120075389	-2.6397977977
C	6.0	1.2977050431	0.7106966233	5.9932462875
C	6.0	0.9434318321	2.2021758613	5.7886245105
H	1.0	1.8327559086	2.8585443895	5.7642751319
H	1.0	0.3229781605	2.5290188653	6.6508220559
H	1.0	0.3395589854	2.3688495295	4.8716272900
C	6.0	2.1854980823	0.5758423408	7.2510542556
H	1.0	1.6664469610	1.0787604738	8.0961132787
H	1.0	3.1731639555	1.0604616350	7.1408950663
H	1.0	2.3429128950	-0.4766623411	7.5557440412
C	6.0	-0.0449261030	-0.0146573353	6.2469247294
H	1.0	0.0582303299	-1.1068408746	6.3840003205
H	1.0	-0.7716007894	0.1881640826	5.4328320094
H	1.0	-0.4873757804	0.3892420760	7.1831287033
C	6.0	-0.2318339930	-2.5397624505	2.5416258932
C	6.0	-1.0680920666	-1.7330884852	3.3569588344
H	1.0	-0.5928505180	-2.9271325218	1.5806855698
H	1.0	0.6743083806	-3.0087300183	2.9494237056
H	1.0	-0.8573558550	-1.6757607283	4.4384186483
H	1.0	-2.1398496367	-1.6181603751	3.1187218376

Transition state **TS2Ga**:

ATOM	CHARGE	X	Y	Z
P	15.0	2.3651518092	0.0744367525	0.0180131398
GA	31.0	0.0348153507	-0.8007464943	-0.5346472301
P	15.0	-2.3673814855	0.0601378279	0.0074847587
C	6.0	2.7981213149	0.3436871471	1.9156353412
C	6.0	4.0211809391	1.2552799644	2.1633725583
H	1.0	4.9476226633	0.8743317705	1.6949757008
H	1.0	4.2032028071	1.2936388139	3.2596639246
H	1.0	3.8632719748	2.2995925128	1.8329732379
C	6.0	1.5518051184	0.9433061891	2.6019185554
H	1.0	0.6605998613	0.3032844162	2.4382438053
H	1.0	1.3214061249	1.9727818969	2.2727114560
H	1.0	1.7344747735	0.9837964023	3.6974811264
C	6.0	3.0562643396	-1.0254541766	2.5852363043
H	1.0	4.0017399946	-1.5021438903	2.2624229353
H	1.0	2.2183297585	-1.7295930069	2.4185386722
H	1.0	3.1385558869	-0.8606249627	3.6810689385
C	6.0	2.5461836950	1.7854842584	-0.9325740577
C	6.0	4.0026854433	2.2312433465	-1.2027484000
H	1.0	4.5382385822	1.5654588898	-1.9057948777
H	1.0	4.6049194464	2.3363318141	-0.2805920111
H	1.0	3.9651572103	3.2331576562	-1.6831296842
C	6.0	1.8715681829	2.8945249534	-0.0908636204
H	1.0	0.8419070514	2.6416811429	0.2213405108
H	1.0	1.8097681596	3.8143019126	-0.7112258426
H	1.0	2.4568130886	3.1534062523	0.8113214382
C	6.0	1.8106872325	1.6797327215	-2.2912615697
H	1.0	2.3709423939	1.0885068622	-3.0378747077
H	1.0	1.6757311672	2.7001842665	-2.7094601235
H	1.0	0.8093060820	1.2099794612	-2.1937128981
C	6.0	-3.1569501472	-0.7275523415	1.6321235669
C	6.0	-2.4569085110	2.0102596216	0.1369656783
C	6.0	-3.4834878238	-2.2166701185	1.3664599432
H	1.0	-4.3350541133	-2.3586718641	0.6741696466
H	1.0	-3.7743332903	-2.6827496511	2.3327039186
H	1.0	-2.6174723780	-2.7892760631	0.9815683072
C	6.0	-2.1056267714	-0.6693887217	2.7648140299
H	1.0	-1.9143694953	0.3579464759	3.1244591117
H	1.0	-1.1425852091	-1.1180201561	2.4516997057
H	1.0	-2.4887574125	-1.2518569197	3.6304084811
C	6.0	-4.4445761470	-0.0228752840	2.1147113911
C	6.0	-4.2658377876	1.0163373618	2.4521406873
H	1.0	-4.8286991639	-0.5792907037	2.9978133225
H	1.0	-5.2536478726	-0.0151816926	1.3605405764
C	6.0	-1.8494382053	2.4232465647	1.4981234588
H	1.0	-1.7455718935	3.5294641351	1.5177906742
H	1.0	-0.8431349406	1.9895722290	1.6582828945
H	1.0	-2.4894140760	2.1446322145	2.3568984120
C	6.0	-3.8783887355	2.6081767539	0.0237143189

H	1.0	-3.7962275519	3.7068747552	0.1752061249
H	1.0	-4.5832612573	2.2268358743	0.7841094997
H	1.0	-4.3228666295	2.4596924050	-0.9789233003
C	6.0	-1.5927651289	2.6390461846	-0.9818152448
H	1.0	-1.3871415498	3.6987694775	-0.7182796864
H	1.0	-2.0950257814	2.6429908493	-1.9644122624
H	1.0	-0.6198532347	2.1304463780	-1.1057384442
C	6.0	3.6613433385	-1.1767905582	-0.7708914862
C	6.0	3.3916037978	-2.6367723540	-0.3379717465
H	1.0	4.1988982312	-3.2680647471	-0.7680854453
H	1.0	2.4391270214	-3.0199302162	-0.7402606461
H	1.0	3.4085977263	-2.7944920590	0.7544198467
C	6.0	3.5358749573	-1.1374104240	-2.3129670780
H	1.0	4.1482413084	-1.9670360322	-2.7274862152
H	1.0	3.9265680673	-0.2017877174	-2.7555260767
H	1.0	2.4931368432	-1.2880937901	-2.6616481989
C	6.0	5.1142898451	-0.8299393671	-0.3641800831
H	1.0	5.7935998372	-1.4926793534	-0.9432824635
H	1.0	5.3153687032	-1.0293263604	0.7064254207
H	1.0	5.4043561326	0.2108817621	-0.5899971659
C	6.0	-3.4444866323	-0.4733575385	-1.5512604159
C	6.0	-3.0897549428	0.4232879760	-2.7598981763
H	1.0	-3.4887341057	1.4512214536	-2.6718266546
H	1.0	-3.5536735888	-0.0252941839	-3.6646516281
H	1.0	-1.9960381916	0.4691823919	-2.9418081009
C	6.0	-4.9653955318	-0.3797606539	-1.2831126265
H	1.0	-5.4928792670	-0.5859664876	-2.2398022058
H	1.0	-5.2934338797	0.6180114968	-0.9389543772
H	1.0	-5.3210862366	-1.1352886553	-0.5564937647
C	6.0	-3.1066047500	-1.9194297977	-1.9832268342
H	1.0	-3.2256158070	-2.6677097895	-1.1787129740
H	1.0	-2.0814846288	-1.9852689900	-2.3969908039
H	1.0	-3.8077440990	-2.2025764328	-2.7975754075
C	6.0	0.1589023218	-2.6651467733	0.7153433550
H	1.0	1.1468861065	-2.9053974015	1.1333049080
H	1.0	-0.6751030433	-2.8662774383	1.4037509834
C	6.0	-0.0581225154	-2.8436921223	-0.7175651184
H	1.0	-1.0654762562	-3.1232180542	-1.0612750034
H	1.0	0.7319699466	-3.2567843455	-1.3676404860

Transition state **TS2In**:

ATOM	CHARGE	X	Y	Z
P	15.0	2.5105193862	0.2006802246	-0.0753643739
IN	49.0	0.0189861314	-0.8362518856	-0.1321644526
P	15.0	-2.4966883800	0.1460402781	0.0398953731
C	6.0	3.0286762949	0.4520790799	1.7932450935
C	6.0	4.3061389685	1.3021721933	1.9817838829
H	1.0	5.1908794842	0.8683500836	1.4787952158
H	1.0	4.5370505040	1.3410660939	3.0685959633
H	1.0	4.1892310352	2.3494194412	1.6437434581
C	6.0	1.8368936884	1.1108753024	2.5262311907
H	1.0	0.9229168020	0.4873497345	2.4174856748
H	1.0	1.6112246236	2.1374835695	2.1849231805
H	1.0	2.0743925754	1.1671252605	3.6102824387
C	6.0	3.2393988890	-0.9299901162	2.4531598346
H	1.0	4.1562932306	-1.4457680481	2.1077968692
H	1.0	2.3640434721	-1.5935515085	2.3028695263
H	1.0	3.3520969459	-0.7735462226	3.5474497298
C	6.0	2.6466489581	1.9006763176	-1.0338652665
C	6.0	4.0915888138	2.2516300211	-1.4628984499
H	1.0	4.5057070466	1.5563715818	-2.2168232507
H	1.0	4.7929137066	2.3077509749	-0.6080409147
H	1.0	4.0720572823	3.2578598378	-1.9347903480
C	6.0	2.1373864555	3.0656048628	-0.1538175970
H	1.0	1.1241126995	2.8991070361	0.2528415475
H	1.0	2.0878641441	3.9765568594	-0.7885264357
H	1.0	2.8165821493	3.2973070670	0.6878120346
C	6.0	1.7483680495	1.8194779252	-2.2922117887
H	1.0	2.0891872593	1.0651951135	-3.0238181201
H	1.0	1.7601998343	2.8068282196	-2.8029178535
H	1.0	0.6940471685	1.5864714760	-2.0389918079
C	6.0	-3.4649688429	-0.8710832018	1.4081374919
C	6.0	-2.5601327825	0.2046667886	0.4803706215
C	6.0	-3.7245647099	-2.3075518741	0.8967108676
H	1.0	-4.4689951615	-2.3470776192	0.0781577835
H	1.0	-4.1419898357	-2.8990393522	1.7396141742
H	1.0	-2.8034332929	-2.8266160087	0.5662498416
C	6.0	-2.5874720986	-0.9732144168	2.6789940892
H	1.0	-2.4724180517	-0.0086418526	3.2040388793
H	1.0	-1.5781870857	-1.3745403564	2.4597164039
H	1.0	-3.0870056148	-1.6702065845	3.3860603936
C	6.0	-4.8184147609	-0.0283760189	1.7864062472
H	1.0	-4.7007198697	0.7577010079	2.2760255013
H	1.0	-5.3193602454	-0.8920387689	2.5245515115
H	1.0	-5.5094632646	-0.1154851814	0.9296838139
C	6.0	-2.1762468282	2.2322091704	1.9671752141
H	1.0	-2.0569962085	3.3201393722	2.1606850199
H	1.0	-1.2151463052	1.7431467628	2.2279043479
C	6.0	-2.9551708187	1.8673050441	2.6628102702
C	6.0	-3.9292650321	2.7177073715	2.2255839510
H	1.0	-3.8579924479	3.7799083346	0.5468141370
H	1.0	-4.7567803923	2.2586123075	0.7971454015
H	1.0	-4.2031916901	2.7275697159	-0.8469167082

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  C         6.0    -1.4924584980     2.7730597313    -0.3652388087
  H         1.0    -1.3156362857     3.7824924265     0.0639616173
  H         1.0    -1.7848268985     2.9117105477    -1.4208163726
  H         1.0    -0.5299517430     2.2278957756    -0.3492229761
  C         6.0     3.6814343589    -1.1045756057    -0.9435532441
  C         6.0     3.3249572301    -2.5323812478    -0.4739216427
  H         1.0     3.9963118808    -3.2404825471    -1.0058136914
  H         1.0     2.2896427142    -2.8058896267    -0.7433210613
  H         1.0     3.4705029047    -2.6976115590     0.6079465723
  C         6.0     3.4428092115    -1.0702433393    -2.4715190133
  H         1.0     4.0133534767    -1.9089894119    -2.9253269291
  H         1.0     3.8000461032    -0.1408663068    -2.9534046607
  H         1.0     2.3742096789    -1.2241425581    -2.7294919823
  C         6.0     5.1744733627    -0.8474794500    -0.6325448520
  H         1.0     5.7753725530    -1.5813554132    -1.2123669017
  H         1.0     5.4114098457    -1.0136453498     0.4361285430
  H         1.0     5.5228943911     0.1603079774    -0.9212266364
  C         6.0    -3.3267363686    -0.1338751901    -1.7196795564
  C         6.0    -2.7712339792     0.9121318600    -2.7122901261
  H         1.0    -3.1443925511     1.9366963816    -2.5214577071
  H         1.0    -3.1104934902     0.6313355656    -3.7321865376
  H         1.0    -1.6613518154     0.9269582196    -2.7332001371
  C         6.0    -4.8691674765    -0.0298072879    -1.6797918401
  H         1.0    -5.2478703690    -0.1074787342    -2.7221975424
  H         1.0    -5.2377135359     0.9298113309    -1.2717825802
  H         1.0    -5.3362400508    -0.8561232941    -1.1095045615
  C         6.0    -2.9351136093    -1.5233227970    -2.2758072759
  H         1.0    -3.3118006292    -2.3620441325    -1.6634562064
  H         1.0    -1.8370808944    -1.6336519816    -2.3849096800
  H         1.0    -3.3896051061    -1.6217736155    -3.2847352792
  C         6.0     0.0781135270    -2.8191564650     0.9711691400
  H         1.0     1.0679037940    -3.1456941638     1.3341685617
  H         1.0    -0.7275767465    -3.1095849114     1.6686495605
  C         6.0    -0.1830482567    -3.0158791657    -0.5062164134
  H         1.0    -1.2136542756    -3.2756078771    -0.8051690017
  H         1.0     0.5576038919    -3.5523244407    -1.1253251483
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Transition state **TS2Tl**:

ATOM	CHARGE	X	Y	Z
	15.0	2.5278353861	0.3430845454	-0.0293790128
TL	81.0	0.0357010825	-0.7809646832	-0.1155827161
P	15.0	-2.5401027340	0.2162267880	0.1138584344
C	6.0	3.0866206150	0.4629034880	1.8383815988
C	6.0	4.3875186861	1.2720399812	2.0465465658
H	1.0	5.2558668233	0.8391045502	1.5153437099
H	1.0	4.6305124049	1.2597848086	3.1313486723
H	1.0	4.2916651896	2.3348107158	1.7534769997
C	6.0	1.9267505003	1.1098402599	2.6306668041
H	1.0	0.9871233955	0.5354197507	2.4833089263
H	1.0	1.7430137057	2.1679055340	2.3704318997
H	1.0	2.1751027075	1.0734273059	3.7130105759
C	6.0	3.2722365875	-0.9613636017	2.4075442541
H	1.0	4.1806585780	-1.4687651786	2.0284389866
H	1.0	2.3872004614	-1.6040801569	2.2168124040
H	1.0	3.3873933870	-0.8804281511	3.5099236339
C	6.0	2.6281918878	2.1097288752	-0.8757333118
C	6.0	4.0500367618	2.4488095082	-1.3845111320
H	1.0	4.4036568335	1.7772007051	-2.1878300557
H	1.0	4.8028188634	2.4611295108	-0.5722453999
H	1.0	4.0196917828	3.4734582383	-1.8144136495
C	6.0	2.2109961416	3.2443706778	0.0875240424
H	1.0	1.2043856146	3.1024353372	0.5178237827
H	1.0	2.1820923771	4.1875715041	-0.4996220127
H	1.0	2.9301249290	3.4056432626	0.9126223991
C	6.0	1.6293097097	2.1100855856	-0.0553731056
H	1.0	1.8181626748	1.3087525952	-2.7928135955
H	1.0	1.7000910009	3.0839647610	-2.5867882828
H	1.0	0.5874481179	1.9982286979	-1.6935216452
C	6.0	-3.6444970891	-1.0924902843	1.0661992942
C	6.0	-2.5704198061	1.9047907624	1.0801063573
C	6.0	-3.8780338029	-2.3197091217	0.1551769672
H	1.0	-4.5390816969	-2.1013388053	-0.7051704780
H	1.0	-4.3846867236	-3.1038883913	0.7578986306
H	1.0	-2.9329463650	-2.7589679500	-0.2208987245
C	6.0	-2.8788158681	-1.5782785593	2.3209229988
H	1.0	-2.8590626537	-0.8312020099	3.1342324221
H	1.0	-1.8353213402	-1.8601240634	2.0799694231
H	1.0	-3.3990417561	-2.4766837389	2.7167514550
C	6.0	-5.0143668330	-0.5199373581	1.4970429384
H	1.0	-4.9235998643	0.3007917661	2.2342548892
H	1.0	-5.5821252317	-1.3351441578	1.9964730628
H	1.0	-5.6306409907	-0.1667660368	0.6490867450
C	6.0	-2.3730730078	1.6446636558	2.5912226211
H	1.0	-2.2032893215	2.6225858275	3.0910794124
H	1.0	-1.4884296282	1.0075764670	2.7949001163
H	1.0	-3.2574856988	1.1852527345	3.0708388096
C	6.0	-3.8576447083	2.7351804478	0.8729469427
H	1.0	-3.7673360150	3.6649918951	1.4756912136
H	1.0	-4.7699605373	2.2113053892	1.2157161504
H	1.0	-4.0056378092	3.0469939948	-0.1787396229
C	6.0	-1.3468304724	2.7137781918	0.6068512519
H	1.0	-1.2524601185	3.6326738501	1.2253211692
H	1.0	-1.4039957508	3.0307413822	-0.4498746303

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  H         1.0    -0.4207106421     2.1208121688     0.7450386912
  C         6.0     3.6704000467    -0.9011056179    -1.0169194454
  C         6.0     3.3248580793    -2.3502009477    -0.6129452808
  H         1.0     3.9580123991    -3.0330261988    -1.2192082382
  H         1.0     2.2730062006    -2.5921118013    -0.8411626664
  H         1.0     3.5229085450    -2.5750700616     0.4490426375
  C         6.0     3.3790636668    -0.7803535818    -2.5324299723
  H         1.0     3.9442509505    -1.5837199577    -3.0519884293
  H         1.0     3.7085595243     0.1791817197    -2.9730880203
  H         1.0     2.3045065847    -0.9317302238    -2.7667190004
  C         6.0     5.1737694043    -0.6646446986    -0.7405644433
  H         1.0     5.7521956566    -1.3703237584    -1.3758855246
  H         1.0     5.4424147215    -0.8880177602     0.3099303084
  H         1.0     5.5192162681     0.3552550988    -0.9873109698
  C         6.0    -3.2194821773     0.4712201558    -1.7054210308
  C         6.0    -2.5735540102     1.7316109661    -2.3242129815
  H         1.0    -2.9103149119     2.6771059766    -1.8572624549
  H         1.0    -2.8685127103     1.7769471397    -3.3945812600
  H         1.0    -1.4658191678     1.6857654654    -2.2950412249
  C         6.0    -4.7582554181     0.6114896143    -1.7606758302
  H         1.0    -5.0460764583     0.8328947991    -2.8113349739
  H         1.0    -5.1461374806     1.4377106343    -1.1350848503
  H         1.0    -5.2813375717    -0.3219103344    -1.4765950449
  C         6.0    -2.7809418061    -0.7233841837    -2.5854689622
  H         1.0    -3.2135435365    -1.6885284076    -2.2664596376
  H         1.0    -1.6767568151    -0.8268440199    -2.6180620597
  H         1.0    -3.1350043142    -0.5324370433    -3.6216508011
  C         6.0     0.0065316563    -3.0098928681     0.5224415199
  H         1.0     0.9756962150    -3.4163987680     0.8596781704
  H         1.0    -0.8345169177    -3.4383575200     1.0969389769
  C         6.0    -0.1780885572    -2.8802643921    -0.9899163615
  H         1.0    -1.1941491988    -3.0341180103    -1.3928769308
  H         1.0     0.5879185548    -3.2977349152    -1.6679071215
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Products of the reactions with ethene

Product **2B**:

ATOM	CHARGE	X	Y	Z
	15.0	-2.0166256611	-0.0173002574	0.0170467079
B	5.0	-0.0683826716	-0.7910626012	0.2047693369
P	15.0	1.9905751734	-0.0622150245	0.0163499317
C	6.0	-2.6728226898	-0.1851671915	-1.8389092118
C	6.0	-3.8992540906	0.7086157058	-2.1443805560
H	1.0	-4.7832635844	0.4605159639	-1.5297052786
H	1.0	-4.1850610699	0.5351586841	-3.2045065349
H	1.0	-3.6962503471	1.7902796018	-2.0489552967
C	6.0	-1.5225483224	0.1892600877	-2.7969485006
H	1.0	-0.6210049456	-0.4270771660	-2.6107284821
H	1.0	-1.2475944610	1.2586082817	-2.7435690394
H	1.0	-1.8519048044	-0.0069808498	-3.8398276713
C	6.0	-3.0856841525	-1.6383903934	-2.1831797311
H	1.0	-3.9810538005	-1.9799744512	-1.6307129354
H	1.0	-2.2713644887	-2.3721888353	-2.0403021067
H	1.0	-3.3537386716	-1.6596638478	-3.2613472493
C	6.0	-2.1651060399	1.8620358424	0.5645141988
C	6.0	-3.5700253558	2.3968895036	0.9355175228
H	1.0	-3.9965178444	1.9226417503	1.8386897002
H	1.0	-4.3020045945	2.3215792310	0.1091150068
H	1.0	-3.4571501914	3.4781491219	1.1691000313
C	6.0	-1.6617333368	2.7591890177	-0.5958404715
H	1.0	-0.7542600668	2.3863706465	-1.0991454197
H	1.0	-1.4242204544	3.7657902204	-0.1904090339
H	1.0	-2.4417309191	2.9016700125	-1.3659276404
C	6.0	-1.2643964998	2.0282088773	1.8161584621
H	1.0	-1.7649852554	1.6791036925	2.7377966189
H	1.0	-1.0298819210	3.1044234281	1.9601139437
H	1.0	-0.3096685415	1.4742856847	1.7374295617
C	6.0	2.9183593052	-1.4488683528	-1.0597193734
C	6.0	2.3527293048	1.6766153007	-0.8609833004
C	6.0	3.0687447269	-2.7404551916	-0.2129097535
H	1.0	3.7664720225	-2.6028631349	0.6355715523
H	1.0	3.5085243299	-3.5263037669	-0.8636115290
H	1.0	2.1206008051	-3.1435875389	0.1844605312
C	6.0	2.1044783777	-1.7413064353	-2.3494737613
H	1.0	2.2962432910	-0.9866364539	-3.1339846162
H	1.0	1.0151340432	-1.7977006307	-2.1846852778
H	1.0	2.4334868758	-2.7201513212	-2.7605310473
C	6.0	4.3419471283	-1.0648022676	-1.5328696130
H	1.0	4.3396630314	-0.2548456445	-2.2862762697
H	1.0	4.7651733999	-1.9585412178	-2.0411703496
H	1.0	5.0365557286	-0.7985236964	-0.7176833493
C	6.0	1.8710861412	1.5713857556	-2.3260355951
H	1.0	1.8913821420	2.5875246733	-2.7744894269
H	1.0	0.8389962965	1.1861267640	-2.4165299363
H	1.0	2.5324288744	0.9356636786	-2.9439135359
C	6.0	3.8365416733	2.1213499672	-0.8812825347
H	1.0	3.8767026829	3.0861325471	-1.4335440263
H	1.0	4.5170404071	1.4259995348	-1.3996413114
H	1.0	4.2394663175	2.3255115152	0.1284925714
C	6.0	1.5795090440	2.8205861088	-0.1529903014
H	1.0	1.3052911447	3.5914788543	-0.9036352950

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H    1.0   2.1960246681   3.3293367837   0.6091115266
H    1.0   0.6538404877   2.4935219007   0.3390947485
C    6.0  -3.2852361423  -1.0300203982   1.1751693670
C    6.0  -3.2312712578  -2.5776685541   1.0497773738
H    1.0  -4.0591220130  -2.9706443330   1.6785766309
H    1.0  -2.3017663550  -3.0351688188   1.4276549009
H    1.0  -3.4159435475  -2.9446744763   0.0249072524
C    6.0  -2.9933797871  -0.6682440426   2.6523745502
H    1.0  -3.5904362789  -1.3449414556   3.3005368933
H    1.0  -3.2947956564   0.3644869044   2.9080404571
H    1.0  -1.9286202402  -0.8004944629   2.9253467160
C    6.0  -4.7513988910  -0.6485513127   0.8420987775
H    1.0  -5.3948524701  -1.0751941020   1.6418249341
H    1.0  -5.0960528353  -1.0960985133  -0.1099735759
H    1.0  -4.9495897057   0.4347791386   0.8151989454
C    6.0   2.9039579157   0.0644220393   1.7935570250
C    6.0   2.5878643336   1.4314937170   2.4430351051
H    1.0   3.0875038173   2.2775275150   1.9395614276
H    1.0   2.9704919496   1.4103902968   3.4858578653
H    1.0   1.5025801420   1.6407138572   2.5041042822
C    6.0   4.4422886894  -0.0605711785   1.6648735941
H    1.0   4.8798104624   0.1661773166   2.6616771688
H    1.0   4.8946854700   0.6462415645   0.9476018225
H    1.0   4.7690215731  -1.0853666201   1.4054611409
C    6.0   2.4512788097  -1.0037166492   2.8157761680
H    1.0   2.6469935225  -2.0428326931   2.4902520910
H    1.0   1.3857384380  -0.9039419477   3.0920490563
H    1.0   3.0504593989  -0.8435998510   3.7379739169
C    6.0  -0.2769922723  -2.3480016040  -0.1970605215
H    1.0  -1.2894819467  -2.6781377476  -0.4665369848
H    1.0   0.4710962651  -2.9590348170  -0.7211265676
C    6.0  -0.0234038940  -2.0165754432   1.2472788722
H    1.0   0.9587698452  -2.3376600378   1.6108287601
H    1.0  -0.7913796161  -2.1936620986   2.0147536028
```

Product 2Al:

```
  ATOM   CHARGE        X               Y               Z
-------------------------------------------------------------
P    15.0   2.3935198957  -0.0111467665  -0.0302412160
AL   13.0   0.0148912107  -0.9309085796   0.0667650692
P    15.0  -2.3745782155   0.0817730360   0.0591690867
C     6.0   2.8813807763   0.5646250923   1.7714471834
C     6.0   4.1503100119   1.4429977926   1.8385162435
H     1.0   5.0564936105   0.9222451630   1.4783352543
H     1.0   4.3299777202   1.7150677090   2.9013757896
H     1.0   4.0466386336   2.3929202221   1.2789195801
C     6.0   1.6885437320   1.3528554208   2.3565216978
H     1.0   0.7507325975   0.7558479964   2.3163831744
H     1.0   1.5187141162   2.3232464426   1.8562418115
H     1.0   1.8912412201   1.5661572245   3.4281107507
C     6.0   3.0693578754  -0.6849458463   2.6647009325
H     1.0   3.9838664997  -1.2553792423   2.4167674393
H     1.0   2.1916606344  -1.3632475063   2.6256014123
H     1.0   3.1773854562  -0.3429325285   3.7166257045
C     6.0   2.5478234384   1.4792564274  -1.2913751671
C     6.0   3.9896798322   1.8047803581  -1.7421058340
H     1.0   4.4568153950   0.9925043297  -2.3295649731
H     1.0   4.6585551318   2.0622138142  -0.8984185010
H     1.0   3.9452725076   2.6959175849  -2.4054109175
C     6.0   1.9474707919   2.7611698326  -0.6751170116
H     1.0   0.9097499838   2.6175721283  -0.3247591894
H     1.0   1.9167894345   3.5424517840  -1.4648855162
H     1.0   2.5505492211   3.1705964808   0.1580751767
C     6.0   1.6887981196   1.1193010581  -2.5262424944
H     1.0   2.0836823916   0.2693382295  -3.1108613055
H     1.0   1.6437146301   1.9982000373  -3.2055042396
H     1.0   0.6480704367   0.8650076721  -2.2361776677
C     6.0  -3.5350608985  -1.2665092956   0.9070234158
C     6.0  -2.6022879197   1.7568955562   1.0352050062
C     6.0  -3.6131238612  -2.5152086059  -0.0032630107
H     1.0  -4.1224968416  -3.3202598234  -0.9665095921
H     1.0  -4.2143993352  -3.2842693822   0.5272495867
H     1.0  -2.6245345510  -2.9657967668  -0.2126635849
C     6.0  -2.9277585289  -1.6917561883   2.2697517784
H     1.0  -3.1565017648  -0.9760217693   3.0786492100
H     1.0  -1.8314741758  -1.8338204015   2.2249432262
H     1.0  -3.3805004616  -2.6630647296   2.5642789514
C     6.0  -4.9756583262  -0.7635612043   1.1616496528
H     1.0  -5.0213230464   0.0554148053   1.9049942230
H     1.0  -5.5521448037  -1.6116564014   1.5910099538
H     1.0  -5.5056937879  -0.4421921191   0.2466570663
C     6.0  -2.5309184079   1.4854745068   2.5560321175
H     1.0  -2.4352800209   2.4620047505   3.0777968377
H     1.0  -1.6527715714   0.8713935063   2.8429499557
H     1.0  -3.4431547976   0.9990169392   2.9485863857
C     6.0  -3.9292414007   2.4831142999   0.7158852753
H     1.0  -4.0061202215   3.3740840630   1.3765934587
H     1.0  -4.8236393883   1.8616962220   0.9048927308
H     1.0  -3.9760852872   2.8549531786  -0.3256472547
C     6.0  -1.4257067790   2.6935590594   0.6976206096
H     1.0  -1.5530027562   3.6434410790   1.2607522066
H     1.0  -1.3534736029   2.9532241231  -0.3731990617
H     1.0  -0.4656280627   2.2531474078   1.0252295556
C     6.0   3.6432159773  -1.4201093486  -0.6177391138
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C    6.0   3.3649485568  -2.7728345078   0.0777744855
H    1.0   4.1604622344  -3.4788026075  -0.2446883806
H    1.0   2.4011131661  -3.2145548672  -0.2282789186
H    1.0   3.4008477377  -2.7267935833   1.1797541785
C    6.0   3.4708198603  -1.6596346806  -2.1365208065
H    1.0   4.0825879175  -2.5457619115  -2.4104277434
H    1.0   3.8315096964  -0.8191144024  -2.7581302363
H    1.0   2.4207057679  -1.8854438742  -2.4100384608
C    6.0   5.1128223658  -1.0371723159  -0.3164603106
H    1.0   5.7644673853  -1.7971469910  -0.8000439817
H    1.0   5.3420468145  -1.0701949278   0.7663871306
H    1.0   5.4173161194  -0.0511541469  -0.7105901722
C    6.0  -2.9286880123   0.3428381041  -1.8092069738
C    6.0  -2.3237327369   1.6607745945  -2.3456860998
H    1.0  -2.7722309346   2.5663332920  -1.8950125335
H    1.0  -2.5201135951   1.7100331897  -3.4381120756
H    1.0  -1.2234993567   1.7059073816  -2.2159952340
C    6.0  -4.4615417074   0.3864833260  -2.0052066926
H    1.0  -4.6645079443   0.5879773036  -3.0794699363
H    1.0  -4.9593943247   1.1858916685  -1.4249019245
H    1.0  -4.9478945124  -0.5786382922  -1.7668900160
C    6.0  -2.3496372059  -0.8019293073  -2.6735748041
H    1.0  -2.7615575858  -1.7959886080  -2.4191324758
H    1.0  -1.2453070916  -0.8689730465  -2.6024129749
H    1.0  -2.6164080532  -0.5993023240  -3.7333454002
C    6.0   0.0303128107  -2.8808919803   0.7218268452
H    1.0   0.9512076136  -3.2252803453   1.1656114630
H    1.0  -0.8564657192  -3.2448913753   1.2150150515
C    6.0  -0.0332847197  -2.7098980867  -0.8144317750
H    1.0  -0.9706087261  -3.0671318483  -1.2782212305
H    1.0   0.8292828544  -3.1023611033  -1.3849876531
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Product 2Ga:

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  ATOM   CHARGE        X               Y               Z
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P    15.0   2.3591960797   0.1055500938   0.0058713502
GA   31.0   0.0472092193  -0.8418724199  -0.2028113791
P    15.0  -2.3483649866   0.0824941546  -0.0158626248
C     6.0   2.8436161048   0.2036779344   1.9043714682
C     6.0   4.0839119964   1.0848572490   2.1775515739
H     1.0   4.9914470226   0.7276148738   1.6557013837
H     1.0   4.3012072746   1.0464654453   3.2671605667
H     1.0   3.9299701211   2.1500932543   1.9211068927
C     6.0   1.6293515326   0.7516348235   2.6869439300
H     1.0   0.7268733687   0.1254079462   2.5216306812
H     1.0   1.3883756104   1.8025849182   2.4453955837
H     1.0   1.8627923934   0.7111816274   3.7726542934
C     6.0   3.1170504777  -1.2181840582   2.4472302207
H     1.0   4.0664516176  -1.6484625583   2.0751651412
H     1.0   2.2863016079  -1.9175998954   2.2284471583
H     1.0   3.2088456960  -1.1500295537   3.5526383605
C     6.0   2.4707096279   1.8850824700  -0.7977282542
C     6.0   3.9011780875   2.3443692585  -1.1646086213
H     1.0   4.3578814973   1.7416061306  -1.9722016023
H     1.0   4.5882514187   2.3591322012  -0.2969882244
H     1.0   3.8342706350   3.3869860128  -1.5444338583
C     6.0   1.8900376339   2.9345077995   0.1800009507
H     1.0   0.9101254733   2.6489482647   0.6026783514
H     1.0   1.7413771619   3.8853204158  -0.3757851117
H     1.0   2.5738514179   3.1571932566   1.0208495367
C     6.0   1.6164518225   1.8724832957  -2.0895460058
H     1.0   2.0724644514   1.2701964078  -2.8954092227
H     1.0   1.5183083142   2.9133572493  -2.4663269525
H     1.0   0.5936925495   1.4767139171  -1.9232048414
C     6.0  -3.2226251686  -1.0217561809   1.3559831123
C     6.0  -2.4918505045   1.9627135965   0.4988706501
C     6.0  -3.4625337965  -2.4397782206   0.7831759202
H     1.0  -4.2532589674  -2.4635608939   0.0088869723
H     1.0  -3.8077785724  -3.0896763542   1.6158704932
H     1.0  -2.5484375984  -2.9040143903   0.3672436886
C     6.0  -2.2819604096  -1.1480455168   2.5797314092
H     1.0  -2.1999821278  -0.2073418471   3.1536492733
H     1.0  -1.2662220712  -1.4769398179   2.2861272666
H     1.0  -2.7073987718  -1.9129042153   3.2643634674
C     6.0  -4.5780463800  -0.4588059923   1.8413059076
H     1.0  -4.4714466067   0.4839146187   2.4125068689
H     1.0  -5.0209744911  -1.2027162215   2.5385953754
H     1.0  -5.3110815130  -0.3013127283   1.0283969411
C     6.0  -1.9733328444   2.1137768646   1.9478026732
H     1.0  -1.8989167514   3.1979414215   2.1804432782
H     1.0  -0.9665912957   1.6734440833   2.0907262626
H     1.0  -2.6577868925   1.6719800742   2.6964709010
C     6.0  -3.9232319619   2.5428665284   0.4169767351
H     1.0  -3.8817598902   3.6002213787   0.7588999498
H     1.0  -4.6535330761   2.0209462480   1.0606019001
H     1.0  -4.3149029588   2.5606367126  -0.6181251255
C     6.0  -1.5912752625   2.8151418719  -0.4220334201
H     1.0  -1.4456534610   3.8112124526   0.0481570557
H     1.0  -2.0325996469   2.9877438960  -1.4180072022
H     1.0  -0.5935154810   2.3678880341  -0.5679110435
C     6.0   3.6197341490  -1.0766343027  -0.9347260165
C     6.0   3.4073450445  -2.5634504276  -0.5652137121
H     1.0   4.1402608279  -3.1558426178  -1.1541588507
H     1.0   2.4050203676  -2.9332066325  -0.8338555059
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H	1.0	3.5949256143	-2.7856099746	0.4992234294
C	6.0	3.3692079966	-0.9463647537	-2.4566545551
H	1.0	3.9704468467	-1.7246423647	-2.9739297187
H	1.0	3.6877942643	0.0293538793	-2.8699308567
H	1.0	2.3057344560	-1.1207370255	-2.7203231590
C	6.0	5.0925782226	-0.7332902317	-0.6059907988
H	1.0	5.7368435390	-1.3744915343	-1.2458787137
H	1.0	5.3497563151	-0.9714954866	0.4440735549
H	1.0	5.3708564629	0.3151494183	-0.8103038995
C	6.0	-3.2810143569	-0.1508852641	-1.7348574401
C	6.0	-2.8539440951	0.9659355084	-2.7148061511
H	1.0	-3.2882466866	1.9535246694	-2.4693323199
H	1.0	-3.2298487624	0.6940258860	-3.7242994087
H	1.0	-1.7514970436	1.0618461084	-2.7951369876
C	6.0	-4.8205692254	-0.1289758972	-1.5855395930
H	1.0	-5.2578686389	-0.1650326128	-2.6067923462
H	1.0	-5.2090502235	0.7836059867	-1.0972417029
H	1.0	-5.2090690308	-1.0124768225	-1.0434583335
C	6.0	-2.8691565926	-1.4836776700	-2.3983093269
H	1.0	-3.0940093906	-2.3728147694	-1.7822369465
H	1.0	-1.7931899344	-1.4948023459	-2.6562682770
H	1.0	-3.4471896024	-1.5856504152	-3.3420066159
C	6.0	0.1440417055	-2.7461309950	0.4938055984
H	1.0	1.1174074578	-3.1026917388	0.8725213341
H	1.0	-0.6794981445	-3.2095300360	1.0643955667
C	6.0	-0.0176334324	-2.6814908831	-1.0252756065
H	1.0	-0.9938600989	-3.0091553540	-1.4165277210
H	1.0	0.7954155646	-3.0575681968	-1.6710349240

H	1.0	3.7613155219	-0.5045693815	-2.9476874878
H	1.0	2.3442770544	-1.5501944727	-2.5616048250
C	6.0	5.1660801973	-0.9037014041	-0.5599733721
H	1.0	5.7636646353	-1.6835052270	-1.0802674276
H	1.0	5.4201930713	-0.9744719016	0.5156136396
H	1.0	5.5077192892	0.0753944029	-0.9401119464
C	6.0	-3.2252322346	0.0760976422	-1.7270979519
C	6.0	-2.6039800065	1.2233996301	-2.5561222984
H	1.0	-2.9369482880	2.2300751964	-2.2401850406
H	1.0	-2.9197786797	1.0933971919	-3.6134976238
H	1.0	-1.4944006040	1.1898737473	-2.5477055692
C	6.0	-4.7664749250	0.1887448516	-1.7679441296
H	1.0	-5.0832020891	0.2357634005	-2.8327965577
H	1.0	-5.1600492887	1.0959644716	-1.2729029182
H	1.0	-5.2669085127	-0.6968178813	-1.3299993599
C	6.0	-2.8031916842	-1.2414601054	-2.4203316160
H	1.0	-3.2176790143	-2.1462023493	-1.9404920196
H	1.0	-1.7005353308	-1.3494845162	-2.4733617730
H	1.0	-3.1933062693	-1.2174488742	-3.4606783365
C	6.0	0.0345079749	-2.8638056460	0.8632426498
H	1.0	0.9940379456	-3.2228434814	1.2728262453
H	1.0	-0.8147091104	-3.1810032226	1.4940412794
C	6.0	-0.1489578886	-2.9502013201	-0.6423943357
H	1.0	-0.1488706155	-3.2341672648	-1.0151710306
H	1.0	0.6448118306	-3.4195457543	-1.2504326710

Product **2In**:

ATOM	CHARGE	X	Y	Z
P	15.0	2.4945633802	0.2057129339	-0.1230818093
IN	49.0	0.0244947070	-0.8140447214	-0.0512536080
P	15.0	-2.4919802325	0.1382872202	0.0956693435
C	6.0	3.0115867520	0.6683303606	1.7029810593
C	6.0	4.3111435096	1.5014714016	1.7823709487
H	1.0	5.1883245762	0.9717954477	1.3661392321
H	1.0	4.5310182847	1.7072798634	2.8524036079
H	1.0	4.2234347638	2.4826973034	1.2781066166
C	6.0	1.8467987810	1.4590735175	2.3415830640
H	1.0	0.8982706564	0.8799409465	2.3001138526
H	1.0	1.6832845310	2.4505837997	1.8819423535
H	1.0	2.0819625239	1.6291412620	3.4142891375
C	6.0	3.1822611026	-0.6287145216	2.5266938730
H	1.0	4.0799794888	-1.2059030520	2.2346921463
H	1.0	2.2877297664	-1.2835934550	2.4679581129
H	1.0	3.3139582056	-0.3435645139	3.5926921964
C	6.0	2.6422238037	1.7728226970	-1.2972675671
C	6.0	4.0866730448	2.0356632320	-1.7869076061
H	1.0	4.4930258024	1.2271719040	-2.4220943226
H	1.0	4.7920811735	2.2195101806	-0.9530051960
H	1.0	4.0710640068	2.9565446008	-2.4091401536
C	6.0	2.1641029548	3.0570430178	-0.5831860865
H	1.0	1.1405289530	2.9666455578	-0.1806204628
H	1.0	2.1451351113	3.8775945566	-1.3325212656
H	1.0	2.8416232091	3.3804617545	0.2291942505
C	6.0	1.7161281007	1.5446433719	-2.5159558955
H	1.0	1.9826788754	0.6498098268	-3.1060221574
H	1.0	1.7962804939	2.4281649716	-3.1848330786
H	1.0	0.6525216282	1.4455117883	-2.2145256846
C	6.0	-3.5309881454	-1.0316328172	1.2772294901
C	6.0	-2.5808622416	1.9613051657	0.7731075584
C	6.0	-3.7016249635	-2.4132892752	0.6055309135
H	1.0	-4.3549556934	-2.3810801670	-0.2873438289
H	1.0	-4.1895090859	-3.0919507740	1.3375247370
H	1.0	-2.7369210379	-2.8783264670	0.3251954348
C	6.0	-2.7632419083	-1.2337967303	2.6083307113
H	1.0	-2.8161238429	-0.3504305356	3.2675622573
H	1.0	-1.6965200774	-1.4913386909	2.4519650558
H	1.0	-3.2381416401	-2.0755985840	3.1570952894
C	6.0	-4.9325678969	-0.4603335613	1.5972841659
H	1.0	-4.8919548937	0.5000970650	2.1462374724
H	1.0	-5.4504785411	-1.1853592576	2.2622747961
H	1.0	-5.5684716046	-0.3286625881	0.7025034383
C	6.0	-2.4114636944	1.9750651124	2.3095752032
H	1.0	-2.2698962542	3.0307493859	2.6274144432
H	1.0	-1.5198030344	1.4076132120	2.6446657378
H	1.0	-3.2993427757	1.5951282430	2.8494214152
C	6.0	-3.8836426564	2.7094601878	0.4093868115
H	1.0	-3.8534490218	3.7110826945	0.8912845467
H	1.0	-4.7941348462	2.1998225718	0.7782283813
H	1.0	-3.9933597139	2.8819574611	-0.6781893218
C	6.0	-1.3673298876	2.7155708295	0.1950300700
H	1.0	-1.3756096940	3.7637506827	0.5652639557
H	1.0	-1.3459255040	2.7508693116	-0.9091821214
H	1.0	-0.4283238713	2.2477988177	0.5518504402
C	6.0	3.6711109845	-1.2020993548	-0.8249145473
C	6.0	3.3414825741	-2.5685420089	-0.1800656530
H	1.0	4.0596982322	-3.3109530839	-0.5900611202
H	1.0	2.3310453125	-2.9222058889	-0.4459482655
H	1.0	3.4495759878	-2.5836582451	0.9178584383
C	6.0	3.4160390725	-1.3635544058	-2.3422348017
H	1.0	3.9837219258	-2.2522594268	-2.6927785000

Product **2Tl**:

ATOM	CHARGE	X	Y	Z
P	15.0	2.5278353861	0.3430845454	-0.0293790128
TL	81.0	0.0357010825	-0.7809646832	-0.1155827161
P	15.0	-2.5401027340	0.2162267880	0.1138584344
C	6.0	3.0866206150	0.4629034880	1.8383815988
C	6.0	4.3875186861	1.2720399812	2.0465465658
H	1.0	5.2558668233	0.8391045502	1.5153437099
H	1.0	4.6305124049	1.2597848086	3.1313486723
H	1.0	4.2916651398	2.3348107158	1.7534769997
C	6.0	1.9267505003	1.1098402599	2.6306668041
H	1.0	0.9871233955	0.5354197507	2.4833089263
H	1.0	1.7430137057	2.1679055340	2.3704318997
H	1.0	2.1751027075	1.0734273059	3.7130105759
C	6.0	3.2722365875	-0.9613636217	2.4075442541
H	1.0	4.1806585780	-1.4687651786	2.0284389866
H	1.0	2.3872004614	-1.6040801569	2.2168124040
H	1.0	3.3873933209	-0.8804281511	3.5099236339
C	6.0	2.6281918678	2.1097288752	-0.8757333118
C	6.0	4.0500367618	2.4488095082	-1.3845111320
H	1.0	4.4036568335	1.7772007051	-2.1878300557
H	1.0	4.8028188634	2.4611295108	-0.5722453999
H	1.0	4.0196917828	3.4734582383	-1.8144136495
C	6.0	2.2109961416	3.2443706778	0.0875240424
H	1.0	1.2043856146	3.1024353372	0.5178237827
H	1.0	1.2820923771	4.1875715041	-0.4996220127
H	1.0	2.9301249290	3.4056432626	0.9126223991
C	6.0	1.6293097097	2.1100855856	-2.0553731056
H	1.0	1.8181626748	1.3087525952	-2.7928135955
H	1.0	1.7000910009	3.0839647610	-2.5867882828
H	1.0	0.5874481179	1.9982286979	-1.6935216452
C	6.0	-3.6444970891	-1.0924902843	1.0661992942
C	6.0	-2.5704198061	1.9047907624	1.0801063573
C	6.0	-3.8780338029	-2.3197091217	0.1551769672
H	1.0	-4.5390816969	-2.1013388053	-0.7051704780
H	1.0	-4.3846867236	-3.1038883913	0.7578986560
H	1.0	-2.9329463650	-2.7589679500	-0.2208987245
C	6.0	-2.8788158681	-1.5782785593	2.3209229988
H	1.0	-2.8590626537	-0.8312020099	3.1342324221
H	1.0	-1.8353213402	-1.8601240634	2.0799649231
H	1.0	-3.3990417561	-2.4766837389	2.7167514550
C	6.0	-5.0143668330	-0.5199373581	1.4970429384
H	1.0	-4.9235998643	0.3007917661	2.2342548892
H	1.0	-5.5821252317	-1.3351414578	1.9964710628
H	1.0	-5.6306409907	-0.1667660368	0.6490867450
C	6.0	-2.3730730078	1.6446636558	2.5912226211
H	1.0	-2.2032893215	2.6225858023	3.0910794124
H	1.0	-1.4884296282	1.0075764670	2.7949001163
H	1.0	-3.2574856988	1.1852527345	3.0708388096
C	6.0	-3.8576447083	2.7351804478	0.8729469427
H	1.0	-3.7673360150	3.6649918061	1.4756912136
H	1.0	-4.7699605373	2.2113053892	1.2157161504
H	1.0	-4.0056378092	3.0469939948	-0.1787396229
C	6.0	-1.3468304724	2.7137781918	0.6068512519
H	1.0	-1.2524601185	3.6326738301	1.2253211692
H	1.0	-1.4039957508	3.0307413822	-0.4498746303
H	1.0	-0.4207106421	2.1208121688	0.7450386912
C	6.0	3.6704000467	-0.9011056179	-1.0169194454
C	6.0	3.3248580793	-2.3502009477	-0.6129452808
H	1.0	3.9580123991	-3.0330261988	-1.2192082382
H	1.0	2.2730062006	-2.5921118013	-0.8411626664
H	1.0	3.5229085450	-2.5750970616	0.4490426375
C	6.0	3.3790366668	-0.7803535818	-2.5324299723
H	1.0	3.9442509505	-1.5837199578	-3.0519884293
H	1.0	3.7085595243	0.1791817198	-2.9730880203
H	1.0	2.3045065846	-0.9317302238	-2.7667190003
C	6.0	5.1737694043	-0.6646446986	-0.7405644433

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H      1.0    5.7521956566   -1.3703237584   -1.3758855246
H      1.0    5.4424147215   -0.8880177602    0.3099303084
H      1.0    5.5192162681    0.3552550988   -0.9873109698
C      6.0   -3.2194821773    0.4712201558   -1.7054210308
C      6.0   -2.5735540102    1.7316109661   -2.3242129815
H      1.0   -2.9103149119    2.6771059766   -1.8572624549
H      1.0   -2.8685127103    1.7769471397   -3.3945812600
H      1.0   -1.4658191678    1.6857654654   -2.2950412249
C      6.0   -4.7582554181    0.6114896143   -1.7606758302
H      1.0   -5.0460764583    0.8328947991   -2.8113349739
H      1.0   -5.1461374806    1.4377106393   -1.1350848503
H      1.0   -5.2813375717   -0.3219103344   -1.4765950449
C      6.0   -2.7809418061   -0.7233841837   -2.5854689622
H      1.0   -3.2135435365   -1.6885284076   -2.2664596376
H      1.0   -1.6767568151   -0.8268440199   -2.6180620597
H      1.0   -3.1350043142   -0.5324370433   -3.6216508011
C      6.0    0.0065316563   -3.0098928681    0.5224415199
H      1.0    0.9756962150   -3.4163987680    0.8596781704
H      1.0   -0.8345169177   -3.4383575200    1.0969389769
C      6.0   -0.1780885572   -2.8802643921   -0.9899163615
H      1.0   -1.1941491988   -3.0341180103   -1.3928769308
H      1.0    0.5879185548   -3.2977349152   -1.6679071215
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