Theoretical Simulation of n-Alkane Cracking on Zeolites

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Supporting Information

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Additional Details for CBMC Simulation

Configurational-bias Monte Carlo (CBMC) is an efficient method for sampling the configurations of chain molecules in dense media. Because most of the simulation box is occupied by the atoms of the zeolite framework, the chance that a location chosen at random will permit a long molecule to be inserted is relatively low. To increase the likelihood of generating an acceptable configuration, chain molecules are instead grown pseudoatom by pseudoatom. First, a given number of trial positions are tested for the first pseudoatom and one of these is selected at random. A given number of trial orientations are generated for the second pseudoatom, and again, one is selected at random according to its Boltzmann factor. This process is repeated until the whole molecule is grown and the overall Rosenbluth weight, $\langle W_{new} \rangle$, is calculated. The Rosenbluth weight of the old configuration, $\langle W_{old} \rangle$, is computed by following the same procedure used to generate the new configuration and using the actual positions of the pseudoatoms as one of the trial orientations. Use of the Rosenbluth weight instead of the Boltzmann weight ensures that detailed balance is obeyed.[1]

In our simulations, we considered only a single molecule moving in the simulation box. The simulation box was formed out of a sufficient number of zeolite unit cells to ensure that the dimensions of the box exceeded twice the cutoff radius. The moves we considered were translation, rotation, and regrowth. Translation moves displaced the molecule by random distance along the x, y, or z directions. The maximum dislpacement distance was adjusted during the simulation to ensure that about 50% of translation moves were accepted. Rotation moves rotated the whole molecule by a random angle around its center of mass. Regrow moves uses the CBMC algorithm to

grow the molecule in a new location in the simulation box, this allowing more efficient sampling of the entire volume compared to just translation and rotation moves.[2,3]

The forcefield parameters were taken from the work of Dubbeldam and coworkers.[3] Zeolite-adsorbate interaction parameters were determined by fitting to the inflection point of experimental isotherms of alkanes in MFI. The parameters for pseudoatom self-interactions were determined by simulations to reproduce the vapor-liquid equilibria. Table S.1 summarizes the parameters used in this work. MR indicated the interaction was calculated using the Lorentz-Berthelot mixing rules.

The alkanes were treated with C-H united atoms connected with flexible bonds. Bond stretching and bending were modeled using a harmonic potential.

$$U_{stretch} = \frac{1}{2} k_{hs} \left(r - r_0 \right)^2 \qquad \text{(S-1)}$$

Parameters for stretching are $k_{hs}/k_b = 96500\ K\ Å^{-2}$ and $r_0 = 1.54\ Å$.

$$U_{bend} = \frac{1}{2} k_{hb} \left(\theta_{ijk} - \theta_0 \right)^2 \qquad \text{(S-2)}$$

Parameters for the bending potential are $k_{hb}/k_b = 62500\ K\ rad^{-2}$ and $\theta_0 = 114°$.

Torsion interactions were modeled using the OPLS[4] torsion potential,

$$U_{torsion} = \frac{1}{2} p_0 + \frac{1}{2} p_1 \left(1 + \cos(\phi_{ijkl}) \right) + \frac{1}{2} p_2 \left(1 - \cos(2\phi_{ijkl}) \right) + \frac{1}{2} p_3 \left(1 + \cos(3\phi_{ijkl}) \right) \qquad \text{(S-3)}$$

with parameters $p_0/k_b = 0.0\ K$, $p_1/k_b = 355.03\ K$, $p_2/k_b = 68.19\ K$, and $p_3/k_b = 791.32\ K$.

T-site locations and distributions of $P_{react}(i,j)$

The configurations of the adsorbed state were used to calculate the distance between the two carbon atoms involved in cracking pathway j and the aluminum atom of the cluster. These distances ranged between 4.2 Å and 5.0 Å. To account for the fact that

more than just the minimum energy configuration is able to react, we counted all configurations for a given pathway where the two carbon atoms of the breaking bond were within 5.0 Å of the T-atom of a given site.

Each zeolite framework has a specific number of T-sites in a crystallographic unit cell. These T-sites may be grouped by their symmetries and each zeolite can have a different number of T-site types. For example, all T-sites in FAU are crystallographically equivalent, but MFI has 12 distinct T-site symmetry types. As a result of this heterogeneity, T-sites of different symmetries will have a different value of $P_{react}(i,j)$ that depends on how accessible that site is to molecules. The distribution of values of $P_{react}(i,j)$ for the cracking paths of n-hexane on MFI and FAU are shown in Figures S.1 and S.2, respectively. There is only one peak for each pathway in Figure S.2, which agrees with the single symmetry type for T-sites in FAU. MFI, which has 12 T-site types, has a distributions of values; however, there are not 12 distinct peaks due to the variance of $P_{react}(i,j)$ around the average value for each T-site type and the fact that some T-sites of different symmetries may have similar values of $P_{react}(i,j)$.

Figure S.3 shows how the value of $\langle p_{react} \rangle$ depends on the distance between the bonds of the propane molecule and the different T-atoms of the MFI framework. The minimum distance is determined by the repulsive part of the Lennard-Jones potential. The value approaches unity as the distance approaches half of the simulation box size, as we should expect. Beyond this distance, the minimum image of the molecule is always captured in the sphere around the T-atom, even if it is separated by the pore walls of the framework. A physically reasonable cutoff radius of 5.0 Å was selected because this

distance corresponded to the maximum distance between cracking C-C bonds and T-atoms in all the adsorbed state structures from the DFT calculations.

The number of T-atoms can be related to an equivalent concentration of acid sites. Given the volume of the unit cell V_{uc} in Å^3 and the bulk density of the zeolite ρ_z in kg m^{-3}, the equivalent concentration of a single acid site in mol kg^{-1} is given by equation S-4.

$$C^{\circ}_{T-site} = \frac{10^{30} \times N_{Si/Al}}{\rho_z V_{uc} N_A} \tag{S-4}$$

N_A is Avogadro's number. Table S.2 gives the values for the zeolites considered in this work.

Brønsted-site Model

An approximate model of the Brønsted site was created by making one of the oxygens of a selected T-site more attractive to the alkane pseudoatoms with a deeper potential well (larger value of epsilon). The parameters for the Brønsted site model were selected to approximate the higher enthalpy of adsorption of n-hexane (about -10 kJ/mol), observed for acidic MFI relative to silicalite.[5,6] The parameters for this work are shown in Table S.3. The heat of adsorption was calculated as described previously. The results using this model are given in Table S.4 for propane and n-hexane.

Experiments measuring the heat of adsorption are conducted at much lower than the temperatures where monomolecular cracking is relevant. At high temperatures the molecule would crack upon adsorption in an acidic zeolite, making estimation of pure component properties difficult. At lower temperatures, the alkane is more likely to be found near the acid site. In fact, as the temperature approaches 0 K, the probability of finding the alkane near the marked acid site approaches 1, as expected, since siting near

the acid site places the molecule in an energy minimum relative to the rest of the zeolite pore. The presence of the acid site provides substantial enhancement to $P_{react}(i,j)$ at lower temperatures. At high temperatures, the molecule has a much smaller preference for siting at the acid site.

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Table S.1: Lennard-Jones parameters used for CBMC simulations. The top number of each interaction pair is ε_{ij}/k_b [K] and the bottom is σ [Å].

	$O_{zeolite}$	CH_3	CH_2
$O_{zeolite}$	-	93.0	60.5
		3.48	3.58
CH_3	93.0	108.0	MR
	3.48	3.76	
CH_2	60.5	MR	56.0
	3.58		3.96

Table S.2: Zeolite physical data and T-site concentrations.

	V_{uc}	ρ_z	$C^{o}_{H^+}$
	Å^3 u.c.$^{-1}$	*kg m^{-3}*	*mol kg^{-1}*
MFI	5332.0	1796.4	0.173
FAU	15677.6	1210.7	0.087

Table S.3: Comparison of Lennard-Jones parameters for zeolite-alkane interactions used in this work.

	Brønsted site model		**siliceous**	
parameter	*CH_2*	*CH_3*	*CH_2*	*CH_3*
σ_{OCHx}	3.58	3.48	3.58	3.48
ε_{OCHx}	400.0	450.0	60.5	93.0

Table S.4: Simulated heat of adsorption for n-alkanes in pure silica MFI and MFI with a Brønsted site model.

	temperature	**ΔH_{ads} (model)**	**ΔH_{ads} (siliceous)**	**$\Delta\Delta H_{ads}$**
	K	*kJ/mol*	*kJ/mol*	*kJ/mol*
propane	298.0	-44.4	-39.1	-5.2
	773.0	-41.1	-37.8	-3.2
n-hexane	298.0	-78.5	-67.9	-10.6
	773.0	-72.1	-64.2	-7.9

Figure S.1: Histogram of *f* for n-hexane bonds in MFI.

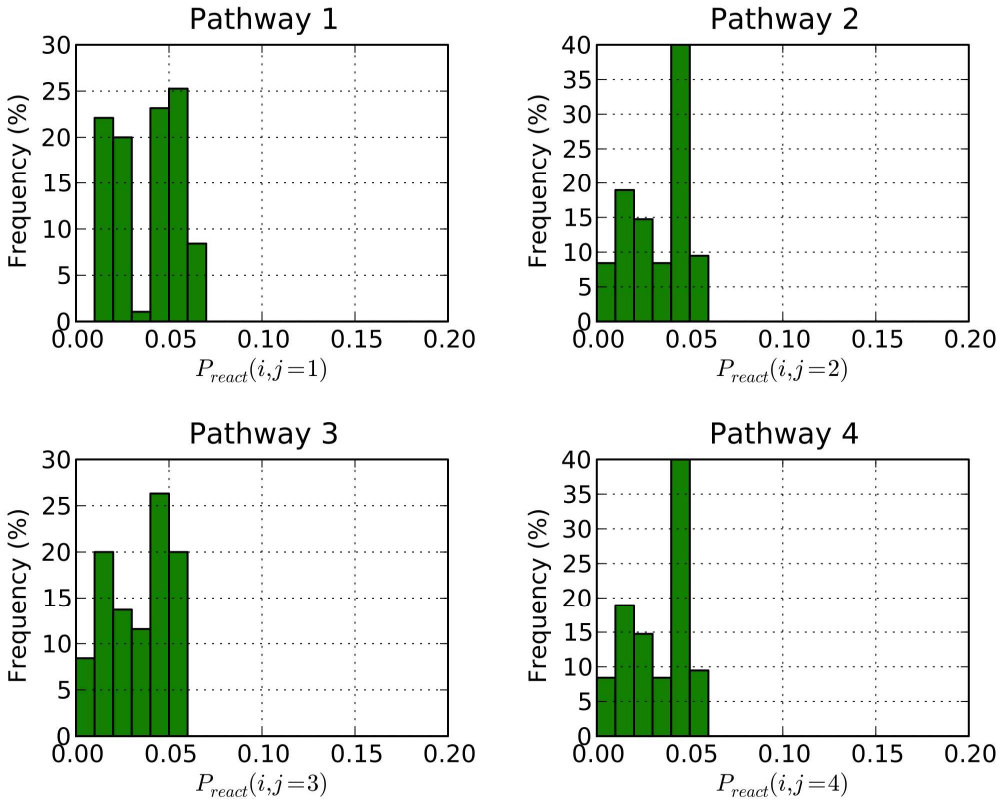


Figure S.2: Histograms of *f* for n-hexane bonds in FAU.

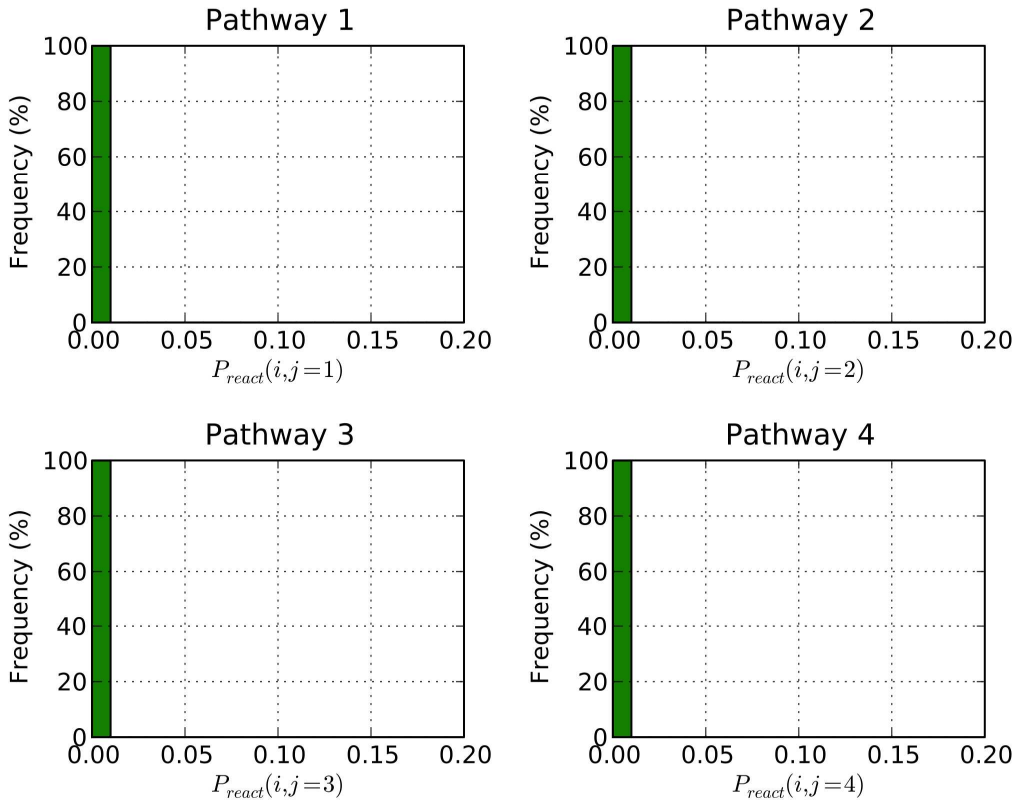
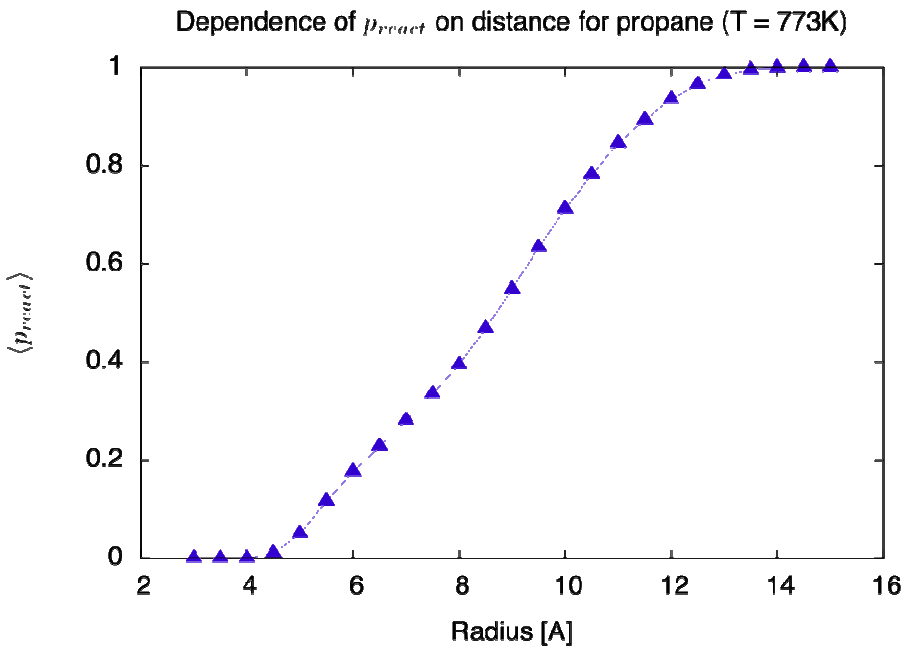


Figure S.3: Effect of cutoff radius on the value of <p_{react}> for propane cracking



Cluster models used in DFT calculations

Figure S.4: T5 cluster model of the Brønsted acid site in H-ZSM-5. Color codes: oxygen (red), silicon (yellow), aluminium (blue), hydrogen (white).

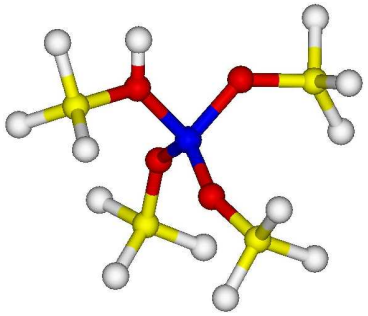
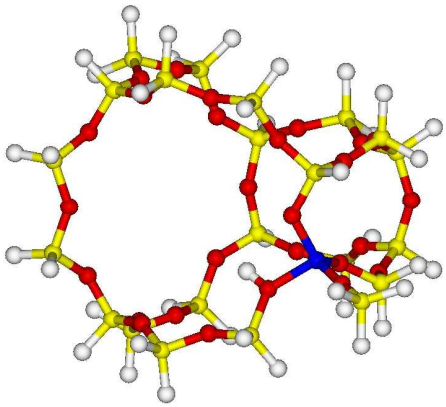


Figure S.5: T23 cluster model of the Brønsted acid site in H-ZSM-5. Color codes: oxygen (red), silicon (yellow), aluminium (blue), hydrogen (white).



DFT calculations applying periodic boundary conditions

DFT calculations applying periodic boundary conditions were performed using the Vienna ab-initio simulation program (VASP).[1-4] The gradient-corrected exchange-correlation functional proposed by Perdew, Burke, and Ernzerhof (PBE)[5,6] was employed. Plane-wave calculations were conducted using the projector-augmented wave (PAW) method.[7,8] The plane-wave basis set kinetic energy cut-off was set to 400 eV. Brillouin-zone sampling was restricted to the gamma point. The unit cell parameters α, β, and γ were fixed to 90° in all calculations as no significant deviation from the orthorhombic system is expected.[9-11] We used the unit cell vector lengths reported by Svelle et al.[12] (a = 20.157 Å, b = 20.033 Å, c = 13.473 Å) which result from optimization of an all-silica unit cell. To create an acidic site, one of the 96 Si atoms in the unit cell was replaced by an Al atom in the T12 site[13] and the resulting negative charge was compensated by a proton bonded to one of the neighbouring framework oxygen atoms. Specifically the Al12-O24(H)-Si3 site (numbering according to ref. 14) was chosen because of its location at the intersection between straight and sinusoidal channels.

Minima on the PBE potential energy surface were located using the conjugate gradient algorithm with fully relaxed atomic positions. Convergence was considered to be achieved when forces were below 10^{-4} eV/Å. Energies were converged to 10^{-5} eV in all cases. Transition structures were located by transferring optimized transition structures from our cluster calculations into the periodic environment and reoptimizing them using the improved-dimer method.[15] Transition structures were considered converged when forces on all atoms were smaller than 0.05 eV/Å. Stationary points found were characterised by harmonic frequencies obtained by diagonalization of the full dynamical

matrices. The force constants were obtained by numerical differentiation of forces with a step size of 0.02 Å. No scaling factor was applied for the frequencies.

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Energies of reactants and transition states

Table S.5: Electronic energies (in Hartree) of reactants (R) and transition states (TS) on the MFI T5-cluster obtained from B3LYP/SV(P) calculations.

Molecule	*E*(R)	*E*(TS)	Products	
propane	-1827.329571	-1827.240220	CH4	C2H4
n-butane	-1866.581530	-1866.494510	CH4	C3H6
	-1866.581600	-1866.502948	C2H6	C2H4
n-pentane	-1905.831511	-1905.745715	CH4	1-C4H8
	-1905.832464	-1905.754464	C2H6	C3H6
	-1905.832842	-1905.755060	C3H8	C2H4
n-hexane	-1945.082167	-1944.997770	CH4	1-C5H10
	-1945.083394	-1945.005488	C2H6	1-C4H8
	-1945.084401	-1945.006540	C3H8	C3H6
	-1945.083500	-1945.006333	C4H10	C2H4

Table S.6: Electronic energies (in Hartree) of reactants (R) and transition states (TS) on the FAU T5-cluster obtained from B3LYP/SV(P) calculations.

Molecule	*E*(R)	*E*(TS)	Products	
propane	-1827.360550	-1827.263846	CH4	C2H4
n-butane	-1866.611439	-1866.519209	CH4	C3H6
	-1866.611141	-1866.529849	C2H6	C2H4
n-pentane	-1905.862207	-1905.770459	CH4	1-C4H8
	-1905.861829	-1905.781983	C2H6	C3H6
	-1905.863714	-1905.782066	C3H8	C2H4
n-hexane	-1945.114010	-1945.022415	CH4	1-C5H10
	-1945.112597	-1945.033058	C2H6	1-C4H8
	-1945.114421	-1945.034128	C3H8	C3H6
	-1945.115649	-1945.034324	C4H10	C2H4

Table S.7: Electronic energies (in Hartree) of reactants (R) and transition states (TS) on the MFI T23-cluster obtained from B3LYP/SV(P) calculations.

Molecule	*E*(R)	*E*(TS)	Products	
propane	-8781.695162	-8781.618353	CH4	C2H4
n-butane	-8820.947494	-8820.869760	CH4	C3H6
	-8820.947494	-8820.871265	C2H6	C2H4

Table S.8: Electronic energies (in eV) of reactants (R) and transition states (TS) obtained from PBE calculations with periodic boundary conditions.

Molecule	*E*(R)	*E*(TS)	Products	
propane	-2339.502099	-2337.710709	CH4	C2H4
n-butane	-2356.000763	-2354.208633	CH4	C3H6

Cartesian coordinates of stationary points obtained from B3LYP/SV(P) calculations for cracking on the MFI T5-cluster

$C_3H_8 \rightarrow CH_4 + C_2H_4$

reactant

H	-0.0397935	-1.7199966	-4.9543747
H	0.4454093	-0.765219	-3.5354134
H	0.5323466	-2.5826874	-3.5152055
H	0.1592678	-1.5371129	-1.7902554
H	2.8272828	-1.51468	-3.7894669
H	2.2600691	-0.6866531	-5.2411117
H	3.5638637	-2.7464791	-5.8531261
H	1.8674261	-2.9260501	-6.3770509
H	2.4416672	-3.7638228	-4.9101225
C	0.6916299	-1.669398	-4.1263571
C	2.5227968	-2.8254906	-5.491341
C	2.1324268	-1.6100591	-4.6455769
Al	0.1120202	0.1172627	-0.0748801
O	0.0595072	-1.556753	-0.8142768
O	-0.0958764	0.8187362	-1.5846478
O	1.6665389	0.1814314	0.5343517
O	-1.1007293	0.1849273	1.0897816
H	-1.1386949	-3.1658171	0.9340632
H	1.2014631	-3.5855833	0.653343
H	-0.0292568	-3.8964624	-1.1921129
H	-0.3102492	3.4464924	-1.1973539
H	-2.1169603	2.2653416	-2.0954151
H	-0.0561772	2.2351267	-3.3947444
H	2.2251902	2.3392429	1.9117505
H	2.0205096	0.2520551	3.09753
H	3.751775	0.3820229	1.4872969
H	-2.4421676	2.3863444	1.8092629
H	-3.6381778	0.4926447	1.1325448
H	-2.3777387	0.4961362	3.1982327
Si	0.00000	-3.019872	0.00000
Si	-0.638226	2.27088	-2.034472
Si	2.392344	0.872496	1.806332
Si	-2.372274	0.908352	1.776808

transition state

H	0.6268506	-2.4121378	-4.2722527
H	-0.4296585	-0.9398735	-3.978403
H	0.1988917	-1.7230003	-2.5825293
H	2.4891529	-1.0160976	-2.5778176
H	1.3643867	0.3895342	-3.1331642
H	2.3645559	-0.584303	-4.415228
H	4.2467487	-0.8341853	-2.193938
H	3.3117616	-2.3398773	-1.7075904
H	2.9381329	-0.7301021	-0.8783962
C	0.474892	-1.5098555	-3.6624269
C	3.3096048	-1.2421979	-1.7858324
C	1.5600326	-0.5543147	-3.6665362
Al	0.1198877	-0.0011125	-0.1254406
O	0.1147453	-1.6056394	-0.7731934
O	0.001516	0.8572621	-1.6033577
O	1.6914443	0.2572332	0.4842157
O	-1.0698194	0.3053347	1.0485074
H	-1.1386949	-3.1658171	0.9340632
H	1.2014631	-3.5855833	0.653343
H	-0.0292568	-3.8964624	-1.1921129
H	-0.3102492	3.4464924	-1.1973539
H	-2.1169603	2.2653416	-2.0954151
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H	3.751775	0.3820229	1.4872969
H	-2.4421676	2.3863444	1.8092629
H	-3.6381778	0.4926447	1.1325448
H	-2.3777387	0.4961362	3.1982327
Si	0.00000	-3.019872	0.000000
Si	-0.638226	2.27088	-2.034472
Si	2.392344	0.872496	1.806332
Si	-2.372274	0.908352	1.776808

$C_4H_{10} \rightarrow CH_4 + C_3H_6$

reactant

H	4.6896163	-2.6908675	-5.1894167
H	4.1134377	-1.8504281	-6.6529679
H	4.2151881	-3.6318383	-6.6297438
H	-0.0488853	-1.7258642	-4.9520622
H	0.4342851	-0.7734771	-3.5317088
H	0.526538	-2.5905457	-3.515629
H	0.1573682	-1.5372852	-1.7905018
H	2.8196707	-1.5160569	-3.7877405
H	2.2490187	-0.6825354	-5.2364318
H	1.824322	-2.9085796	-6.3516714
H	2.3953218	-3.7441261	-4.9015649
C	0.6829003	-1.6756428	-4.1246287
C	3.9618197	-2.7452939	-6.0206938
C	2.5244399	-2.8185482	-5.4976001
C	2.1228711	-1.6089769	-4.6436896
Al	0.1120376	0.1171422	-0.0748759
O	0.0594464	-1.5568171	-0.8142501
O	-0.0964097	0.8186025	-1.5845548
O	1.6665755	0.1813624	0.5343606
O	-1.1005314	0.1850561	1.090022
H	-1.1386949	-3.1658171	0.9340632
H	1.2014631	-3.5855833	0.653343
H	-0.0292568	-3.8964624	-1.1921129
H	-0.3102492	3.4464924	-1.1973539
H	-2.1169603	2.2653416	-2.0954151
H	-0.0561772	2.2351267	-3.3947444
H	2.2251902	2.3392429	1.9117505
H	2.0205096	0.2520551	3.09753
H	3.751775	0.3820229	1.4872969
H	-2.4421676	2.3863444	1.8092629
H	-3.6381778	0.4926447	1.1325448
H	-2.3777387	0.4961362	3.1982327
Si	0.00000	-3.019872	0.00000
Si	-0.638226	2.27088	-2.034472
Si	2.392344	0.872496	1.806332
Si	-2.372274	0.908352	1.776808

transition state

H	1.6033582	-3.4184734	-4.1372774
H	1.0599697	-2.5270354	-5.5921916
H	-0.1170939	-3.4104357	-4.5774014
H	-0.3184363	-0.9458023	-3.9834533
H	0.2567359	-1.7611213	-2.6170426
H	2.6516867	-1.0832953	-2.6089561
H	1.3514187	0.3272957	-2.9794722
H	2.3825845	-0.4559929	-4.3818087
H	4.3684725	-0.9338226	-2.0942881
H	3.3655985	-2.4001379	-1.6370239
H	2.9850282	-0.7696331	-0.8728281
C	0.7941411	-2.7904268	-4.5521491
C	0.5737088	-1.5596493	-3.6847054
C	3.3905703	-1.3053703	-1.7502034
C	1.5920131	-0.5406418	-3.6201879
Al	0.1212186	-0.0052665	-0.1245523
O	0.1121124	-1.6072409	-0.7730802
O	0.0038896	0.8578203	-1.6024151
O	1.690952	0.2595553	0.4841984
O	-1.0711253	0.3069539	1.0458577
H	-1.1386949	-3.1658171	0.9340632
H	1.2014631	-3.5855833	0.653343
H	-0.0292568	-3.8964624	-1.1921129
H	-0.3102492	3.4464924	-1.1973539
H	-2.1169603	2.2653416	-2.0954151
H	-0.0561772	2.2351267	-3.3947444
H	2.2251902	2.3392429	1.9117505
H	2.0205096	0.2520551	3.09753
H	3.751775	0.3820229	1.4872969
H	-2.4421676	2.3863444	1.8092629
H	-3.6381778	0.4926447	1.1325448
H	-2.3777387	0.4961362	3.1982327
Si	0.00000	-3.019872	0.00000
Si	-0.638226	2.27088	-2.034472
Si	2.392344	0.872496	1.806332
Si	-2.372274	0.908352	1.776808

$C_4H_{10} \rightarrow C_2H_6 + C_2H_4$

reactant

H	4.9441618	-0.8358654	-0.8730036
H	5.9029521	-0.9046654	-2.3790871
H	5.6345722	-2.3872189	-1.4225245
H	2.0692542	-1.3771279	-4.7235059
H	1.4236642	0.1892631	-4.2065406
H	1.172326	-1.3017177	-3.2010457
H	0.3143635	0.192622	-2.3712877
H	2.9774799	0.1953358	-2.2030488
H	3.8853909	0.1026678	-3.7217788
H	4.1139558	-2.391202	-3.4216655
H	3.1710991	-2.2957402	-1.9251106
C	1.8926361	-0.743955	-3.8343228
C	5.1601194	-1.4504092	-1.7666942
C	3.8818292	-1.7330057	-2.560726
C	3.1906981	-0.4612082	-3.0687729
Al	0.16661	-0.0798484	-0.0378019
O	0.1152942	-1.5998	-0.7572489
O	-0.042372	0.7469762	-1.6445364
O	1.6929385	0.4270594	0.4164178
O	-1.0744323	0.422223	0.9671402
H	-1.1386949	-3.1658171	0.9340632
H	1.2014631	-3.5855833	0.653343
H	-0.0292568	-3.8964624	-1.1921129
H	-0.3102492	3.4464924	-1.1973539
H	-2.1169603	2.2653416	-2.0954151
H	-0.0561772	2.2351267	-3.3947444
H	2.2251902	2.3392429	1.9117505
H	2.0205096	0.2520551	3.09753
H	3.751775	0.3820229	1.4872969
H	-2.4421676	2.3863444	1.8092629
H	-3.6381778	0.4926447	1.1325448
H	-2.3777387	0.4961362	3.1982327
Si	0.00000	-3.019872	0.00000
Si	-0.638226	2.27088	-2.034472
Si	2.392344	0.872496	1.806332
Si	-2.372274	0.908352	1.776808

transition state

H	2.9774286	2.2278533	-2.5642624
H	4.0747887	1.3165418	-3.6599803
H	4.4344932	1.4427237	-1.9136933
H	2.1019434	-2.4608369	-3.7400819
H	0.654919	-1.9701112	-4.6697959
H	0.5951388	-1.9838008	-2.8735634
H	1.6259671	0.1571202	-2.5505273
H	0.8117502	0.3775651	-3.8791451
H	2.4366858	-0.0569759	-4.4842353
H	3.3835627	-0.874158	-2.4799048
H	2.4748344	0.0817599	-1.2630817
C	1.2354134	-1.7775763	-3.7482307
C	3.6208176	1.3362349	-2.6540037
C	2.8582035	0.0741507	-2.3190883
C	1.6543426	-0.327185	-3.7658963
Al	0.1118127	-0.0120419	-0.1235444
O	0.1219452	-1.5999034	-0.7508827
O	0.0710945	0.8783492	-1.6060715
O	1.6950728	0.3071398	0.455571
O	-1.0580458	0.3475796	1.0442844
H	-1.1386949	-3.1658171	0.9340632
H	1.2014631	-3.5855833	0.653343
H	-0.0292568	-3.8964624	-1.1921129
H	-0.3102492	3.4464924	-1.1973539
H	-2.1169603	2.2653416	-2.0954151
H	-0.0561772	2.2351267	-3.3947444
H	2.2251902	2.3392429	1.9117505
H	2.0205096	0.2520551	3.09753
H	3.751775	0.3820229	1.4872969
H	-2.4421676	2.3863444	1.8092629
H	-3.6381778	0.4926447	1.1325448
H	-2.3777387	0.4961362	3.1982327
Si	0.00000	-3.019872	0.00000
Si	-0.638226	2.27088	-2.034472
Si	2.392344	0.872496	1.806332
Si	-2.372274	0.908352	1.776808

$C_5H_{12} \rightarrow CH_4 + 1\text{-}C_4H_8$

reactant

H	4.7533549	-1.1794311	-3.4320572
H	4.5699503	-2.9166371	-3.8007487
H	5.0543102	-2.3908149	-2.1644995
H	2.6730143	-3.053997	-2.1173116
H	2.8109253	-1.3107413	-1.8219503
H	1.1406108	-0.9923514	-6.3346984
H	1.117454	0.7578396	-5.9804079
H	-0.0154358	-0.3314567	-5.1434308
H	0.2765677	-1.5364367	-1.7639148
H	1.9037495	0.3215809	-3.6335463
H	3.0621542	-0.3098762	-4.8181111
H	2.0775536	-2.62528	-4.5222552
H	0.901584	-1.9779723	-3.3955623
C	4.4057824	-2.1453534	-3.0244929
C	1.0181948	-0.2449253	-5.5279647
C	2.9341545	-2.0906016	-2.5987161
C	1.949355	-1.8366139	-3.7540632
C	2.0440368	-0.4531688	-4.4104392
Al	0.1113446	0.1215127	-0.0736186
O	0.0434016	-1.553337	-0.8115874
O	-0.0760162	0.8262521	-1.5840706
O	1.668767	0.1737862	0.5350543
O	-1.098015	0.1879022	1.0927764
H	-1.1386949	-3.1658171	0.9340632
H	1.2014631	-3.5855833	0.653343
H	-0.0292568	-3.8964624	-1.1921129
H	-0.3102492	3.4464924	-1.1973539
H	-2.1169603	2.2653416	-2.0954151
H	-0.0561772	2.2351267	-3.3947444
H	2.2251902	2.3392429	1.9117505
H	2.0205096	0.2520551	3.09753
H	3.751775	0.3820229	1.4872969
H	-2.4421676	2.3863444	1.8092629
H	-3.6381778	0.4926447	1.1325448
H	-2.3777387	0.4961362	3.1982327
Si	0.000000	-3.019872	0.000000
Si	-0.638226	2.27088	-2.034472
Si	2.392344	0.872496	1.806332
Si	-2.372274	0.908352	1.776808

transition state

H	1.5914366	-4.8324161	-3.3989645
H	3.0578334	-3.9678568	-2.8882734
H	3.0957479	-4.9814143	-4.3479087
H	2.9281371	-2.5648366	-5.0490578
H	1.5179427	-3.500621	-5.5360023
H	0.5248187	-1.5401934	-4.7565893
H	0.3310972	-2.5940145	-3.3587669
H	1.8366858	-1.3934976	-1.9561428
H	0.945468	-0.2377954	-2.7445211
H	2.5068008	-0.4044209	-3.6816475
H	3.2693538	-0.4150703	-1.3365063
H	3.7469618	-1.799771	-2.4843264
H	2.8407766	-2.1346735	-0.9425727
C	2.4707426	-4.2768284	-3.7710985
C	2.0405687	-3.0957107	-4.6508481
C	1.0945896	-2.0874192	-3.9744922
C	3.0412025	-1.4063499	-1.7474732
C	1.683242	-0.9408964	-3.1971194
Al	0.1121557	-0.0023781	-0.101827
O	0.2345963	-1.6083363	-0.7449679
O	-0.0716219	0.8301914	-1.5847642
O	1.6888591	0.3248938	0.4598894
O	-1.075269	0.2500629	1.0836869
H	-1.1386949	-3.1658171	0.9340632
H	1.2014631	-3.5855833	0.653343
H	-0.0292568	-3.8964624	-1.1921129
H	-0.3102492	3.4464924	-1.1973539
H	-2.1169603	2.2653416	-2.0954151
H	-0.0561772	2.2351267	-3.3947444
H	2.2251902	2.3392429	1.9117505
H	2.0205096	0.2520551	3.09753
H	3.751775	0.3820229	1.4872969
H	-2.4421676	2.3863444	1.8092629
H	-3.6381778	0.4926447	1.1325448
H	-2.3777387	0.4961362	3.1982327
Si	0.000000	-3.019872	0.000000
Si	-0.638226	2.27088	-2.034472
Si	2.392344	0.872496	1.806332
Si	-2.372274	0.908352	1.776808

$C_5H_{12} \rightarrow C_2H_6 + C_3H_6$

reactant

H	2.2588707	-2.6375501	-4.9864757
H	2.6726719	-1.1557338	-5.8918825
H	0.9678332	-1.6622942	-5.729581
H	4.7210709	-0.9321146	-0.828497
H	5.7697235	-1.0723155	-2.2685323
H	5.3976377	-2.5181357	-1.2907738
H	1.4089513	0.2231788	-4.1903343
H	1.0830294	-1.2725417	-3.2462358
H	0.2976304	0.1850042	-2.374338
H	2.9430345	0.1376028	-2.3043669
H	3.8667618	-0.0702634	-3.8011175
H	4.0088892	-2.5445895	-3.3715546
H	2.9710176	-2.3633211	-1.9469993
C	1.9356225	-1.6036321	-5.199416
C	1.8163563	-0.7727239	-3.9156797
C	4.9740655	-1.5784655	-1.6893467
C	3.7395085	-1.8479492	-2.5549674
C	3.1288642	-0.5662948	-3.1386859
Al	0.1668639	-0.0793132	-0.0381279
O	0.1118041	-1.5995905	-0.7569998
O	-0.0431464	0.7467541	-1.6446543
O	1.6939706	0.4246238	0.4166155
O	-1.0733614	0.4231208	0.9681941
H	-1.1386949	-3.1658171	0.9340632
H	1.2014631	-3.5855833	0.653343
H	-0.0292568	-3.8964624	-1.1921129
H	-0.3102492	3.4464924	-1.1973539
H	-2.1169603	2.2653416	-2.0954151
H	-0.0561772	2.2351267	-3.3947444
H	2.2251902	2.3392429	1.9117505
H	2.0205096	0.2520551	3.09753
H	3.751775	0.3820229	1.4872969
H	-2.4421676	2.3863444	1.8092629
H	-3.6381778	0.4926447	1.1325448
H	-2.3777387	0.4961362	3.1982327
Si	0.000000	-3.019872	0.000000
Si	-0.638226	2.27088	-2.034472
Si	2.392344	0.872496	1.806332
Si	-2.372274	0.908352	1.776808

transition state

H	2.4110691	-2.9747154	-2.8038041
H	2.7040549	-2.7826209	-4.5652557
H	1.3588366	-3.792128	-3.9657836
H	3.0430368	2.1620573	-2.6496048
H	4.1107249	1.1635868	-3.6935515
H	4.4467444	1.3265726	-1.9453903
H	0.3834803	-1.6699213	-4.7527519
H	0.2420101	-1.732925	-2.9808234
H	1.5769889	0.1580654	-2.5290364
H	0.9053989	0.5330888	-3.9472325
H	2.4546549	-0.1710576	-4.4854765
H	3.2848641	-0.9541201	-2.4624387
H	2.4361053	0.0771271	-1.2846854
C	1.9208336	-2.8597294	-3.7867876
C	0.9661725	-1.6639824	-3.8096446
C	3.6418479	1.2363889	-2.6967509
C	2.8052718	0.0237667	-2.3453454
C	1.6183386	-0.2936267	-3.7864062
Al	0.1123311	-0.0109897	-0.1226587
O	0.1274707	-1.5990527	-0.7469649
O	0.0698324	0.8733105	-1.6117057
O	1.6939417	0.3144197	0.4532089
O	-1.0603832	0.3481255	1.0407895
H	-1.1386949	-3.1658171	0.9340632
H	1.2014631	-3.5855833	0.653343
H	-0.0292568	-3.8964624	-1.1921129
H	-0.3102492	3.4464924	-1.1973539
H	-2.1169603	2.2653416	-2.0954151
H	-0.0561772	2.2351267	-3.3947444
H	2.2251902	2.3392429	1.9117505
H	2.0205096	0.2520551	3.09753
H	3.751775	0.3820229	1.4872969
H	-2.4421676	2.3863444	1.8092629
H	-3.6381778	0.4926447	1.1325448
H	-2.3777387	0.4961362	3.1982327
Si	0.000000	-3.019872	0.000000
Si	-0.638226	2.27088	-2.034472
Si	2.392344	0.872496	1.806332
Si	-2.372274	0.908352	1.776808

$C_5H_{12} \rightarrow C_3H_8 + C_2H_4$

reactant

H	2.5722841	0.8839723	-3.004987
H	3.6461856	0.4664114	-4.3466424
H	1.3948346	-3.319946	-4.9876436
H	-0.1779641	-2.5180223	-5.2456723
H	0.3445869	-2.9534507	-3.5913673
H	0.2252119	0.1575752	-2.3793497
H	0.6290293	-0.4755192	-4.0408739
H	1.6696045	-0.8223501	-5.4117955
H	3.3238942	-1.976198	-3.8772327
H	2.2922851	-1.5944082	-2.4922072
H	5.2389945	-0.6483577	-2.6776168
H	4.1423363	-0.155009	-1.3526847
H	4.9855897	1.0823905	-2.3231194
C	4.4829169	0.099444	-2.3727672
C	0.6938559	-2.5743927	-4.5687791
C	3.3040017	0.1253505	-3.3495987
C	2.6001645	-1.23106	-3.4916642
C	1.3769437	-1.2128803	-4.4177508
Al	0.1674904	-0.0822538	-0.036462
O	0.1096939	-1.6006553	-0.7621997
O	-0.0511825	0.7428297	-1.6427942
O	1.693782	0.4214641	0.4177588
O	-1.0728409	0.4173107	0.9718532
H	-1.1386949	-3.1658171	0.9340632
H	1.2014631	-3.5855833	0.653343
H	-0.0292568	-3.8964624	-1.1921129
H	-0.3102492	3.4464924	-1.1973539
H	-2.1169603	2.2653416	-2.0954151
H	-0.0561772	2.2351267	-3.3947444
H	2.2251902	2.3392429	1.9117505
H	2.0205096	0.2520551	3.09753
H	3.751775	0.3820229	1.4872969
H	-2.4421676	2.3863444	1.8092629
H	-3.6381778	0.4926447	1.1325448
H	-2.3777387	0.4961362	3.1982327
Si	0.000000	-3.019872	0.000000
Si	-0.638226	2.27088	-2.034472
Si	2.392344	0.872496	1.806332
Si	-2.372274	0.908352	1.776808

transition state

H	2.9472623	2.1446008	-2.6357378
H	3.9034285	1.2311606	-3.8255968
H	1.9724913	-2.5091421	-3.7917573
H	0.5038296	-1.9996035	-4.6772238
H	0.4987334	-2.0160018	-2.8798634
H	1.5540323	0.1296896	-2.587526
H	0.7100252	0.3424581	-3.8906254
H	2.3063029	-0.106721	-4.5485357
H	3.3011089	-0.9483003	-2.575662
H	2.4543639	0.0309002	-1.3386634
H	5.5095173	0.5138394	-1.9967361
H	4.5506144	1.4283068	-0.7989519
H	5.3952823	2.291204	-2.1177405
C	4.8304666	1.3765947	-1.8654379
C	1.1139391	-1.8156035	-3.7731648
C	3.5912157	1.2563071	-2.7653017
C	2.7978539	0.0114833	-2.405771
C	1.5497563	-0.3692548	-3.8004111
Al	0.1156138	-0.00997	-0.122279
O	0.122603	-1.5989746	-0.7482961
O	0.0645333	0.8728917	-1.6103822
O	1.6984572	0.3128387	0.4517848
O	-1.0571423	0.3500939	1.0434384
H	-1.1386949	-3.1658171	0.9340632
H	1.2014631	-3.5855833	0.653343
H	-0.0292568	-3.8964624	-1.1921129
H	-0.3102492	3.4464924	-1.1973539
H	-2.1169603	2.2653416	-2.0954151
H	-0.0561772	2.2351267	-3.3947444
H	2.2251902	2.3392429	1.9117505
H	2.0205096	0.2520551	3.09753
H	3.751775	0.3820229	1.4872969
H	-2.4421676	2.3863444	1.8092629
H	-3.6381778	0.4926447	1.1325448
H	-2.3777387	0.4961362	3.1982327
Si	0.000000	-3.019872	0.000000
Si	-0.638226	2.27088	-2.034472
Si	2.392344	0.872496	1.806332
Si	-2.372274	0.908352	1.776808

$C_6H_{14} \rightarrow CH_4 + 1\text{-}C_5H_{10}$

reactant

H	6.5823238	-1.8655819	-3.667435
H	6.6901767	-0.3919002	-4.6678283
H	5.3426897	-1.5301323	-4.9046785
H	4.5913023	0.5087618	-3.594868
H	5.8677908	0.2358278	-2.4119779
H	4.8473114	-1.8908683	-1.6752295
H	3.7509292	-0.5189138	-1.4740173
H	1.3092313	-2.6242975	-5.050544
H	0.2973606	-1.1544284	-4.9414282
H	0.3661892	-2.3117288	-3.5863157
H	0.1331658	-1.5262465	-1.7862806
H	1.7846111	-0.2278573	-3.1380676
H	2.6964557	-0.5417772	-4.6145708
H	3.5900774	-2.6711696	-3.6786507
H	2.5668204	-2.5190162	-2.2527785
C	5.9867873	-1.0603476	-4.1384713
C	5.172163	-0.2891771	-3.0937441
C	0.9751935	-1.8161601	-4.3736217
C	4.2352079	-1.1579046	-2.2369674
C	3.1381719	-1.9252038	-2.9957805
C	2.1610391	-1.0424585	-3.7867003
Al	0.1127332	0.1218287	-0.072596
O	0.0529315	-1.5532726	-0.8115983
O	-0.1019301	0.8160659	-1.5841104
O	1.6718518	0.1839945	0.5281158
O	-1.0942334	0.1886533	1.0972837
H	-1.1386949	-3.1658171	0.9340632
H	1.2014631	-3.5855833	0.653343
H	-0.0292568	-3.8964624	-1.1921129
H	-0.3102492	3.4464924	-1.1973539
H	-2.1169603	2.2653416	-2.0954151
H	-0.0561772	2.2351267	-3.3947444
H	2.2251902	2.3392429	1.9117505
H	2.0205096	0.2520551	3.09753
H	3.751775	0.3820229	1.4872969
H	-2.4421676	2.3863444	1.8092629
H	-3.6381778	0.4926447	1.1325448
H	-2.3777387	0.4961362	3.1982327
Si	0.000000	-3.019872	0.000000
Si	-0.638226	2.27088	-2.034472
Si	2.392344	0.872496	1.806332
Si	-2.372274	0.908352	1.776808

transition state

H	4.2699275	-4.7952223	-4.9065706
H	2.8094682	-5.7032611	-5.3853304
H	3.6484849	-6.1032669	-3.8619913
H	1.5782817	-4.7749677	-3.3641603
H	3.023826	-3.8870437	-2.8900771
H	2.8869898	-2.5677934	-5.0848617
H	1.4712141	-3.5212047	-5.5277603
H	0.4893408	-1.5426929	-4.7558171
H	0.3187421	-2.5816668	-3.3436231
H	1.9038519	-1.3919514	-2.0038692
H	0.9449299	-0.2244345	-2.7545471
H	2.5021527	-0.4100766	-3.722747
H	3.2418925	-0.380289	-1.2871165
H	3.8113075	-1.7053568	-2.4689156
H	2.9000124	-2.1351941	-0.9442698
C	3.3471332	-5.2692053	-4.5210153
C	2.4702366	-4.2626255	-3.7710936
C	2.009184	-3.0962081	-4.6601422
C	1.073265	-2.084669	-3.9778589
C	3.0819333	-1.3752144	-1.7231124
C	1.6676462	-0.9259492	-3.2339415
Al	0.1132599	-0.0041538	-0.1047768
O	0.2223514	-1.6086813	-0.7447192
O	-0.0650052	0.8314782	-1.5882821
O	1.6894462	0.3259273	0.4593068
O	-1.0729338	0.259173	1.0807151
H	-1.1386949	-3.1658171	0.9340632
H	1.2014631	-3.5855833	0.653343
H	-0.0292568	-3.8964624	-1.1921129
H	-0.3102492	3.4464924	-1.1973539
H	-2.1169603	2.2653416	-2.0954151
H	-0.0561772	2.2351267	-3.3947444
H	2.2251902	2.3392429	1.9117505
H	2.0205096	0.2520551	3.09753
H	3.751775	0.3820229	1.4872969
H	-2.4421676	2.3863444	1.8092629
H	-3.6381778	0.4926447	1.1325448
H	-2.3777387	0.4961362	3.1982327
Si	0.000000	-3.019872	0.000000
Si	-0.638226	2.27088	-2.034472
Si	2.392344	0.872496	1.806332
Si	-2.372274	0.908352	1.776808

$C_6H_{14} \rightarrow C_2H_6 + 1\text{-}C_4H_8$

reactant

H	2.5246735	-0.009035	-6.5359361
H	2.8132785	-1.6526221	-7.1673886
H	3.8980431	-0.973238	-5.9306114
H	2.2821431	-2.6341303	-4.9039314
H	0.9169734	-1.7407455	-5.5706423
H	4.73723	-0.9134952	-0.7926054
H	5.8045977	-0.9653926	-2.2243081
H	5.479804	-2.4562591	-1.2987828
H	1.4262653	0.2253657	-4.1692383
H	1.1243704	-1.2653748	-3.2052863
H	0.3142398	0.1929543	-2.3741017
H	2.9414678	0.1388796	-2.2537557
H	3.879493	0.0112125	-3.7449523
H	4.1136801	-2.4674386	-3.3947168
H	3.0554691	-2.3745464	-1.9775556
C	2.8431082	-1.030997	-6.2542546
C	1.9387609	-1.6158737	-5.1645873
C	1.8467067	-0.7638751	-3.8848035
C	5.0236478	-1.5210273	-1.6710226
C	3.8090623	-1.8087712	-2.5588972
C	3.1557416	-0.5327883	-3.1073122
Al	0.1664155	-0.0791314	-0.0389305
O	0.1117569	-1.5996903	-0.7568079
O	-0.0408091	0.7476778	-1.6452523
O	1.6938073	0.4234846	0.4171351
O	-1.0737675	0.4242773	0.9668797
H	-1.1386949	-3.1658171	0.9340632
H	1.2014631	-3.5855833	0.653343
H	-0.0292568	-3.8964624	-1.1921129
H	-0.3102492	3.4464924	-1.1973539
H	-2.1169603	2.2653416	-2.0954151
H	-0.0561772	2.2351267	-3.3947444
H	2.2251902	2.3392429	1.9117505
H	2.0205096	0.2520551	3.09753
H	3.751775	0.3820229	1.4872969
H	-2.4421676	2.3863444	1.8092629
H	-3.6381778	0.4926447	1.1325448
H	-2.3777387	0.4961362	3.1982327
Si	0.000000	-3.019872	0.000000
Si	-0.638226	2.27088	-2.034472
Si	2.392344	0.872496	1.806332
Si	-2.372274	0.908352	1.776808

transition state

H	2.5710354	-2.8585915	-5.8751948
H	3.6372679	-3.8301929	-4.8279989
H	3.7636434	-2.0603998	-4.813778
H	2.4863024	-2.9128956	-2.7686468
H	1.3765182	-3.7773756	-3.809824
H	2.9954209	2.2135788	-2.6344431
H	4.0901485	1.2514426	-3.6839624
H	4.4215752	1.4130272	-1.9347856
H	0.4529325	-1.698182	-4.7475197
H	0.303223	-1.7466896	-2.9750148
H	1.5853314	0.1764921	-2.5273603
H	0.9004084	0.5195883	-3.9401377
H	2.469846	-0.1213181	-4.4839381
H	3.3242823	-0.8947509	-2.4638239
H	2.445279	0.1032942	-1.2826081
C	3.0441152	-2.8998766	-4.8757212
C	1.9951102	-2.8638679	-3.758891
C	1.0301899	-1.6694163	-3.8005411
C	3.6195268	1.3052242	-2.6867064
C	2.8158532	0.0680177	-2.3436108
C	1.6433203	-0.280595	-3.7823653
Al	0.1126611	-0.0111842	-0.1232414
O	0.1250298	-1.5990709	-0.7469618
O	0.0724142	0.8747756	-1.6114056
O	1.6941835	0.3139309	0.453465
O	-1.0599398	0.3499836	1.0400925
H	-1.1386949	-3.1658171	0.9340632
H	1.2014631	-3.5855833	0.653343
H	-0.0292568	-3.8964624	-1.1921129
H	-0.3102492	3.4464924	-1.1973539
H	-2.1169603	2.2653416	-2.0954151
H	-0.0561772	2.2351267	-3.3947444
H	2.2251902	2.3392429	1.9117505
H	2.0205096	0.2520551	3.09753
H	3.751775	0.3820229	1.4872969
H	-2.4421676	2.3863444	1.8092629
H	-3.6381778	0.4926447	1.1325448
H	-2.3777387	0.4961362	3.1982327
Si	0.000000	-3.019872	0.000000
Si	-0.638226	2.27088	-2.034472
Si	2.392344	0.872496	1.806332
Si	-2.372274	0.908352	1.776808

$C_6H_{14} \rightarrow C_3H_8 + C_3H_6$

reactant

H	2.2895758	-2.632914	-4.968057
H	2.6988365	-1.1533148	-5.8791827
H	0.9964433	-1.6704031	-5.7243617
H	4.6790706	-0.8746613	-0.8261046
H	5.7345938	-0.999991	-2.2428168
H	1.4166149	0.2265882	-4.1927092
H	1.0935835	-1.2663192	-3.2431782
H	0.3012	0.1865634	-2.3741494
H	2.9396713	0.1593431	-2.2970505
H	3.873064	-0.0498598	-3.7872423
H	4.0343484	-2.5201382	-3.3454429
H	2.9788228	-2.3442805	-1.9317196
H	5.9438611	-3.5037988	-1.8735909
H	4.8757509	-3.3769977	-0.4502973
H	6.4753432	-2.5865009	-0.4374639
C	5.601828	-2.8211139	-1.0726533
C	1.9606162	-1.6024174	-5.1887525
C	1.8282792	-0.7653939	-3.910337
C	4.9748346	-1.54977	-1.6522047
C	3.7489579	-1.8226704	-2.5338059
C	3.1349317	-0.5473502	-3.1265375
Al	0.1667874	-0.0793188	-0.0382645
O	0.1119329	-1.5996585	-0.7569304
O	-0.0424274	0.7469679	-1.6447369
O	1.6942052	0.4235138	0.416893
O	-1.073349	0.4236206	0.9678493
H	-1.1386949	-3.1658171	0.9340632
H	1.2014631	-3.5855833	0.653343
H	-0.0292568	-3.8964624	-1.1921129
H	-0.3102492	3.4464924	-1.1973539
H	-2.1169603	2.2653416	-2.0954151
H	-0.0561772	2.2351267	-3.3947444
H	2.2251902	2.3392429	1.9117505
H	2.0205096	0.2520551	3.09753
H	3.751775	0.3820229	1.4872969
H	-2.4421676	2.3863444	1.8092629
H	-3.6381778	0.4926447	1.1325448
H	-2.3777387	0.4961362	3.1982327
Si	0.000000	-3.019872	0.000000
Si	-0.638226	2.27088	-2.034472
Si	2.392344	0.872496	1.806332
Si	-2.372274	0.908352	1.776808

$C_6H_{14} \rightarrow C_4H_{10} + C_2H_4$

reactant

H	6.0177972	-0.5670077	-3.7496868
H	5.3199979	-1.8452369	-2.717633
H	6.434039	-0.649047	-2.0163168
H	4.0430228	-0.0922222	-1.4019703
H	4.8070415	1.1878138	-2.3489832
H	-0.2518283	-2.526788	-5.2308733
H	0.3027625	-2.965287	-3.587888
H	1.3226275	-3.3353145	-5.0056916
H	2.5334925	0.8722319	-3.1128203
H	3.638731	0.4169531	-4.4161768
H	0.2202332	0.1559913	-2.3805451
H	2.2754831	-1.6051534	-2.5247193
H	3.2691959	-2.0080387	-3.9315967
H	1.5997345	-0.8391769	-5.4340077
H	0.5876033	-0.4880804	-4.0431596
C	5.6109927	-0.779362	-2.742197
C	4.4362172	0.1466727	-2.4084835
C	3.2752744	0.1057043	-3.4157267
C	0.6334833	-2.5871479	-4.5720569
C	1.3249569	-1.2285499	-4.4344071
C	2.5668213	-1.2517526	-3.5329467
Al	0.1672483	-0.0822998	-0.0369638
O	0.1092964	-1.6008242	-0.7625553
O	-0.0512341	0.7426777	-1.6431953
O	1.6933074	0.4210042	0.4182875
O	-1.0731785	0.416952	0.9715029
H	-1.1386949	-3.1658171	0.9340632
H	1.2014631	-3.5855833	0.653343
H	-0.0292568	-3.8964624	-1.1921129
H	-0.3102492	3.4464924	-1.1973539
H	-2.1169603	2.2653416	-2.0954151
H	-0.0561772	2.2351267	-3.3947444
H	2.2251902	2.3392429	1.9117505
H	2.0205096	0.2520551	3.09753
H	3.751775	0.3820229	1.4872969
H	-2.4421676	2.3863444	1.8092629
H	-3.6381778	0.4926447	1.1325448
H	-2.3777387	0.4961362	3.1982327
Si	0.00000	-3.01987	0.00000
Si	-0.638226	2.27088	-2.034472
Si	2.392344	0.872496	1.806332
Si	-2.372274	0.908352	1.776808

transition state

H	6.2730388	0.4813424	-2.8657365
H	5.5382849	-0.3776201	-1.4780035
H	6.7084417	0.9251694	-1.1941942
H	4.3593659	1.7489716	-0.7788453
H	5.1526603	2.6409083	-2.0842522
H	0.6375824	-2.0546835	-4.6482828
H	0.6251531	-2.0498657	-2.8520969
H	2.1258734	-2.4825667	-3.754286
H	2.8584081	2.2005591	-2.7272156
H	3.9497798	1.2955739	-3.8036151
H	1.6010024	0.1411588	-2.5882045
H	2.4868831	0.0978241	-1.3192508
H	3.3744392	-0.8599899	-2.5504895
H	2.3435496	-0.0714877	-4.5342975
H	0.7250698	0.3025535	-3.8744878
C	5.8715589	0.611431	-1.842584
C	4.746046	1.6505752	-1.8093552
C	3.5712289	1.3581076	-2.765741
C	1.2352314	-1.831411	-3.7447874
C	1.5983299	-0.3672108	-3.7876809
C	2.8418842	0.0822574	-2.382955
Al	0.1153033	-0.0105488	-0.1234354
O	0.1245711	-1.5997937	-0.7488013
O	0.062948	0.8747564	-1.6078847
O	1.6983906	0.3137884	0.451998
O	-1.0565738	0.3478194	1.045244
H	-1.1386949	-3.1658171	0.9340632
H	1.2014631	-3.5855833	0.653343
H	-0.0292568	-3.8964624	-1.1921129
H	-0.3102492	3.4464924	-1.1973539
H	-2.1169603	2.2653416	-2.0954151
H	-0.0561772	2.2351267	-3.3947444
H	2.2251902	2.3392429	1.9117505
H	2.0205096	0.2520551	3.09753
H	3.751775	0.3820229	1.4872969
H	-2.4421676	2.3863444	1.8092629
H	-3.6381778	0.4926447	1.1325448
H	-2.3777387	0.4961362	3.1982327
Si	0.00000	-3.01987	0.00000
Si	-0.638226	2.27088	-2.034472
Si	2.392344	0.872496	1.806332
Si	-2.372274	0.908352	1.776808

Cartesian coordinates of stationary points obtained from B3LYP/SV(P) calculations for cracking on the FAU T5-cluster

$C_3H_8 \rightarrow CH_4 + C_2H_4$

reactant

H	13.2989347	12.6103164	11.5436359
H	12.4583989	11.0520666	11.78785
H	14.2158434	11.0927479	11.5071374
H	15.3548097	9.7811395	12.6260835
H	13.6439175	10.7196431	13.9819167
H	12.7283928	12.2254045	13.986436
H	14.9916298	12.5858842	14.9999345
H	14.8521841	13.5371117	13.4941117
H	15.786614	12.0215514	13.5112635
C	13.3800821	11.6151224	12.0189481
C	14.872321	12.5101764	13.9044746
C	13.6064991	11.7305448	13.5312403
Al	15.6233856	7.5206845	13.552105
O	16.048188	9.0958793	12.5587245
O	14.3355439	8.2084599	14.4337809
O	15.1679575	6.3858955	12.3868771
O	17.0882103	7.2117454	14.3689721
H	14.261262	7.181994	16.821028
H	17.136502	7.983422	16.899535
H	16.821028	4.562989	11.642257
H	16.032721	6.207816	10.008052
H	17.917006	8.277972	10.837739
H	14.474215	4.587002	10.840828
H	18.757316	8.816198	15.341029
H	18.777365	6.450061	16.070678
H	18.648939	9.795929	12.502615
H	17.115578	10.624785	10.861752
H	12.596385	6.450061	15.303072
H	12.616434	8.816198	16.032721
Si	17.94378	7.62533	15.70319
Si	13.42997	7.62533	15.67056
Si	15.67056	5.39428	11.19892
Si	17.47367	9.42844	11.66903

transition state

H	13.461594	11.5227377	11.2715416
H	12.8950692	9.8183768	11.6102455
H	14.6026382	10.0804885	11.6659212
H	15.0910701	11.0937942	13.7874269
H	13.7096059	9.8139654	13.9018818
H	13.0142465	11.6028039	13.7693305
H	15.113031	12.2695387	15.1868745
H	15.35095	12.8957485	13.4883225
H	16.5978857	11.8017842	14.2372548
C	13.6369486	10.6158706	11.869297
C	15.5270478	12.0654053	14.1883172
C	13.5175601	10.7447879	13.3029335
Al	15.6676668	7.6524607	13.444395
O	16.1001129	9.118019	12.522579
O	14.2943089	8.2214332	14.4041551
O	15.1658894	6.3862209	12.3941692
O	17.0028028	7.1981157	14.4442112
H	14.261262	7.181994	16.821028
H	17.136502	7.983422	16.899535
H	16.821028	4.562989	11.642257
H	16.032721	6.207816	10.008052
H	17.917006	8.277972	10.837739
H	14.474215	4.587002	10.840828
H	18.757316	8.816198	15.341029
H	18.777365	6.450061	16.070678
H	18.648939	9.795929	12.502615
H	17.115578	10.624785	10.861752
H	12.596385	6.450061	15.303072
H	12.616434	8.816198	16.032721
Si	17.94378	7.62533	15.70319
Si	13.42997	7.62533	15.67056
Si	15.67056	5.39428	11.19892
Si	17.47367	9.42844	11.66903

$C_4H_{10} \rightarrow CH_4 + C_3H_6$

reactant

H	13.1069655	12.3035071	9.8900767
H	11.3962188	11.8456424	10.1037519
H	12.4036904	11.0060437	8.8946128
H	12.1256975	9.5304812	10.8728006
H	13.8138055	10.0120127	10.7299694
H	15.3646334	9.789962	12.6423788
H	12.9461763	10.0402458	13.0896498
H	11.742593	11.2548581	12.6512397
H	13.7237039	12.2847681	13.8152678
H	13.5768582	12.9336361	12.1610909
H	14.8114247	11.7164448	12.5233412
C	12.4093369	11.4462163	9.9081343
C	12.8003006	10.4024305	10.9597369
C	13.7637547	12.0149486	12.7450536
C	12.764181	10.8988709	12.4155378
Al	15.6231347	7.5210532	13.5519077
O	16.0476363	9.095512	12.5574271
O	14.3359807	8.2084088	14.4342125
O	15.168744	6.3846667	12.3878746
O	17.0878774	7.2116514	14.3692641
H	14.261262	7.181994	16.821028
H	17.136502	7.983422	16.899535
H	16.821028	4.562989	11.642257
H	16.032721	6.207816	10.008052
H	17.917006	8.277972	10.837739
H	14.474215	4.587002	10.840828
H	18.757316	8.816198	15.341029
H	18.777365	6.450061	16.070678
H	18.648939	9.795929	12.502615
H	17.115578	10.624785	10.861752
H	12.596385	6.450061	15.303072
H	12.616434	8.816198	16.032721
Si	17.94378	7.62533	15.70319
Si	13.42997	7.62533	15.67056
Si	15.67056	5.39428	11.19892
Si	17.47367	9.42844	11.66903

transition state

H	13.6968559	10.5870609	9.5465662
H	12.0066973	10.0192463	9.358252
H	13.3371462	9.206396	8.4865302
H	12.6690189	7.7960823	10.4708108
H	14.3127514	8.3717449	10.6882627
H	13.6585662	10.1800422	12.1395715
H	13.0726036	8.5525857	12.8166989
H	11.8176328	9.6765586	11.9933114
H	13.2342462	10.7494586	13.8880835
H	13.5718725	11.9344282	12.5021082
H	14.9054162	10.7525464	13.1202938
C	13.0591532	9.6899837	9.4378749
C	13.2725817	8.7275456	10.6040451
C	13.8330466	10.9898799	13.002475
C	12.7938322	9.1711907	11.941449
Al	15.6817995	7.6505118	13.4580718
O	16.1079853	9.0958851	12.5188462
O	14.2624368	8.1647739	14.3647762
O	15.1513192	6.413017	12.3641094
O	17.0039884	7.1649026	14.4523627
H	14.261262	7.181994	16.821028
H	17.136502	7.983422	16.899535
H	16.821028	4.562989	11.642257
H	16.032721	6.207816	10.008052
H	17.917006	8.277972	10.837739
H	14.474215	4.587002	10.840828
H	18.757316	8.816198	15.341029
H	18.777365	6.450061	16.070678
H	18.648939	9.795929	12.502615
H	17.115578	10.624785	10.861752
H	12.596385	6.450061	15.303072
H	12.616434	8.816198	16.032721
Si	17.94378	7.62533	15.70319
Si	13.42997	7.62533	15.67056
Si	15.67056	5.39428	11.19892
Si	17.47367	9.42844	11.66903

$C_4H_{10} \rightarrow C_2H_6 + C_2H_4$

reactant

H	12.8862575	10.8089113	13.9282816
H	11.7076621	11.7911955	13.0419077
H	13.4553224	12.1231342	12.8677243
H	11.7918585	8.6953327	9.7119053
H	11.0737518	7.4338267	10.7505743
H	12.8402093	7.6817716	10.7462996
H	14.0893422	9.1528177	14.0320826
H	11.8243804	8.686587	12.8065173
H	10.7162964	9.6588862	11.8338477
H	12.629152	10.9158136	10.8348224
H	13.7896875	9.916023	11.707842
C	11.8660456	8.2022594	10.6991763
C	12.7039316	11.3187681	12.9574497
C	12.7718606	10.3474682	11.7740589
C	11.7328975	9.2186496	11.8366798
Al	15.7924058	7.5982045	13.3621907
O	16.1380433	9.0848589	12.565568
O	14.3289942	8.2601008	14.3534636
O	15.1312979	6.3430343	12.4260744
O	16.9420682	7.1133503	14.5194694
H	14.261262	7.181994	16.821028
H	17.136502	7.983422	16.899535
H	16.821028	4.562989	11.642257
H	16.032721	6.207816	10.008052
H	17.917006	8.277972	10.837739
H	14.474215	4.587002	10.840828
H	18.757316	8.816198	15.341029
H	18.777365	6.450061	16.070678
H	18.648939	9.795929	12.502615
H	17.115578	10.624785	10.861752
H	12.596385	6.450061	15.303072
H	12.616434	8.816198	16.032721
Si	17.94378	7.62533	15.70319
Si	13.42997	7.62533	15.67056
Si	15.67056	5.39428	11.19892
Si	17.47367	9.42844	11.66903

transition state

H	2.289022	-3.0393919	-2.8805513
H	2.523843	-2.8421378	-4.6502493
H	1.1856055	-3.8356279	-4.0095955
H	3.0071842	2.0680441	-2.7114073
H	3.9270455	1.0780228	-3.8656939
H	0.2140959	-1.696647	-4.7522424
H	0.1343065	-1.763721	-2.9764691
H	1.5044838	0.1217145	-2.5710185
H	0.7957108	0.4943675	-3.9642266
H	2.3125179	-0.2290927	-4.5557199
H	3.1967985	-1.037941	-2.5674981
H	2.4138193	0.0111854	-1.3631477
H	5.4746218	0.3246344	-2.000825
H	4.5526008	1.3182715	-0.8379528
H	5.4555272	2.1022268	-2.1677301
C	4.8402906	1.2250514	-1.8995525
C	1.7668214	-2.9121741	-3.8454574
C	0.8294219	-1.7025117	-3.8300337
C	3.6060242	1.1443194	-2.8097254
C	2.7412246	-0.0496048	-2.4341146
C	1.5024714	-0.3414272	-3.8250139
Al	0.1163144	-0.0087446	-0.1216094
O	0.1292276	-1.5982571	-0.744482
O	0.0618003	0.8671692	-1.6164558
O	1.6972732	0.3202642	0.4495074
O	-1.0597747	0.3499485	1.039774
H	-1.1386949	-3.1658171	0.9340632
H	1.2014631	-3.5855833	0.653343
H	-0.0292568	-3.8964624	-1.1921129
H	-0.3102492	3.4464924	-1.1973539
H	-2.1169603	2.2653416	-2.0954151
H	-0.0561772	2.2351267	-3.3947444
H	2.2251902	2.3392429	1.9117505
H	2.0205096	0.2520551	3.09753
H	3.751775	0.3820229	1.4872969
H	-2.4421676	2.3863444	1.8092629
H	-3.6381778	0.4926447	1.1325448
H	-2.3777387	0.4961362	3.1982327
Si	0.000000	-3.019872	0.000000
Si	-0.638226	2.27088	-2.034472
Si	2.392344	0.872496	1.806332
Si	-2.372274	0.908352	1.776808

transition state

H	13.4022645	11.072095	14.8297382
H	12.1913494	11.8960073	13.7781331
H	13.903902	12.4013649	13.7528881
H	12.7250775	8.8719139	10.4324307
H	11.4952002	7.7589601	11.0964771
H	13.2131438	7.5518894	11.5622567
H	13.2841457	9.3983812	13.0925363
H	11.8823997	8.6585428	13.4344784
H	11.4482905	10.0123977	12.3469063
H	13.3701785	10.9052076	11.7121204
H	14.6317028	10.1516991	12.753351
C	12.4329362	8.2984964	11.3286253
C	13.2302463	11.5280944	13.8411896
C	13.5912122	10.573653	12.7330516
C	12.1594985	9.1951951	12.5119898
Al	15.6759815	7.6386364	13.4588793
O	16.1184975	9.0859319	12.538557
O	14.2488275	8.1935161	14.3575296
O	15.1406488	6.3865962	12.3878293
O	16.9816473	7.1552345	14.4731456
H	14.261262	7.181994	16.821028
H	17.136502	7.983422	16.899535
H	16.821028	4.562989	11.642257
H	16.032721	6.207816	10.008052
H	17.917006	8.277972	10.837739
H	14.474215	4.587002	10.840828
H	18.757316	8.816198	15.341029
H	18.777365	6.450061	16.070678
H	18.648939	9.795929	12.502615
H	17.115578	10.624785	10.861752
H	12.596385	6.450061	15.303072
H	12.616434	8.816198	16.032721
Si	17.94378	7.62533	15.70319
Si	13.42997	7.62533	15.67056
Si	15.67056	5.39428	11.19892
Si	17.47367	9.42844	11.66903

$C_5H_{12} \rightarrow CH_4 + 1\text{-}C_4H_8$

reactant

H	10.3151273	11.2165559	9.8841158
H	10.8950276	12.6921048	9.0652367
H	10.9173362	12.5946357	10.8422689
H	13.2386106	12.2441122	9.8825849
H	12.6351137	10.9372376	8.8654188
H	12.1076986	9.5358944	10.8393368
H	13.8147731	9.9617433	10.7450725
H	15.3624776	9.7882482	12.6380751
H	12.9383217	10.0242488	13.0684142
H	11.7335042	11.2332111	12.6377524
H	13.7142868	12.2609363	13.8074667
H	13.5544125	12.9275946	12.1616049
H	14.7981672	11.714826	12.5017831
C	11.0823362	12.013136	9.9168262
C	12.4956297	11.423648	9.8494595
C	12.8085845	10.3865793	10.9420714
C	13.7499954	12.0033063	12.7340682
C	12.7553142	10.8850845	12.397597
Al	15.6231015	7.5210844	13.5520039
O	16.0478046	9.0955357	12.5576829
O	14.3358055	8.208273	14.434122
O	15.1688773	6.3846892	12.3878787
O	17.0879195	7.2115996	14.3692462
H	14.261262	7.181994	16.821028
H	17.136502	7.983422	16.899535
H	16.821028	4.562989	11.642257
H	16.032721	6.207816	10.008052
H	17.917006	8.277972	10.837739
H	14.474215	4.587002	10.840828
H	18.757316	8.816198	15.341029
H	18.777365	6.450061	16.070678
H	18.648939	9.795929	12.502615
H	17.115578	10.624785	10.861752
H	12.596385	6.450061	15.303072
H	12.616434	8.816198	16.032721
Si	17.94378	7.62533	15.70319
Si	13.42997	7.62533	15.67056
Si	15.67056	5.39428	11.19892
Si	17.47367	9.42844	11.66903

transition state

H	10.9688166	9.2788337	8.9896874
H	11.6032931	10.7681378	8.2455549
H	11.2353644	10.74057	9.9811631
H	13.7457529	10.5485099	9.5661494
H	13.4762868	9.1613589	8.5182729
H	12.6429905	7.7940115	10.4568655
H	14.2959922	8.3448481	10.6890698
H	13.655356	10.164759	12.1339985
H	13.0729581	8.5362462	12.8091296
H	11.8089773	9.6572361	12.0054069
H	13.2323987	10.7355316	13.8809153
H	13.5406483	11.9219609	12.489436
H	14.8962668	10.7639612	13.1023554
C	11.6474701	10.1373015	9.1503867
C	13.0835482	9.6732251	9.4142708
C	13.261693	8.7152201	10.5989076
C	13.8195166	10.9823765	12.9893022
C	12.7847459	9.1557982	11.9378136
Al	15.6820556	7.6511517	13.458013
O	16.1081576	9.0958558	12.518662
O	14.2622567	8.1638753	14.3645745
O	15.1519114	6.4126682	12.3645001
O	17.0040741	7.1647304	14.4524414
H	14.261262	7.181994	16.821028
H	17.136502	7.983422	16.899535
H	16.821028	4.562989	11.642257
H	16.032721	6.207816	10.008052
H	17.917006	8.277972	10.837739
H	14.474215	4.587002	10.840828
H	18.757316	8.816198	15.341029
H	18.777365	6.450061	16.070678
H	18.648939	9.795929	12.502615
H	17.115578	10.624785	10.861752
H	12.596385	6.450061	15.303072
H	12.616434	8.816198	16.032721
Si	17.94378	7.62533	15.70319
Si	13.42997	7.62533	15.67056
Si	15.67056	5.39428	11.19892
Si	17.47367	9.42844	11.66903

$C_5H_{12} \rightarrow C_2H_6 + C_3H_6$

reactant

H	12.344584	9.318583	9.0540095
H	10.5818581	9.1429195	9.2735765
H	11.5519987	7.7739742	8.6662427
H	12.9468789	10.8003561	13.9202754
H	11.7653212	11.8031243	13.0629829
H	13.5144233	12.0910679	12.8305934
H	11.0086643	7.3563885	11.0452095
H	12.7480564	7.6180722	10.8901361
H	14.0867072	9.1512206	14.030198
H	11.7821224	8.7349097	12.8821067
H	10.6819383	9.6844934	11.8780547
H	12.5969402	10.8959612	10.8398474
H	13.7577776	9.8679394	11.6799247
C	11.5519049	8.619814	9.3772995
C	11.7678163	8.127162	10.8124165
C	12.7468229	11.3062681	12.9506514
C	12.7531167	10.3247972	11.7733989
C	11.6897436	9.2219915	11.8891104
Al	15.7922003	7.5983086	13.3622579
O	16.1374375	9.0843752	12.5642797
O	14.3297077	8.2600633	14.3541279
O	15.1314709	6.3421423	12.4268069
O	16.9426435	7.1135742	14.518935
H	14.261262	7.181994	16.821028
H	17.136502	7.983422	16.899535
H	16.821028	4.562989	11.642257
H	16.032721	6.207816	10.008052
H	17.917006	8.277972	10.837739
H	14.474215	4.587002	10.840828
H	18.757316	8.816198	15.341029
H	18.777365	6.450061	16.070678
H	18.648939	9.795929	12.502615
H	17.115578	10.624785	10.861752
H	12.596385	6.450061	15.303072
H	12.616434	8.816198	16.032721
Si	17.94378	7.62533	15.70319
Si	13.42997	7.62533	15.67056
Si	15.67056	5.39428	11.19892
Si	17.47367	9.42844	11.66903

transition state

H	13.9581148	9.2758196	10.2915209
H	12.2932818	9.793195	9.8497055
H	12.8827472	8.1640583	9.4241087
H	13.3930112	11.1145263	15.0080023
H	12.2562089	11.9985538	13.929153
H	13.9809792	12.4558321	13.9918939
H	11.3938132	7.9251699	11.3881756
H	13.060245	7.556344	11.871587
H	13.382239	9.4674528	13.2180241
H	11.8558628	8.9399725	13.5967102
H	11.5562046	10.2260421	12.3956175
H	13.5104218	11.0327602	11.887088
H	14.691364	10.2312405	12.9455328
C	12.9085739	8.9440273	10.2038662
C	12.3989354	8.3718501	11.5288303
C	13.2814925	11.6002557	14.0248519
C	13.6555827	10.6587527	12.9061838
C	12.2051971	9.3793829	12.6485823
Al	15.6765026	7.636961	13.4556633
O	16.1166557	9.085057	12.5361711
O	14.2508423	8.202846	14.3588242
O	15.1429644	6.379383	12.3946603
O	16.9790616	7.1572287	14.4749722
H	14.261262	7.181994	16.821028
H	17.136502	7.983422	16.899535
H	16.821028	4.562989	11.642257
H	16.032721	6.207816	10.008052
H	17.917006	8.277972	10.837739
H	14.474215	4.587002	10.840828
H	18.757316	8.816198	15.341029
H	18.777365	6.450061	16.070678
H	18.648939	9.795929	12.502615
H	17.115578	10.624785	10.861752
H	12.596385	6.450061	15.303072
H	12.616434	8.816198	16.032721
Si	17.94378	7.62533	15.70319
Si	13.42997	7.62533	15.67056
Si	15.67056	5.39428	11.19892
Si	17.47367	9.42844	11.66903

$C_5H_{12} \rightarrow C_3H_8 + C_2H_4$

reactant

H	13.6507622	12.8083754	11.582687
H	14.8672228	11.8051494	12.418404
H	13.9087373	13.0048581	13.337386
H	13.0203054	10.7011778	13.7614054
H	11.8138349	11.6703126	12.9329825
H	11.4845432	8.3675866	9.8507569
H	10.8159768	7.2268901	11.0496992
H	12.5838527	7.4020111	10.8778032
H	14.0604057	9.1390579	14.0143109
H	11.7781152	8.6113735	12.9211116
H	10.6326217	9.5513931	11.9611141
H	12.4941703	10.6450851	10.71693
H	13.6907594	9.6507011	11.5500838
C	13.866531	12.2626413	12.5197229
C	11.6266733	7.9551776	10.8671214
C	12.8024761	11.1941343	12.7845355
C	12.7028337	10.135064	11.6779829
C	11.6277337	9.0667687	11.9204287
Al	15.7907454	7.6011092	13.3626298
O	16.1350617	9.087611	12.5624343
O	14.328165	8.2595251	14.3536036
O	15.1321772	6.3442411	12.425676
O	16.9425419	7.11602	14.517843
H	14.261262	7.181994	16.821028
H	17.136502	7.983422	16.899535
H	16.821028	4.562989	11.642257
H	16.032721	6.207816	10.008052
H	17.917006	8.277972	10.837739
H	14.474215	4.587002	10.840828
H	18.757316	8.816198	15.341029
H	18.777365	6.450061	16.070678
H	18.648939	9.795929	12.502615
H	17.115578	10.624785	10.861752
H	12.596385	6.450061	15.303072
H	12.616434	8.816198	16.032721
Si	17.94378	7.62533	15.70319
Si	13.42997	7.62533	15.67056
Si	15.67056	5.39428	11.19892
Si	17.47367	9.42844	11.66903

transition state

H	14.040196	13.2690297	12.7421924
H	15.2180292	12.4390246	13.8016188
H	13.9325995	13.4534549	14.5145007
H	13.3630192	11.0255579	14.7790104
H	12.1723473	11.8479949	13.7368834
H	12.6621033	8.8210637	10.4351751
H	11.4550521	7.7046629	11.1340611
H	13.1826913	7.520272	11.571843
H	13.260201	9.3723809	13.0925008
H	11.8668301	8.6353942	13.4507232
H	11.4125118	9.9761114	12.3590698
H	13.3236625	10.8615011	11.6796878
H	14.6005721	10.1216452	12.7116641
C	14.1599852	12.7390358	13.7046063
C	12.3909488	8.2562008	11.3431005
C	13.2263646	11.5207457	13.8027228
C	13.5583864	10.5393855	12.7010999
C	12.1314183	9.165193	12.5207727
Al	15.6756272	7.6395065	13.4587032
O	16.1197825	9.0870925	12.5402218
O	14.2466249	8.1923299	14.35569
O	15.1411812	6.3867623	12.3878215
O	16.9806206	7.1555431	14.4739613
H	14.261262	7.181994	16.821028
H	17.136502	7.983422	16.899535
H	16.821028	4.562989	11.642257
H	16.032721	6.207816	10.008052
H	17.917006	8.277972	10.837739
H	14.474215	4.587002	10.840828
H	18.757316	8.816198	15.341029
H	18.777365	6.450061	16.070678
H	18.648939	9.795929	12.502615
H	17.115578	10.624785	10.861752
H	12.596385	6.450061	15.303072
H	12.616434	8.816198	16.032721
Si	17.94378	7.62533	15.70319
Si	13.42997	7.62533	15.67056
Si	15.67056	5.39428	11.19892
Si	17.47367	9.42844	11.66903

$C_6H_{14} \rightarrow CH_4 + 1\text{-}C_5H_{10}$

reactant

H	11.4404497	13.6748185	8.6064403
H	9.7234899	13.1943812	8.6768098
H	10.8697546	12.2684122	7.6700938
H	10.3424821	11.0478844	9.833083
H	10.8948701	12.4479349	10.7597042
H	13.2148586	12.1633078	9.8198509
H	12.6554742	10.8210549	8.8218798
H	12.1216039	9.4546176	10.8239216
H	13.8222273	9.9030821	10.733235
H	15.359328	9.7856754	12.6320608
H	12.9278927	10.0009858	13.0468331
H	11.7104867	11.1854065	12.5838863
H	13.6678223	12.263825	13.7451395
H	13.5148591	12.8920517	12.0835714
H	14.769954	11.7021958	12.4615676
C	10.7567704	12.8052116	8.6307588
C	11.0635757	11.8889643	9.8194559
C	12.4910341	11.3244864	9.7945483
C	12.8087445	10.3176698	10.9131158
C	13.7162931	11.9830447	12.6780383
C	12.7382138	10.8457292	12.3576366
Al	15.6231771	7.5210874	13.5521074
O	16.0479356	9.0955506	12.5578548
O	14.3357163	8.2080854	14.4340309
O	15.1689433	6.3847592	12.3878558
O	17.0880946	7.2116294	14.3691337
H	14.261262	7.181994	16.821028
H	17.136502	7.983422	16.899535
H	16.821028	4.562989	11.642257
H	16.032721	6.207816	10.008052
H	17.917006	8.277972	10.837739
H	14.474215	4.587002	10.840828
H	18.757316	8.816198	15.341029
H	18.777365	6.450061	16.070678
H	18.648939	9.795929	12.502615
H	17.115578	10.624785	10.861752
H	12.596385	6.450061	15.303072
H	12.616434	8.816198	16.032721
Si	17.94378	7.62533	15.70319
Si	13.42997	7.62533	15.67056
Si	15.67056	5.39428	11.19892
Si	17.47367	9.42844	11.66903

transition state

H	12.1756708	11.9284418	7.9733088
H	10.5185672	11.3300285	7.6871041
H	11.9128983	10.4749229	6.9734038
H	11.0123005	9.2444568	8.9989399
H	11.2529487	10.6937199	9.9860504
H	13.7499658	10.5567765	9.5734164
H	13.5056088	9.1677356	8.5199013
H	12.6459486	7.7966019	10.4513984
H	14.298479	8.343826	10.6923274
H	13.6529336	10.1665702	12.1326484
H	13.0707551	8.5356031	12.8063945
H	11.8083382	9.6572542	12.0011288
H	13.2309416	10.7319465	13.8815271
H	13.5393284	11.921978	12.4933063
H	14.8947721	10.7622939	13.1032999
C	11.5608292	11.014748	7.8716492
C	11.6612512	10.1340241	9.1210075
C	13.09696	9.6750269	9.4125602
C	13.2655029	8.7165038	10.5973066
C	13.8180666	10.9809465	12.9905218
C	12.784091	9.1557926	11.9351765
Al	15.6819475	7.6512296	13.4581048
O	16.1084404	9.0958487	12.518963
O	14.2622775	8.1638247	14.364697
O	15.1520703	6.4125759	12.3645933
O	17.0040443	7.1646249	14.4525316
H	14.261262	7.181994	16.821028
H	17.136502	7.983422	16.899535
H	16.821028	4.562989	11.642257
H	16.032721	6.207816	10.008052
H	17.917006	8.277972	10.837739
H	14.474215	4.587002	10.840828
H	18.757316	8.816198	15.341029
H	18.777365	6.450061	16.070678
H	18.648939	9.795929	12.502615
H	17.115578	10.624785	10.861752
H	12.596385	6.450061	15.303072
H	12.616434	8.816198	16.032721
Si	17.94378	7.62533	15.70319
Si	13.42997	7.62533	15.67056
Si	15.67056	5.39428	11.19892
Si	17.47367	9.42844	11.66903

$C_6H_{14} \rightarrow C_2H_6 + 1\text{-}C_4H_8$

reactant

H	9.4857184	8.794588	9.2389318
H	10.2811486	9.7355269	7.9483659
H	10.2007958	10.3874721	9.6021618
H	13.5723596	12.1521584	12.9262539
H	12.5095719	9.4618415	9.0992362
H	11.8049506	7.9096057	8.655799
H	12.9948435	10.8298734	13.9712118
H	11.8209434	11.86889	13.1469958
H	11.0194438	7.5098076	10.9646457
H	12.7713059	7.726534	10.8828569
H	14.0895212	9.1537168	14.033852
H	11.8115503	8.8106083	12.8624985
H	10.7241449	9.8016525	11.8935117
H	12.6510765	11.0314202	10.8953647
H	13.8007453	9.9653404	11.7028332
C	10.3418309	9.4599573	9.0169887
C	11.6752383	8.7736993	9.3345352
C	11.8091254	8.2644489	10.7800576
C	12.7990884	11.3691967	13.0189365
C	12.7999645	10.4275197	11.8095176
C	11.7267399	9.3310627	11.8860498
Al	15.7919943	7.5985596	13.3621644
O	16.137756	9.084935	12.5648675
O	14.3293509	8.2603108	14.3539706
O	15.1314703	6.3426606	12.4264332
O	16.9424849	7.113851	14.5189091
H	14.261262	7.181994	16.821028
H	17.136502	7.983422	16.899535
H	16.821028	4.562989	11.642257
H	16.032721	6.207816	10.008052
H	17.917006	8.277972	10.837739
H	14.474215	4.587002	10.840828
H	18.757316	8.816198	15.341029
H	18.777365	6.450061	16.070678
H	18.648939	9.795929	12.502615
H	17.115578	10.624785	10.861752
H	12.596385	6.450061	15.303072
H	12.616434	8.816198	16.032721
Si	17.94378	7.62533	15.70319
Si	13.42997	7.62533	15.67056
Si	15.67056	5.39428	11.19892
Si	17.47367	9.42844	11.66903

transition state

H	10.9759819	9.6387431	9.3940528
H	12.3981878	10.2992776	8.5461912
H	11.9388667	10.9459696	10.1332405
H	14.0200136	12.458863	14.03739
H	13.9315606	9.3348809	10.3147777
H	12.9935377	8.090178	9.5098283
H	13.4261321	11.1086554	15.0382565
H	12.2914374	12.0159169	13.9768447
H	11.3949313	7.9570889	11.4061936
H	13.0657228	7.5976982	11.8812475
H	13.3914108	9.4881162	13.2267788
H	11.8615454	8.9735798	13.6042712
H	11.5703397	10.2712327	12.4172597
H	13.5297998	11.0691466	11.9167089
H	14.7070456	10.2409623	12.9586567
C	12.00671	10.0139591	9.5384929
C	12.9004656	8.9542896	10.1914068
C	12.3999737	8.4089904	11.5377486
C	13.3140203	11.6084261	14.0622922
C	13.6750509	10.6784501	12.9295287
C	12.2124256	9.4171817	12.6587735
Al	15.676336	7.6370533	13.4560325
O	16.118071	9.0858016	12.5381215
O	14.2520589	8.2038591	14.3602942
O	15.1437474	6.3796677	12.3945822
O	16.9793391	7.1568425	14.4750046
H	14.261262	7.181994	16.821028
H	17.136502	7.983422	16.899535
H	16.821028	4.562989	11.642257
H	16.032721	6.207816	10.008052
H	17.917006	8.277972	10.837739
H	14.474215	4.587002	10.840828
H	18.757316	8.816198	15.341029
H	18.777365	6.450061	16.070678
H	18.648939	9.795929	12.502615
H	17.115578	10.624785	10.861752
H	12.596385	6.450061	15.303072
H	12.616434	8.816198	16.032721
Si	17.94378	7.62533	15.70319
Si	13.42997	7.62533	15.67056
Si	15.67056	5.39428	11.19892
Si	17.47367	9.42844	11.66903

$C_6H_{14} \rightarrow C_3H_8 + C_3H_6$

reactant

H	13.7294002	12.901813	11.7125909
H	14.9343761	11.8471797	12.5005976
H	13.9955563	13.0197995	13.4731169
H	12.1328046	9.1821223	9.0381157
H	10.3827118	9.0596269	9.3672373
H	11.2795964	7.649437	8.7418314
H	13.0768728	10.7128679	13.8019672
H	11.8813338	11.7325897	13.0208157
H	10.8692725	7.3123545	11.1610125
H	12.6029053	7.5198457	10.8934248
H	14.0614465	9.1412231	14.0172432
H	11.7880635	8.7168784	12.9064691
H	10.6612983	9.6750546	11.9409899
H	12.5434217	10.8015374	10.7639007
H	13.7230573	9.745554	11.5465609
C	13.9405027	12.3137459	12.6247496
C	11.3437545	8.5136004	9.4275024
C	11.6335612	8.0541219	10.8605866
C	12.8626646	11.2496859	12.8475482
C	12.7434683	10.2408267	11.6964003
C	11.6528806	9.1802225	11.9074164
Al	15.7901181	7.6016594	13.3626291
O	16.1350555	9.0881198	12.5623957
O	14.3275274	8.2596377	14.353345
O	15.1328445	6.3443172	12.4256798
O	16.9423948	7.1168072	14.5176739
H	14.261262	7.181994	16.821028
H	17.136502	7.983422	16.899535
H	16.821028	4.562989	11.642257
H	16.032721	6.207816	10.008052
H	17.917006	8.277972	10.837739
H	14.474215	4.587002	10.840828
H	18.757316	8.816198	15.341029
H	18.777365	6.450061	16.070678
H	18.648939	9.795929	12.502615
H	17.115578	10.624785	10.861752
H	12.596385	6.450061	15.303072
H	12.616434	8.816198	16.032721
Si	17.94378	7.62533	15.70319
Si	13.42997	7.62533	15.67056
Si	15.67056	5.39428	11.19892
Si	17.47367	9.42844	11.66903

transition state

H	14.1858514	13.3743962	13.0730132
H	15.2918004	12.4845809	14.1596688
H	13.9905924	13.4983621	14.8428611
H	13.9410523	9.2789479	10.2866193
H	12.2736051	9.7920551	9.8509686
H	12.8656195	8.1645971	9.4224816
H	13.3610047	11.0727172	14.9855827
H	12.2434647	11.9591942	13.9207353
H	11.3845501	7.9203608	11.3911017
H	13.0534584	7.5569096	11.869343
H	13.3713876	9.4667136	13.2187753
H	11.8502533	8.934815	13.5984684
H	11.5428752	10.2214893	12.4015379
H	13.4932162	11.0333828	11.8822885
H	14.6808447	10.22895	12.9326657
C	14.2452141	12.8079139	14.0202794
C	12.892176	8.9442429	10.2025578
C	12.3884497	8.3703642	11.5289959
C	13.2865838	11.6067524	14.0228976
C	13.6446139	10.655776	12.8997693
C	12.1959551	9.3769443	12.6503259
Al	15.6759448	7.6379236	13.4557047
O	16.1178714	9.0860908	12.5375471
O	14.250366	8.202899	14.3588289
O	15.1436432	6.3799103	12.3944156
O	16.978702	7.1577034	14.4752514
H	14.261262	7.181994	16.821028
H	17.136502	7.983422	16.899535
H	16.821028	4.562989	11.642257
H	16.032721	6.207816	10.008052
H	17.917006	8.277972	10.837739
H	14.474215	4.587002	10.840828
H	18.757316	8.816198	15.341029
H	18.777365	6.450061	16.070678
H	18.648939	9.795929	12.502615
H	17.115578	10.624785	10.861752
H	12.596385	6.450061	15.303072
H	12.616434	8.816198	16.032721
Si	17.94378	7.62533	15.70319
Si	13.42997	7.62533	15.67056
Si	15.67056	5.39428	11.19892
Si	17.47367	9.42844	11.66903

$C_6H_{14} \rightarrow C_4H_{10} + C_2H_4$

reactant

H	14.3256573	12.8461857	14.6314017
H	13.0836172	13.8606237	13.8493058
H	14.8073041	14.0869364	13.4461646
H	13.6621392	12.8209122	11.6028272
H	14.8871958	11.808234	12.3795178
H	13.0945022	10.7180619	13.7770777
H	11.8683938	11.7022473	12.9936485
H	11.4553294	8.4615064	9.856096
H	10.7980221	7.30624	11.0473842
H	12.5639818	7.4683507	10.845774
H	14.0613385	9.1404241	14.0163546
H	11.8058508	8.64926	12.9241227
H	10.653233	9.6167588	12.0008603
H	12.5035509	10.7118985	10.7416169
H	13.7045042	9.6931556	11.5394735
C	14.0381705	13.3282762	13.6774882
C	13.9116949	12.3017485	12.548404
C	11.6119919	8.0302737	10.862464
C	12.8519804	11.2250464	12.8119564
C	12.7241232	10.1853378	11.6907886
C	11.6426531	9.1234677	11.9343657
Al	15.7904214	7.6013215	13.3626922
O	16.1351406	9.0877322	12.5623631
O	14.3283465	8.2595753	14.3539125
O	15.1323286	6.3444627	12.4254841
O	16.9428002	7.1163086	14.5175456
H	14.261262	7.181994	16.821028
H	17.136502	7.983422	16.899535
H	16.821028	4.562989	11.642257
H	16.032721	6.207816	10.008052
H	17.917006	8.277972	10.837739
H	14.474215	4.587002	10.840828
H	18.757316	8.816198	15.341029
H	18.777365	6.450061	16.070678
H	18.648939	9.795929	12.502615
H	17.115578	10.624785	10.861752
H	12.596385	6.450061	15.303072
H	12.616434	8.816198	16.032721
Si	17.94378	7.62533	15.70319
Si	13.42997	7.62533	15.67056
Si	15.67056	5.39428	11.19892
Si	17.47367	9.42844	11.66903

transition state

H	14.0237386	13.331023	15.8108391
H	12.8559068	14.1617034	14.7447014
H	14.5788861	14.6266168	14.7170485
H	14.0520443	13.2108463	12.7140134
H	15.2074949	12.3875181	13.7739411
H	13.3476311	11.0302617	14.7834395
H	12.1679768	11.8552003	13.7302798
H	12.6409531	8.8186964	10.4490946
H	11.4402398	7.7047694	11.1629491
H	13.171893	7.5205959	11.5831306
H	13.2706863	9.3593983	13.1138742
H	11.8695013	8.6411362	13.4704299
H	11.4094473	9.9779922	12.3819383
H	13.3216987	10.8436631	11.6836676
H	14.5925503	10.1152303	12.7206269
C	13.8881818	13.7696225	14.805335
C	14.1604823	12.7363724	13.7083648
C	12.3782212	8.2564406	11.3611441
C	13.2195264	11.5185004	13.8016344
C	13.5481348	10.5268112	12.7084412
C	12.1324641	9.1698824	12.5394046
Al	15.6761375	7.6390264	13.4580509
O	16.1205166	9.0865459	12.5410784
O	14.2451657	8.1930098	14.3539417
O	15.1412627	6.385736	12.3887147
O	16.9789556	7.1548747	14.4756595
H	14.261262	7.181994	16.821028
H	17.136502	7.983422	16.899535
H	16.821028	4.562989	11.642257
H	16.032721	6.207816	10.008052
H	17.917006	8.277972	10.837739
H	14.474215	4.587002	10.840828
H	18.757316	8.816198	15.341029
H	18.777365	6.450061	16.070678
H	18.648939	9.795929	12.502615
H	17.115578	10.624785	10.861752
H	12.596385	6.450061	15.303072
H	12.616434	8.816198	16.032721
Si	17.94378	7.62533	15.70319
Si	13.42997	7.62533	15.67056
Si	15.67056	5.39428	11.19892
Si	17.47367	9.42844	11.66903

Cartesian coordinates of stationary points obtained from B3LYP/SV(P) calculations for cracking on the MFI T23-cluster

$C_3H_8 \rightarrow CH_4 + C_2H_4$

reactant

H	4.5669842	-23.645373	19.5615878
H	4.1448438	-24.6577991	18.160515
H	5.5984811	-23.6102784	18.1160682
H	7.4231227	-24.939767	16.2900964
H	6.2614692	-26.0257592	18.5211393
H	5.170329	-26.1124329	19.9012234
H	7.5390532	-25.7802132	20.6790273
H	6.5530379	-24.365158	21.1222718
H	7.6651094	-24.2743078	19.7317339
C	4.9927353	-24.2769973	18.7596844
C	6.9575169	-24.9362724	20.2656784
C	5.8312665	-25.4194123	19.3455311
O	7.6447797	-22.515381	16.1559656
Al	9.1363362	-23.2803274	16.3838923
O	8.3941831	-24.9601697	16.1789852
Si	10.9984125	-22.4989714	18.6750242
O	10.6974737	-22.644424	20.2724274
Si	11.1391118	-23.3280798	21.6561324
O	11.6225135	-24.8968276	21.5151451
Si	11.1324812	-26.4532268	21.6283579
O	9.8376513	-26.6368036	22.5889884
Si	9.1621091	-27.3010923	23.9207147
O	7.568894	-26.9250683	23.9014263
Si	6.1854407	-26.4654643	24.6241427
O	5.8987245	-24.8977947	24.3772033
Si	6.1824219	-23.3267628	24.6236572
O	4.8956279	-22.5564849	24.0059542
Si	4.3529242	-21.0209737	23.8994524
Si	7.132118	-21.0924865	15.6074703
O	10.3032695	-23.143206	15.165214
Si	10.9807215	-22.4704847	13.8519634
O	9.7749336	-23.2697883	17.9527753
Si	9.1526178	-26.4691536	16.2349544
O	7.8304199	-27.3737889	16.1075457
Si	7.1259021	-28.7485464	15.5896032
O	5.6722187	-28.7633348	16.3073381
Si	4.149924	-29.355397	16.2262328
O	3.3097181	-28.6610876	17.4330819
Si	2.1874251	-28.667569	18.608958
O	1.3721261	-27.2662038	18.6192776
Si	0.3430861	-26.4317206	17.656988
O	0.8558824	-24.89711	17.756579
Si	0.3451147	-23.357194	17.659806
O	1.3639923	-22.5283197	18.6314364
Si	2.1918466	-21.1291839	18.6004871
O	2.8880194	-20.9146451	20.0454945
Si	2.4513411	-20.4425613	21.552171
O	3.7755213	-20.8640329	22.3958421
Si	4.1484551	-20.432233	16.21962
O	3.2917313	-21.1483413	17.4137152

O	5.6703499	-20.9534052	16.3170258
O	9.859708	-26.6688293	17.6616771
Si	11.015539	-27.305315	18.645074
O	10.6063657	-27.0065323	20.1847829
O	4.9026547	-27.2438428	24.0045968
Si	4.3554494	-28.7762579	23.9026588
O	3.7791995	-28.9383106	22.3973958
Si	2.4523294	-29.3570438	21.5585122
O	2.8875817	-28.8852803	20.0493231
O	9.832832	-23.2269343	22.6185883
Si	9.1615695	-22.5026135	23.9203577
O	7.5637431	-22.8663398	23.9031458
H	12.266803	-26.659059	18.287513
H	12.27153	-27.250951	22.099389
H	9.157408	-28.803271	23.861244
H	9.907894	-26.587045	25.009014
H	5.367066	-29.791205	24.150016
H	3.293202	-28.99206	24.85544
H	7.969768	-29.861989	15.960069
H	1.2322	-29.728691	18.399937
H	0.428942	-26.78058	16.218725
H	-1.000227	-26.588332	18.242393
H	3.519301	-29.026022	14.963281
H	2.34716	-30.805536	21.646024
H	1.16586	-28.772582	22.04891
H	4.261163	-30.806312	16.277826
H	6.271807	-26.78867	26.036663
H	11.07541	-28.756115	18.493167
H	10.101653	-26.55658	15.124677
H	7.067465	-28.675256	14.144806
H	10.292676	-22.899389	12.62458
H	12.368134	-22.895881	13.890981
H	10.972595	-20.996732	13.826247
H	12.266811	-23.140949	18.287496
H	9.907894	-23.212955	25.009014
H	6.271809	-23.011334	26.036664
H	12.271531	-22.549059	22.099401
H	0.428952	-23.019382	16.218711
H	-1.000218	-23.211608	18.242381
H	1.232262	-20.071225	18.399884
H	1.16584	-21.027349	22.04888
H	3.293197	-20.80798	24.855446
H	3.519314	-20.773972	14.963268
H	7.067475	-21.124751	14.14479
H	5.367066	-20.008796	24.150018
H	7.969784	-19.938014	15.960046
H	11.07543	-21.043885	18.493137
H	2.347198	-18.994431	21.646032
H	4.261183	-18.993679	16.277806
H	9.157409	-20.996728	23.861244

transition state

H	4.8081988	-23.7275134	18.9951481
H	4.172697	-24.5059479	17.525051
H	5.5389808	-23.3534299	17.3979272
H	7.3690079	-24.9672573	17.9139168
H	6.2677133	-25.807599	17.1912728
H	5.6983981	-26.1255712	18.8321651
H	7.8522003	-25.818721	19.5673309
H	6.8928931	-24.2683157	19.8530254
H	8.3148753	-24.2408418	18.80292
C	5.095883	-24.1505669	18.0174382
C	7.4574613	-24.8865852	19.1458273
C	6.037421	-25.3282722	18.1588996
O	7.6628549	-22.4624108	16.236459
Al	9.0894311	-23.3810586	16.3503829
O	8.3731856	-24.977491	16.3516407
Si	10.9891257	-22.4998336	18.6516702
O	10.6863701	-22.6818902	20.2549152
Si	11.1437924	-23.3299281	21.6487517
O	11.6258562	-24.8997858	21.5418754
Si	11.1347084	-26.4590572	21.6169346
O	9.8295023	-26.6424326	22.5743673
Si	9.1671911	-27.3003461	23.9150208
O	7.5720143	-26.9166414	23.8946442
Si	6.1894102	-26.4661417	24.6244945
O	5.8968823	-24.8983512	24.3709453
Si	6.1862644	-23.3275601	24.6242303
O	4.9019528	-22.5554709	24.0009877
Si	4.3529664	-21.0205957	23.8995279
Si	7.1487569	-21.0897252	15.6089717
O	10.2909791	-23.1214077	15.1749387
Si	10.9748498	-22.4720186	13.859613
O	9.7374857	-23.2400175	17.9503897
Si	9.1344322	-26.3880067	16.2285352
O	7.8766467	-27.4148561	16.1426499
Si	7.1529507	-28.737708	15.5872758
O	5.6821108	-28.7474398	16.3041254
Si	4.1706329	-29.352696	16.2184459
O	3.331504	-28.6587341	17.4388251
Si	2.1950879	-28.6729767	18.5996576
O	1.3844769	-27.2658099	18.6090801
Si	0.3441471	-26.433596	17.656021
O	0.8615077	-24.898006	17.7590013
Si	0.3452338	-23.3582419	17.6585301
O	1.3758309	-22.5327112	18.6229701
Si	2.1948411	-21.1261825	18.5954911
O	2.8879421	-20.9241403	20.0458447
Si	2.4509606	-20.4429908	21.5510423
O	3.7751353	-20.8695992	22.3943765
Si	4.1550484	-20.4294698	16.2128067
O	3.3039752	-21.1496528	17.4179617

O	5.6702994	-20.9533472	16.3085271
O	9.8520148	-26.7101088	17.661314
Si	11.0128166	-27.30895	18.6220192
O	10.5973043	-26.9807375	20.1700118
O	4.9092463	-27.2452339	23.9980521
Si	4.3551114	-28.7770853	23.901995
O	3.7777893	-28.9328558	22.3955895
Si	2.4512057	-29.3571519	21.5562489
O	2.8868963	-28.8789002	20.0484843
O	9.8273018	-23.2173923	22.6055132
Si	9.1660846	-22.502636	23.916969
O	7.5668888	-22.8748914	23.8961095
H	12.266803	-26.659059	18.287513
H	12.27153	-27.250951	22.099389
H	9.157408	-28.803271	23.861244
H	9.907894	-26.587045	25.009014
H	5.367066	-29.791205	24.150016
H	3.293202	-28.99206	24.85544
H	7.969768	-29.861989	15.960069
H	1.2322	-29.728691	18.399937
H	0.428942	-26.78058	16.218725
H	-1.000227	-26.588332	18.242393
H	3.519301	-29.026022	14.963281
H	2.34716	-30.805536	21.646024
H	1.16586	-28.772582	22.04891
H	4.261163	-30.806312	16.277826
H	6.271807	-26.78867	26.036663
H	11.07541	-28.756115	18.493167
H	10.101653	-26.55658	15.124677
H	7.067465	-28.675256	14.144806
H	10.292676	-22.899389	12.62458
H	12.368134	-22.895881	13.890981
H	10.972595	-20.996732	13.826247
H	12.266811	-23.140949	18.287496
H	9.907894	-23.212955	25.009014
H	6.271809	-23.011334	26.036664
H	12.271531	-22.549059	22.099401
H	0.428952	-23.019382	16.218711
H	-1.000218	-23.211608	18.242381
H	1.232262	-20.071225	18.399884
H	1.16584	-21.027349	22.04888
H	3.293197	-20.80798	24.855446
H	3.519314	-20.773972	14.963268
H	7.067475	-21.124751	14.14479
H	5.367066	-20.008796	24.150018
H	7.969784	-19.938014	15.960046
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H	2.347198	-18.994431	21.646032
H	4.261183	-18.993679	16.277806
H	9.157409	-20.996728	23.861244

$C_4H_{10} \rightarrow CH_4 + C_3H_6$
reactant

H	4.5782934	-25.1211878	21.5927992
H	3.8852797	-26.215568	20.3661363
H	2.9741349	-24.7801035	20.9017493
H	3.9015743	-24.2615422	18.6971064
H	4.7364023	-23.2728261	19.8983586
H	7.4334492	-24.9471873	16.4084919
H	6.2881623	-24.1472421	18.2069899
H	5.8151675	-25.8313452	18.5612089
H	8.0342485	-25.2248774	19.6197998
H	6.8359111	-25.6389131	20.8688961
H	7.2468788	-23.9332987	20.552879
C	3.9859049	-25.1544066	20.6612831
C	4.6120274	-24.313966	19.5432525
C	7.0756454	-24.9134495	20.0709763
C	5.9632842	-24.8303649	19.0190046
O	7.653061	-22.5088472	16.1630107
Al	9.1395123	-23.284225	16.3801694
O	8.3881635	-24.9631626	16.1904201
Si	10.9990248	-22.4991809	18.6735799
O	10.6972012	-22.6428974	20.2714011
Si	11.1393139	-23.327238	21.6542867
O	11.622281	-24.8961198	21.5142546
Si	11.1325957	-26.4524999	21.6285172
O	9.8386023	-26.6350692	22.5897565
Si	9.1622781	-27.3003716	23.9196794
O	7.5685825	-26.9217152	23.8971726
Si	6.1856507	-26.4658344	24.6238414
O	5.895799	-24.8981785	24.3779825
Si	6.1830193	-23.3270589	24.6234521
O	4.896085	-22.5562188	24.0068081
Si	4.3527261	-21.0209077	23.8991489
Si	7.1331339	-21.0925872	15.6081749
O	10.3031233	-23.1564263	15.1579931
Si	10.9807583	-22.4719041	13.8507963
O	9.7817402	-23.2735786	17.9477052
Si	9.1530768	-26.4688015	16.2362925
O	7.836016	-27.3812141	16.1172354
Si	7.1267573	-28.7485935	15.5901763
O	5.6724715	-28.7617194	16.3079099
Si	4.1509089	-29.3549278	16.2258743
O	3.3125026	-28.6586214	17.4336991
Si	2.1879164	-28.6685863	18.6075292
O	1.3714323	-27.2678912	18.6201107
Si	0.3432893	-26.4321327	17.6575711
O	0.855523	-24.8971104	17.7585534
Si	0.3449207	-23.3571412	17.6601089
O	1.3641271	-22.5283214	18.6329378
Si	2.1926287	-21.1286872	18.5998075
O	2.8883919	-20.9092302	20.0442513
Si	2.4511636	-20.4420596	21.5522998

O	3.7761884	-20.8650073	22.3947809
Si	4.1497612	-20.4330346	16.2192656
O	3.2920613	-21.1505226	17.4128107
O	5.6701584	-20.9569478	16.3165693
O	9.8630393	-26.668673	17.6624204
Si	11.0174191	-27.3060974	18.6455343
O	10.6066923	-27.0050257	20.1845589
O	4.9031594	-27.2447911	24.0049136
Si	4.3550164	-28.7770376	23.9020358
O	3.7799998	-28.9411186	22.3965843
Si	2.4517213	-29.357738	21.5587268
O	2.887553	-28.8931044	20.0471841
O	9.8323445	-23.2254718	22.6168068
Si	9.1622511	-22.5027355	23.9200188
O	7.5646036	-22.8689443	23.9013457
H	12.266803	-26.659059	18.287513
H	12.27153	-27.250951	22.099389
H	9.157408	-28.803271	23.861244
H	9.907894	-26.587045	25.009014
H	5.367066	-29.791205	24.150016
H	3.293202	-28.99206	24.85544
H	7.969768	-29.861989	15.960069
H	1.2322	-29.728691	18.399937
H	0.428942	-26.78058	16.218725
H	-1.000227	-26.588332	18.242393
H	3.519301	-29.026022	14.963281
H	2.34716	-30.805536	21.646024
H	1.16586	-28.772582	22.04891
H	4.261163	-30.806312	16.277826
H	6.271807	-26.78867	26.036663
H	11.07541	-28.756115	18.493167
H	10.101653	-26.55658	15.124677
H	7.067465	-28.675256	14.144806
H	10.292676	-22.899389	12.62458
H	12.368134	-22.895881	13.890981
H	10.972595	-20.996732	13.826247
H	12.266811	-23.140949	18.287496
H	9.907894	-23.212955	25.009014
H	6.271809	-23.011334	26.036664
H	12.271531	-22.549059	22.099401
H	0.428952	-23.019382	16.218711
H	-1.000218	-23.211608	18.242381
H	1.232262	-20.071225	18.399884
H	1.16584	-21.027349	22.04888
H	3.293197	-20.80798	24.855446
H	3.519314	-20.773972	14.963268
H	7.067475	-21.124751	14.14479
H	5.367066	-20.008796	24.150018
H	7.969784	-19.938014	15.960046
H	11.07543	-21.043885	18.493137
H	2.347198	-18.994431	21.646032
H	4.261183	-18.993679	16.277806
H	9.157409	-20.996728	23.861244

transition state

H	5.0063909	-24.1178603	20.5958823
H	4.0378774	-25.5245197	20.0521948
H	3.400904	-23.8677978	19.8912583
H	4.0794328	-24.6183738	17.6764652
H	5.1843479	-23.3328337	18.1545932
H	7.3429303	-24.919809	17.8299792
H	6.2097931	-25.3386998	16.9713098
H	5.8597686	-26.3665291	18.3609344
H	7.8653122	-25.9271479	19.3801503
H	6.87672	-24.4612109	19.8721951
H	8.2562051	-24.2653627	18.7941486
C	4.3138795	-24.480182	19.8129613
C	4.8827253	-24.3682037	18.3953775
C	7.4261444	-24.971233	19.0744316
C	6.0227999	-25.3229153	18.0613442
O	7.6600308	-22.4688321	16.2380609
Al	9.0945869	-23.3751157	16.3524279
O	8.3805745	-24.973484	16.3345617
Si	10.9878282	-22.500214	18.6522803
O	10.6884628	-22.6760552	20.2566559
Si	11.1440812	-23.3298117	21.647821
O	11.6251158	-24.8998971	21.5377105
Si	11.1344991	-26.4591895	21.6157134
O	9.8313787	-26.6421723	22.5756125
Si	9.1678548	-27.3003743	23.9148618
O	7.5724846	-26.9172258	23.8953993
Si	6.1900929	-26.4661506	24.6242526
O	5.8969154	-24.8983919	24.3698175
Si	6.1875541	-23.3279378	24.6233559
O	4.9037953	-22.5564805	23.9962235
Si	4.353671	-21.0214322	23.8994027
Si	7.1490696	-21.0940878	15.6119207
O	10.295924	-23.1129467	15.1788102
Si	10.9760381	-22.4705384	13.8589727
O	9.7354653	-23.2420902	17.9544401
Si	9.1366148	-26.388398	16.2269646
O	7.8802177	-27.4154557	16.1441321
Si	7.1544102	-28.7359976	15.5881991
O	5.6831673	-28.7475418	16.3056788
Si	4.1721621	-29.3530605	16.2178181
O	3.3332193	-28.6599482	17.4394157
Si	2.196364	-28.6730314	18.5995364
O	1.3872347	-27.264347	18.6075862
Si	0.3443487	-26.4335117	17.6561241
O	0.8612322	-24.8971243	17.7625779
Si	0.344311	-23.3576329	17.6581114
O	1.3753443	-22.5305508	18.62296
Si	2.1960812	-21.1230308	18.5936805
O	2.8844542	-20.924313	20.0463969
Si	2.4504273	-20.4424006	21.5523141

O	3.774611	-20.8704528	22.3942097
Si	4.1580677	-20.4298611	16.21192
O	3.3055106	-21.1506336	17.4178501
O	5.6715778	-20.9535621	16.312607
O	9.8554574	-26.707392	17.6590468
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O	4.9090029	-27.2447131	23.9985094
Si	4.3555836	-28.7765628	23.9024725
O	3.7777084	-28.9325616	22.3960635
Si	2.4512971	-29.3567647	21.5571235
O	2.8861168	-28.8736592	20.0500719
O	9.8283349	-23.2190535	22.6060927
Si	9.1673513	-22.5027761	23.9163356
O	7.5679017	-22.8744898	23.8965127
H	12.266803	-26.659059	18.287513
H	12.27153	-27.250951	22.099389
H	9.157408	-28.803271	23.861244
H	9.907894	-26.587045	25.009014
H	5.367066	-29.791205	24.150016
H	3.293202	-28.99206	24.85544
H	7.969768	-29.861989	15.960069
H	1.2322	-29.728691	18.399937
H	0.428942	-26.78058	16.218725
H	-1.000227	-26.588332	18.242393
H	3.519301	-29.026022	14.963281
H	2.34716	-30.805536	21.646024
H	1.16586	-28.772582	22.04891
H	4.261163	-30.806312	16.277826
H	6.271807	-26.78867	26.036663
H	11.07541	-28.756115	18.493167
H	10.101653	-26.55658	15.124677
H	7.067465	-28.675256	14.144806
H	10.292676	-22.899389	12.62458
H	12.368134	-22.895881	13.890981
H	10.972595	-20.996732	13.826247
H	12.266811	-23.140949	18.287496
H	9.907894	-23.212955	25.009014
H	6.271809	-23.011334	26.036664
H	12.271531	-22.549059	22.099401
H	0.428952	-23.019382	16.218711
H	-1.000218	-23.211608	18.242381
H	1.232262	-20.071225	18.399884
H	1.16584	-21.027349	22.04888
H	3.293197	-20.80798	24.855446
H	3.519314	-20.773972	14.963268
H	7.067475	-21.124751	14.14479
H	5.367066	-20.008796	24.150018
H	7.969784	-19.938014	15.960046
H	11.07543	-21.043885	18.493137
H	2.347198	-18.994431	21.646032
H	4.261183	-18.993679	16.277806
H	9.157409	-20.996728	23.861244

$C_4H_{10} \rightarrow C_2H_6 + C_2H_4$
reactant

H	4.5782934	-25.1211878	21.5927992
H	3.8852797	-26.215568	20.3661363
H	2.9741349	-24.7801035	20.9017493
H	3.9015743	-24.2615422	18.6971064
H	4.7364023	-23.2728261	19.8983586
H	7.4334492	-24.9471873	16.4084919
H	6.2881623	-24.1472421	18.2069899
H	5.8151675	-25.8313452	18.5612089
H	8.0342485	-25.2248774	19.6197998
H	6.8359111	-25.6389131	20.8688961
H	7.2468788	-23.9332987	20.552879
C	3.9859049	-25.1544066	20.6612831
C	4.6120274	-24.313966	19.5432525
C	7.0756454	-24.9134495	20.0709763
C	5.9632842	-24.8303649	19.0190046
O	7.653061	-22.5088472	16.1630107
Al	9.1395123	-23.284225	16.3801694
O	8.3881635	-24.9631626	16.1904201
Si	10.9990248	-22.4991809	18.6735799
O	10.6972012	-22.6428974	20.2714011
Si	11.1393139	-23.327238	21.6542867
O	11.622281	-24.8961198	21.5142546
Si	11.1325957	-26.4524999	21.6285172
O	9.8386023	-26.6350692	22.5897565
Si	9.1622781	-27.3003716	23.9196794
O	7.5685825	-26.9217152	23.8971726
Si	6.1856507	-26.4658344	24.6238414
O	5.895799	-24.8981785	24.3779825
Si	6.1830193	-23.3270589	24.6234521
O	4.896085	-22.5562188	24.0068081
Si	4.3527261	-21.0209077	23.8991489
Si	7.1331339	-21.0925872	15.6081749
O	10.3031233	-23.1564263	15.1579931
Si	10.9807583	-22.4719041	13.8507963
O	9.7817402	-23.2735786	17.9477052
Si	9.1530768	-26.4688015	16.2362925
O	7.836016	-27.3812141	16.1172354
Si	7.1267573	-28.7485935	15.5901763
O	5.6724715	-28.7617194	16.3079099
Si	4.1509089	-29.3549278	16.2258743
O	3.3125026	-28.6586214	17.4336991
Si	2.1879164	-28.6685863	18.6075292
O	1.3714323	-27.2678912	18.6201107
Si	0.3432893	-26.4321327	17.6575711
O	0.855523	-24.8971104	17.7585534
Si	0.3449207	-23.3571412	17.6601089
O	1.3641271	-22.5283214	18.6329378
Si	2.1926287	-21.1286872	18.5998075
O	2.8883919	-20.9092302	20.0442513
Si	2.4511636	-20.4420596	21.5522998

O	3.7761884	-20.8650073	22.3947809
Si	4.1497612	-20.4330346	16.2192656
O	3.2920613	-21.1505226	17.4128107
O	5.6701584	-20.9569478	16.3165693
O	9.8630393	-26.668673	17.6624204
Si	11.0174191	-27.3060974	18.6455343
O	10.6066923	-27.0050257	20.1845589
O	4.9031594	-27.2447911	24.0049136
Si	4.3550164	-28.7770376	23.9020358
O	3.7799998	-28.9411186	22.3965843
Si	2.4517213	-29.357738	21.5587268
O	2.887553	-28.8931044	20.0471841
O	9.8323445	-23.2254718	22.6168068
Si	9.1622511	-22.5027355	23.9200188
O	7.5646036	-22.8689443	23.9013457
H	12.266803	-26.659059	18.287513
H	12.27153	-27.250951	22.099389
H	9.157408	-28.803271	23.861244
H	9.907894	-26.587045	25.009014
H	5.367066	-29.791205	24.150016
H	3.293202	-28.99206	24.85544
H	7.969768	-29.861989	15.960069
H	1.2322	-29.728691	18.399937
H	0.428942	-26.78058	16.218725
H	-1.000227	-26.588332	18.242393
H	3.519301	-29.026022	14.963281
H	2.34716	-30.805536	21.646024
H	1.16586	-28.772582	22.04891
H	4.261163	-30.806312	16.277826
H	6.271807	-26.78867	26.036663
H	11.07541	-28.756115	18.493167
H	10.101653	-26.55658	15.124677
H	7.067465	-28.675256	14.144806
H	10.292676	-22.899389	12.62458
H	12.368134	-22.895881	13.890981
H	10.972595	-20.996732	13.826247
H	12.266811	-23.140949	18.287496
H	9.907894	-23.212955	25.009014
H	6.271809	-23.011334	26.036664
H	12.271531	-22.549059	22.099401
H	0.428952	-23.019382	16.218711
H	-1.000218	-23.211608	18.242381
H	1.232262	-20.071225	18.399884
H	1.16584	-21.027349	22.04888
H	3.293197	-20.80798	24.855446
H	3.519314	-20.773972	14.963268
H	7.067475	-21.124751	14.14479
H	5.367066	-20.008796	24.150018
H	7.969784	-19.938014	15.960046
H	11.07543	-21.043885	18.493137
H	2.347198	-18.994431	21.646032
H	4.261183	-18.993679	16.277806
H	9.157409	-20.996728	23.861244

transition state

H	4.5217922	-23.8878338	18.6821662
H	4.1612133	-24.5650506	17.0844849
H	5.449529	-23.3329455	17.2494775
H	7.2201932	-25.0273369	17.6510952
H	6.2393431	-25.7885967	16.9366195
H	5.6115214	-26.2002688	18.4886561
H	7.7318676	-25.9510825	19.2598583
H	8.1060106	-24.2991869	18.7070025
H	7.4007523	-24.2337318	21.03328
H	5.8035645	-24.9518031	20.6635079
H	6.2402797	-23.321317	20.0432413
C	7.2867191	-24.9699795	19.0410136
C	5.9777854	-25.3361959	17.9167744
C	6.6216456	-24.3326737	20.256291
C	4.979665	-24.2048866	17.732642
O	7.6553701	-22.4725396	16.2216512
Al	9.0875297	-23.3804162	16.3553813
O	8.3613222	-24.9824117	16.3641287
Si	10.9890195	-22.4987172	18.6511913
O	10.6876476	-22.6769585	20.2554958
Si	11.1440814	-23.3298487	21.6458624
O	11.6269584	-24.8995537	21.5402645
Si	11.1347143	-26.4582214	21.6171299
O	9.8305423	-26.6386317	22.5764876
Si	9.1678054	-27.3000151	23.914996
O	7.5728071	-26.9154208	23.8957855
Si	6.1894879	-26.4663606	24.624364
O	5.8951431	-24.8987885	24.3707424
Si	6.1858984	-23.3283416	24.6237753
O	4.9028394	-22.5548251	24.0003267
Si	4.3529824	-21.0202791	23.8993515
Si	7.1487768	-21.0904707	15.6078306
O	10.277712	-23.1421329	15.1616515
Si	10.9724696	-22.4750959	13.8601378
O	9.7432033	-23.230996	17.9421493
Si	9.1359856	-26.3917527	16.2304426
O	7.8710896	-27.4099765	16.1337687
Si	7.1514756	-28.7396055	15.5862338
O	5.6811526	-28.7466045	16.3034879
Si	4.1690581	-29.3529302	16.2192179
O	3.3323	-28.657409	17.4399725
Si	2.1944323	-28.6724773	18.6006081
O	1.3833354	-27.2660876	18.6094776
Si	0.3436897	-26.4333451	17.6559932
O	0.8596123	-24.8979508	17.7579752
Si	0.3457058	-23.3577236	17.6588866
O	1.3771462	-22.5330202	18.6234733
Si	2.1952434	-21.1258404	18.5956281
O	2.8887154	-20.922958	20.0456008
Si	2.451043	-20.4429057	21.5508045

O	3.7754128	-20.869066	22.3942211
Si	4.1553936	-20.4286043	16.2126332
O	3.3026759	-21.1472268	17.4167897
O	5.6721386	-20.9486167	16.3104426
O	9.8556552	-26.7232355	17.6550736
Si	11.0150444	-27.3105836	18.6249811
O	10.5990468	-26.9836783	20.1713133
O	4.9097552	-27.2452857	23.9967204
Si	4.3552686	-28.7770691	23.9019102
O	3.7775389	-28.9332872	22.3957843
Si	2.451048	-29.3574031	21.5566997
O	2.8865123	-28.8802379	20.0485937
O	9.8254438	-23.2211484	22.6038135
Si	9.1671128	-22.5032003	23.9162973
O	7.5680972	-22.8793221	23.8951623
H	12.266803	-26.659059	18.287513
H	12.27153	-27.250951	22.099389
H	9.157408	-28.803271	23.861244
H	9.907894	-26.587045	25.009014
H	5.367066	-29.791205	24.150016
H	3.293202	-28.99206	24.85544
H	7.969768	-29.861989	15.960069
H	1.2322	-29.728691	18.399937
H	0.428942	-26.78058	16.218725
H	-1.000227	-26.588332	18.242393
H	3.519301	-29.026022	14.963281
H	2.34716	-30.805536	21.646024
H	1.16586	-28.772582	22.04891
H	4.261163	-30.806312	16.277826
H	6.271807	-26.78867	26.036663
H	11.07541	-28.756115	18.493167
H	10.101653	-26.55658	15.124677
H	7.067465	-28.675256	14.144806
H	10.292676	-22.899389	12.62458
H	12.368134	-22.895881	13.890981
H	10.972595	-20.996732	13.826247
H	12.266811	-23.140949	18.287496
H	9.907894	-23.212955	25.009014
H	6.271809	-23.011334	26.036664
H	12.271531	-22.549059	22.099401
H	0.428952	-23.019382	16.218711
H	-1.000218	-23.211608	18.242381
H	1.232262	-20.071225	18.399884
H	1.16584	-21.027349	22.04888
H	3.293197	-20.80798	24.855446
H	3.519314	-20.773972	14.963268
H	7.067475	-21.124751	14.14479
H	5.367066	-20.008796	24.150018
H	7.969784	-19.938014	15.960046
H	11.07543	-21.043885	18.493137
H	2.347198	-18.994431	21.646032
H	4.261183	-18.993679	16.277806
H	9.157409	-20.996728	23.861244

Cartesian coordinates of stationary points optimized with periodic DFT (PBE/400 ev). The cell parameters of the orthorhombic MFI unit cell are *a* = 20.157 Å, *b* = 20.033 Å, *c* = 13.473 Å.

$C_3H_8 \rightarrow CH_4 + C_2H_4$

Reactant

Si	8.64122	1.17565	2.00416
Si	1.63088	18.95725	8.73801
Si	11.71817	11.20231	11.51012
Si	18.72795	8.94265	4.74027
Si	11.70688	18.97553	11.52717
Si	18.72158	1.15105	4.78943
Si	8.63492	8.96344	1.9843
Si	1.64423	11.1846	8.71461
Si	6.22231	0.60585	3.94746
Si	4.0461	19.51698	10.68765
Si	14.10205	10.55386	9.58333
Si	16.30767	9.57894	2.81092
Si	14.14836	19.5661	9.61679
Si	16.26179	0.57948	2.84255
Si	6.22584	9.51816	3.93871
Si	4.05502	10.63627	10.67046
Si	5.78155	1.3511	6.92711
Si	4.48674	18.78382	0.19059
Si	14.6027	11.26572	6.6184
Si	15.8666	8.8677	13.30351
Si	14.59053	18.91596	6.63326
Si	15.87149	1.35819	13.34907
Si	5.7618	8.77112	6.91177
Si	4.47916	11.35485	0.15798
Si	2.57005	1.38348	6.93901
Si	7.69578	18.75984	0.19699
Si	17.78289	11.34365	6.55865
Si	12.66035	8.77074	13.29812
Si	17.79326	18.76584	6.60993
Si	12.66432	1.36744	13.34922
Si	2.54835	8.72368	6.9115
Si	7.68684	11.39739	0.15147
Si	1.52575	0.62818	4.10357
Si	8.74624	19.51947	10.84159
Si	18.86707	10.698	9.38268
Si	11.5926	9.47787	2.64171
Si	18.82405	19.50042	9.44514
Si	11.60333	0.63856	2.7121
Si	1.5169	9.47381	4.07547
Si	8.78828	10.63657	10.80835
Si	3.702	1.13958	2.05616
Si	6.57022	18.99456	8.80007
Si	16.62174	11.17412	11.36288
Si	13.79145	8.96936	4.66476
Si	16.66535	19.00002	11.5062
Si	13.77312	1.21967	4.74651
Si	3.71283	8.98281	2.04651
Si	6.57665	11.15088	8.80082
Si	8.56945	16.61122	2.24589

Si	1.67003	3.50847	8.99844
Si	11.77739	6.58068	11.24155
Si	18.63757	13.51908	4.46675
Si	11.75034	3.5089	11.30202
Si	18.67142	16.61236	4.56169
Si	8.53619	13.51156	2.21436
Si	1.66721	6.61605	8.98957
Si	6.19785	17.46947	4.14435
Si	4.06716	2.65413	10.87222
Si	14.09503	7.4123	9.35436
Si	16.34198	12.76734	2.50353
Si	14.14007	2.70749	9.39675
Si	16.26319	17.412	2.64553
Si	6.19426	12.68008	4.14432
Si	4.06001	7.46621	10.87058
Si	5.54409	16.62924	7.10386
Si	4.73953	3.50323	0.35483
Si	14.83525	6.66252	6.38959
Si	15.581	13.49962	13.06504
Si	14.81309	3.53681	6.44276
Si	15.58916	16.61188	13.16743
Si	5.55146	13.51434	7.10529
Si	4.7392	6.6182	0.34021
Si	2.42898	16.60072	6.97744
Si	7.85529	3.53836	0.24297
Si	17.94072	6.60767	6.52869
Si	12.4635	13.54794	13.29224
Si	17.91543	3.52371	6.5521
Si	12.48575	16.61217	13.27816
Si	2.43728	13.53819	6.96109
Si	7.85945	6.5944	0.20869
Si	1.44021	17.49598	4.12087
Si	8.8337	2.64105	10.8595
Si	18.9249	7.53615	9.37975
Si	11.43927	12.62577	2.64647
Si	18.91586	2.62922	9.41795
Si	11.47451	17.50815	2.65949
Si	1.44829	12.63255	4.11597
Si	8.86031	7.47548	10.8332
Si	3.73692	16.64554	2.30581
Si	6.53487	3.48395	9.03417
Si	16.59375	6.67898	11.19564
Si	16.61555	3.5218	11.24007
Si	13.76364	16.75444	4.53507
Si	3.73738	13.47846	2.30574
Si	6.52767	6.64691	9.03358
Al	13.8221	13.38891	4.42242
O	7.40933	1.24655	3.05152
O	2.86287	18.87913	9.78538
O	13.00675	11.27647	10.53262
O	17.46698	8.91187	3.72738
O	12.94379	18.92014	10.48095
O	17.48248	1.12533	3.74851
O	7.3974	8.87325	3.02732
O	2.91447	11.26718	9.71342
O	6.17079	1.40724	5.3561
O	4.08771	18.71219	12.09539
O	14.09966	11.32059	8.16363
O	16.29805	8.79126	1.389
O	14.22003	18.77203	8.19831
O	16.24964	1.41731	1.45308

O	6.17387	8.71058	5.34583
O	4.03332	11.44934	12.07493
O	4.17298	1.21557	7.12864
O	6.09498	18.95327	0.37562
O	16.20893	10.96763	6.56129
O	14.25514	9.03832	13.15036
O	16.19229	18.977	6.38933
O	14.26513	1.18451	13.14792
O	4.15119	8.90669	7.08778
O	6.08714	11.15507	0.27759
O	2.17823	1.41786	5.36732
O	8.10305	18.71765	12.10226
O	18.3211	11.5123	8.08303
O	12.22722	8.65796	1.3822
O	18.14847	18.71247	8.18818
O	12.28551	1.40911	1.45261
O	2.14356	8.67004	5.34459
O	8.14739	11.43775	12.07108
O	2.22471	1.12433	2.72751
O	8.0525	19.02294	9.46245
O	18.11516	11.21243	10.72615
O	12.3057	8.98609	4.01386
O	18.13801	18.99514	10.82579
O	12.2883	1.13546	4.09858
O	2.23302	8.98471	2.70634
O	8.07089	11.10394	9.4302
O	4.79768	0.76999	3.19553
O	5.47655	19.35049	9.94519
O	15.5883	10.64147	10.22866
O	14.85968	9.39273	3.51683
O	15.56368	19.3807	10.37543
O	14.8513	0.7998	3.60955
O	4.79521	9.37565	3.19102
O	5.51174	10.80032	9.977
O	7.35698	16.71131	3.31095
O	2.89514	3.4056	10.0509
O	12.95451	6.56057	10.12718
O	17.57907	13.52002	3.24883
O	12.95778	3.42535	10.22833
O	17.47017	16.75841	3.48469
O	7.32245	13.45616	3.28725
O	2.89673	6.71503	10.03692
O	6.20286	16.85757	5.64063
O	4.0809	3.27272	12.36542
O	14.10959	6.93082	7.81225
O	16.42783	13.19062	0.93371
O	14.11875	3.2995	7.89029
O	16.25581	16.76289	1.16936
O	6.21184	13.29396	5.64165
O	4.04613	6.84846	12.36592
O	3.98066	17.09195	7.07314
O	6.30412	3.04423	0.32531
O	16.39559	7.12262	6.48273
O	14.0212	13.06518	13.26905
O	16.3614	3.02442	6.50584
O	14.03743	17.11619	13.22854
O	3.98887	13.05337	7.07247
O	6.30233	7.0695	0.25966
O	1.93099	16.68353	5.43657
O	8.36434	3.45996	12.17865
O	18.49563	6.71012	8.04901

O	11.86315	13.47164	1.31451
O	18.46737	3.42276	8.07401
O	11.94926	16.71164	1.33472
O	1.96354	13.46481	5.41269
O	8.39042	6.64888	12.15012
O	2.21054	16.92079	2.80772
O	8.05783	3.22416	9.55352
O	18.10628	6.96469	10.6648
O	12.18488	13.21207	3.93731
O	18.12829	3.23371	10.70768
O	12.26635	16.89654	3.95919
O	2.20509	13.20132	2.78823
O	8.0545	6.9162	9.53332
O	4.74976	17.21663	3.44921
O	5.50769	2.90487	10.15975
O	15.54989	7.13897	10.03138
O	14.93965	13.22686	3.1321
O	15.57893	3.00312	10.09267
O	14.84532	17.04045	3.38291
O	4.73197	12.91623	3.46887
O	5.50901	7.2061	10.17673
O	6.51369	19.06108	4.20222
O	3.75772	1.06188	10.94259
O	13.70867	8.98518	9.4275
O	16.59817	11.15871	2.61629
O	13.87099	1.10638	9.35156
O	16.42994	19.02095	2.55068
O	6.52843	11.09267	4.20284
O	3.759	9.05965	10.92904
O	1.77418	19.07016	4.32255
O	8.47644	1.07214	11.06749
O	18.59243	9.10863	9.15902
O	11.83092	11.06193	2.38448
O	18.55735	1.05646	9.23699
O	11.857	19.07527	2.51639
O	1.7851	11.05927	4.32112
O	8.54185	9.04883	11.05751
O	8.75505	2.58068	1.19567
O	1.51926	17.55286	7.92604
O	11.58695	12.6219	12.2872
O	18.82814	7.51772	5.5221
O	11.59328	17.55272	12.3025
O	18.78403	2.58162	5.55521
O	8.74082	7.56869	1.15424
O	1.51727	12.58268	7.89292
O	8.45328	19.99375	0.93741
O	1.8285	0.13593	7.6708
O	11.85989	9.99861	12.5959
O	18.60376	10.14071	5.8343
O	11.90778	0.12093	12.63061
O	18.57556	19.99882	5.89918
O	8.44649	10.1928	0.93432
O	1.80107	9.96463	7.64879
O	8.16871	17.35449	0.85662
O	2.06888	2.77882	7.59961
O	12.26174	7.37358	12.5725
O	18.04933	12.7405	5.76952
O	12.16823	2.75944	12.68396
O	18.25232	17.35795	5.94797
O	8.07639	12.82921	0.81005
O	2.06735	7.3259	7.58297

O	3.95501	2.62604	1.46567
O	6.33328	17.50419	8.21292
O	16.22036	12.67578	11.82315
O	14.09041	7.46601	5.20113
O	16.39823	17.5194	12.10057
O	14.01979	2.7225	5.28561
O	3.9895	7.49344	1.47354
O	6.33625	12.64553	8.22146
O	3.75618	0.04115	0.85792
O	6.49661	0.05336	7.59749
O	16.59902	10.15863	12.63483
O	13.84694	10.005	5.91025
O	16.62239	0.07067	12.69878
O	13.88069	0.19838	6.01303
O	3.75572	10.06617	0.83505
O	6.46343	10.06962	7.59236
O	3.99393	17.40516	0.89266
O	6.30646	2.72387	7.61664
O	16.33348	7.49232	12.57485
O	14.25039	12.66014	5.91803
O	16.36446	2.73345	12.6414
O	13.99484	17.58872	5.89181
O	4.02322	12.72916	0.89364
O	6.27426	7.40086	7.61785
O	20.09828	0.94702	3.96348
O	10.33583	19.22157	10.70136
O	0.29736	10.97394	9.5915
O	10.01012	9.15721	2.81248
O	0.25171	19.1838	9.5584
O	10.02	0.95397	2.82829
O	20.0945	9.15648	3.89463
O	10.36894	10.96555	10.64006
O	19.99855	17.2915	3.91152
O	10.43403	2.81725	10.63753
O	0.3587	7.32541	9.65175
O	9.82002	12.74317	2.83587
O	0.35611	2.80726	9.65978
O	9.88553	17.31789	2.90723
O	20.00806	12.82556	3.93581
O	10.45285	7.26582	10.5887
O	8.88988	15.06531	1.90544
O	1.35313	5.0597	8.67003
O	11.44459	5.05325	11.67519
O	18.93337	15.05627	4.91325
O	3.97849	15.06371	2.06848
O	6.2835	5.06351	8.79281
O	16.4083	5.10075	11.52468
O	13.94364	15.1612	5.09381
O	5.67967	15.07365	7.52982
O	4.60807	5.06155	0.77252
O	14.73886	5.09032	6.02339
O	15.67784	15.07567	12.67771
O	2.28106	15.06778	7.48663
O	8.00309	5.07038	0.75663
O	18.0445	5.0586	6.0468
O	12.35522	15.08461	12.76216
H	12.91636	14.93501	9.3647
H	13.45489	15.85987	7.96395
H	12.93288	14.13818	7.79159
H	13.92848	15.09673	6.07736
H	11.12299	15.72143	6.96895

H	11.13115	16.54032	8.52778
H	9.22597	14.91343	8.39268
H	10.36672	14.41083	9.65841
H	10.36186	13.5803	8.08831
C	10.25292	14.56287	8.57349
C	11.28621	15.55913	8.04873
C	12.72464	15.0991	8.29236

Transition state

Si	8.60022	1.19479	2.01144
Si	1.62742	18.97019	8.76911
Si	11.70987	11.18083	11.59354
Si	18.71118	8.96638	4.80842
Si	11.69576	18.94712	11.54518
Si	18.70865	1.17193	4.77592
Si	8.61906	8.95142	2.03786
Si	1.6175	11.19767	8.77325
Si	6.20005	0.61854	3.97069
Si	4.04388	19.53	10.72267
Si	14.09341	10.5557	9.64574
Si	16.28415	9.56335	2.87338
Si	14.09443	19.55511	9.60252
Si	16.28433	0.57184	2.81325
Si	6.21165	9.52507	3.98496
Si	4.03964	10.64165	10.71
Si	5.74817	1.35428	6.94442
Si	4.4769	18.78218	0.21683
Si	14.57397	11.31065	6.67809
Si	15.84398	8.80756	13.37987
Si	14.58124	18.95227	6.6067
Si	15.85337	1.31514	13.32602
Si	5.75194	8.79933	6.96746
Si	4.46379	11.35137	0.21241
Si	2.53596	1.37743	6.93819
Si	7.69084	18.75108	0.22064
Si	17.76012	11.36801	6.63315
Si	12.6357	8.72087	13.36493
Si	17.7865	18.80205	6.61133
Si	12.64327	1.37771	13.31982
Si	2.54321	8.7506	6.96705
Si	7.67339	11.39897	0.22143
Si	1.49291	0.63027	4.0982
Si	8.7427	19.50434	10.86201
Si	18.841	10.67844	9.45389
Si	11.57538	9.46623	2.70144
Si	18.83878	19.48927	9.44612
Si	11.54875	0.70307	2.6546
Si	1.50542	9.48939	4.13047
Si	8.77057	10.65821	10.86953
Si	3.69246	1.14607	2.08243
Si	6.5542	19.00963	8.83245
Si	16.6078	11.13267	11.45789
Si	13.76909	8.99278	4.75395
Si	16.62446	18.9628	11.44207
Si	13.7783	1.22084	4.66101
Si	3.69426	8.98261	2.10332
Si	6.57118	11.17668	8.85094

Si	8.57848	16.62541	2.28133
Si	1.64939	3.50599	9.0039
Si	11.74507	6.58308	11.28739
Si	18.62455	13.52493	4.54507
Si	11.73971	3.51827	11.22612
Si	18.62792	16.61334	4.55052
Si	8.53457	13.5224	2.27536
Si	1.66351	6.61193	9.02298
Si	6.19346	17.48233	4.16839
Si	4.03499	2.66791	10.90817
Si	14.09419	7.42301	9.41439
Si	16.30954	12.74215	2.58177
Si	14.09219	2.69996	9.35035
Si	16.26806	17.40922	2.62026
Si	6.1794	12.68834	4.18004
Si	4.04257	7.46449	10.91191
Si	5.52206	16.64605	7.12492
Si	4.71248	3.5156	0.37068
Si	14.81001	6.64757	6.44576
Si	15.57719	13.49164	13.14312
Si	14.80723	3.50918	6.38463
Si	15.57403	16.60411	13.14666
Si	5.53141	13.52617	7.14768
Si	4.71825	6.63047	0.3847
Si	2.40306	16.60971	7.00876
Si	7.8271	3.54538	0.2207
Si	17.92511	6.60971	6.57343
Si	12.45842	13.53557	13.38678
Si	17.91788	3.532	6.53363
Si	12.46907	16.59883	13.32405
Si	2.41924	13.54645	7.01642
Si	7.83509	6.60394	0.23589
Si	1.40784	17.49851	4.14774
Si	8.82005	2.62751	10.85476
Si	18.90948	7.51528	9.42796
Si	11.43409	12.60536	2.72893
Si	18.88976	2.61862	9.4076
Si	11.47298	17.59157	2.6618
Si	1.43577	12.64719	4.1662
Si	8.84427	7.4974	10.86412
Si	3.72253	16.64883	2.34023
Si	6.49886	3.48583	9.06146
Si	16.58702	6.66616	11.25077
Si	16.5644	3.50683	11.20692
Si	13.77899	16.73158	4.51136
Si	3.71799	13.4873	2.34281
Si	6.51252	6.65326	9.07634
Al	13.81472	13.49788	4.51321
O	7.35597	1.27036	3.04393
O	2.88238	18.90103	9.78938
O	12.98529	11.26703	10.59683
O	17.45847	8.91605	3.787
O	12.93384	18.85672	10.49636
O	17.44629	1.17196	3.76368
O	7.37761	8.86484	3.07747
O	2.88841	11.2835	9.77338
O	6.1769	1.41549	5.38331
O	4.06824	18.71097	12.1229
O	14.10764	11.35717	8.24454
O	16.24116	8.73247	1.47412
O	14.08764	18.82199	8.15005

O	16.32029	1.3815	1.40571
O	6.16426	8.73607	5.40246
O	4.03223	11.43361	12.12548
O	4.13954	1.18395	7.10351
O	6.08799	18.92565	0.39289
O	16.18163	11.02037	6.59148
O	14.23234	8.95347	13.18873
O	16.19259	19.10601	6.51324
O	14.24153	1.12655	13.22324
O	4.14418	8.96323	7.14507
O	6.0728	11.16649	0.35417
O	2.12252	1.4226	5.37281
O	8.10101	18.70589	12.12559
O	18.26479	11.49922	8.17339
O	12.22352	8.63453	1.45601
O	18.24382	18.68808	8.16075
O	12.17047	1.52088	1.39242
O	2.14196	8.6931	5.39997
O	8.1231	11.44393	12.13746
O	2.20549	1.1263	2.72854
O	8.04512	19.01652	9.47893
O	18.10017	11.15709	10.81707
O	12.28835	9.01597	4.08668
O	18.11177	18.9621	10.79615
O	12.2848	1.146	4.03125
O	2.21373	8.9854	2.76122
O	8.06272	11.15532	9.49401
O	4.75854	0.77143	3.24912
O	5.48576	19.37178	9.99788
O	15.56649	10.62318	10.31904
O	14.85182	9.39931	3.61494
O	15.54815	19.34375	10.28235
O	14.83287	0.77791	3.50922
O	4.77653	9.38004	3.24738
O	5.49377	10.82573	10.01329
O	7.36349	16.72649	3.347
O	2.86485	3.39362	10.06537
O	12.95369	6.59718	10.21118
O	17.54498	13.47131	3.35241
O	12.90226	3.50116	10.0978
O	17.46692	16.69305	3.42733
O	7.31662	13.47981	3.347
O	2.88294	6.69979	10.08486
O	6.20263	16.87893	5.67087
O	4.01226	3.29687	12.39792
O	14.11834	6.88259	7.89239
O	16.40925	13.23295	1.02792
O	14.09596	3.1592	7.80074
O	16.27829	16.8201	1.11615
O	6.18569	13.29057	5.68349
O	4.01404	6.87632	12.41853
O	3.95874	17.09799	7.07751
O	6.2741	3.05552	0.2811
O	16.37351	7.10229	6.51437
O	14.01523	13.05838	13.34082
O	16.3662	3.0381	6.45557
O	14.01877	17.09358	13.23115
O	3.97199	13.06207	7.14097
O	6.28008	7.08557	0.29208
O	1.88632	16.69699	5.47583
O	8.35819	3.46948	12.1629

O	18.45661	6.68845	8.10499
O	11.88079	13.48086	1.42024
O	18.44565	3.40659	8.06152
O	11.95365	16.71251	1.38596
O	1.96263	13.46986	5.4648
O	8.37204	6.6748	12.18086
O	2.19837	16.91012	2.85155
O	8.0236	3.18003	9.54812
O	18.10245	6.94745	10.72253
O	12.1612	13.12362	4.05745
O	18.08073	3.21776	10.68583
O	12.28135	17.15869	4.00269
O	2.18868	13.2252	2.83933
O	8.0414	6.93431	9.56425
O	4.74723	17.21753	3.47598
O	5.48088	2.93805	10.21136
O	15.54655	7.18597	10.1083
O	14.90421	13.14934	3.22078
O	15.52723	3.03331	10.03928
O	14.8404	17.06966	3.32727
O	4.72182	12.92407	3.49893
O	5.49688	7.18638	10.23469
O	6.50663	19.07467	4.21919
O	3.75331	1.07118	10.9895
O	13.69761	8.99556	9.43419
O	16.58321	11.12986	2.6128
O	13.78868	1.10559	9.45123
O	16.51334	19.01517	2.57562
O	6.52389	11.10272	4.22732
O	3.74881	9.06016	10.93764
O	1.74613	19.0746	4.32943
O	8.4849	1.05734	11.09594
O	18.58713	9.08922	9.20839
O	11.78294	11.04569	2.40063
O	18.54919	1.04133	9.23416
O	11.76299	19.15454	2.34741
O	1.78455	11.07501	4.35917
O	8.51455	9.0693	11.08506
O	8.71271	2.58197	1.17641
O	1.50756	17.55858	7.97214
O	11.58228	12.5857	12.39917
O	18.81956	7.54879	5.60187
O	11.57221	17.53527	12.3419
O	18.8033	2.60311	5.5393
O	8.71658	7.56189	1.19785
O	1.49549	12.59595	7.9494
O	8.43384	19.99075	0.96524
O	1.79604	0.13693	7.68311
O	11.8489	9.95213	12.64744
O	18.57537	10.16667	5.89743
O	11.88653	0.12142	12.61508
O	18.58101	20.02025	5.88725
O	8.43522	10.18999	0.9953
O	1.77786	9.9785	7.70679
O	8.17421	17.34966	0.88321
O	2.05895	2.77614	7.60857
O	12.19005	7.3251	12.66171
O	18.08271	12.77295	5.88265
O	12.2449	2.75236	12.5652
O	18.14293	17.39393	5.89386
O	8.07557	12.82916	0.87692

O	2.0832	7.34439	7.63407
O	3.96305	2.63298	1.5012
O	6.29989	17.52196	8.24274
O	16.2247	12.63498	11.92765
O	14.04323	7.48466	5.29538
O	16.3355	17.47817	12.01617
O	14.05852	2.73121	5.17278
O	3.97616	7.49277	1.53317
O	6.33733	12.66995	8.26063
O	3.77172	0.05448	0.88028
O	6.47629	0.07245	7.63446
O	16.57051	10.10783	12.72133
O	13.82209	10.02669	6.00034
O	16.5648	0.02675	12.63774
O	13.87647	0.21928	5.94127
O	3.7416	10.06171	0.88781
O	6.47971	10.08534	7.64924
O	3.96665	17.41501	0.92809
O	6.22408	2.73703	7.64677
O	16.34492	7.43981	12.65679
O	14.17746	12.70137	6.01191
O	16.29465	2.6902	12.58657
O	14.10764	17.60014	5.85546
O	3.98992	12.72709	0.93374
O	6.24074	7.41989	7.67096
O	20.06932	0.95031	3.92589
O	10.32648	19.17745	10.70607
O	0.26998	10.98136	9.64662
O	9.99431	9.12723	2.86988
O	0.26926	19.20514	9.62178
O	9.97064	1.01635	2.85828
O	20.0808	9.18077	3.96628
O	10.35405	10.98606	10.71781
O	19.9695	17.29699	3.9298
O	10.41505	2.80351	10.60531
O	0.34612	7.30414	9.68294
O	9.81186	12.75851	2.91452
O	0.32681	2.81621	9.65892
O	9.88911	17.33819	2.94248
O	19.99607	12.83826	3.99968
O	10.43886	7.2981	10.62495
O	8.89563	15.07331	1.95993
O	1.35444	5.0612	8.67296
O	11.39463	5.04176	11.64892
O	18.91501	15.07349	4.95369
O	3.9724	15.069	2.09488
O	6.28591	5.07062	8.82007
O	16.37354	5.08141	11.52625
O	13.73814	15.20207	5.00202
O	5.67012	15.09061	7.5524
O	4.59428	5.07022	0.80503
O	14.69495	5.08255	6.0531
O	15.66372	15.05366	12.69898
O	2.26528	15.07985	7.52928
O	7.97144	5.07023	0.75467
O	18.05757	5.07462	6.05699
O	12.32369	15.06233	12.8268
H	11.50427	14.18592	9.17518
H	13.13198	14.81941	9.51646
H	12.93355	13.51869	8.32725
H	12.45921	15.11179	6.35964

H	13.333	15.83757	7.30305
H	11.81119	16.40747	7.95093
H	10.76965	15.86348	5.96449
H	10.52306	14.48426	7.14322
H	11.442	14.20832	5.66307
C	11.19568	14.97609	6.43708
C	12.34179	15.49496	7.66117
C	12.4742	14.43269	8.72396

$C_4H_{10} \rightarrow CH_4 + C_3H_6$

Reactant

Si	8.66952	1.17161	2.04013
Si	1.65847	18.94977	8.77434
Si	11.74985	11.19679	11.5369
Si	18.76041	8.93084	4.76802
Si	11.73479	18.96931	11.55286
Si	18.75143	1.15265	4.82103
Si	8.66554	8.95922	2.01967
Si	1.67317	11.18153	8.74896
Si	6.25197	0.60172	3.98681
Si	4.07176	19.5127	10.72437
Si	14.1339	10.54586	9.60616
Si	16.34624	9.56624	2.8382
Si	14.17727	19.56593	9.64249
Si	16.30005	0.58476	2.87163
Si	6.25809	9.5141	3.97576
Si	4.08231	10.6321	10.70476
Si	5.80907	1.34794	6.96382
Si	4.51595	18.77818	0.22758
Si	14.64039	11.27069	6.64549
Si	15.89422	8.86205	13.33167
Si	14.62223	18.90085	6.66269
Si	15.89554	1.35363	13.37992
Si	5.7916	8.76634	6.94778
Si	4.50984	11.35223	0.19144
Si	2.59621	1.37555	6.97277
Si	7.7264	18.75591	0.23143
Si	17.81801	11.33499	6.58645
Si	12.68836	8.76556	13.32665
Si	17.82476	18.76011	6.63834
Si	12.68915	1.35752	13.37874
Si	2.57776	8.72126	6.945
Si	7.71841	11.39384	0.18555
Si	1.5514	0.62573	4.1338
Si	8.7731	19.50892	10.87152
Si	18.89861	10.69033	9.41438
Si	11.62368	9.47467	2.67336
Si	18.85347	19.50011	9.47614
Si	11.63139	0.62933	2.74711
Si	1.54614	9.46769	4.10619
Si	8.81878	10.63833	10.83804
Si	3.73495	1.13685	2.09384
Si	6.59176	18.98782	8.8349
Si	16.64912	11.16797	11.39157
Si	13.82751	8.97339	4.69327
Si	16.69142	19.00036	11.53588

Si	13.80776	1.20559	4.77304
Si	3.74722	8.97886	2.0814
Si	6.60147	11.14905	8.83562
Si	8.60061	16.60805	2.28447
Si	1.70019	3.50402	9.03372
Si	11.80887	6.57523	11.27179
Si	18.66313	13.51304	4.49413
Si	11.7827	3.50221	11.3317
Si	18.69661	16.60579	4.59268
Si	8.56569	13.50821	2.24974
Si	1.69927	6.61071	9.02234
Si	6.22461	17.46578	4.18029
Si	4.09571	2.64919	10.90835
Si	14.12676	7.40443	9.37826
Si	16.37733	12.74576	2.52515
Si	14.16977	2.70587	9.41951
Si	16.30196	17.42545	2.67102
Si	6.22332	12.67543	4.17956
Si	4.08972	7.46294	10.90412
Si	5.55874	16.62463	7.13488
Si	4.77147	3.49918	0.38895
Si	14.87004	6.65437	6.41662
Si	15.61553	13.49415	13.09444
Si	14.84822	3.533	6.46971
Si	15.62251	16.6099	13.19895
Si	5.56827	13.50934	7.13564
Si	4.77099	6.61465	0.37252
Si	2.44733	16.59669	7.00884
Si	7.88878	3.53368	0.27699
Si	17.97664	6.60042	6.56273
Si	12.497	13.54312	13.32428
Si	17.95162	3.52091	6.5923
Si	12.51641	16.60748	13.31115
Si	2.45762	13.53175	6.98967
Si	7.89169	6.59209	0.23978
Si	1.45925	17.49188	4.15046
Si	8.86705	2.63217	10.89192
Si	18.95809	7.52861	9.41401
Si	11.46979	12.62389	2.67989
Si	18.94747	2.62839	9.45652
Si	11.50618	17.4963	2.69878
Si	1.46991	12.62735	4.14318
Si	8.89307	7.4746	10.86252
Si	3.76408	16.641	2.34203
Si	6.56379	3.47921	9.07362
Si	16.62218	6.67379	11.22252
Si	16.63983	3.51672	11.2677
Si	13.80756	16.75296	4.55502
Si	3.76733	13.47363	2.33995
Si	6.55696	6.64278	9.06965
Al	13.85977	13.37316	4.44019
O	7.43805	1.23966	3.08796
O	2.89029	18.87167	9.82195
O	13.03674	11.26438	10.55657
O	17.49822	8.88847	3.75648
O	12.97258	18.92345	10.50817
O	17.50816	1.14928	3.78395
O	7.42958	8.86908	3.06435
O	2.94494	11.26631	9.7459
O	6.20344	1.40591	5.39402
O	4.11479	18.70955	12.13286

O	14.13794	11.32269	8.19124
O	16.32594	8.77808	1.41679
O	14.25378	18.7659	8.22809
O	16.27734	1.42365	1.48289
O	6.20606	8.70597	5.3825
O	4.05992	11.44452	12.1095
O	4.19987	1.21325	7.15999
O	6.1248	18.94003	0.41252
O	16.24409	10.95801	6.59126
O	14.28286	9.03551	13.1793
O	16.22365	18.96945	6.41779
O	14.28999	1.16811	13.18294
O	4.18079	8.90355	7.12107
O	6.11816	11.15441	0.30758
O	2.20218	1.41011	5.40166
O	8.13067	18.712	12.136
O	18.35779	11.50132	8.11043
O	12.25479	8.65753	1.41058
O	18.18124	18.71389	8.21637
O	12.30627	1.3948	1.48093
O	2.17224	8.66829	5.37828
O	8.182	11.43375	12.10624
O	2.25588	1.12357	2.76122
O	8.07494	19.0094	9.49548
O	18.14236	11.20706	10.75448
O	12.34219	8.97957	4.04132
O	18.16377	18.99517	10.85487
O	12.32148	1.13835	4.12654
O	2.26695	8.97933	2.73958
O	8.09656	11.11326	9.46466
O	4.82633	0.76602	3.2368
O	5.50265	19.3482	9.98277
O	15.6175	10.62989	10.25807
O	14.8966	9.39805	3.54603
O	15.59076	19.38818	10.40681
O	14.8831	0.77871	3.63505
O	4.82788	9.37192	3.22727
O	5.54076	10.79349	10.01415
O	7.3837	16.7105	3.34419
O	2.92864	3.40381	10.08268
O	12.98715	6.5587	10.15865
O	17.59389	13.51777	3.28522
O	12.99012	3.42057	10.25772
O	17.48568	16.74903	3.52575
O	7.35164	13.45074	3.32197
O	2.93074	6.70832	10.06756
O	6.22681	16.84931	5.67488
O	4.10661	3.26547	12.4027
O	14.14064	6.91005	7.84001
O	16.46917	13.17449	0.95699
O	14.14571	3.30463	7.9152
O	16.29658	16.77137	1.19691
O	6.23774	13.2921	5.67566
O	4.07455	6.84617	12.39993
O	3.99747	17.09452	7.09401
O	6.33648	3.04198	0.35419
O	16.4305	7.1121	6.51764
O	14.05567	13.06401	13.30448
O	16.39697	3.02439	6.54654
O	14.06933	17.10799	13.26858
O	4.00786	13.0404	7.09234

O	6.33403	7.06531	0.28854
O	1.93802	16.6823	5.47205
O	8.40366	3.44755	12.21529
O	18.53109	6.70243	8.08293
O	11.89306	13.46579	1.3455
O	18.50087	3.42822	8.11562
O	11.97245	16.71072	1.36471
O	1.97446	13.45947	5.44409
O	8.42448	6.6518	12.18218
O	2.237	16.9116	2.84414
O	8.08785	3.221	9.59039
O	18.13712	6.95683	10.6973
O	12.2171	13.21273	3.97004
O	18.15621	3.22605	10.74709
O	12.30464	16.87012	3.98964
O	2.23435	13.19687	2.82033
O	8.08516	6.91182	9.56544
O	4.77659	17.21628	3.48351
O	5.53915	2.89848	10.20093
O	15.58237	7.13688	10.05586
O	14.96035	13.17667	3.14026
O	15.61059	2.999	10.11313
O	14.86968	17.08873	3.39715
O	4.76127	12.90778	3.50184
O	5.541	7.20611	10.21345
O	6.54179	19.05701	4.24397
O	3.78111	1.05779	10.97596
O	13.74163	8.97852	9.43742
O	16.65972	11.14144	2.63896
O	13.90011	1.10506	9.36786
O	16.50152	19.0306	2.57537
O	6.56004	11.08854	4.24061
O	3.78337	9.05555	10.96099
O	1.79359	19.06622	4.34849
O	8.5081	1.06302	11.09368
O	18.62485	9.10076	9.19239
O	11.86072	11.05958	2.42088
O	18.59038	1.05642	9.26612
O	11.88914	19.0645	2.56775
O	1.8068	11.0545	4.3502
O	8.57577	9.04919	11.08032
O	8.78446	2.58046	1.23834
O	1.54159	17.54312	7.96711
O	11.62575	12.61477	12.31709
O	18.86473	7.51116	5.5579
O	11.63007	17.54623	12.32868
O	18.8227	2.57363	5.60305
O	8.77078	7.56461	1.18941
O	1.54036	12.57929	7.92769
O	8.47846	19.99641	0.96643
O	1.85939	0.12432	7.70302
O	11.88588	9.98938	12.61919
O	18.63592	10.13432	5.85599
O	11.92833	0.11611	12.6564
O	18.60397	19.98887	5.91781
O	8.47493	10.18843	0.97
O	1.83127	9.96245	7.68239
O	8.20891	17.35586	0.89511
O	2.09195	2.76843	7.63615
O	12.29198	7.36569	12.60495
O	18.08308	12.73383	5.80037

O	12.20153	2.75329	12.71415
O	18.28506	17.34911	5.98287
O	8.10883	12.8248	0.84509
O	2.09613	7.32373	7.61652
O	3.99215	2.62296	1.50424
O	6.34444	17.49973	8.24644
O	16.2452	12.67102	11.84646
O	14.13111	7.47313	5.23518
O	16.42119	17.51776	12.12441
O	14.06615	2.70503	5.31525
O	4.02491	7.48991	1.5081
O	6.35074	12.64165	8.255
O	3.79128	0.03817	0.89606
O	6.52145	0.04886	7.6342
O	16.62665	10.1551	12.66611
O	13.87446	10.0195	5.93087
O	16.65174	0.06733	12.73263
O	13.90497	0.17493	6.0329
O	3.79011	10.06286	0.87073
O	6.49405	10.06362	7.63035
O	4.01746	17.40076	0.92826
O	6.33307	2.7196	7.65626
O	16.35927	7.48778	12.60051
O	14.30631	12.67152	5.94551
O	16.37811	2.72965	12.66728
O	14.03707	17.56256	5.92815
O	4.05343	12.72672	0.9265
O	6.30121	7.39456	7.65311
O	20.12513	0.95013	3.98944
O	10.36149	19.20713	10.7289
O	0.32816	10.96695	9.62816
O	10.04163	9.15343	2.84646
O	0.2804	19.18227	9.59481
O	10.04748	0.94207	2.8638
O	20.12555	9.14384	3.92022
O	10.39861	10.97112	10.66623
O	20.01811	17.28723	3.93298
O	10.46723	2.80851	10.66728
O	0.39152	7.31822	9.68848
O	9.85114	12.74289	2.87229
O	0.38709	2.80765	9.70236
O	9.91806	17.30646	2.95245
O	20.03021	12.82018	3.95285
O	10.48547	7.26246	10.61844
O	8.91647	15.06213	1.94011
O	1.38573	5.05477	8.70007
O	11.47602	5.04708	11.70314
O	18.96157	15.04952	4.94128
O	4.00992	15.05936	2.10656
O	6.31081	5.05892	8.83358
O	16.43251	5.09599	11.55041
O	14.03051	15.15321	5.08352
O	5.6801	15.06876	7.56283
O	4.63967	5.05802	0.80459
O	14.77124	5.08421	6.03754
O	15.7166	15.07196	12.71541
O	2.30784	15.06199	7.5148
O	8.03655	5.06746	0.78491
O	18.08263	5.05259	6.07847
O	12.38602	15.07982	12.79652
H	11.40152	13.79759	8.91922

H	11.98783	13.93504	7.27089
H	11.3259	16.38342	7.26003
H	10.69002	16.20006	8.89209
H	8.85625	16.02267	7.18039
H	9.02356	14.48928	8.06434
H	9.68175	14.64235	6.42111
H	13.67145	15.71897	8.06766
H	13.90173	14.13401	8.86329
H	13.09795	15.4737	9.71247
H	14.16054	15.08257	6.05503
C	9.53345	15.17786	7.37246
C	10.86541	15.65252	7.94939
C	11.84897	14.50923	8.20413
C	13.2034	14.9736	8.73699

Transition state

Si	8.59557	1.19932	2.01564
Si	1.62679	18.96844	8.77396
Si	11.71187	11.17892	11.59429
Si	18.71272	8.9617	4.80825
Si	11.70009	18.95356	11.55499
Si	18.71181	1.16871	4.78499
Si	8.61329	8.94838	2.03933
Si	1.61862	11.19925	8.77467
Si	6.19686	0.62011	3.97295
Si	4.04507	19.52931	10.72463
Si	14.09266	10.54933	9.63918
Si	16.28596	9.5658	2.87736
Si	14.09567	19.5552	9.59981
Si	16.28017	0.5676	2.83005
Si	6.2082	9.52384	3.98775
Si	4.03906	10.64161	10.71315
Si	5.74805	1.35358	6.94933
Si	4.47651	18.78118	0.22074
Si	14.58014	11.30357	6.67136
Si	15.847	8.81348	13.37951
Si	14.58717	18.94327	6.60902
Si	15.85655	1.31422	13.33824
Si	5.74924	8.7995	6.97074
Si	4.46363	11.35082	0.21518
Si	2.53616	1.37469	6.94165
Si	7.69059	18.74965	0.22929
Si	17.76421	11.36193	6.63102
Si	12.63712	8.71809	13.3644
Si	17.79021	18.80118	6.61884
Si	12.64458	1.38673	13.33007
Si	2.53946	8.75183	6.96651
Si	7.67309	11.39894	0.22418
Si	1.49395	0.6308	4.09926
Si	8.74257	19.50436	10.86915
Si	18.84347	10.68013	9.4543
Si	11.56834	9.45131	2.69834
Si	18.83889	19.48774	9.4538
Si	11.54203	0.71334	2.66008
Si	1.50264	9.48585	4.12758
Si	8.77089	10.65908	10.87127

Si	3.6911	1.1471	2.08377
Si	6.55711	19.00885	8.83565
Si	16.60552	11.13675	11.45018
Si	13.76785	8.98694	4.7445
Si	16.6212	18.96363	11.44511
Si	13.77025	1.21759	4.67284
Si	3.69413	8.98079	2.1051
Si	6.56945	11.17726	8.85513
Si	8.57817	16.62359	2.2874
Si	1.64858	3.50612	9.00297
Si	11.74681	6.58192	11.28
Si	18.62446	13.52631	4.54701
Si	11.73795	3.51822	11.23228
Si	18.62911	16.61075	4.55955
Si	8.53338	13.52001	2.27847
Si	1.66114	6.61203	9.02345
Si	6.19022	17.48419	4.16828
Si	4.03463	2.66766	10.90767
Si	14.09461	7.4141	9.40977
Si	16.30647	12.74938	2.59158
Si	14.09745	2.7006	9.35981
Si	16.26495	17.39969	2.63225
Si	6.17859	12.68689	4.1836
Si	4.0408	7.4643	10.91264
Si	5.5212	16.64758	7.12685
Si	4.71025	3.51544	0.36859
Si	14.81474	6.6464	6.43996
Si	15.58209	13.49059	13.14983
Si	14.80866	3.51149	6.39148
Si	15.58099	16.60397	13.15659
Si	5.53023	13.526	7.14988
Si	4.71687	6.63	0.38219
Si	2.40287	16.61126	7.01138
Si	7.82341	3.5457	0.21726
Si	17.92789	6.60857	6.57526
Si	12.45628	13.53498	13.39723
Si	17.91682	3.52882	6.53891
Si	12.46888	16.60008	13.3423
Si	2.41787	13.54634	7.01649
Si	7.8327	6.6032	0.23161
Si	1.40724	17.49884	4.14933
Si	8.82001	2.62722	10.85451
Si	18.90855	7.51509	9.43287
Si	11.42874	12.58725	2.73297
Si	18.88867	2.61787	9.41444
Si	11.46643	17.60501	2.67121
Si	1.43292	12.64478	4.16535
Si	8.84577	7.49854	10.86319
Si	3.71956	16.6485	2.34121
Si	6.49884	3.48648	9.06374
Si	16.5847	6.66236	11.25457
Si	16.56965	3.50329	11.22327
Si	13.77063	16.72826	4.51224
Si	3.71825	13.4872	2.34625
Si	6.51171	6.65374	9.07977
Al	13.80336	13.49435	4.5151
O	7.35017	1.27758	3.04673
O	2.88242	18.8986	9.79361
O	12.98571	11.25979	10.59365
O	17.45397	8.91254	3.79458
O	12.93403	18.86618	10.50067

O	17.4456	1.16541	3.77776
O	7.37007	8.86138	3.07653
O	2.89033	11.284	9.77374
O	6.17315	1.41355	5.38721
O	4.07276	18.71205	12.12583
O	14.10292	11.34405	8.23464
O	16.26063	8.7489	1.46951
O	14.09127	18.81193	8.15208
O	16.32537	1.36677	1.4171
O	6.164	8.73618	5.40598
O	4.02969	11.4332	12.12901
O	4.13969	1.18158	7.11208
O	6.08739	18.922	0.40346
O	16.18724	11.00438	6.59488
O	14.23391	8.96202	13.20409
O	16.19758	19.11273	6.51809
O	14.24341	1.13909	13.23403
O	4.14081	8.96068	7.14516
O	6.07261	11.16439	0.35482
O	2.12702	1.41842	5.37505
O	8.09804	18.70962	12.13339
O	18.27244	11.49759	8.16961
O	12.21095	8.61776	1.45112
O	18.24371	18.68616	8.16922
O	12.17179	1.53228	1.40248
O	2.13814	8.69288	5.39942
O	8.12432	11.44295	12.14065
O	2.2038	1.13025	2.72931
O	8.04701	19.01308	9.48589
O	18.0987	11.16817	10.81205
O	12.28466	9.00463	4.08258
O	18.11043	18.96108	10.80341
O	12.27767	1.14235	4.0411
O	2.2122	8.98013	2.75969
O	8.062	11.15649	9.49645
O	4.75502	0.77247	3.25244
O	5.48625	19.37059	9.99874
O	15.56715	10.6273	10.30891
O	14.84511	9.38749	3.59848
O	15.5486	19.34876	10.28368
O	14.82814	0.79331	3.51771
O	4.77118	9.37951	3.25369
O	5.49471	10.82496	10.01956
O	7.3582	16.72429	3.3478
O	2.86628	3.39266	10.06168
O	12.94889	6.58621	10.19652
O	17.54312	13.48536	3.35463
O	12.90483	3.49471	10.1095
O	17.4658	16.68623	3.43886
O	7.31479	13.47852	3.34951
O	2.88452	6.70016	10.08063
O	6.19812	16.88188	5.67131
O	4.0067	3.29738	12.39727
O	14.12217	6.87994	7.88609
O	16.41515	13.21442	1.03017
O	14.10983	3.18437	7.81818
O	16.2948	16.83156	1.11977
O	6.18787	13.28731	5.68764
O	4.00589	6.87544	12.41918
O	3.9581	17.10104	7.08403
O	6.27105	3.05421	0.27438

O	16.37723	7.10363	6.51213
O	14.01655	13.07037	13.34638
O	16.36589	3.03316	6.45178
O	14.02266	17.0812	13.2513
O	3.97078	13.06158	7.13935
O	6.27787	7.08516	0.28079
O	1.88812	16.70058	5.47824
O	8.35769	3.47206	12.16065
O	18.45716	6.69135	8.10738
O	11.8801	13.46856	1.43039
O	18.43674	3.4043	8.0697
O	11.95307	16.71894	1.40304
O	1.95807	13.46536	5.46598
O	8.37683	6.67322	12.17937
O	2.19493	16.90613	2.85315
O	8.02497	3.18072	9.54721
O	18.09927	6.94616	10.72574
O	12.15562	13.09073	4.0668
O	18.08395	3.21656	10.69569
O	12.28153	17.19571	4.01507
O	2.18805	13.22539	2.84064
O	8.04184	6.93467	9.56431
O	4.74352	17.22163	3.47563
O	5.48254	2.93751	10.21473
O	15.54364	7.17245	10.10863
O	14.8996	13.17188	3.21857
O	15.5284	3.02102	10.06312
O	14.83524	17.03503	3.32266
O	4.72031	12.92468	3.50433
O	5.49782	7.18709	10.24014
O	6.50721	19.07611	4.21675
O	3.75341	1.07079	10.98947
O	13.70073	8.98731	9.43613
O	16.58036	11.13757	2.64482
O	13.79192	1.10511	9.43318
O	16.49568	19.0076	2.60984
O	6.52272	11.10113	4.22809
O	3.74665	9.06009	10.9394
O	1.74778	19.0747	4.32522
O	8.48191	1.05774	11.09683
O	18.58761	9.09015	9.21605
O	11.77418	11.02988	2.39131
O	18.55018	1.03999	9.24209
O	11.74455	19.16614	2.34026
O	1.78059	11.0719	4.35413
O	8.51411	9.07007	11.08509
O	8.70769	2.58142	1.17256
O	1.50588	17.55701	7.97653
O	11.59134	12.58433	12.40025
O	18.82412	7.54434	5.60182
O	11.58371	17.54215	12.35438
O	18.80661	2.59996	5.54865
O	8.71048	7.56152	1.19594
O	1.49495	12.59914	7.95401
O	8.43326	19.98755	0.97765
O	1.79564	0.13464	7.68721
O	11.85029	9.94952	12.6475
O	18.5845	10.16345	5.8967
O	11.89194	0.12943	12.62278
O	18.59106	20.01602	5.89593
O	8.43475	10.19155	1.00116

O	1.77823	9.9834	7.70451
O	8.17751	17.34711	0.88721
O	2.05565	2.77443	7.60799
O	12.20663	7.32422	12.64916
O	18.07769	12.76799	5.87912
O	12.24066	2.76014	12.5765
O	18.14358	17.39096	5.90328
O	8.07273	12.83076	0.87812
O	2.07464	7.34797	7.63477
O	3.96334	2.63304	1.50076
O	6.30267	17.52223	8.24307
O	16.21595	12.63574	11.92511
O	14.04692	7.48184	5.29013
O	16.32689	17.47952	12.01698
O	14.04263	2.72489	5.19721
O	3.98084	7.49243	1.53432
O	6.33255	12.6707	8.26629
O	3.77065	0.05352	0.88328
O	6.48071	0.07416	7.6396
O	16.57064	10.1092	12.71045
O	13.82377	10.02699	5.9853
O	16.55965	0.02508	12.64301
O	13.8702	0.20313	5.94234
O	3.74183	10.06152	0.89122
O	6.47526	10.08645	7.65315
O	3.96179	17.41391	0.92843
O	6.22273	2.73842	7.64882
O	16.33874	7.44189	12.65708
O	14.19935	12.69868	6.00563
O	16.30928	2.69015	12.60694
O	14.13382	17.58491	5.85536
O	3.99201	12.72668	0.93761
O	6.23802	7.42047	7.67494
O	20.07024	0.95129	3.93055
O	10.3271	19.17854	10.71981
O	0.27242	10.98043	9.64981
O	9.98753	9.11591	2.87455
O	0.26956	19.20367	9.62816
O	9.96563	1.03315	2.86508
O	20.0788	9.17486	3.96027
O	10.35442	10.98682	10.72049
O	19.96794	17.29848	3.9365
O	10.41619	2.7998	10.60907
O	0.34474	7.30109	9.68921
O	9.80719	12.74811	2.91606
O	0.32635	2.81803	9.66001
O	9.88486	17.33904	2.95449
O	19.99321	12.83663	3.99807
O	10.44089	7.30283	10.62369
O	8.89947	15.07107	1.96871
O	1.35461	5.06134	8.67144
O	11.38944	5.04344	11.64661
O	18.92174	15.07152	4.96401
O	3.97332	15.0687	2.09819
O	6.28431	5.07124	8.82449
O	16.37606	5.07863	11.53805
O	13.68673	15.19855	4.99763
O	5.6679	15.09125	7.5519
O	4.59434	5.07008	0.80357
O	14.70285	5.08202	6.04373
O	15.68302	15.05319	12.71491

O	2.26604	15.08013	7.52775
O	7.96642	5.0702	0.7526
O	18.05837	5.07181	6.06371
O	12.30594	15.06418	12.85182
H	11.61494	14.23712	9.22885
H	12.80213	13.47583	8.14998
H	12.38339	15.13964	6.32421
H	13.2567	15.88754	7.23371
H	11.75293	16.38586	7.97207
H	10.63322	15.83694	6.02414
H	10.5011	14.42147	7.17702
H	11.37186	14.22142	5.6572
H	14.62534	14.93163	9.03223
H	13.83655	14.05518	10.35562
H	13.47336	15.77299	10.10097
C	11.12151	14.96214	6.45742
C	12.29497	15.49882	7.62772
C	12.54162	14.41625	8.6586
C	13.68318	14.82315	9.58887