Electronic Supplementary Information

Trimethyloxonium ion - a zeolite confined mobile and efficient methyl carrier at low temperature: a DFT study coupled with microkinetic analysis

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Content

S1. Model and methods

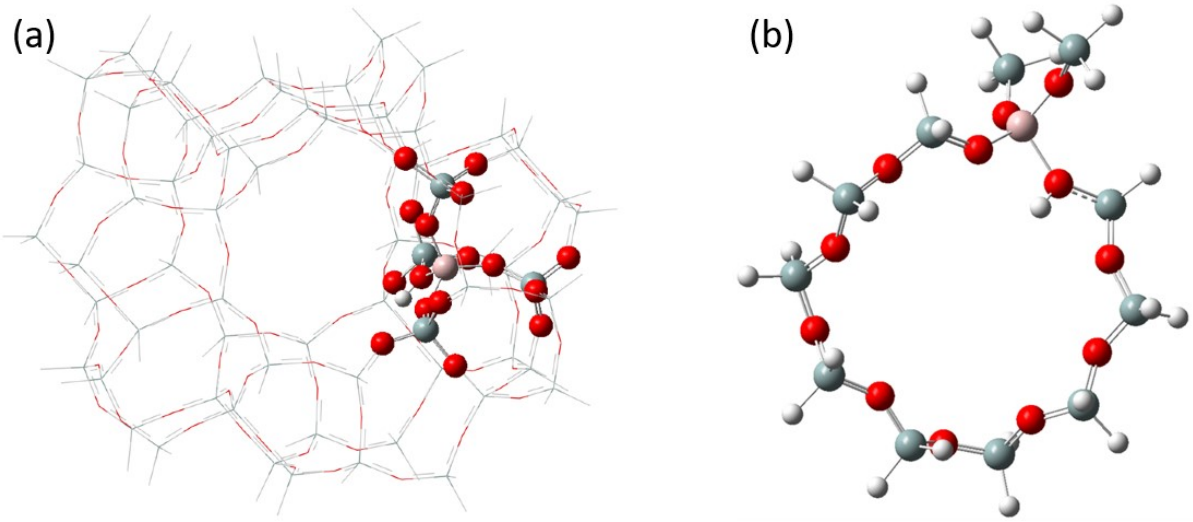


Fig. S1 (a) 68T and (b) 12T cluster models of H-ZSM-5 for DFT and *ab initio* calculations.

Models and Methods test

In order to verify the reliability of the model and method used in this work, calculations were carried out at DFT and ab inito level of theory. The calculated thermodynamic, kinetic and microkinetic data were compared with available experimental and theoretical results. The ωB97X-D/6-311+G(2df,2p)//B3LYP/6-311G(d,p) calculations performed in this work was denoted as ωB//B3. The quasi-rigid-rotor harmonic (QRRHO) approximation was denoted as *. PBE[1] calculations with D3-Becke-Jonson dispersion corrections[2] (PBE-D3) over both 68T cluster and periodic models were denoted as PBE-cluster*and PBE-PBC*, respectively. The electronic energies of active site (12T) and reacting species were improved at DLPNO-CCSD(T)/def2-TZVP (with the respective def2-TZVP/C auxiliary basis set) level[3] using PBE-D3 optimized structures by employing ONIOM strategy with 68T cluster model (ONIOM(DLPNO-CCSD(T)/def2-TZVP:PBE-D3/6-311G(d,p)), denoted as ONIOM-cluster*). To obtain improved energies for periodic model, we also applied hybrid QM/QM method[4] that combines PBE-D3 for the full periodic system with ωB97X-D for 68T and reacting species based on PBE-D3 optimized structures (hybrid(ωB97X-D:PBE-D3), denoted as Hybrid-PBC*).

PBE-D3 calculations with periodic boundary condition were performed with plane-wave kinetic energy cutoff of 600 eV and Γ-point using the Vienna Ab Initio Package (VASP)[5, 6]. For calculations over cluster models, Gaussian software was employed, except for DLPNO-CCSD(T) calculations with ORCA[7].

(1) Thermodynamics:

Firstly, to verify the calculated thermodynamic properties, the methanol adsorption enthalpy was tested and compared with experimental results available. As shown in Table S1, the methanol adsorption enthalpy calculated at ωB//B3 level over 68T cluster (-100 kJ/mol) is in good agreement with the experimental results reported by Pope (-104 kJ/mol, Si/Al = 37) at 323 K[8]. Besides, the calculated methanol adsorption enthalpies at ONIOM-cluster* and Hybrid-PBC* levels are -97 and -104 kJ/mol, respectively, quite similar to the value at ωB//B3 level. The adsorption enthalpy obtained by PBE-cluster* (-137 kJ/mol) and PBE-PBC* (-121 kJ/mol) are lower than the experimental value at 323 K, while close to the theoretical value (-117 kJ/mol) reported by de Wispelaere at PBE-D3 level[9] as well as experimental result (-115±5 kJ/mol, Si/Al = 26) obtained at 400 K[10] . These demonstrate that the methanol adsorption enthalpy calculated at ωB//B3 level over 68T cluster model was not only consistent with the results corrected at DLPNO-CCSD(T) level over ONIOM-cluster* model as well as at ωB97X-D level over hybrid-PBC* periodic model, but also in very good agreement with experimental data within chemical accuracy.

Table S1 Adsorption enthalpies of methanol at 323 K.

CH_3OH	ΔH_{ads}, kJ/mol
Exp.[8]	–104
ωB//B3	–100
PBE-PBC*	–121
PBE-cluster*	–137
ONIOM-cluster*	–97
Hybrid-PBC*	–104

Besides, The methanol adsorption enthalpies and entropies were tested on the 68T cluster with 5T around the Al center relaxed and only terminal H fixed (Table S2); it is found that the results obtained at 68T(5T-relaxed)-ωB97X-D/6-311+G(2df,2p)//B3LYP/6-311G(d,p) level (–100 kJ mol-1and −189 J·mol-1·K-1) are much closer to the experimental results (–104 kJ mol-1 and −185 J·mol-1·K-1)[8], compared to the results computed with fully optimized 68T(H-fixed) cluster model at ωB97XD/6-311+G(2df,2p)//ωB97XD/6-311G(d,p) level (–101 kJ mol-1 and −145 J·mol-1·K-1) and periodic PBE+D calculations with QRRHO approximation (–116 kJ mol-1 and −163 J·mol-1·K-1)[11] (Table S2).

Table S2 Calculated adsorption enthalpies and entropies of methanol at 323 K.

CH_3OH	ΔH_{ads}, kJ mol^{-1}	ΔS_{ads}, J·mol^{-1}·K^{-1}
Exp.[4, 8]	–104 (323 K)	−185 (323 K)
PBE+D (pbc)[11]	–116 (300 K)	−163 (300 K)
68T(5T-relaxed)-ωB97XD/6-311+G(2df,2p) //B3LYP/6-311G(d,p)	–100 (323 K)	–189 (323 K)
68T(H-fixed)-ωB97XD/6-311+G(2df,2p) //ωB97XD/6-311G(d,p)	–101 (323 K)	–145 (323 K)

(2) Kinetics:

Secondly, the kinetics of ethene methylation by CH_3OH was compared with experimental as well as theoretical results at different levels of theory. As summarized in Table S3, the calculated enthalpy barrier for ethene methylation by CH_3OH in this work (101 kJ/mol) agrees well with the available experimental value (104 kJ/mol),[4, 12] and that calculated over ONIOM-cluster* (99 kJ/mol) and hybrid-PBC* (80 kJ/mol) at 623 K. It also accords well with the theoretical results obtained with harmonic (104 kJ/mol, denoted as Harmonic-Svelle)[13] and anharmonic (105 kJ/mol, denoted as Anharmonic-Hybrid)[4] vibrational energies; the latter performed at hybrid(MP2:PBE+D) level reported by Sauer is within chemical accuracy[4]. In addition, the rate

constant calculated in this work (1.0×10^{-6} mbar^{-1} s^{-1}) is close to those obtained at Anharmonic-Hybrid (6.1×10^{-5} mbar^{-1} s^{-1})[4], ONIOM-cluster* (3.9×10^{-7} mbar^{-1} s^{-1}) and hybrid-PBC* (3.0×10^{-5} mbar^{-1} s^{-1}). The deviation from experimental value (2.0×10^{-4} mbar^{-1} s^{-1})[12] is probably due to the ignorance of methylation reactions that contributed by CH_3OCH_3 which is produced by methanol dehydration.

Table S3 Enthalpy barriers and rate constants for methylation of ethene by methanol at 623 K.

Ethene methylation by CH_3OH	$\Delta H^{\ddagger}$, kJ/mol	k, mbar^{-1} s^{-1}
Exp.[12]	104	2.0×10^{-4}
Harmonic, van Speybroeck[14]	94	1.3×10^{-4}
Harmonic, Svelle[13]	104	7.2×10^{-6}
Harmonic-Hybrid[4]	113	4.8×10^{-9}
Anharmonic-Hybrid[4]	105	6.1×10^{-5}
This work	101	1.0×10^{-6}
ONIOM-cluster*	99	3.9×10^{-7}
Hybrid-PBC*	80	3.0×10^{-5}

Apart from this, as shown in Table S4, the apparent energy, enthalpy and Gibbs free energy barriers ($\Delta E_{app}^{\neq}$, $\Delta G_{app}^{\neq}$ and $\Delta H_{app}^{\neq}$) for ethene methylation by CH_3OH, CH_3OCH_3, Z-CH_3 and $Z^-\ldots(CH_3)_3O^+$ as well as the Gibbs free energy span ($\Delta G_{span}^{\neq}$) are also computed and compared among various tested models and methods at 323 and 623 K. It could be found that $\Delta G_{span}^{\neq}$ at ωB//B3 are quite similar to those obtained at ONIOM-cluster* and hybrid-PBC*, and the differences are within 7 kJ/mol. Moreover, PBE-D3 calculations on both cluster and periodic models underestimate the barriers, consistent with Sauer and coworkers' results[4]. Therefore, the employed computational methods over 68T cluster in this work are kinetically reliable.

As mentioned by reviewer, the low frequencies introduce errors to the entropies.[15] Herein, quasi-rigid-rotor harmonic oscillator (QRRHO) treatment proposed by Grimme[16] is tested to evaluate the error of low frequencies to the entropy correction by using Shermo software[17]. It is found that the difference of the rate-determining $\Delta G_{span}^{\neq}$ between RRHO and QRRHO approximation for ωB//B3, ωB//B3*, ONIOM-cluster* and ONIOM-periodic* are quite small and the maximum is 9 kJ/mol, which indicates that the RRHO approach in this work is reasonable.

Table S4 The calculated apparent energy, enthalpy and Gibbs free energy barriers ($\Delta E_{app}^{\neq}$, $\Delta G_{app}^{\neq}$ and $\Delta H_{app}^{\neq}$) for ethene methylation by CH_3OH, CH_3OCH_3, Z-CH_3 and $Z^-\cdots(CH_3)_3O^+$ as well as the Gibbs free energy span ($\Delta G_{span}^{\neq}$) at 323 and 623 K.

Energies (kJ/mol)		**wB//B3 (This work)**	wB//B3*	**ONIOM-cluster***	**Hybrid-PBC***	PBE-cluster*	PBE-PBC*
$\Delta E_{app}^{\neq}$ (CH_3OH)		**90**	90	**88**	**73**	54	66
$\Delta E_{app}^{\neq}$ (CH_3OCH_3)		**86**	86	**88**	**81**	50	72
$\Delta E_{app}^{\neq}$ (Z-CH_3)		**67**	67	**64**	**56**	23	35
$\Delta E_{app}^{\neq}$ ($Z^-\cdots(CH_3)_3O^+$)		**40**	40	**57**	**56**	3	26
323 K	$\Delta H_{app}^{\neq}$ (CH_3OH)	**96**	96	**94**	**77**	60	70
	$\Delta H_{app}^{\neq}$ (CH_3OCH_3)	**93**	93	**94**	**88**	56	79
	$\Delta H_{app}^{\neq}$ (Z-CH_3)	**67**	67	**65**	**51**	25	30
	$\Delta H_{app}^{\neq}$ ($Z^-\cdots(CH_3)_3O^+$)	**39**	39	**55**	**52**	2	21
623 K	$\Delta H_{app}^{\neq}$ (CH_3OH)	**101**	101	**99**	**80**	65	72
	$\Delta H_{app}^{\neq}$ (CH_3OCH_3)	**97**	97	**98**	**92**	60	83
	$\Delta H_{app}^{\neq}$ (Z-CH_3)	**70**	70	**71**	**50**	31	28
	$\Delta H_{app}^{\neq}$ ($Z^-\cdots(CH_3)_3O^+$)	**43**	43	**59**	**53**	5	22
323 K	$\Delta G_{app}^{\neq}$ (CH_3OH)	**144**	146	**145**	**128**	111	121
	$\Delta G_{app}^{\neq}$ (CH_3OCH_3)	**143**	144	**144**	**134**	106	125
	$\Delta G_{app}^{\neq}$ (Z-CH_3)	**112**	116	**112**	**113**	72	91
	$\Delta G_{app}^{\neq}$ ($Z^-\cdots(CH_3)_3O^+$)	**90**	90	**108**	**103**	54	72
	$\Delta G_{span}^{\neq}$	**166**	157	**167**	**162**	147	137
623 K	$\Delta G_{app}^{\neq}$ (CH_3OH)	**187**	194	**194**	**175**	160	168
	$\Delta G_{app}^{\neq}$ (CH_3OCH_3)	**188**	192	**193**	**176**	155	166
	$\Delta G_{app}^{\neq}$ (Z-CH_3)	**153**	165	**158**	**172**	118	149
	$\Delta G_{app}^{\neq}$ ($Z^-\cdots(CH_3)_3O^+$)	**137**	138	**157**	**150**	103	119
	$\Delta G_{span}^{\neq}$	**179**	179	**174**	**172**	172	149

wB//B3: ωB97X-D/6-311+G(2df,2p)//B3LYP/6-311G(d,p) over 68T cluster; ωB//B3*: ωB//B3 with QRRHO approximation; ONIOM-cluster*: ONIOM(DLPNO-CCSD(T)/def2-TZVP (12T): PBE-D3/def2-TZVP) over 68T cluster with QRRHO approximation; Hybrid-PBC*: hybrid(ωB97X-D/6-311+G(2df,2p)//B3LYP/6-311G(d,p) (68T): PBE-D3) over periodic model with QRRHO approximation; PBE-cluster*: PBE-D3/6-311G(d,p) over 68T cluster with QRRHO approximation; PBE-PBC*: PBE-D3 calculations with QRRHO approximation over periodic model.

(3) Microkinetic modeling:

Thirdly, in order to test the sensitivity of the microkinetic results with respect to the input DFT data, especially entropies, the microkinetic modeling was carried out on the basis of DFT data obtained by ONIOM-cluster* and Hybrid-PBC*. As listed in Tables S5 and S6, on the one hand, methylation rates by these four types of methyl donors are qualitatively same and decreases in the order of Z-CH_3 > Z^-…$(CH_3)_3O^+$ > CH_3OCH_3 > CH_3OH; on the other hand, the calculated propene production rates are very close and accord well with the experimental results under different condition.[12, 18, 19] All these suggest that our microkinetic modeling analyses are qualitatively reliable and not much sensitive to the DFT results calculated by cluster or periodic models.

Table S5 Methylation rates of various methyl donors [mol·mol$(H^+)^{-1}$·h^{-1})] at 623 K and 1 bar (50 mbar ethene, 50 mbar CH_3OCH_3)

	CH_3OH	$(CH_3)_2O$	Z-CH_3	Z^-…$(CH_3)_3O^+$
this work	2.45×10^{-6}	5.99×10^{-2}	2.72×10^{2}	2.67×10^{0}
ONIOM-cluster*	2.83×10^{-6}	3.39×10^{-2}	4.38×10^{2}	1.69×10^{-1}
Hybrid-PBC*	3.46×10^{-7}	1.26×10^{-2}	9.20×10^{0}	1.37×10^{-1}

Table S6 Propene production rate [mol(propene) mol$(H^+)^{-1}$·h^{-1}]

	Exp.	This work	ONIOM-cluster*	Hybrid-PBC*
370 K, C_2H_4/CH_3OCH_3 = 5 mbar/210-520 mbar	3×10^{-4}	1×10^{-4}	2×10^{-5}	2×10^{-5}
623K, C_2H_4/CH_3OH = 50 mbar/50 mbar	35	6	14	8
623K, $C_2H_4/CH_3OH/CH_3OCH_3/H_2O$ = 50 mbar/16.7 mbar/16.7 mbar/16.7 mbar	/	31	70	9

Therefore, the calculations at ωB//B3 (ωB97X-D/6-311+G(2df,2p)//B3LYP/6-311G(d,p)) level of theory with 5T-relaxed 68T cluster including RRHO approximation are reasonable and reliable.

S2. Methylation of ethene

S2.1 CH_3OH and CH_3OCH_3 *via* the concerted mechanism

With respect to the concerted mechanism, CH_3OH or CH_3OCH_3 molecule first forms an end-on physisorption complex with the Brønsted acid site. Then, the adsorbed CH_3OH or CH_3OCH_3 methylates co-adsorbed alkene or aromatic species. Then, the C–O bond in CH_3OH or CH_3OCH_3 molecule is significantly prolonged, causing methyl cation in CH_3OH or CH_3OCH_3 electrophilic attack the double bond of alkene. Simultaneously, the proton transfer from acidic site to adsorbed CH_3OH or CH_3OCH_3 with H_2O or CH_3OH generated. The methyl group is transformed into an inverted umbrella-like configuration through typical S_N2 mechanism.[20] For the stepwise mechanism, Z–CH_3 is first formed. Then, it attacks unsaturated alkenes or aromatics, leading to the crack of C–O bond of Z–CH_3 and the simultaneous methylation of the alkenes to form carbenium ions through an umbrella-like inversion (also the S_N2 mechanism).

Table S7 Computed intrinsic and apparent Gibbs free energy barriers ($\Delta G_{int}^{\neq}$ and $\Delta G_{app}^{\neq}$, kJ/mol) as well as the Gibbs free energy span ($\Delta G_{span}^{\neq}$, kJ/mol) for the formation of CH_3OCH_3, Z–CH_3 and $Z^{-}\cdots(CH_3)_3O^{+}$ during methanol dehydration process over H-ZSM-5 at 323 and 623 K.

CH_3OCH_3 formation	373 K			623 K		
	$\Delta G_{int}^{\neq}$	$\Delta G_{app}^{\neq}$	$\Delta G_{span}^{\neq}$	$\Delta G_{int}^{\neq}$	$\Delta G_{app}^{\neq}$	$\Delta G_{span}^{\neq}$
via $2CH_3OH$	123	117	164	130	160	176
Z–CH_3 formation	373 K			623 K		
	$\Delta G_{int}^{\neq}$	$\Delta G_{app}^{\neq}$	$\Delta G_{span}^{\neq}$	$\Delta G_{int}^{\neq}$	$\Delta G_{app}^{\neq}$	$\Delta G_{span}^{\neq}$
via **CH_3OCH_3**	**106**	**178**	**191**	**105**	**164**	**164**
via CH_3OH	168	168	215	165	165	181
via $2CH_3OH$	150	127	173	150	165	181
$Z^{-}\cdots(CH_3)_3O^{+}$ formation	373 K			623 K		
	$\Delta G_{int}^{\neq}$	$\Delta G_{app}^{\neq}$	$\Delta G_{span}^{\neq}$	$\Delta G_{int}^{\neq}$	$\Delta G_{app}^{\neq}$	$\Delta G_{span}^{\neq}$
via CH_3OH + CH_3OCH_3	106	109	142	110	146	152
via $2CH_3OCH_3$	**125**	**112**	**125**	136	142	142
via Z–CH_3 + CH_3OCH_3	84	73	151	**93**	**109**	**125**

S2.2 Gibbs free energy profiles for methylation of ethene

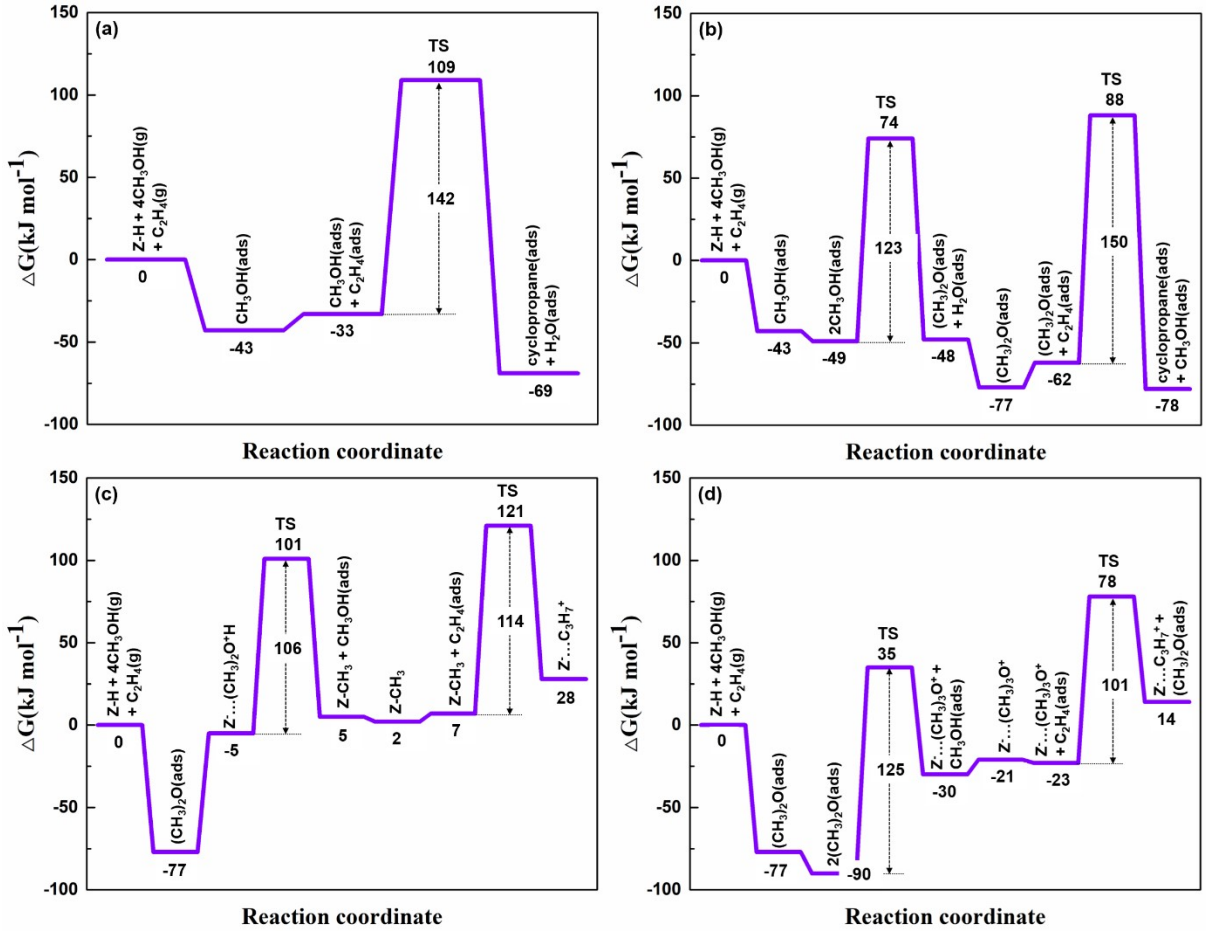


Fig. S2 Gibbs free energy profiles for methylation of ethene on H-ZSM-5 at 373 K with (a) CH_3OH, (b) CH_3OCH_3, (c) Z-CH_3, and (d) $(CH_3)_3O^+$ by taking [ZH + 4CH_3OH(g) + C_2H_4(g)]) as the reference state.

S2.3 Structure of $Z^-\cdots(CH_3)_3O^+$

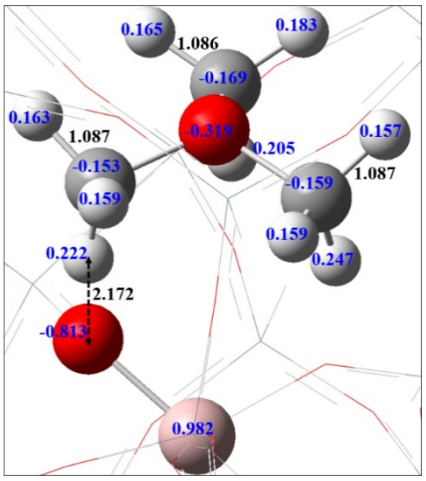
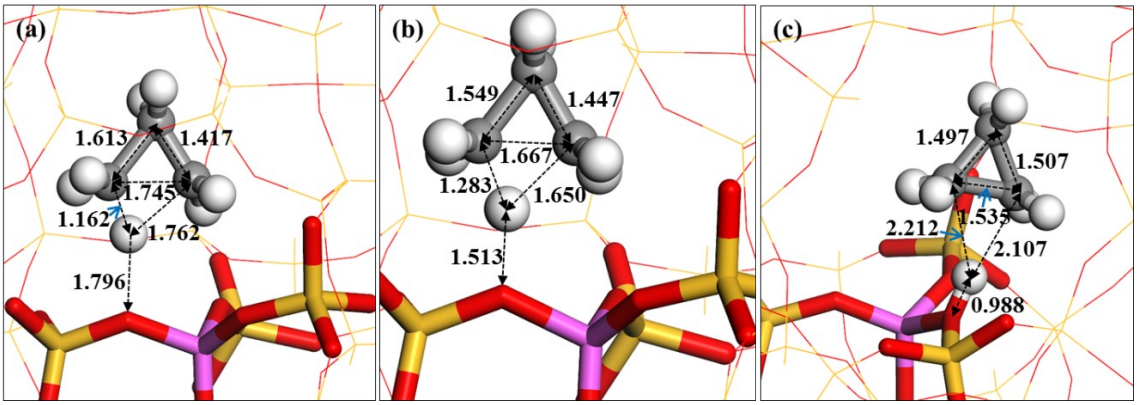


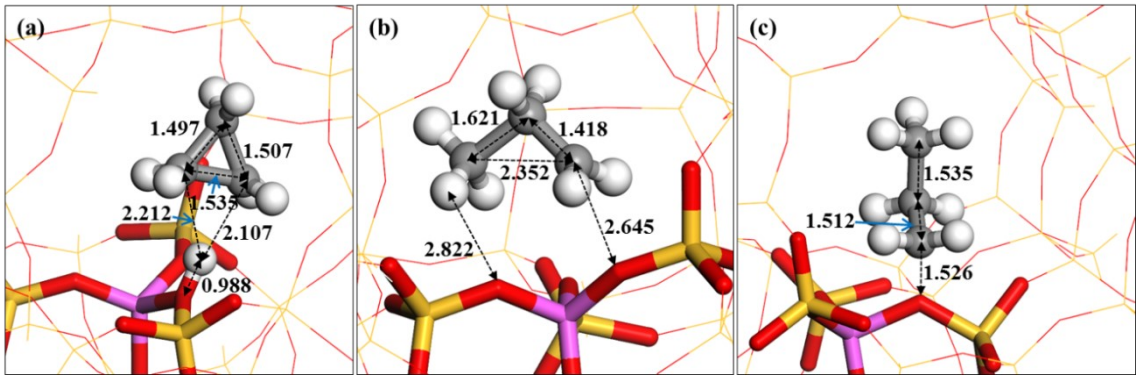
Fig. S3 The structure of $Z^-\cdots(CH_3)_3O^+$ in zeolite with the Mulliken charge in blue and the bonding distances

in black (Å). The color is schemed as follows: red for O, pink for Al, grey for C and white for H.

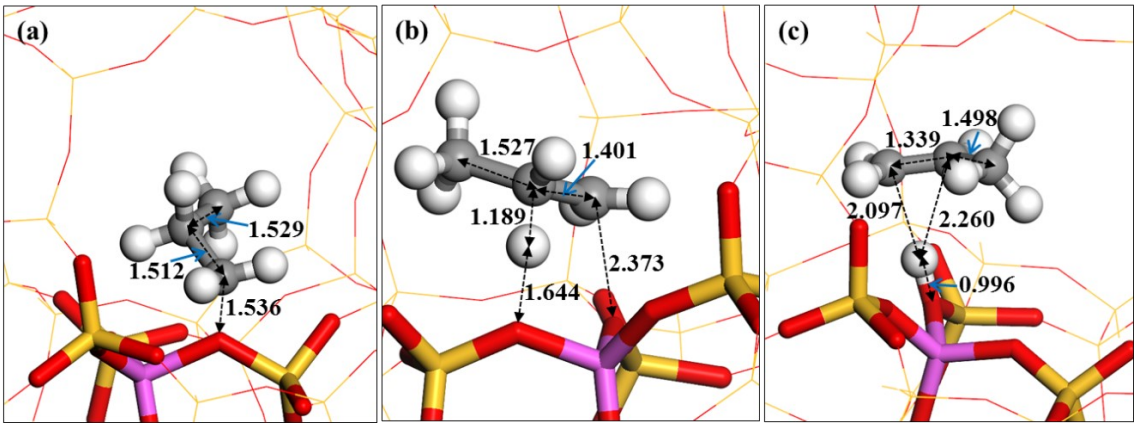
S3. $C_3H_7^+$ conversion



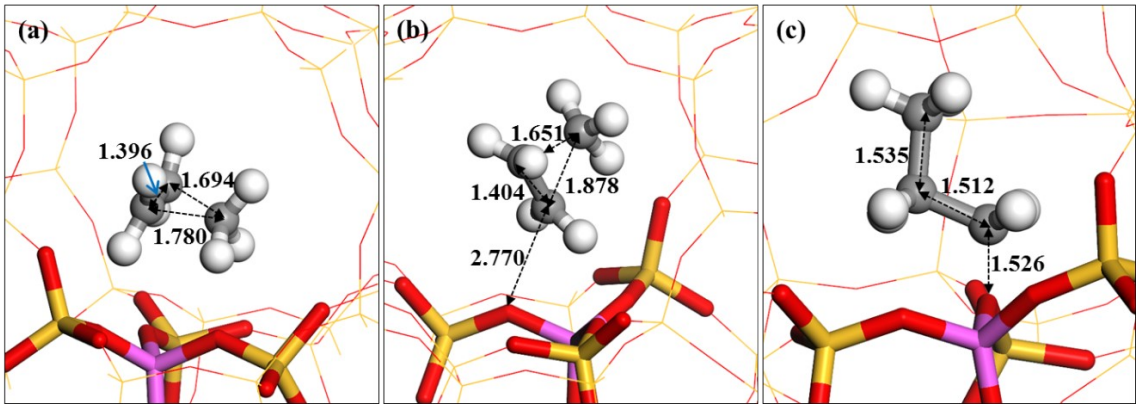
Cyclopropane formation: (a) initial state (IS, [Z$^-$···$C_3H_7^+$]), (b) transition state (TS, [Z···H···C_3H_7]‡) and (c) final state (FS, [ZH + cyclopropane])



Formation of Z-$CH_2CH_2CH_3$ from cyclopropane: (a) initial state (IS, [ZH + cyclopropane]), (b) transition state (TS, [Z···$CH_2CH_2CH_3$]‡) and (c) final state (FS, [Z–$CH_2CH_2CH_3$])



Formation of CH_2=CH-CH_3: (a) initial state (IS, [Z–$CH_2CH_2CH_3$]), (b) transition state (TS, [Z···H···$CHCH_2(CH_3)$]‡) and (c) final state (FS, [ZH + CH_2=CH–CH_3])



Formation of Z–$CH_2CH_2CH_3$ from $Z^-\cdots C_3H_7^+$: (a) initial state (IS, [$Z^-\cdots C_3H_7^+$]), (b) transition state (TS, [Z···$CH_2CH_2CH_3$]‡) and (c) final state (FS, [Z–$CH_2CH_2CH_3$])

Fig. S4 Optimized structures for the conversion of $C_3H_7^+$ species over H-ZSM-5 (The bonding distances are in Å unit and the color is schemed as follows: red, yellow, pink, grey and white for O, Si, Al, C and H, respectively).

Although Z–$CH(CH_3)_2$ is slightly more stable than Z–$CH_2CH_2CH_3$, the stability of corresponding cations are largely different. *Iso*-propyl ion ($CH_3CH^+CH_3$) shows much higher

stability than *n*-propyl ion ($CH_3CH_2CH_2^+$), due to the hyperconjugation of C–H bond.[21] The poorly stable secondary carbenium ions can be considered as transient species despite of the presence of a significant amount during the reaction process.[22-24] The net charge of +1 of *iso*-propyl cation is delocalized over one carbon atom and six hydrogen atoms, and the C–C bond distance is as short as 1.440 Å (Fig. S4). Beckham and coworkers reported that the amount of *iso*-propyl cations is negligible inside zeolites at high temperatures.[25]

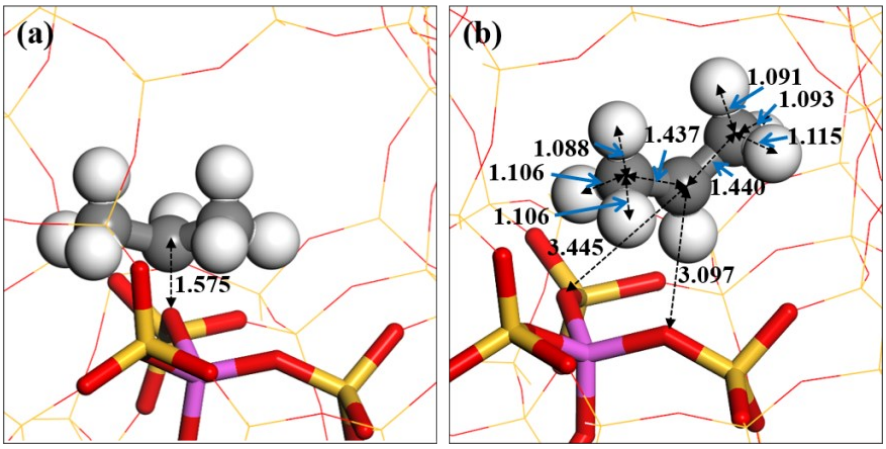


Fig. S5 Optimized structures of (a) *iso*-propoxy species (Z-$CH(CH_3)_2$) and (b) *iso*-propyl ion ($CH_3CH^+CH_3$) over H-ZSM-5 zeolite (Atom coloring: yellow (Si), red (O), white (H), pink (Al), and grey (C).; the bonding distance unit is angstroms (Å)).

Fig. S6 depicts the optimized geometrical parameters and structures of TS for deprotonation of Z–$CH_2CH_2CH_3$ and Z–$CH(CH_3)_2$. Firstly, the C–O bond of Z–$CH(CH_3)_2$ is weaker than that of Z–$CH_2CH_2CH_3$ indicated by the C–O bond distance (1.578 vs. 1.526 Å), similar to *i*-butoxide and *n*-butoxide[26]. Secondly, the proton in the TS of *iso*-propyl ion deprotonation is stabilized by forming a three-membered ring (3-MR) with two carbon atoms, whereas this 3-MR ring is not formed in the TS of *n*-propyl deprotonation. Thirdly, Z–$CH(CH_3)_2$ deprotonates through a secondary carbenium ion TS, while Z–$CH_2CH_2CH_3$ does *via* a primary carbenium

ion TS. Fourthly, the six hydrogen atoms of *iso*-propyl ion make its deprotonation probability be three times as large as that of *n*-propyl ion. If their concentrations are the same, the deprotonation rate of *iso*-propyl ions would be 2.5×10^4 times of that of *n*-propyl ions. Thus, the above results suggest that Z–$CH(CH_3)_2$ is not only thermodynamically more favored, but also its further deprotonation into propene is kinetically far more prominent, compared to Z–$CH_2CH_2CH_3$.

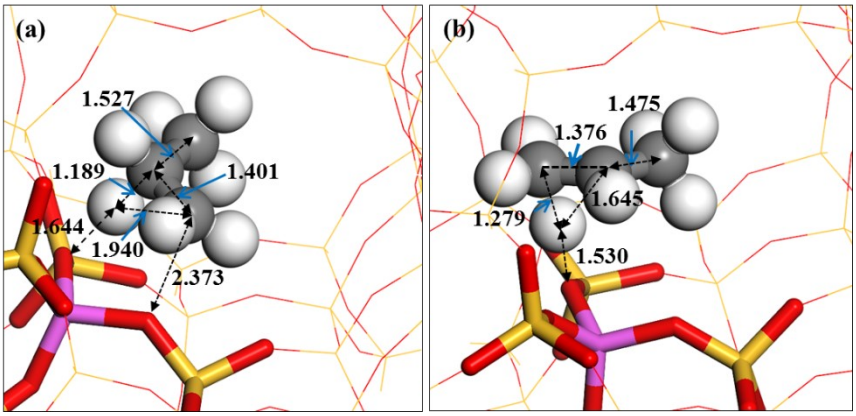


Fig. S6 Optimized structures for deprotonation TS of (a) *n*-propyl and (b) *iso*-propyl ions over H-ZSM-5 (The bonding distances are in Å unit and the color is schemed as follows: red, yellow, pink, grey and white for O, Si, Al, C and H, respectively).

Table S8 Computed intrinsic Gibbs free energy barriers ($\Delta G_{int}^{\neq}$, kJ/mol) for the isomerization of Z–$CH(CH_3)_2$ to Z–$CH_2CH_2CH_3$ and the reversal reaction at 623 K over H-ZSM-5 optimized at ONIOM2[ωB97XD/6-31+G(d,p):ωB97XD/3-21G] and B3LYP/6-311G(d,p) levels.

Isomerization reaction	ONIOM2 [ωB97XD/6-31+G(d,p): ωB97XD/3-21G]	B3LYP/6-311G(d,p)
Z-$CH_2CH_2CH_3$ → Z-$CH(CH_3)_2$	95	96
Z-$CH(CH_3)_2$ → Z-$CH_2CH_2CH_3$	86	94

S4. Microkinetic model

To avoid zero proton coverage, an arbitrary proton source was introduced in the model.[9, 27] Based on a list of electronic energies and frequencies obtained by DFT-D calculations, CatMAP computed the free energies of all intermediate species and transition states, from which rate coefficients of all reaction and adsorption/desorption steps were calculated. With a set of coupled differential equations obtained from expressions (S1 – S39), the coverages of all species at steady-state conditions were determined with the sum of active sites assumed to be 1. The concentration of CH_3OCH_3 and ethene fixed at 0.05/0.5/0.95 and 0.05, respectively, corresponds to a partial pressure of 50/500/950 and 50 mbar for the cofeeding of CH_3OCH_3 and ethene at atmospheric pressure (1 bar), which approximately mimics the experimental feed composition consisting of reactants and inert carrier gas He at very low conversion level.[9] The partial pressures are defined as the concentration times the total pressure and total and partial pressures change simultaneously with the concentration fixed. Our model did not consider the inert carrier gas.

H* represents a Brønsted acid site (BAS) of the zeolite and X.H* signifies molecule X directly interacting with the BAS. The elementary reaction steps equations are listed below.

$CH_3OH(g) + H^* \leftrightarrow CH_3OH.H^*$, (S1)

$CH_3OH.H^* \leftrightarrow CH_3\text{-}OH\text{-}H^* \leftrightarrow H_2O.CH_3^*$, (S2)

$H_2O.CH_3^* \leftrightarrow CH_3^* + H_2O(g)$, (S3)

$CH_3OH(g) + CH_3OH.H^* \leftrightarrow CH_3OH.CH_3OH.H^*$, (S4)

$CH_3OH.CH_3OH.H^* \leftrightarrow [CH_3OH\text{-}CH_3OH\text{-}H^*]^{\ddagger} \leftrightarrow (CH_3)_2O.H_2O.H^*$, (S5)

$(CH_3)_2O.H_2O.H^* \leftrightarrow (CH_3)_2O.H^* + H_2O(g)$, (S6)

1 $(CH_3)_2O.H^* \leftrightarrow H^* + (CH_3)_2O(g)$, (S7)

2 $(CH_3)_2O.H^* \leftrightarrow CH_3O(H)CH_3^*$, (S8)

3 $CH_3O(H)CH_3^* \leftrightarrow [CH_3O(H)\text{-}CH_3^*]^{\ddagger} \leftrightarrow CH_3OH.CH_3^*$, (S9)

4 $CH_3OH.CH_3^* \leftrightarrow CH_3^* + CH_3OH(g)$, (S10)

5 $CH_3OH(g) + CH_3OH.H^* \leftrightarrow CH_3OH.HOCH_3.H^*$, (S11)

6 $CH_3OH.HOCH_3.H^* \leftrightarrow [CH_3OH\text{-}HOCH_3\text{-}H^*]^{\ddagger} \leftrightarrow CH_3OH.H_2O.CH_3^*$, (S12)

7 $CH_3OH.H_2O.CH_3^* \leftrightarrow CH_3^* + CH_3OH(g) + H_2O(g)$, (S13)

8 $(CH_3)_2O(g) + CH_3OH.H^* \leftrightarrow (CH_3)_2O.CH_3OH.H^*$, (S14)

9 $(CH_3)_2O.CH_3OH.H^* \leftrightarrow (CH_3)_2O\text{-}CH_3\text{-}OH\text{-}H^* \leftrightarrow H_2O.(CH_3)_3O^*$, (S15)

10 $H_2O.(CH_3)_3O^* \leftrightarrow H_2O\ (g) + (CH_3)_3O^*$, (S16)

11 $(CH_3)_2O(g) + (CH_3)_2O.H^* \leftrightarrow (CH_3)_2O.(CH_3)_2O.H^*$, (S17)

12 $(CH_3)_2O.(CH_3)_2O.H^* \leftrightarrow [(CH_3)_2O\text{-}(CH_3)_2O\text{-}H^*]^{\ddagger} \leftrightarrow CH_3OH.(CH_3)_3O^*$, (S18)

13 $CH_3OH.(CH_3)_3O^* \leftrightarrow CH_3OH(g) + (CH_3)_3O^*$, (S19)

14 $(CH_3)_2O(g) + CH_3^* \leftrightarrow (CH_3)_2O.CH_3^*$, (S20)

15 $(CH_3)_2O.CH_3^* \leftrightarrow [(CH_3)_2O\text{-}CH_3^*]^{\ddagger} \leftrightarrow (CH_3)_3O^*$, (S21)

16 $C_2H_4(g) + CH_3OH.H^* \leftrightarrow C_2H_4.CH_3OH.H^*$, (S22)

17 $C_2H_4.CH_3OH.H^* \leftrightarrow [C_2H_4\text{-}CH_3OH\text{-}H^*]^{\ddagger} \leftrightarrow C_3H_7.H_2O^*$, (S23)

18 $C_3H_7.H_2O^* \leftrightarrow C_3H_7^* + H_2O(g)$, (S24)

19 $C_2H_4(g) + (CH_3)_2O.H^* \leftrightarrow C_2H_4.(CH_3)_2O.H^*$, (S25)

20 $C_2H_4.(CH_3)_2O.H^* \leftrightarrow [C_2H_4\text{-}(CH_3)_2O\text{-}H^*]^{\ddagger} \leftrightarrow CH_3OH.C_3H_7^*$, (S26)

21 $CH_3OH.C_3H_7^* \leftrightarrow C_3H_7^* + CH_3OH(g)$, (S27)

22 $C_2H_4(g) + CH_3^* \leftrightarrow C_2H_4.CH_3^*$, (S28)

$C_2H_4.CH_3^* \leftrightarrow [C_2H_4\text{-}CH_3^*]^{\ddagger} \leftrightarrow C_3H_7^*$, (S29)

$C_2H_4(g) + (CH_3)_3O^* \leftrightarrow C_2H_4.(CH_3)_3O^*$, (S30)

$C_2H_4.(CH_3)_3O^* \leftrightarrow [C_2H_4\text{-}(CH_3)_3O^*]^{\ddagger} \leftrightarrow (CH_3)_2O.C_3H_7^*$, (S31)

$(CH_3)_2O.C_3H_7^* \leftrightarrow C_3H_7^* + (CH_3)_2O(g)$, (S32)

$C_3H_7^* \leftrightarrow [CH_2C(H_2)\text{-}CH_3^*]^{\ddagger} \leftrightarrow CH_3CH_2CH_2^*$ (S33)

$CH_3CH_2CH_2^* \leftrightarrow [CH_3C(H)\text{-}H\text{-}CH_2^*]^{\ddagger} \leftrightarrow (CH_3)_2CH^*$, (S34)

$(CH_3)_2CH^* \leftrightarrow CH_3CHCH_3^*$, (S35)

$CH_3CHCH_3^* \leftrightarrow [CH_3CHC(H_2)\text{-}H^*]^{\ddagger} \leftrightarrow CH_3CHCH_2.H^*$, (S36)

$CH_3CHCH_2.H^* \leftrightarrow H^* + CH_3CHCH_2(g)$, (S37)

$H_2(g) + 2^* \rightarrow 2H^*$ (S38)

Reaction (38) illustrates the source of protons. To avoid the model solution of zero proton coverage, the electronic chemisorption energy of H at the oxygen of the acid site was set to 2.0 eV by setting the reference energy of the zeolite accordingly, as handled by Brogaard and De Wispelaere *et al.*[9, 27] Even though this is an arbitrary selection, some cross checks were performed to prove that it doesn't have an effect on the outcome of the microkinetic model. The concentration of hydrogen gas was set to 10^{-5}, but varying different values did not change the results.[9, 27] Steps denoted with a ‡ sign are considered as activated, all other steps are barrierless. Reactions S1 to S38 give rise to a set of rate equations S39-S76, which in turn result in a set of coupled differential equations S77-S105. It should be noted that the sum of all coverages of the adsorbed intermediate equals 1 (S106).

$$r_1 = k_1^f\, p(CH_3OH)\theta(H) - k_1^r \theta(CH_3OH.H) \quad \text{(S39)}$$

$$r_2 = k_2^f \theta(CH_3OH.H) - k_2^r \theta(H_2O.CH_3) \quad \text{(S40)}$$

1 $$r_3 = k_3^f \theta(H_2O.CH_3) - k_3^r \theta(CH_3)\, p(H_2O)$$ (S41)

2 $$r_4 = k_4^f \theta(CH_3OH.H)\, p(CH_3OH) - k_4^r \theta(CH_3OH.CH_3OH.H)$$ (S42)

3 $$r_5 = k_5^f \theta(CH_3OH.\ CH_3OH.\ H) - k_5^r \theta[(CH_3)_2O.\ H_2O.\ H)]$$ (S43)

4 $$r_6 = k_6^f \theta[(CH_3)_2O.\ H_2O.\ H)] - k_6^r \theta[(CH_3)_2O.\ H)]\, p(H_2O)$$ (S44)

5 $$r_7 = k_7^f \theta[(CH_3)_2O.\ H] - k_7^r \theta(H)\, p[(CH_3)_2O]$$ (S45)

6 $$r_8 = k_8^f \theta[(CH_3)_2O.\ H] - k_8^r \theta[CH_3O(H)CH_3]$$ (S46)

7 $$r_9 = k_9^f \theta[CH_3O(H)CH_3] - k_9^r \theta(CH_3OH.\ CH_3)$$ (S47)

8 $$r_{10} = k_{10}^f \theta(CH_3OH.\ CH_3) - k_{10}^r \theta(CH_3)\, p(CH_3OH)$$ (S48)

9 $$r_{11} = k_{11}^f \theta(CH_3OH.\ H)\, p(CH_3OH) - k_{11}^r \theta(CH_3OH.\ HOCH_3.\ H)$$ (S49)

10 $$r_{12} = k_{12}^f \theta(CH_3OH.\ HOCH_3.\ H) - k_{12}^r \theta(CH_3OH.\ H_2O.\ CH_3)$$ (S50)

11 $$r_{13} = k_{13}^f \theta(CH_3OH.\ H_2O.\ CH_3) - k_{13}^r \theta(CH_3)\, p(CH_3OH)\, p(H_2O)$$ (S51)

12 $$r_{14} = k_{14}^f \theta(CH_3OH.\ H)\, p[(CH_3)_2O] - k_{14}^r \theta[(CH_3)_2O.CH_3OH.H]$$ (S52)

13 $$r_{15} = k_{15}^f \theta[(CH_3)_2O.CH_3OH.H] - k_{15}^r \theta[H_2O.(CH_3)_3O]$$ (S53)

14 $$r_{16} = k_{16}^f \theta[H_2O.(CH_3)_3O] - k_{16}^r \theta[(CH_3)_3O]\, p(H_2O)$$ (S54)

15 $$r_{17} = k_{17}^f \theta[(CH_3)_2O.\ H]\, p[(CH_3)_2O] - k_{17}^r \theta[(CH_3)_2O.\ (CH_3)_2O.\ H]$$ (S55)

16 $$r_{18} = k_{18}^f \theta[(CH_3)_2O.\ (CH_3)_2O.\ H] - k_{18}^r \theta[CH_3OH.\ (CH_3)_3O]$$ (S56)

17 $$r_{19} = k_{19}^f \theta[CH_3OH.\ (CH_3)_3O] - k_{19}^r \theta[(CH_3)_3O]\, p(CH_3OH)$$ (S57)

18 $$r_{20} = k_{20}^f \theta(CH_3)\, p[(CH_3)_2O] - k_{20}^r \theta[(CH_3)_2O.\ CH_3]$$ (S58)

19 $$r_{21} = k_{21}^f \theta[(CH_3)_2O.\ CH_3] - k_{21}^r \theta[(CH_3)_3O]$$ (S59)

20 $$r_{22} = k_{22}^f \theta(CH_3OH.\ H)\, p(C_2H_4) - k_{22}^r \theta(C_2H_4.\ CH_3OH.\ H)$$ (S60)

21 $$r_{23} = k_{23}^f \theta(C_2H_4.\ CH_3OH.\ H) - k_{23}^r \theta(C_3H_7.\ H_2O)$$ (S61)

22 $$r_{24} = k_{24}^f \theta(C_3H_7.\ H_2O) - k_{24}^r \theta(C_3H_7)\, p(H_2O)$$ (S62)

$$r_{25} = k_{25}^{f}\theta[(CH_3)_2O.H]p(C_2H_4) - k_{25}^{r}\theta[C_2H_4.(CH_3)_2O.H] \quad \text{(S63)}$$

$$r_{26} = k_{26}^{f}\theta[C_2H_4.(CH_3)_2O.H] - k_{26}^{r}\theta(CH_3OH.C_3H_7) \quad \text{(S64)}$$

$$r_{27} = k_{27}^{f}\theta(CH_3OH.C_3H_7) - k_{27}^{r}\theta(C_3H_7)p(CH_3OH) \quad \text{(S65)}$$

$$r_{28} = k_{28}^{f}\theta(CH_3)p(C_2H_4) - k_{28}^{r}\theta(C_2H_4.CH_3) \quad \text{(S66)}$$

$$r_{29} = k_{29}^{f}\theta(C_2H_4.CH_3) - k_{29}^{r}\theta(C_3H_7) \quad \text{(S67)}$$

$$r_{30} = k_{30}^{f}\theta[(CH_3)_3O]p(C_2H_4) - k_{30}^{r}\theta[C_2H_4.(CH_3)_3O] \quad \text{(S68)}$$

$$r_{31} = k_{31}^{f}\theta[C_2H_4.(CH_3)_3O] - k_{31}^{r}\theta[(CH_3)_2O.C_3H_7] \quad \text{(S69)}$$

$$r_{32} = k_{32}^{f}\theta[(CH_3)_2O.C_3H_7] - k_{32}^{r}\theta(C_3H_7)p[(CH_3)_2O] \quad \text{(S70)}$$

$$r_{33} = k_{33}^{f}\theta(C_3H_7) - k_{33}^{r}\theta(CH_3CH_2CH_2) \quad \text{(S71)}$$

$$r_{34} = k_{34}^{f}\theta(CH_3CH_2CH_2) - k_{34}^{r}\theta[(CH_3)_2CH] \quad \text{(S72)}$$

$$r_{35} = k_{35}^{f}\theta[(CH_3)_2CH] - k_{35}^{r}\theta(CH_3CHCH_3) \quad \text{(S73)}$$

$$r_{36} = k_{36}^{f}\theta(CH_3CHCH_3) - k_{36}^{r}\theta(CH_3CHCH_2.H) \quad \text{(S74)}$$

$$r_{37} = k_{37}^{f}\theta(CH_3CHCH_2.H) - k_{37}^{r}\theta(H)p(CH_3CHCH_2) \quad \text{(S75)}$$

$$r_{38} = k_{38}^{f}p(H_2)\theta(*)^2 - k_{38}^{r}\theta(H)^2 \quad \text{(S76)}$$

$$\frac{d}{dt}\theta(H) = r_7 + 2r_{38} + r_{37} - r_1 \quad \text{(S77)}$$

$$\frac{d}{dt}\theta(CH_3OH.H) = r_1 - r_2 - r_4 - r_{11} - r_{14} - r_{22} \quad \text{(S78)}$$

$$\frac{d}{dt}\theta(CH_3OH.CH_3OH.H) = r_4 - r_5 \quad \text{(S79)}$$

$$\frac{d}{dt}\theta[(CH_3)_2O.H_2O.H] = r_5 - r_6 \quad \text{(S80)}$$

$$\frac{d}{dt}\theta[(CH_3)_2O.H] = r_6 - r_7 - r_8 - r_{17} - r_{25} \quad \text{(S81)}$$

$$\frac{d}{dt}\theta[CH_3O(H)CH_3] = r_8 - r_9 \quad \text{(S82)}$$

$$\frac{d}{dt}\theta(CH_3OH.CH_3) = r_9 - r_{10} \quad \text{(S83)}$$

$$\frac{d}{dt}\theta(H_2O.CH_3) = r_2 - r_3 \quad \text{(S84)}$$

1 $$\frac{d}{dt}\theta(CH_3) = r_3 + r_{10} + r_{13} - r_{20} - r_{28}$$ (S85)

2 $$\frac{d}{dt}\theta(CH_3OH.\ HOCH_3.\ H) = r_{11} - r_{12}$$ (S86)

3 $$\frac{d}{dt}\theta(CH_3OH.\ H_2O.\ CH_3) = r_{12} - r_{13}$$ (S87)

4 $$\frac{d}{dt}\theta[(CH_3)_2O.\ (CH_3)_2O.\ H] = r_{17} - r_{18}$$ (S88)

5 $$\frac{d}{dt}\theta[CH_3OH.\ (CH_3)_3O] = r_{18} - r_{19}$$ (S89)

6 $$\frac{d}{dt}\theta[(CH_3)_2O.CH_3OH.H] = r_{14} - r_{15}$$ (S90)

7 $$\frac{d}{dt}\theta[\mathrm{H}_2O.(CH_3)_3O] = r_{15} - r_{16}$$ (S91)

8 $$\frac{d}{dt}\theta[(CH_3)_3O] = r_{16} + r_{19} + r_{21} - r_{30}$$ (S92)

9 $$\frac{d}{dt}\theta[(CH_3)_2O.\ CH_3] = r_{20} - r_{21}$$ (S93)

10 $$\frac{d}{dt}\theta(C_2H_4.\ CH_3OH.\ H) = r_{22} - r_{23}$$ (S94)

11 $$\frac{d}{dt}\theta(C_3H_7.\ H_2O) = r_{23} - r_{24}$$ (S95)

12 $$\frac{d}{dt}\theta(C_3H_7) = r_{24} + r_{27} + r_{29} + r_{32} - r_{33}$$ (S96)

13 $$\frac{d}{dt}\theta[C_2H_4.\ (CH_3)_2O.\ H] = r_{25} - r_{26}$$ (S97)

14 $$\frac{d}{dt}\theta(CH_3OH.\ C_3H_7) = r_{26} - r_{27}$$ (S98)

15 $$\frac{d}{dt}\theta(C_2H_4.\ CH_3) = r_{28} - r_{29}$$ (S99)

16 $$\frac{d}{dt}\theta[C_2H_4.\ (CH_3)_3O] = r_{30} - r_{31}$$ (S100)

17 $$\frac{d}{dt}\theta[(CH_3)_2O.\ C_3H_7] = r_{31} - r_{32}$$ (S101)

18 $$\frac{d}{dt}\theta(CH_3CH_2CH_2) = r_{33} - r_{34}$$ (S102)

19 $$\frac{d}{dt}\theta[(CH_3)_2CH] = r_{34} - r_{35}$$ (S103)

20 $$\frac{d}{dt}\theta(CH_3CHCH_3) = r_{35} - r_{36}$$ (S104)

21 $$\frac{d}{dt}\theta(CH_3CHCH_2.\ H) = r_{36} - r_{37}$$ (S105)

22 $\sum\theta(j)$=1, $\theta(j)$ is the coverage of the adsorbed intermediate j (S106)

S5. The stability of Z–CH_3 at high temperatures

Fig. S5 shows the formation energy $\Delta_r E$ ($\Delta_r G$, $\Delta_r H$ and $-T\Delta_r S$) of all the four types of methyl donors in the range of 298 – 723 K. Three gaseous methanol molecules and zeolite framework ($3CH_3OH$ (g) + ZH) are taken as the reference state to calculate the formation energies of other species by eqs. (S34) – (S37).

$ZH + 3CH_3OH\ (g) = ZH\cdots CH_3OH + 2CH_3OH\ (g)$;

$$\Delta_r E(ZH\cdots CH_3OH) = E(ZH\cdots CH_3OH) - [E(ZH) + E(CH_3OH, g)] \quad (S34)$$

$ZH + 3CH_3OH\ (g) = ZH\cdots CH_3OCH_3 + H_2O\ (g) + CH_3OH\ (g)$;

$$\Delta_r E(ZH\cdots CH_3OCH_3) = E(ZH\cdots CH_3OCH_3) + E(H_2O, g) - [E(ZH) + 2E(CH_3OH, g)] \quad (S35)$$

$ZH + 3CH_3OH\ (g) = Z\text{-}CH_3 + H_2O\ (g) + 2CH_3OH\ (g)$;

$$\Delta_r E(Z\text{-}CH_3) = E(Z\text{-}CH_3) + E(H_2O, g) - [E(ZH) + E(CH_3OH, g)] \quad (S36)$$

$ZH + 3CH_3OH\ (g) = Z^-\cdots(CH_3)_3O^+ + 2H_2O\ (g)$;

$$\Delta_r E(Z^-\cdots(CH_3)_3O^+) = E(Z^-\cdots(CH_3)_3O^+) + 2E(H_2O, g) - [E(ZH) + 3E(CH_3OH, g)] \quad (S37)$$

The formation Gibbs free energies of all the methyl donors are largely influenced by the reaction temperature except for Z–CH_3 (Fig. S5). In the temperature region from 298 to 723 K, the formation Gibbs free energies of $ZH\cdots CH_3OH$, $ZH\cdots CH_3OCH_3$ and $Z^-\cdots(CH_3)_3O^+$ species enhance by 63.6, 64.1 and 72.8 kJ/mol, respectively, whereas that of Z–CH_3 increases by only 4.1 kJ/mol. It was found that the entropy losses ($-T\Delta_r S$) were 59.6, 59.3, 62.3 and 2.1 kJ/mol, while the formation enthalpies were enlarged by only 4.0, 4.8, 10.6 and 2.0 kJ/mol for $ZH\cdots CH_3OH$, $ZH\cdots CH_3OCH_3$, $Z^-\cdots(CH_3)_3O^+$ and Z-CH_3 species, respectively. This shows that the significant increase of the formation Gibbs free energies mainly results from the entropy

losses, whereas the changes of the formation enthalpies are much less important. For Z-CH_3, the number of gas phase species keeps constant for its formation reaction resulting in little entropy loss with the temperature.

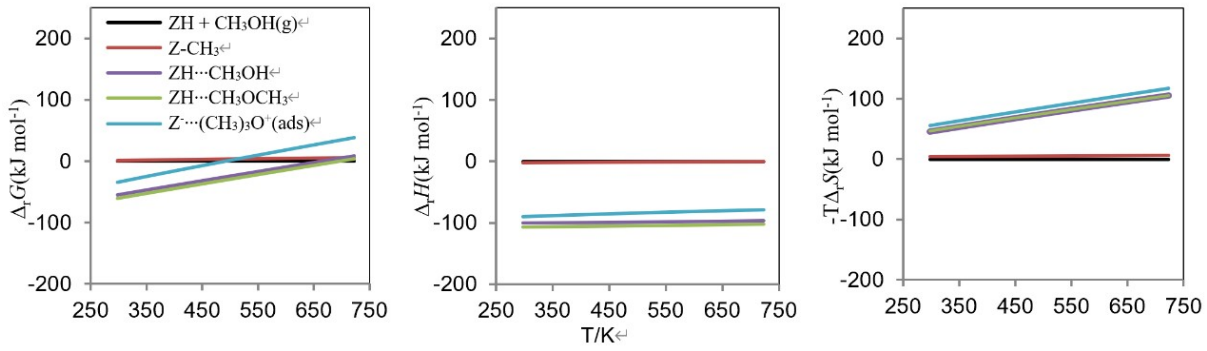


Fig. S7 Dependence of the formation energy $\Delta_r E$ ($\Delta_r G$, $\Delta_r H$ and $-T\Delta_r S$) of CH_3OH and its derived methyl donors from [Z-H + 4CH_3OH(g)] on the reaction temperature.

S6. Degree of rate control

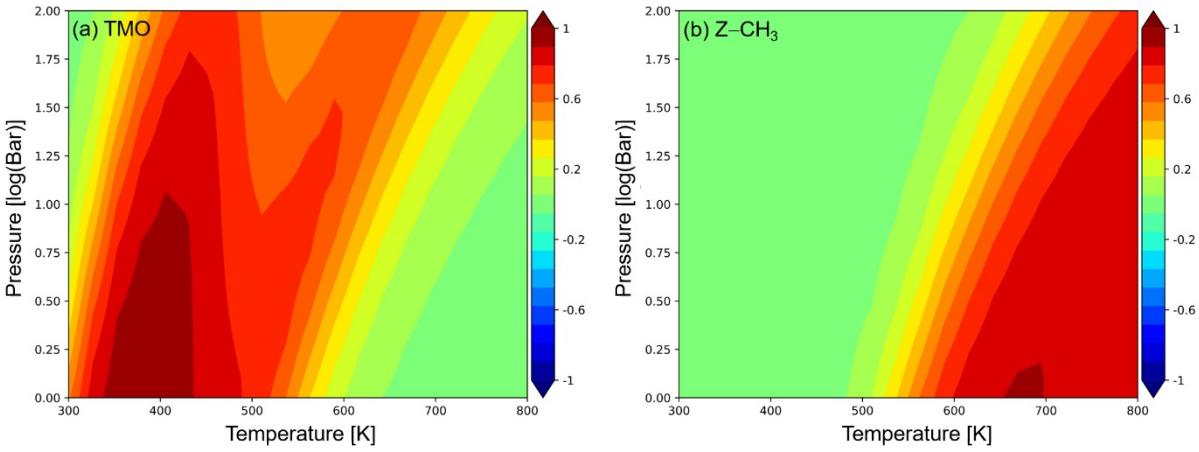


Fig. S8 DRC for propene formation *via* the transition state of methylation by (a) $Z^{-}\cdots(CH_3)_3O^{+}$and (b) Z-CH_3 (50 mbar ethene, 500 mbar CH_3OCH_3).

S7. Coverages

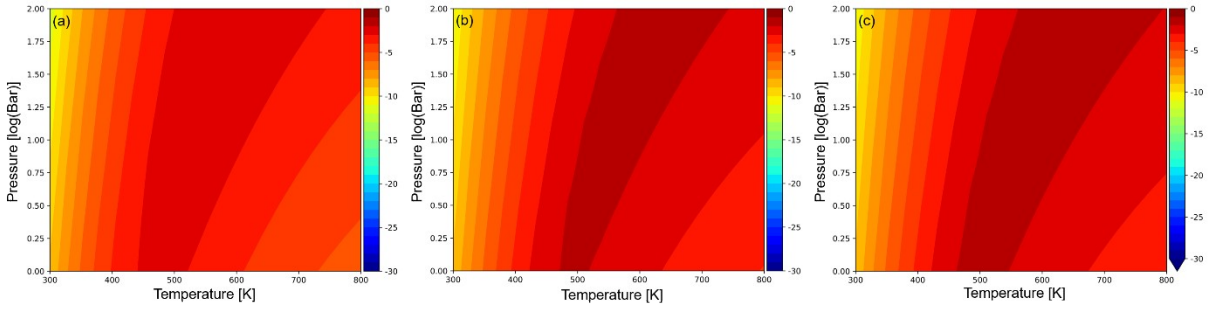


Fig. S9 Coverages of $Z^{-}\cdots(CH_3)_3O^{+}$ at the feed of (a) 50 mbar ethene and 50 mbar CH_3OCH_3 (b) 50 mbar ethene and 500 mbar CH_3OCH_3 and (c) 50 mbar ethene and 950 mbar CH_3OCH_3.

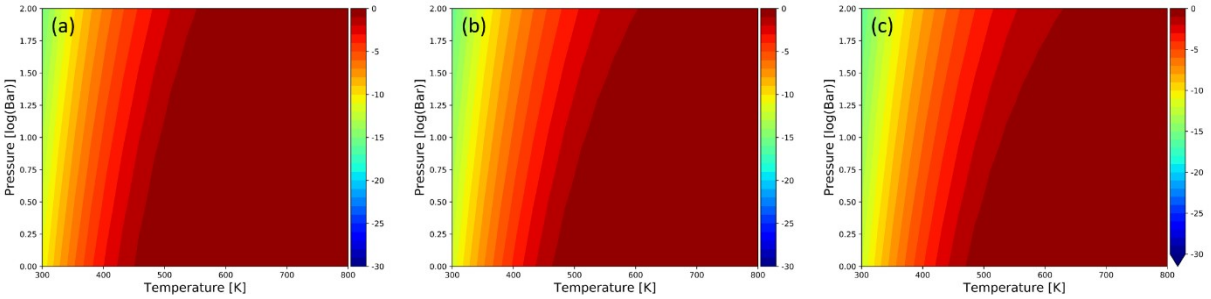


Fig. S10 Coverages of Z-CH_3 at the feed of (a) 50 mbar ethene and 50 mbar CH_3OCH_3 (b) 50 mbar ethene and 500 mbar CH_3OCH_3 and (c) 50 mbar ethene and 950 mbar CH_3OCH_3.

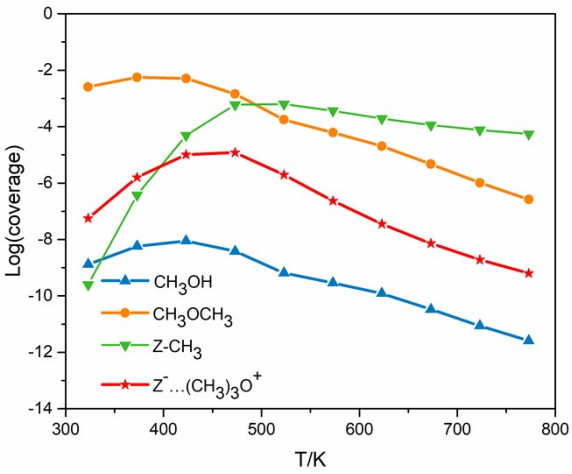


Fig. S11 Relationship between the coverages (log(coverage)) of co-adsorbed ethene and various methyl donors and reaction temperature with the feed of 50 mbar ethene and 50 mbar CH_3OCH_3.

S8. CH_3OH and ethene co-feeding

At the feed of 50 mbar ethene and 50 mbar CH_3OH, from Fig. S10 it can be concluded that Z-CH_3 is the active methylation species and both the transition state of Z-CH_3 formation from methanol dimer and ethene methylation *via* Z-CH_3 shows large sensitivity values for propene formation. Therefore, the rate of propene formation is determined by Z-CH_3 formation and methylation.

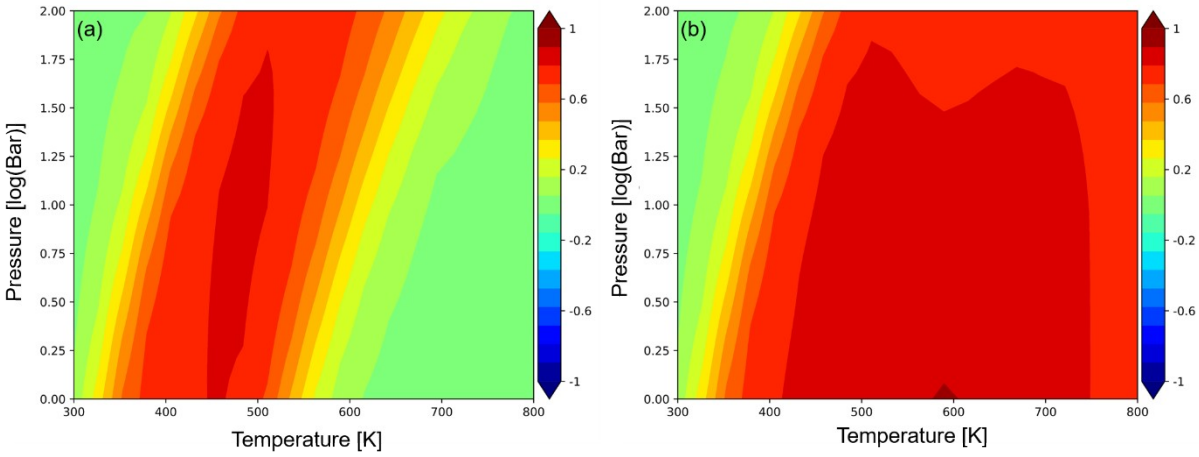


Fig. S12 DRC for propene formation *via* the transition state of (a) Z-CH_3 formation from two CH_3OH and (b) methylation by Z-CH_3 (50 mbar ethene, 50 mbar CH_3OH)

S9. Microkinetic input file (.mkm CatMAP)

Microkinetic model file (.mkm)

rxn_expressions :

CH_4_g ↔ CH_4_g,	#1
2*_s+H_2_g ↔ 2H*,	#2
CH_3OH_g + H* ↔ CH_3OHH*,	#3, MeOH ads
CH_3OH_g+CH_3OHH* ↔ CH_3OHCH_3OHH*,	#4, 2MeOH ads
CH_3OHCH_3OHH* ↔ CH_3OH-CH_3OH-H* ↔ $(CH_3)_2OH_2OH$*,	#5, DME formation
$(CH_3)_2OH_2OH$* ↔ $(CH_3)_2OH$* + H_2O_g,	#6
$(CH_3)_2OH$* ↔ H* + $(CH_3)_2O$_g,	#7
$(CH_3)_2OH$* ↔ $CH_3O(H)CH_3$*,	#8, protonation of DME
$CH_3O(H)CH_3$* ↔ $CH_3O(H)$-CH_3* ↔ CH_3OHCH_3*,	#9, ZCH_3 formation via DME
CH_3OHCH_3* ↔ CH_3* + CH_3OH_g,	#10
CH_3OH_g + CH_3OHH* ↔ $CH_3OHHOCH_3H$*,	#11, ZCH_3_$CH_3OHHOCH_3H$*
$CH_3OHHOCH_3H$* ↔ CH_3OH-$HOCH_3$-H* ↔ $CH_3OHH_2OCH_3$*,	#12, ZCH_3_formation via $CH_3OHHOCH_3H$*
$CH_3OHH_2OCH^3$* ↔ CH_3* + CH_3OH_g + H_2O_g,	#13
CH_3OHH* ↔ CH_3-OH-H* ↔ H_2OCH_3*,	#14, ZCH_3 formation via MeOH
H_2OCH_3* <-> CH_3* + H_2O_g,	#15
$(CH_3)_2O$_g + CH_3OHH* <-> $(CH_3)_2OCH_3OHH$*,	#16
$(CH_3)_2OCH_3OHH$* <-> $(CH_3)_2O$-CH_3-OHH* -> $H_2O(CH_3)_3O$*,	#17, TMO formation via MeOH&DME
$H_2O(CH_3)_3O$* <-> H_2O_g + $(CH_3)_3O$*,	#18
$(CH_3)_2O$_g + $(CH_3)_2OH$* ↔ $(CH_3)_2O(CH_3)_2OH$*,	#19
$(CH_3)_2O(CH_3)_2OH$ ↔ $(CH_3)_2O$-$(CH_3)_2O$-H* ↔ $CH_3OH(CH_3)_3O$*,	#20, TMO formation *via* 2DME
$CH_3OH(CH_3)_3O$* ↔ CH_3OH_g + $(CH_3)_3O$*,	#21
$(CH_3)_2O$_g + CH_3* ↔ $(CH_3)_2OCH_3$*,	#22
$(CH_3)_2OCH_3$* ↔ $(CH_3)_2O$-CH_3* ↔ $(CH_3)_3O$*,	#23, TMO formation via

DME+CH_3

C_2H_4_g + CH_3OHH^* ↔ $C_2H_4CH_3OHH^*$, #24

$C_2H_4CH_3OHH^*$ ↔ C_2H_4-CH_3OH-H* ↔ $C_3H_7H_2O^*$, #25, methylation by MeOH

$C_3H_7H_2O^*$ ↔ $C_3H_7^*$ + H_2O_g, #26

C_2H_4_g + $(CH_3)_2OH^*$ ↔ $C_2H_4(CH_3)_2OH^*$, #27

$C_2H_4(CH_3)_2OH^*$ ↔ C_2H_4-$(CH_3)_2O$-H* ↔ $CH_3OHC_3H_7^*$, #28, methylation by DME

$CH_3OHC_3H_7^*$ ↔ $C_3H_7^*$ + CH_3OH_g, #29

C_2H_4_g + CH_3^* ↔ $C_2H_4CH_3^*$, #30

$C_2H_4CH_3^*$ ↔ C_2H_4-CH_3^* ↔ $C_3H_7^*$, #31, methylation by Z-CH_3

C_2H_4_g + $(CH_3)_3O^*$ ↔ $C_2H_4(CH_3)_3O^*$, #32

$C_2H_4(CH_3)_3O^*$ ↔ C_2H_4-$(CH_3)_3O^*$ ↔ $(CH_3)_2OC_3H_7^*$, #33, methylation by TMO^+

$(CH_3)_2OC_3H_7^*$ ↔ $C_3H_7^*$ + $(CH_3)_2O$_g, #34

$C_3H_7^*$ ↔ $CH_2C(H_2)$-CH_3^* ↔ CH_3CH_2CH, #35, C_3H_7 conversion

$CH_3CH_2CH_2^*$ ↔ $CH_3C(H)$-H-CH_2^* ↔ $(CH_3)_2CH^*$, #36, C_3H_7 conversion

$(CH_3)_2CH^*$ ↔ $CH_3CHCH_3^*$, #37, C_3H_7 conversion

$CH_3CHCH_3^*$ ↔ $CH_3CHC(H_2)$-H* ↔ $CH_3CHCH_2H^*$, #38, C_3H_7 conversion

$CH_3CHCH_2H^*$ ↔ H* + CH_3CHCH_2_g, #39

```
surface_names = ['ZSM-5']

scaler = 'ThermodynamicScaler'

descriptor_names= ['temperature','logPressure'] #descriptor names
descriptor_ranges = [[300,800],[0, 2]]

resolution = 20

species_definitions = {}
delta = 1e-5
species_definitions['s'] = {'site_names': ['000'], 'total':1}

DME : C2H4 = 50 : 50 mbar
species_definitions['(CH3)2O_g'] = {'concentration':0.05 - delta}
species_definitions['CH4_g'] = {'concentration': delta }
species_definitions['H2_g'] = {'concentration': delta }
species_definitions['CH3OH_g'] = {'concentration':delta} #define the gas pressures
```

```
species_definitions[' C2H4_g'] = {'concentration':0.05 - delta}
species_definitions['H2O_g'] = {'concentration':delta}
species_definitions['CH3CHCH2_g'] = {'concentration':delta}

DME : C2H4 = 500 : 50 mbar
species_definitions['(CH3)2O_g'] = {'concentration':0.50 - delta}
species_definitions['CH4_g'] = {'concentration': delta }
species_definitions['H2_g'] = {'concentration': delta }
species_definitions['CH3OH_g'] = {'concentration':delta} #define the gas pressures
species_definitions['C2H4_g'] = {'concentration':0.05 - delta}
species_definitions['H2O_g'] = {'concentration':delta}
species_definitions['CH3CHCH2_g'] = {'concentration':delta}

DME : C2H4 = 950 : 50 mbar
species_definitions['(CH3)2O_g'] = {'concentration':0.95 - delta}
species_definitions['CH4_g'] = {'concentration': delta }
species_definitions['H2_g'] = {'concentration': delta }
species_definitions['CH3OH_g'] = {'concentration':delta} #define the gas pressures
species_definitions['C2H4_g'] = {'concentration':0.05 - delta}
species_definitions['H2O_g'] = {'concentration':delta}
species_definitions['CH3CHCH2_g'] = {'concentration':delta}

MeOH : C2H4 = 50 : 50 mbar
species_definitions['(CH3)2O_g'] = {'concentration': delta}
species_definitions['CH4_g'] = {'concentration': delta }
species_definitions['H2_g'] = {'concentration': delta }
species_definitions['CH3OH_g'] = {'concentration': 0.05 - delta } #define the gas pressures
species_definitions['C2H4_g'] = {'concentration' : 0.05 - delta}
species_definitions['H2O_g'] = {'concentration':delta}
species_definitions['CH3CHCH2_g'] = {'concentration':delta}

MeOH : C2H4 = 500 : 50 mbar
species_definitions['(CH3)2O_g'] = {'concentration': delta}
species_definitions['CH4_g'] = {'concentration': delta }
species_definitions['H2_g'] = {'concentration': delta }
species_definitions['CH3OH_g'] = {'concentration': 0.50 - delta } #define the gas pressures
species_definitions['C2H4_g'] = {'concentration' : 0.05 - delta}
species_definitions['H2O_g'] = {'concentration':delta}
species_definitions['CH3CHCH2_g'] = {'concentration':delta}

MeOH : C2H4 = 950 : 50 mbar
species_definitions['(CH3)2O_g'] = {'concentration': delta}
species_definitions['CH4_g'] = {'concentration': delta }
species_definitions['H2_g'] = {'concentration': delta }
```

```
species_definitions['CH3OH_g'] = {'concentration': 0.95 - delta } #define the gas pressures
species_definitions['C2H4_g'] = {'concentration' : 0.05 - delta}
species_definitions['H2O_g'] = {'concentration':delta}
species_definitions['CH3CHCH2_g'] = {'concentration':delta}

MeOH : (CH3)2O = 1 : 1
species_definitions['(CH3)2O_g'] = {'concentration': 0.0167}
species_definitions['CH4_g'] = {'concentration': delta }
species_definitions['H2_g'] = {'concentration': delta }
species_definitions['CH3OH_g'] = {'concentration': 0.0167 } #define the gas pressures
species_definitions['C2H4_g'] = {'concentration' : 0.05 - delta}
species_definitions['H2O_g'] = {'concentration':0.0167}
species_definitions['CH3CHCH2_g'] = {'concentration':delta}

MeOH : (CH3)2O = 1 : 2.7
species_definitions['(CH3)2O_g'] = {'concentration': 0.021}
species_definitions['CH4_g'] = {'concentration': delta }
species_definitions['H2_g'] = {'concentration': delta }
species_definitions['CH3OH_g'] = {'concentration': 0.0078 } #define the gas pressures
species_definitions['C2H4_g'] = {'concentration' : 0.05 - delta}
species_definitions['H2O_g'] = {'concentration':0.021}
species_definitions['CH3CHCH2_g'] = {'concentration':delta}



gas_thermo_mode = "ideal_gas"
adsorbate_thermo_mode = "HO_approximation"

decimal_precision = 200
tolerance = 1e-70
max_rootfinding_iterations = 100
max_bisections = 10


```

S10. Cartesian coordinates for all the optimized structures

C2H4(gas)

C	0.00000000	0.66357800	0.00000000
H	-0.92247900	1.23476800	0.00000000
H	0.92248400	1.23476600	0.00000000
C	0.00000000	-0.66357800	0.00000000
H	0.92247900	-1.23476800	0.00000000
H	-0.92248400	-1.23476600	0.00000000

C3H6(gas)

C	-3.07626709	1.94456888	-0.03037173
H	-2.55295066	2.79748796	0.41594328
H	-3.12521490	2.13641887	-1.10807661
H	-4.09659568	1.92788515	0.35989569
C	-2.35587512	0.66005929	0.25618905
H	-1.32960495	0.59939945	-0.10261410
C	-2.87122121	-0.38210310	0.90081606
H	-3.88980218	-0.37088891	1.27796948
H	-2.29605508	-1.28432404	1.07561887

CH3OCH3(gas)

O	0.00000000	0.00000000	-0.57792242
C	0.00000000	1.17305269	0.20647927
H	0.89212515	1.23361277	0.84820321
H	0.00000000	2.02190203	-0.47824728
H	-0.89212515	1.23361277	0.84820321
C	0.00000000	-1.17305269	0.20647927
H	0.00000000	-2.02190203	-0.47824728
H	0.89212515	-1.23361277	0.84820321
H	-0.89212515	-1.23361277	0.84820321

CH4(gas)

C	-0.66831683	-0.80445548	0.00000000
H	-0.30483718	-1.83257081	-0.00000092
H	-0.30481775	-0.29040495	0.89037018
H	-0.30481925	-0.29040388	-0.89037018
H	-1.75879314	-0.80444226	0.00000092

cyclopropane(gas)

C	-2.29718092	1.02950471	0.00000000
C	-0.78948325	1.02972547	0.00000000
C	-1.54331018	2.33525454	0.00000000
H	-2.80680400	0.73507176	-0.90949287
H	-2.80680400	0.73507176	0.90949287
H	-0.27958402	0.73559829	-0.90948261
H	-0.27958402	0.73559829	0.90948261
H	-1.54301752	2.92392630	0.90946315
H	-1.54301752	2.92392630	-0.90946315

H2(gas)

H	-0.25024339	0.59466019	0.00000000
H	-0.99441685	0.59466019	0.00000000

H2O(gas)

O	-0.97664688	0.95147275	0.00000000
H	-0.01605936	0.99914075	0.00000000
H	-1.25236374	1.87287432	0.00000000

Z-CH(CH3)2-deprotonation-TS-oniom

Si	-3.85140190	2.10933183	3.01246781
Si	-3.82813746	-0.75562299	-1.82459544
Si	-7.28058561	-0.35673777	1.59881828
Si	-3.44891735	-2.85489295	2.49346667
Al	-4.27280496	-0.26922623	1.09803156
O	-3.24543517	-1.44463874	1.79723380
O	-5.88709937	-0.85229315	1.01273483
O	-3.95693905	1.30807574	1.66717298
O	-3.64485847	0.08030269	-0.48714449
O	-2.44838241	2.91187009	3.04448403
O	-3.03888479	-2.15204711	-1.77932468
O	-5.34743505	-1.07606508	-2.25922715
O	-3.09188970	0.22942894	-2.85029546
O	-5.09845227	3.12693203	3.08870154
O	-7.92172653	0.91754391	0.85250730
O	-8.36453872	-1.51778246	1.36161698
O	-4.46630231	-3.91546548	1.78433636
O	-7.24230829	0.03295916	3.17146743
O	-4.00204245	-2.72577178	4.01433456
O	-3.92035041	1.25602298	4.37598565

1	O	-1.97311496	-3.51906086	2.44563143
2	O	-2.43622664	-2.92105696	6.14995529
3	Si	1.28267429	4.51491494	3.29968909
4	Si	-1.77949690	4.28911248	3.58393771
5	Si	-6.36816227	3.87477774	2.43089279
6	Si	3.47244400	2.72089500	4.43808400
7	Si	4.31383600	-0.21946000	4.38101800
8	Si	-1.05132321	-4.82305068	2.25880916
9	Si	1.81370399	-4.41550612	3.36558283
10	Si	4.09470200	-2.55191500	2.43892000
11	Si	6.60283800	-4.28991900	3.00216600
12	Si	4.87431700	-3.78673200	-5.15224700
13	Si	7.39251500	-5.58607300	-4.60606200
14	O	6.12638100	-4.67628000	-4.82250600
15	Si	-6.40401043	-1.53453500	-6.09611864
16	Si	-2.60271992	-4.19708927	-5.21814719
17	Si	-3.30772221	-1.46375326	-6.39965635
18	O	-2.55585598	-2.80976689	-5.99217253
19	O	-4.87496259	-1.71355575	-6.45613429
20	O	-1.17604534	-4.84123322	-5.26239740
21	Si	-0.28637900	-6.18255600	-5.22203600
22	Si	2.65060800	-5.77009100	-4.38363900
23	O	1.22145200	-5.72512400	-5.07027500
24	O	3.54630100	-4.65299600	-5.10103400
25	Si	-8.01730785	-3.63239219	-1.85122955
26	Si	2.11626100	3.24456800	-4.24992600
27	Si	-0.82177590	2.83025780	-5.08903338
28	Si	-4.68102800	5.41078100	-5.95857600
29	Si	-1.78249400	5.79093000	-5.05880900
30	O	0.60793700	2.78618200	-4.40251600
31	O	-1.71695586	1.71442595	-4.37096947
32	O	-5.10606069	4.14728132	-5.10539766
33	O	-3.33259700	6.00463200	-5.36388900
34	O	-1.47949700	4.24772400	-4.83911000
35	O	2.27288800	4.13234000	-2.93860500
36	O	-1.47310500	6.60394700	-3.72315900
37	Si	-0.32701100	7.27710000	-2.83776400
38	Si	4.73430200	7.18106200	-3.12366000
39	O	6.09355500	6.70936600	-2.43825900
40	Si	6.97257300	5.57640600	-1.75173200
41	O	6.65340200	4.15702600	-2.38154100
42	Si	8.23338000	-1.40447300	-3.37666500
43	Si	9.40160800	1.42263100	-3.04203600
44	Si	6.81359500	3.12473200	-3.57948700

1	Si	4.43209300	1.25836300	-4.25359800
2	O	9.03612400	-0.11181500	-2.87625900
3	O	8.11373900	2.26301700	-3.36743500
4	O	5.54354200	2.17444600	-3.59756700
5	O	3.00481700	1.90164300	-4.20940500
6	Si	-5.56319608	2.64733445	-4.86570093
7	O	8.21942900	-5.07574200	-3.35719400
8	Si	2.19942600	5.56874600	-2.26523100
9	O	0.98757000	6.38209600	-2.89494300
10	O	3.53113700	6.37368400	-2.49126100
11	Si	3.53341300	-1.74327700	6.99222300
12	Si	6.63865000	6.08528000	1.27259000
13	O	5.29926200	-3.38253100	3.06465600
14	O	6.14251300	4.93557800	2.24570300
15	Si	8.08141300	-2.92084000	5.30161600
16	Si	7.27576300	0.05489300	5.29634300
17	Si	8.58853400	2.66166400	4.32135300
18	Si	6.00796600	4.35248800	3.71720500
19	O	7.97144800	-1.35601300	5.08937300
20	O	8.21209400	1.14396600	4.58715800
21	O	7.29170500	3.51571300	4.07726000
22	O	4.72993300	3.41446000	3.77174100
23	O	3.54126100	1.15694500	4.16312000
24	O	5.86545800	0.05316900	4.58099200
25	O	7.71967600	-3.66934800	3.94523100
26	O	4.07587600	-1.08128400	3.06154000
27	O	3.69564900	-0.98635200	5.62508200
28	O	2.11091800	3.26388900	3.88628500
29	Si	4.42729600	-3.05877600	-0.57370600
30	Si	6.93423200	-4.79476700	0.00135000
31	O	5.70682500	-4.00353300	-0.62643200
32	Si	8.91499400	-4.19116400	-2.24804200
33	Si	5.13684900	-1.47361200	-3.07245000
34	O	8.81846100	-2.64672600	-2.58184100
35	O	4.38513100	-0.12910500	-3.47962500
36	O	6.70421200	-1.22494200	-3.01467400
37	O	8.24704500	-4.47299100	-0.83097000
38	O	4.59352600	-1.87026400	-1.62744700
39	O	4.76969300	-2.62296800	-4.10186600
40	Si	-5.64069475	6.87326175	2.73314543
41	Si	-2.60555779	7.04513037	2.39477462
42	O	-0.23907845	4.07700299	3.26867795
43	O	-5.91996210	5.38731758	2.26388478
44	O	-4.17652500	7.29057100	2.27892100

1	O	-2.31812630	5.52581452	2.75663647
2	O	1.74551900	4.93603400	1.83768300
3	O	-1.99084900	7.39284500	0.96576000
4	Si	-0.65960500	7.78396200	0.17486200
5	Si	1.86808900	6.07370600	0.73551900
6	Si	4.21899700	7.96640100	1.54368300
7	O	0.58000600	7.00304800	0.79605900
8	O	3.14938400	6.95546600	0.96635700
9	O	5.67479700	7.34740000	1.35373600
10	O	-0.90653500	7.37953200	-1.35117500
11	O	1.98850200	5.34591000	-0.68938600
12	O	6.65664000	5.50023000	-0.19987900
13	O	4.26037100	-2.37103800	0.85999800
14	O	7.20553700	-4.33511900	1.51561400
15	O	-2.94087163	-0.31660510	-5.36985195
16	Si	-3.04552009	0.84691491	-4.31884252
17	O	-4.29706577	1.73746182	-4.64940635
18	Si	-7.65049585	1.91033255	-2.74969485
19	Si	-6.78257485	-1.05069522	-3.01441139
20	Si	-5.49048183	-5.33983412	-1.27885074
21	Si	-2.95575256	-3.72774310	-2.13722656
22	O	-7.52024345	0.33655713	-2.80248181
23	O	-7.71572983	-2.18970335	-2.41670338
24	O	-6.70224100	-4.52663500	-1.90848500
25	O	-4.15855336	-4.53504301	-1.50488596
26	O	-6.55458304	-1.33264122	-4.54831802
27	O	-2.92941443	-3.96941281	-3.68597771
28	O	-6.48306621	2.60192897	-3.57035249
29	O	-1.59698653	-4.19991773	-1.45135481
30	Si	-1.60672386	-4.17048790	6.73615897
31	Si	1.45423000	-3.94675700	6.45201500
32	O	-0.08555100	-3.73327800	6.76737200
33	O	2.21638900	-2.62637000	6.94345500
34	O	0.39371838	-4.32663938	2.66768072
35	O	2.72264300	-3.26062100	2.76373500
36	O	1.68468900	-4.20214300	4.92307200
37	O	-1.85436700	-5.36177100	5.72713600
38	O	-1.54714803	-5.97315460	3.23213321
39	Si	-1.68176907	-6.55620284	4.70364628
40	Si	-0.71707767	-5.33235025	-0.76552881
41	Si	2.32989300	-5.20217700	-1.30962100
42	O	0.79823700	-4.94310600	-0.99601000
43	O	3.13098100	-3.88288800	-0.93415200
44	O	2.54199100	-5.50858300	-2.84122900

1	O	-0.78479600	-6.99171200	-3.95964700
2	O	-1.03640900	-6.75170400	-1.39508300
3	Si	-0.87612400	-7.78396800	-2.59304700
4	Si	-8.40602829	3.26445766	4.73448021
5	Si	-7.60019102	0.28892862	4.73923042
6	Si	-3.79675618	-2.37719087	5.59757740
7	Si	-4.63875973	0.56504616	5.65447881
8	Si	-7.98394403	2.41850415	0.27466909
9	Si	-8.35008993	-3.12540275	1.16155102
10	Si	-5.82192078	-4.83489615	1.72215760
11	O	-8.29604248	1.69965044	4.94667827
12	O	-3.86591586	-0.81333454	5.87302101
13	O	-6.19009273	0.28992359	5.45508240
14	O	-7.10973356	-3.90555095	1.78244008
15	O	-7.45966486	3.76695220	3.57224667
16	O	-6.99486124	3.38115956	1.05709674
17	O	-7.55578147	2.41979662	-1.25078205
18	O	-8.59624556	-3.52905367	-0.36469922
19	O	-5.70103540	-5.56269859	0.29714298
20	O	-1.03358098	-5.40936588	0.78672468
21	H	-5.71819200	6.49169800	-5.95831600
22	H	-8.98649000	2.25879400	-3.33121300
23	H	-0.44571300	9.26221600	0.28867200
24	H	-0.04115900	8.64608800	-3.37453700
25	H	8.00722100	6.55577900	1.65953500
26	H	8.40798500	5.94503100	-1.97028900
27	H	9.48112700	2.69419800	3.11869500
28	H	9.32187600	3.20112400	5.51099400
29	H	10.38943300	1.57418600	-4.15783100
30	H	10.01865300	1.87423800	-1.75384100
31	H	-9.59856617	-3.49179096	1.90350168
32	H	-0.43429200	-7.01887900	-6.45599600
33	H	-2.04306000	-4.56776700	8.11305700
34	H	10.36852400	-4.55088000	-2.29083400
35	H	-3.65465318	-5.06431445	-5.83908835
36	H	-6.61497400	7.85822200	2.16328400
37	H	-5.78069800	6.97173700	4.22133100
38	H	-4.49839200	5.01771600	-7.39246800
39	H	-0.96606300	6.35542800	-6.18074500
40	H	4.75923500	6.94995700	-4.60355600
41	H	4.60055400	8.64981500	-2.86147500
42	H	6.90013400	3.87476800	-4.87329900
43	H	8.25953600	-5.54336400	-5.82695000
44	H	6.96088900	-7.00259800	-4.37981500

1	H	-7.15472645	-2.74347549	-6.56370188
2	H	-6.95636831	-0.36166865	-6.84658550
3	H	-9.09228200	-4.26333100	-2.68211100
4	H	-5.42109100	-6.69484200	-1.91393400
5	H	-2.07551200	-8.68125400	-2.61014800
6	H	0.36117100	-8.60395300	-2.39120900
7	H	-0.46016200	-7.35251200	5.04633400
8	H	-2.88873400	-7.44196900	4.75506400
9	H	4.19652100	9.26567100	0.79852800
10	H	3.92103600	8.22741100	2.98843500
11	H	-8.06587200	3.96873100	6.01210000
12	H	-9.80329700	3.53866500	4.26932800
13	H	-9.39996725	2.88922060	0.41620092
14	H	-8.47605453	-0.72945485	5.40327175
15	H	-5.93724287	-5.90774951	2.76113936
16	H	-4.98682741	-3.03348811	6.22846756
17	H	3.27408700	-7.11172000	-4.61855200
18	H	6.62819000	-6.26114600	-0.01201900
19	H	6.24887400	-5.68307500	3.42376500
20	H	9.47867000	-3.19504700	5.76674200
21	H	1.96509100	-5.11677100	7.23571900
22	H	2.42921500	-5.75472300	3.09817100
23	H	2.82619500	-6.35957600	-0.49845400
24	H	-2.02640400	7.97055300	3.42042300
25	H	-6.34603356	2.16422888	-6.04799461
26	H	5.84456500	5.48325800	4.68605600
27	H	4.97783000	-3.21458500	-6.53275600
28	H	-0.71755700	2.58127900	-6.56253900
29	H	-2.79684000	-1.09222300	-7.75784800
30	H	3.36197700	-0.75169100	8.10188400
31	H	7.09546400	0.35583700	6.75272200
32	H	-4.41465311	1.37330220	6.89554916
33	H	1.51691100	5.64353900	4.25647700
34	H	3.45890800	2.99711400	5.91035300
35	H	8.37714000	-1.59728400	-4.85522400
36	H	4.74115600	1.04293100	-5.70346600
37	H	2.58844700	4.01119100	-5.44699100
38	H	4.73601000	-2.60462900	7.22918500
39	H	7.18458100	-3.39692600	6.40298100
40	H	-1.99916145	4.53460743	5.04545124
41	C	-1.38679295	1.73413231	-0.50499097
42	H	-1.17485286	1.71512690	-1.57353812
43	H	-1.72898373	2.66507156	-0.06199169
44	C	-0.91195896	0.73631978	0.31414930

1	H	-2.38744903	0.94635845	-0.38263852
2	C	-0.33929296	-0.54274632	-0.14537063
3	H	0.63507556	-0.67235230	0.34312093
4	H	-0.96867420	-1.36795090	0.21085559
5	H	-0.22065443	-0.59487352	-1.22821339
6	H	-1.06943292	0.85008093	1.38771680
7				
8				
9	Z-CH(CH3)2-oniom			
10	Si	-3.87040115	2.15671093	3.03765230
11	Si	-3.83939372	-0.74495681	-1.81952310
12	Si	-7.25118341	-0.36605024	1.60791347
13	Si	-3.46184761	-2.86773477	2.51279690
14	Al	-4.30600117	-0.23587938	1.05704190
15	O	-3.08653107	-1.40945272	1.77459441
16	O	-5.83288480	-0.99651711	1.20082318
17	O	-4.08479746	1.26517021	1.77247467
18	O	-3.70746692	0.05664974	-0.48123694
19	O	-2.45794047	2.92658644	3.03332377
20	O	-3.05908486	-2.15430719	-1.76724537
21	O	-5.36793646	-1.10188655	-2.25098906
22	O	-3.13911769	0.21758657	-2.87255702
23	O	-5.10823449	3.17803222	3.11271575
24	O	-7.78608571	0.91943022	0.79996434
25	O	-8.36196873	-1.49328256	1.32696337
26	O	-4.49730305	-3.83352553	1.75237629
27	O	-7.29119961	0.05702532	3.16544360
28	O	-4.03137947	-2.61198710	3.98921406
29	O	-3.89744759	1.32010973	4.41618076
30	O	-2.01462417	-3.53375130	2.51744632
31	O	-2.44745500	-2.89255700	6.15093700
32	Si	1.27565900	4.53394600	3.28197500
33	Si	-1.78653300	4.31109200	3.56665600
34	Si	-6.37585500	3.89573200	2.41417600
35	Si	3.46435000	2.74171700	4.42514900
36	Si	4.30414900	-0.19923200	4.37576900
37	Si	-1.06313100	-4.80570900	2.26510600
38	Si	1.80180500	-4.39651400	3.37102300
39	Si	4.08391300	-2.53658800	2.43969700
40	Si	6.59105600	-4.27449000	3.00765800
41	Si	4.86350300	-3.79147700	-5.14818000
42	Si	7.38067600	-5.59076600	-4.59712100
43	O	6.11505600	-4.68084900	-4.81602900
44	Si	-6.41350700	-1.53558100	-6.09885900

1	Si	-2.61377200	-4.19794700	-5.21366700
2	Si	-3.31716600	-1.46730600	-6.40229200
3	O	-2.56603400	-2.81265300	-5.99127200
4	O	-4.88454000	-1.71641700	-6.45827000
5	O	-1.18743300	-4.84299700	-5.25612200
6	Si	-0.29848800	-6.18467000	-5.21221400
7	Si	2.63865100	-5.77163200	-4.37463300
8	O	1.20957800	-5.72766600	-5.06150700
9	O	3.53501200	-4.65688400	-5.09484000
10	Si	-8.02827100	-3.62160600	-1.84856000
11	Si	2.10919200	3.24363200	-4.26430500
12	Si	-0.82900300	2.82875500	-5.10258500
13	Si	-4.68677300	5.40910600	-5.97914500
14	Si	-1.78811000	5.79000900	-5.08011500
15	O	0.60063200	2.78567200	-4.41583800
16	O	-1.72481600	1.71522300	-4.38165500
17	O	-5.11256600	4.14805200	-5.12273200
18	O	-3.33807100	6.00376200	-5.38588100
19	O	-1.48597000	4.24721300	-4.85639500
20	O	2.26618900	4.13471100	-2.95527300
21	O	-1.47839300	6.60631300	-3.74654700
22	Si	-0.33200900	7.28113300	-2.86279900
23	Si	4.72927600	7.18160600	-3.14800700
24	O	6.08821400	6.71094800	-2.46126900
25	Si	6.96655700	5.57929200	-1.77173500
26	O	6.64666900	4.15846000	-2.39789500
27	Si	8.22370900	-1.40645500	-3.37848100
28	Si	9.39344500	1.42087100	-3.05107100
29	Si	6.80640300	3.12298100	-3.59315100
30	Si	4.42394400	1.25616700	-4.26263400
31	O	9.02711300	-0.11294200	-2.88135400
32	O	8.10606000	2.26111100	-3.37875600
33	O	5.53583500	2.17334100	-3.60888100
34	O	2.99701400	1.90033400	-4.22023000
35	Si	-5.57053100	2.64899100	-4.87917800
36	O	8.20776100	-5.07765300	-3.34950700
37	Si	2.19345100	5.57289500	-2.28562600
38	O	0.98209100	6.38527000	-2.91754700
39	O	3.52561800	6.37652200	-2.51362400
40	Si	3.52267500	-1.71586000	6.99084200
41	Si	6.63265300	6.09617500	1.25123000
42	O	5.28796800	-3.36623600	3.06768500
43	O	6.13580900	4.94926600	2.22727300
44	Si	8.07017900	-2.90026600	5.30368400

1	Si	7.26614600	0.07588000	5.29063700
2	Si	8.58041700	2.67940500	4.30901500
3	Si	6.00082000	4.37006100	3.70026800
4	O	7.96108200	-1.33593400	5.08738100
5	O	8.20313000	1.16260500	4.57871600
6	O	7.28407300	3.53352300	4.06260000
7	O	4.72227200	3.43287100	3.75712200
8	O	3.53234000	1.17702300	4.15424100
9	O	5.85590200	0.07307000	4.57517100
10	O	7.70815100	-3.65208700	3.94921000
11	O	4.06583300	-1.06434000	3.05850600
12	O	3.68543900	-0.96256500	5.62176000
13	O	2.10316600	3.28402000	3.87182900
14	Si	4.41648800	-3.05142800	-0.57157800
15	Si	6.92243100	-4.78728600	0.00818700
16	O	5.69550800	-3.99701300	-0.62174700
17	Si	8.90371200	-4.19058400	-2.24258800
18	Si	5.12711500	-1.47312400	-3.07435600
19	O	8.80804700	-2.64696300	-2.58039300
20	O	4.37616200	-0.12926700	-3.48507600
21	O	6.69460800	-1.22515600	-3.01708800
22	O	8.23549000	-4.46837900	-0.82484900
23	O	4.58345300	-1.86573800	-1.62837800
24	O	4.75942200	-2.62494100	-4.10082500
25	Si	-5.64645000	6.89462300	2.70866100
26	Si	-2.61109600	7.06395000	2.37010800
27	O	-0.24636900	4.09674400	3.25179500
28	O	-5.92622900	5.40754800	2.24325200
29	O	-4.18195100	7.30994200	2.25350100
30	O	-2.32460300	5.54537000	2.73590500
31	O	1.73885000	4.95105400	1.81887300
32	O	-1.99610800	7.40762900	0.94026900
33	Si	-0.66458400	7.79597400	0.14847600
34	Si	1.86213300	6.08580200	0.71377800
35	Si	4.21400000	7.97930600	1.51724300
36	O	0.57455000	7.01599700	0.77180000
37	O	3.14388700	6.96746100	0.94244300
38	O	5.66947900	7.35902400	1.32902500
39	O	-0.91160400	7.38772800	-1.37653000
40	O	1.98227100	5.35425400	-0.70922800
41	O	6.65045100	5.50730500	-0.21971800
42	O	4.24981400	-2.35989000	0.86032600
43	O	7.19385700	-4.32386600	1.52128000
44	O	-2.94974000	-0.31768200	-5.37544000

1	Si	-3.05398600	0.84867000	-4.32782300
2	O	-4.30491000	1.73901700	-4.66037300
3	Si	-7.65834200	1.91856700	-2.76126300
4	Si	-6.79235300	-1.04375900	-3.01818500
5	Si	-5.50229900	-5.32897000	-1.27166400
6	Si	-2.96662700	-3.72041500	-2.13402400
7	O	-7.52905900	0.34465000	-2.81057500
8	O	-7.72593500	-2.18061600	-2.41807200
9	O	-6.71373100	-4.51669100	-1.90351600
10	O	-4.17013900	-4.52532100	-1.49963600
11	O	-6.56403200	-1.32957400	-4.55159400
12	O	-2.94045900	-3.96614100	-3.68211600
13	O	-6.49055100	2.60741000	-3.58382200
14	O	-1.60825500	-4.19166400	-1.44702600
15	Si	-1.61877300	-4.14091900	6.74066900
16	Si	1.44234100	-3.91960100	6.45616100
17	O	-0.09735000	-3.70447000	6.77083100
18	O	2.20517600	-2.59836100	6.94424700
19	O	0.38196300	-4.30866700	2.67262300
20	O	2.71144100	-3.24370600	2.76622700
21	O	1.67279200	-4.17907000	4.92790400
22	O	-1.86696300	-5.33469000	5.73466100
23	O	-1.55992900	-5.95266000	3.24128700
24	Si	-1.69490700	-6.53187100	4.71428000
25	Si	-0.72914400	-5.32266000	-0.75780300
26	Si	2.31798300	-5.19558700	-1.30212300
27	O	0.78644100	-4.93487300	-0.98931700
28	O	3.11975600	-3.87576600	-0.93000200
29	O	2.53004500	-5.50607200	-2.83291400
30	O	-0.79745200	-6.99028500	-3.94777700
31	O	-1.04915300	-6.74350100	-1.38386500
32	Si	-0.88932700	-7.77895000	-2.57913900
33	Si	-8.41383500	3.29250100	4.71913500
34	Si	-7.60956400	0.31662100	4.73165100
35	Si	-3.80792500	-2.34945400	5.59759300
36	Si	-4.64805000	0.59295700	5.64657600
37	Si	-7.99183300	2.43486000	0.26154000
38	Si	-8.36095800	-3.10663600	1.16275000
39	Si	-5.83375500	-4.81617900	1.72792500
40	O	-8.30489000	1.72811500	4.93532100
41	O	-3.87595500	-0.78477000	5.86853500
42	O	-6.19964300	0.31894600	5.44762300
43	O	-7.12114900	-3.88576200	1.78576500
44	O	-7.46708900	3.79151600	3.55568900

1	O	-7.00212200	3.39887900	1.04148500
2	O	-7.56361300	2.43192400	-1.26389000
3	O	-8.60742200	-3.51398800	-0.36249300
4	O	-5.71358400	-5.54755900	0.30483400
5	O	-1.04584300	-5.39542300	0.79442100
6	H	-5.72335000	6.49058400	-5.98177400
7	H	-8.99417200	2.26627100	-3.34400400
8	H	-0.44989800	9.27440100	0.25847700
9	H	-0.04536700	8.64857200	-3.40308900
10	H	8.00144700	6.56693100	1.63707400
11	H	8.40218800	5.94657000	-1.99112200
12	H	9.47313000	2.70834000	3.10635400
13	H	9.31395100	3.22154500	5.49731900
14	H	10.38144700	1.56900000	-4.16716900
15	H	10.01062500	1.87547700	-1.76399600
16	H	-9.60983400	-3.47040700	1.90550200
17	H	-0.44675000	-7.02410500	-6.44401700
18	H	-2.05542700	-4.53440900	8.11850200
19	H	10.35705000	-4.55119900	-2.28432300
20	H	-3.66611800	-5.06617600	-5.83245600
21	H	-6.62008100	7.87861600	2.13618400
22	H	-5.78646200	6.99700900	4.19659100
23	H	-4.50422900	5.01223100	-7.41199900
24	H	-0.97127700	6.35115700	-6.20343800
25	H	4.75420900	6.94665700	-4.62729700
26	H	4.59630400	8.65110500	-2.88963700
27	H	6.89346000	3.86961700	-4.88889300
28	H	8.24782500	-5.55168900	-5.81804000
29	H	6.94826100	-7.00646600	-4.36724500
30	H	-7.16486900	-2.74533200	-6.56337700
31	H	-6.96516300	-0.36438000	-6.85240400
32	H	-9.10356300	-4.25409300	-2.67802800
33	H	-5.43375900	-6.68560100	-1.90324100
34	H	-2.08920100	-8.67562600	-2.59402000
35	H	0.34750500	-8.59908200	-2.37507100
36	H	-0.47378200	-7.32794400	5.05913600
37	H	-2.90237700	-7.41683500	4.76788800
38	H	4.19229300	9.27665400	0.76872500
39	H	3.91605800	8.24421700	2.96128800
40	H	-8.07342000	3.99989100	5.99493100
41	H	-9.81093000	3.56625900	4.25312700
42	H	-9.40762900	2.90661000	0.40173100
43	H	-8.48604900	-0.69968400	5.39822500
44	H	-5.94989600	-5.88610600	2.76975500

1	H	-4.99820700	-3.00339900	6.22969400
2	H	3.26142100	-7.11420300	-4.60601800
3	H	6.61559300	-6.25352800	-0.00141200
4	H	6.23629900	-5.66635800	3.43283100
5	H	9.46724700	-3.17402700	5.76963900
6	H	1.95250000	-5.08786000	7.24293500
7	H	2.41662900	-5.73677400	3.10709300
8	H	2.81358700	-6.35115200	-0.48792000
9	H	-2.03155800	7.99170900	3.39342500
10	H	-6.35352700	2.16324800	-6.06031200
11	H	5.83795100	5.50342400	4.66617500
12	H	4.96744500	-3.22296300	-6.53015700
13	H	-0.72478900	2.57589800	-6.57543800
14	H	-2.80596600	-1.09955700	-7.76141300
15	H	3.35168400	-0.72131100	8.09791800
16	H	7.08588700	0.38069200	6.74621600
17	H	-4.42372200	1.40486000	6.88536300
18	H	1.51042100	5.66494300	4.23580700
19	H	3.45083900	3.02175400	5.89669700
20	H	8.36749000	-1.60317100	-4.85652300
21	H	4.73301400	1.03681400	-5.71191300
22	H	2.58189600	4.00689700	-5.46330900
23	H	4.72478400	-2.57724900	7.23013800
24	H	7.17299400	-3.37301200	6.40620000
25	H	-2.00631100	4.55985200	5.02736600
26	C	-0.72839314	-1.53344180	0.82575115
27	H	-1.25466051	-2.03617138	0.01273930
28	H	-0.10535122	-2.25037131	1.36293421
29	C	-1.66216852	-0.78764503	1.76031521
30	H	-0.06149502	-0.79708836	0.36746720
31	H	-1.88132351	0.19459846	1.34199228
32	C	-1.15751969	-0.64239810	3.17742071
33	H	-0.89912696	-1.60383738	3.62786184
34	H	-0.24390568	-0.03994143	3.13312488
35	H	-1.86547104	-0.11630620	3.82007736
36				
37				
38	Z-CH(CH3)2			
39	Si	-3.86790134	2.17318764	3.05399193
40	Si	-3.83384576	-0.75101477	-1.84595760
41	Si	-7.29673243	-0.35822753	1.61585155
42	Si	-3.45232303	-2.86045657	2.50598545
43	Al	-4.31341912	-0.20809805	1.06381553
44	O	-3.09184466	-1.37588116	1.80073107

1	O	-5.84475555	-0.94573349	1.25531654
2	O	-4.04106680	1.29524633	1.76653454
3	O	-3.73466717	0.03440266	-0.49260152
4	O	-2.45346624	2.93960677	3.04837581
5	O	-3.04655261	-2.16010078	-1.77141129
6	O	-5.36004889	-1.08874596	-2.28574545
7	O	-3.09975496	0.21302230	-2.88229089
8	O	-5.10094264	3.19768673	3.09848649
9	O	-7.79211911	0.92715343	0.79211193
10	O	-8.37292986	-1.50578425	1.29806972
11	O	-4.51409440	-3.81945519	1.77371122
12	O	-7.34567605	0.02918139	3.17795653
13	O	-3.97348905	-2.61842909	3.99924865
14	O	-3.90512633	1.29028135	4.40563827
15	O	-1.99715640	-3.52079009	2.46045122
16	O	-2.44745500	-2.89255700	6.15093700
17	Si	1.27565900	4.53394600	3.28197500
18	Si	-1.78653300	4.31109200	3.56665600
19	Si	-6.37585500	3.89573200	2.41417600
20	Si	3.46435000	2.74171700	4.42514900
21	Si	4.30414900	-0.19923200	4.37576900
22	Si	-1.06313100	-4.80570900	2.26510600
23	Si	1.80180500	-4.39651400	3.37102300
24	Si	4.08391300	-2.53658800	2.43969700
25	Si	6.59105600	-4.27449000	3.00765800
26	Si	4.86350300	-3.79147700	-5.14818000
27	Si	7.38067600	-5.59076600	-4.59712100
28	O	6.11505600	-4.68084900	-4.81602900
29	Si	-6.41350700	-1.53558100	-6.09885900
30	Si	-2.61377200	-4.19794700	-5.21366700
31	Si	-3.31716600	-1.46730600	-6.40229200
32	O	-2.56603400	-2.81265300	-5.99127200
33	O	-4.88454000	-1.71641700	-6.45827000
34	O	-1.18743300	-4.84299700	-5.25612200
35	Si	-0.29848800	-6.18467000	-5.21221400
36	Si	2.63865100	-5.77163200	-4.37463300
37	O	1.20957800	-5.72766600	-5.06150700
38	O	3.53501200	-4.65688400	-5.09484000
39	Si	-8.02827100	-3.62160600	-1.84856000
40	Si	2.10919200	3.24363200	-4.26430500
41	Si	-0.82900300	2.82875500	-5.10258500
42	Si	-4.68677300	5.40910600	-5.97914500
43	Si	-1.78811000	5.79000900	-5.08011500
44	O	0.60063200	2.78567200	-4.41583800

1	O	-1.72481600	1.71522300	-4.38165500
2	O	-5.11256600	4.14805200	-5.12273200
3	O	-3.33807100	6.00376200	-5.38588100
4	O	-1.48597000	4.24721300	-4.85639500
5	O	2.26618900	4.13471100	-2.95527300
6	O	-1.47839300	6.60631300	-3.74654700
7	Si	-0.33200900	7.28113300	-2.86279900
8	Si	4.72927600	7.18160600	-3.14800700
9	O	6.08821400	6.71094800	-2.46126900
10	Si	6.96655700	5.57929200	-1.77173500
11	O	6.64666900	4.15846000	-2.39789500
12	Si	8.22370900	-1.40645500	-3.37848100
13	Si	9.39344500	1.42087100	-3.05107100
14	Si	6.80640300	3.12298100	-3.59315100
15	Si	4.42394400	1.25616700	-4.26263400
16	O	9.02711300	-0.11294200	-2.88135400
17	O	8.10606000	2.26111100	-3.37875600
18	O	5.53583500	2.17334100	-3.60888100
19	O	2.99701400	1.90033400	-4.22023000
20	Si	-5.57053100	2.64899100	-4.87917800
21	O	8.20776100	-5.07765300	-3.34950700
22	Si	2.19345100	5.57289500	-2.28562600
23	O	0.98209100	6.38527000	-2.91754700
24	O	3.52561800	6.37652200	-2.51362400
25	Si	3.52267500	-1.71586000	6.99084200
26	Si	6.63265300	6.09617500	1.25123000
27	O	5.28796800	-3.36623600	3.06768500
28	O	6.13580900	4.94926600	2.22727300
29	Si	8.07017900	-2.90026600	5.30368400
30	Si	7.26614600	0.07588000	5.29063700
31	Si	8.58041700	2.67940500	4.30901500
32	Si	6.00082000	4.37006100	3.70026800
33	O	7.96108200	-1.33593400	5.08738100
34	O	8.20313000	1.16260500	4.57871600
35	O	7.28407300	3.53352300	4.06260000
36	O	4.72227200	3.43287100	3.75712200
37	O	3.53234000	1.17702300	4.15424100
38	O	5.85590200	0.07307000	4.57517100
39	O	7.70815100	-3.65208700	3.94921000
40	O	4.06583300	-1.06434000	3.05850600
41	O	3.68543900	-0.96256500	5.62176000
42	O	2.10316600	3.28402000	3.87182900
43	Si	4.41648800	-3.05142800	-0.57157800
44	Si	6.92243100	-4.78728600	0.00818700

1	O	5.69550800	-3.99701300	-0.62174700
2	Si	8.90371200	-4.19058400	-2.24258800
3	Si	5.12711500	-1.47312400	-3.07435600
4	O	8.80804700	-2.64696300	-2.58039300
5	O	4.37616200	-0.12926700	-3.48507600
6	O	6.69460800	-1.22515600	-3.01708800
7	O	8.23549000	-4.46837900	-0.82484900
8	O	4.58345300	-1.86573800	-1.62837800
9	O	4.75942200	-2.62494100	-4.10082500
10	Si	-5.64645000	6.89462300	2.70866100
11	Si	-2.61109600	7.06395000	2.37010800
12	O	-0.24636900	4.09674400	3.25179500
13	O	-5.92622900	5.40754800	2.24325200
14	O	-4.18195100	7.30994200	2.25350100
15	O	-2.32460300	5.54537000	2.73590500
16	O	1.73885000	4.95105400	1.81887300
17	O	-1.99610800	7.40762900	0.94026900
18	Si	-0.66458400	7.79597400	0.14847600
19	Si	1.86213300	6.08580200	0.71377800
20	Si	4.21400000	7.97930600	1.51724300
21	O	0.57455000	7.01599700	0.77180000
22	O	3.14388700	6.96746100	0.94244300
23	O	5.66947900	7.35902400	1.32902500
24	O	-0.91160400	7.38772800	-1.37653000
25	O	1.98227100	5.35425400	-0.70922800
26	O	6.65045100	5.50730500	-0.21971800
27	O	4.24981400	-2.35989000	0.86032600
28	O	7.19385700	-4.32386600	1.52128000
29	O	-2.94974000	-0.31768200	-5.37544000
30	Si	-3.05398600	0.84867000	-4.32782300
31	O	-4.30491000	1.73901700	-4.66037300
32	Si	-7.65834200	1.91856700	-2.76126300
33	Si	-6.79235300	-1.04375900	-3.01818500
34	Si	-5.50229900	-5.32897000	-1.27166400
35	Si	-2.96662700	-3.72041500	-2.13402400
36	O	-7.52905900	0.34465000	-2.81057500
37	O	-7.72593500	-2.18061600	-2.41807200
38	O	-6.71373100	-4.51669100	-1.90351600
39	O	-4.17013900	-4.52532100	-1.49963600
40	O	-6.56403200	-1.32957400	-4.55159400
41	O	-2.94045900	-3.96614100	-3.68211600
42	O	-6.49055100	2.60741000	-3.58382200
43	O	-1.60825500	-4.19166400	-1.44702600
44	Si	-1.61877300	-4.14091900	6.74066900

1	Si	1.44234100	-3.91960100	6.45616100
2	O	-0.09735000	-3.70447000	6.77083100
3	O	2.20517600	-2.59836100	6.94424700
4	O	0.38196300	-4.30866700	2.67262300
5	O	2.71144100	-3.24370600	2.76622700
6	O	1.67279200	-4.17907000	4.92790400
7	O	-1.86696300	-5.33469000	5.73466100
8	O	-1.55992900	-5.95266000	3.24128700
9	Si	-1.69490700	-6.53187100	4.71428000
10	Si	-0.72914400	-5.32266000	-0.75780300
11	Si	2.31798300	-5.19558700	-1.30212300
12	O	0.78644100	-4.93487300	-0.98931700
13	O	3.11975600	-3.87576600	-0.93000200
14	O	2.53004500	-5.50607200	-2.83291400
15	O	-0.79745200	-6.99028500	-3.94777700
16	O	-1.04915300	-6.74350100	-1.38386500
17	Si	-0.88932700	-7.77895000	-2.57913900
18	Si	-8.41383500	3.29250100	4.71913500
19	Si	-7.60956400	0.31662100	4.73165100
20	Si	-3.80792500	-2.34945400	5.59759300
21	Si	-4.64805000	0.59295700	5.64657600
22	Si	-7.99183300	2.43486000	0.26154000
23	Si	-8.36095800	-3.10663600	1.16275000
24	Si	-5.83375500	-4.81617900	1.72792500
25	O	-8.30489000	1.72811500	4.93532100
26	O	-3.87595500	-0.78477000	5.86853500
27	O	-6.19964300	0.31894600	5.44762300
28	O	-7.12114900	-3.88576200	1.78576500
29	O	-7.46708900	3.79151600	3.55568900
30	O	-7.00212200	3.39887900	1.04148500
31	O	-7.56361300	2.43192400	-1.26389000
32	O	-8.60742200	-3.51398800	-0.36249300
33	O	-5.71358400	-5.54755900	0.30483400
34	O	-1.04584300	-5.39542300	0.79442100
35	H	-5.72335000	6.49058400	-5.98177400
36	H	-8.99417200	2.26627100	-3.34400400
37	H	-0.44989800	9.27440100	0.25847700
38	H	-0.04536700	8.64857200	-3.40308900
39	H	8.00144700	6.56693100	1.63707400
40	H	8.40218800	5.94657000	-1.99112200
41	H	9.47313000	2.70834000	3.10635400
42	H	9.31395100	3.22154500	5.49731900
43	H	10.38144700	1.56900000	-4.16716900
44	H	10.01062500	1.87547700	-1.76399600

1	H	-9.60983400	-3.47040700	1.90550200
2	H	-0.44675000	-7.02410500	-6.44401700
3	H	-2.05542700	-4.53440900	8.11850200
4	H	10.35705000	-4.55119900	-2.28432300
5	H	-3.66611800	-5.06617600	-5.83245600
6	H	-6.62008100	7.87861600	2.13618400
7	H	-5.78646200	6.99700900	4.19659100
8	H	-4.50422900	5.01223100	-7.41199900
9	H	-0.97127700	6.35115700	-6.20343800
10	H	4.75420900	6.94665700	-4.62729700
11	H	4.59630400	8.65110500	-2.88963700
12	H	6.89346000	3.86961700	-4.88889300
13	H	8.24782500	-5.55168900	-5.81804000
14	H	6.94826100	-7.00646600	-4.36724500
15	H	-7.16486900	-2.74533200	-6.56337700
16	H	-6.96516300	-0.36438000	-6.85240400
17	H	-9.10356300	-4.25409300	-2.67802800
18	H	-5.43375900	-6.68560100	-1.90324100
19	H	-2.08920100	-8.67562600	-2.59402000
20	H	0.34750500	-8.59908200	-2.37507100
21	H	-0.47378200	-7.32794400	5.05913600
22	H	-2.90237700	-7.41683500	4.76788800
23	H	4.19229300	9.27665400	0.76872500
24	H	3.91605800	8.24421700	2.96128800
25	H	-8.07342000	3.99989100	5.99493100
26	H	-9.81093000	3.56625900	4.25312700
27	H	-9.40762900	2.90661000	0.40173100
28	H	-8.48604900	-0.69968400	5.39822500
29	H	-5.94989600	-5.88610600	2.76975500
30	H	-4.99820700	-3.00339900	6.22969400
31	H	3.26142100	-7.11420300	-4.60601800
32	H	6.61559300	-6.25352800	-0.00141200
33	H	6.23629900	-5.66635800	3.43283100
34	H	9.46724700	-3.17402700	5.76963900
35	H	1.95250000	-5.08786000	7.24293500
36	H	2.41662900	-5.73677400	3.10709300
37	H	2.81358700	-6.35115200	-0.48792000
38	H	-2.03155800	7.99170900	3.39342500
39	H	-6.35352700	2.16324800	-6.06031200
40	H	5.83795100	5.50342400	4.66617500
41	H	4.96744500	-3.22296300	-6.53015700
42	H	-0.72478900	2.57589800	-6.57543800
43	H	-2.80596600	-1.09955700	-7.76141300
44	H	3.35168400	-0.72131100	8.09791800

1	H	7.08588700	0.38069200	6.74621600
2	H	-4.42372200	1.40486000	6.88536300
3	H	1.51042100	5.66494300	4.23580700
4	H	3.45083900	3.02175400	5.89669700
5	H	8.36749000	-1.60317100	-4.85652300
6	H	4.73301400	1.03681400	-5.71191300
7	H	2.58189600	4.00689700	-5.46330900
8	H	4.72478400	-2.57724900	7.23013800
9	H	7.17299400	-3.37301200	6.40620000
10	H	-2.00631100	4.55985200	5.02736600
11	C	-0.76648094	-1.36178478	0.74696657
12	H	-1.31064796	-1.62227941	-0.15847146
13	H	-0.25149809	-2.23424051	1.14165561
14	C	-1.66437138	-0.70493778	1.77084585
15	H	-0.00652850	-0.62373545	0.47245815
16	H	-1.93802802	0.28669563	1.42209925
17	C	-1.10922111	-0.61769319	3.17466714
18	H	-0.81390270	-1.59364141	3.55825590
19	H	-0.21583282	0.01212119	3.13117735
20	H	-1.81157322	-0.14398368	3.85960255
21				
22				
23	Z-CH2CH2CH3-deprotonation-TS			
24	Si	-0.02352452	0.03229728	-0.02145632
25	Si	-0.07238511	-0.01005533	5.65041952
26	Si	3.72323023	-0.03702736	2.48974138
27	Si	1.04570933	-3.88945915	2.97667669
28	Al	0.77060582	-0.82297289	2.86283945
29	O	0.26669448	-2.49191626	2.83552952
30	O	2.44628932	-0.69978160	3.18379110
31	O	0.08405123	-0.00625670	1.54404452
32	O	-0.24739531	-0.14548778	4.07911916
33	O	-1.57627960	0.14255904	-0.44781190
34	O	-0.36522324	-1.43737398	6.33204910
35	O	1.37255007	0.50928157	6.16355903
36	O	-1.24601464	1.00940674	6.02325829
37	O	0.82387152	1.28788686	-0.55549270
38	O	3.73085594	1.56573421	2.50654925
39	O	5.02010497	-0.47223023	3.32703483
40	O	2.19885680	-4.01286519	4.10737799
41	O	3.87643975	-0.50901838	0.95223721
42	O	1.75736613	-4.29567540	1.58786397
43	O	0.55946248	-1.28558880	-0.74651095
44	O	-0.16340416	-4.90299060	3.35252804

1	C	-2.08390943	-2.41757198	2.51972237
2	H	-1.77682645	-2.28914144	1.48969079
3	H	-1.98713794	-3.41441374	2.93466814
4	C	-2.66244815	-1.35579979	3.22814443
5	H	-1.64334518	-0.84003381	3.55873742
6	H	-3.03144663	-0.55973624	2.57423998
7	C	-3.46654997	-1.61706212	4.49994867
8	H	-3.58399906	-0.69217820	5.06496924
9	H	-4.46177941	-1.99339220	4.25284003
10	H	-2.96595982	-2.34378746	5.14206794
11	O	0.80120000	-6.00640000	-0.15260000
12	Si	-5.49760000	-0.02110000	-1.47430000
13	Si	-2.51950000	0.76950000	-1.59090000
14	Si	1.67330000	2.63520000	-0.36440000
15	Si	-6.77250000	-2.79180000	-1.55910000
16	Si	-6.65860000	-5.43650000	-0.02630000
17	Si	-0.62810000	-6.20850000	4.15930000
18	Si	-3.21920000	-7.43500000	2.98450000
19	Si	-6.09540000	-6.32220000	2.83000000
20	Si	-7.79180000	-8.89230000	3.21140000
21	Si	-7.85690000	-4.02790000	9.99880000
22	Si	-9.54690000	-6.64300000	10.42590000
23	O	-8.68790000	-5.35140000	10.15840000
24	Si	1.78780000	2.30220000	9.72780000
25	Si	-0.76980000	-1.62740000	10.29930000
26	Si	-1.17800000	1.38380000	9.93890000
27	O	-1.38700000	-0.16320000	10.26480000
28	O	0.35020000	1.77510000	10.12160000
29	O	-1.90930000	-2.64050000	10.65650000
30	Si	-2.31670000	-4.06080000	11.29600000
31	Si	-5.02660000	-5.18350000	10.35000000
32	O	-3.83590000	-4.30830000	10.92640000
33	O	-6.34110000	-4.27000000	10.39930000
34	Si	4.73290000	-0.80100000	7.13550000
35	Si	-7.29070000	2.20560000	5.67640000
36	Si	-4.57940000	3.32750000	6.62400000
37	Si	-1.94070000	7.20800000	6.08700000
38	Si	-4.59330000	6.04430000	5.10460000
39	O	-5.77090000	2.45290000	6.04720000
40	O	-3.26560000	2.41450000	6.57330000
41	O	-0.99450000	5.94280000	5.99240000
42	O	-3.27080000	6.91960000	5.26710000
43	O	-4.35770000	4.58890000	5.69440000
44	O	-7.46660000	2.24720000	4.09540000

1	O	-4.88400000	5.95910000	3.53970000
2	Si	-5.99570000	5.67090000	2.42990000
3	Si	-10.73910000	3.90040000	2.70070000
4	O	-11.73290000	2.70740000	2.34160000
5	Si	-12.07420000	1.15480000	2.31840000
6	O	-11.45520000	0.42330000	3.58130000
7	Si	-11.39460000	-4.15760000	7.24580000
8	Si	-13.29570000	-2.46030000	5.52120000
9	Si	-11.50890000	0.09760000	5.13610000
10	Si	-8.83680000	-0.22830000	6.67330000
11	O	-12.44950000	-3.64190000	6.15630000
12	O	-12.41530000	-1.16550000	5.38290000
13	O	-10.03410000	-0.20050000	5.63860000
14	O	-7.69650000	0.78430000	6.31660000
15	Si	-0.05970000	4.78730000	6.54670000
16	O	-10.24280000	-7.11800000	9.08650000
17	Si	-7.71660000	3.11370000	2.78820000
18	O	-6.95550000	4.50240000	2.92570000
19	O	-9.24950000	3.38730000	2.56950000
20	Si	-4.97250000	-7.60980000	-1.50390000
21	Si	-11.35590000	0.26280000	-0.54610000
22	O	-6.84510000	-7.72030000	2.70470000
23	O	-10.35620000	-0.94150000	-0.80140000
24	Si	-9.16490000	-9.40520000	0.52820000
25	Si	-9.33470000	-6.71560000	-0.96890000
26	Si	-11.54680000	-4.63200000	-1.45310000
27	Si	-9.77590000	-2.05450000	-1.77500000
28	O	-9.58580000	-8.00560000	-0.07990000
29	O	-10.67690000	-5.84320000	-0.91270000
30	O	-10.64710000	-3.36120000	-1.66840000
31	O	-8.28390000	-2.37400000	-1.34130000
32	O	-6.40440000	-3.94670000	-0.53100000
33	O	-8.15250000	-5.87130000	-0.34420000
34	O	-8.84920000	-9.23940000	2.07860000
35	O	-6.41640000	-5.42400000	1.54900000
36	O	-5.61290000	-6.41590000	-0.70840000
37	O	-5.77370000	-1.60340000	-1.35130000
38	Si	-6.81090000	-5.43360000	5.68340000
39	Si	-8.50460000	-8.00720000	6.05360000
40	O	-7.72180000	-6.63160000	6.20070000
41	Si	-10.95800000	-7.17850000	7.67890000
42	Si	-8.42890000	-3.23820000	7.03330000
43	O	-11.40780000	-5.74300000	7.18590000
44	O	-8.21960000	-1.69260000	6.70790000

1	O	-9.95660000	-3.63110000	6.85010000
2	O	-9.98360000	-7.83070000	6.60240000
3	O	-7.53000000	-4.04100000	5.99020000
4	O	-7.92320000	-3.54700000	8.50450000
5	Si	0.12370000	4.64450000	-2.14540000
6	Si	-2.82300000	3.84600000	-1.95510000
7	O	-3.94890000	0.19040000	-1.21850000
8	O	0.75580000	3.76930000	-0.98750000
9	O	-1.45550000	4.66540000	-1.97180000
10	O	-2.55360000	2.34860000	-1.49990000
11	O	-6.33220000	0.83850000	-0.42850000
12	O	-3.77030000	4.57610000	-0.90140000
13	Si	-5.28020000	4.78230000	-0.42350000
14	Si	-7.00390000	2.22870000	-0.05400000
15	Si	-9.63060000	2.52380000	-1.72000000
16	O	-6.07880000	3.41370000	-0.57020000
17	O	-8.42830000	2.36750000	-0.70540000
18	O	-10.83220000	1.58900000	-1.25000000
19	O	-5.20960000	5.26350000	1.09860000
20	O	-7.15700000	2.26930000	1.54270000
21	O	-11.46650000	0.47770000	1.01990000
22	O	-6.60040000	-5.49380000	4.09960000
23	O	-8.61720000	-8.44720000	4.51360000
24	O	-1.68270000	1.69080000	8.46850000
25	Si	-1.74890000	2.17160000	6.97410000
26	O	-0.91870000	3.49570000	6.81430000
27	Si	2.50950000	3.95250000	5.10420000
28	Si	2.56680000	1.37880000	6.82680000
29	Si	3.01120000	-3.35760000	7.49350000
30	Si	-0.01130000	-2.57110000	7.40600000
31	O	2.86460000	2.66320000	5.94600000
32	O	3.90010000	0.51780000	6.89190000
33	O	3.77240000	-1.96900000	7.63100000
34	O	1.47830000	-3.08400000	7.27480000
35	O	2.15450000	1.79120000	8.29130000
36	O	-0.24970000	-2.04670000	8.86410000
37	O	1.05380000	4.47370000	5.45680000
38	O	-1.00420000	-3.76440000	7.04720000
39	Si	0.52350000	-7.58780000	-0.03030000
40	Si	-2.45310000	-8.37930000	0.08690000
41	O	-1.02440000	-7.79970000	-0.28570000
42	O	-3.48040000	-7.82240000	-1.00870000
43	O	-2.05280000	-6.52240000	3.54850000
44	O	-4.53620000	-6.55020000	2.91500000

1	O	-2.87430000	-7.94910000	1.53380000
2	O	0.93450000	-7.98310000	1.44400000
3	O	0.37160000	-7.41290000	3.90390000
4	Si	0.95190000	-8.52590000	2.93030000
5	Si	-1.34640000	-5.31660000	7.02370000
6	Si	-4.32960000	-6.05610000	7.41270000
7	O	-2.92290000	-5.44190000	7.01850000
8	O	-5.41450000	-5.45960000	6.41750000
9	O	-4.71840000	-5.65910000	8.88780000
10	O	-1.36620000	-5.12610000	10.61890000
11	O	-0.72730000	-6.04810000	8.28660000
12	Si	-0.78110000	-6.37380000	9.84140000
13	Si	4.19160000	1.79580000	-2.03250000
14	Si	4.36130000	-0.89370000	-0.53530000
15	Si	1.79910000	-4.81760000	0.05480000
16	Si	1.68500000	-2.17150000	-1.47840000
17	Si	3.22790000	3.06050000	2.23970000
18	Si	5.44850000	-1.68950000	4.28210000
19	Si	3.72400000	-4.24270000	4.65120000
20	O	4.61250000	0.39620000	-1.42440000
21	O	1.43100000	-3.66270000	-0.97330000
22	O	3.17920000	-1.73800000	-1.16010000
23	O	4.64900000	-3.05760000	4.13510000
24	O	2.93690000	2.40530000	-1.28880000
25	O	2.15280000	3.10900000	1.07410000
26	O	2.54300000	3.62290000	3.55350000
27	O	5.51820000	-1.20780000	5.80380000
28	O	3.57090000	-4.20200000	6.24790000
29	O	-0.73790000	-5.99420000	5.72550000
30	H	-1.30770000	8.45280000	5.54490000
31	H	3.53900000	4.98890000	5.43620000
32	H	-5.91550000	5.84190000	-1.27060000
33	H	-6.78570000	6.92250000	2.19890000
34	H	-12.70540000	-0.03450000	-1.12450000
35	H	-13.56750000	1.03610000	2.31350000
36	H	-12.61360000	-4.36250000	-0.43650000
37	H	-12.17550000	-5.02190000	-2.75570000
38	H	-14.47190000	-2.17020000	6.40220000
39	H	-13.77040000	-2.92530000	4.17860000
40	H	6.86450000	-1.88260000	3.83330000
41	H	-2.15040000	-4.10050000	12.78420000
42	H	1.31010000	-8.39770000	-1.01480000
43	H	-12.21020000	-7.97290000	7.89080000
44	H	0.36340000	-1.65380000	11.27870000

1	H	0.62130000	6.05740000	-2.14750000
2	H	0.50140000	4.07440000	-3.47820000
3	H	-2.25700000	7.49990000	7.52180000
4	H	-5.73850000	6.73170000	5.78280000
5	H	-10.96700000	4.40130000	4.09400000
6	H	-11.01960000	5.00810000	1.73210000
7	H	-12.06290000	1.27880000	5.87220000
8	H	-10.59640000	-6.34750000	11.45320000
9	H	-8.66420000	-7.73420000	10.94950000
10	H	2.77450000	1.81970000	10.74640000
11	H	1.80020000	3.79900000	9.78440000
12	H	5.77540000	-0.53010000	8.17660000
13	H	3.24710000	-4.17500000	8.72650000
14	H	0.61160000	-6.65520000	10.31590000
15	H	-1.64370000	-7.57580000	10.07620000
16	H	0.12290000	-9.76940000	3.03170000
17	H	2.36090000	-8.82750000	3.33990000
18	H	-10.15040000	3.92860000	-1.73450000
19	H	-9.16390000	2.16210000	-3.09680000
20	H	3.89500000	1.63920000	-3.49250000
21	H	5.32300000	2.73990000	-1.76330000
22	H	4.42880000	3.88350000	1.88700000
23	H	5.61650000	-1.70970000	-0.58830000
24	H	4.35730000	-5.55350000	4.29820000
25	H	3.22920000	-5.21290000	-0.15130000
26	H	-5.23700000	-6.37850000	11.22840000
27	H	-7.76830000	-9.07120000	6.80850000
28	H	-6.95230000	-10.08460000	3.55430000
29	H	-10.29630000	-10.34930000	0.25900000
30	H	-2.42150000	-9.87450000	0.00040000
31	H	-3.42900000	-8.60990000	3.88980000
32	H	-4.28320000	-7.54880000	7.29620000
33	H	-3.45780000	3.89970000	-3.31080000
34	H	0.59910000	5.23700000	7.81470000
35	H	-9.79240000	-1.54060000	-3.18200000
36	H	-8.38790000	-2.95530000	10.89960000
37	H	-4.87450000	3.78240000	8.02040000
38	H	-2.02270000	2.13730000	10.92000000
39	H	-4.91220000	-7.27130000	-2.96190000
40	H	-8.98790000	-7.09310000	-2.37650000
41	H	1.45750000	-2.18460000	-2.95900000
42	H	-5.88650000	0.35320000	-2.87170000
43	H	-6.57060000	-3.25690000	-2.96870000
44	H	-11.74490000	-3.66940000	8.61800000

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 1  H   -9.32890000   0.16850000    8.03140000
 2  H   -8.19140000   3.21540000    6.31880000
 3  H   -5.78340000  -8.84910000   -1.27830000
 4  H   -7.97590000  -9.98270000   -0.17660000
 5  H   -2.11760000   0.35870000   -2.97420000
 6
 7
 8  Z-CH2CH2CH3-to-Z-CH(CH3)2-TS
 9  Si -0.02925819   0.02158213   -0.01731236
10  Si -0.07165848  -0.00588159   5.64848673
11  Si 3.71542050   -0.03169756   2.48700899
12  Si 1.04178338   -3.88641660   2.97903699
13  Al 0.73691235   -0.83466538   2.88317281
14  O   0.28286505   -2.49419839   2.89124862
15  O   2.42396616   -0.66927461   3.16140159
16  O   0.02658353   -0.03297893   1.54983197
17  O  -0.20291416   -0.03222418   4.08019023
18  O  -1.58689135   0.15822008   -0.43401923
19  O  -0.37119389   -1.44893031   6.31136235
20  O   1.35292043   0.50820242    6.21724445
21  O  -1.28245799   0.98299049    6.03566119
22  O   0.81847553   1.28889941    -0.52638951
23  O   3.75051106   1.57352940    2.50106351
24  O   5.00696997   -0.47517200   3.33089280
25  O   2.20484531   -4.03863209   4.10460010
26  O   3.88120909   -0.50035731   0.94881808
27  O   1.75440131   -4.28714966   1.58268355
28  O   0.55557798   -1.27266704   -0.76975826
29  O  -0.15043876   -4.92022534   3.34878199
30  O   0.80120900   -6.00640500   -0.15261600
31  Si -5.49759800   -0.02111700   -1.47430200
32  Si -2.51954000   0.76953400    -1.59086900
33  Si 1.67326300    2.63520200    -0.36440700
34  Si -6.77250000   -2.79180000   -1.55910000
35  Si -6.65860000   -5.43650000   -0.02630000
36  Si -0.62808300   -6.20855200   4.15932100
37  Si -3.21919800   -7.43499000   2.98448000
38  Si -6.09540000   -6.32220000   2.83000000
39  Si -7.79180000   -8.89230000   3.21140000
40  Si -7.85690000   -4.02790000   9.99880000
41  Si -9.54690000   -6.64300000   10.42590000
42  O   -8.68790000   -5.35140000   10.15840000
43  Si 1.78779800    2.30220900    9.72779700
44  Si -0.76979100   -1.62741000   10.29930600
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1	Si	-1.17799800	1.38379600	9.93889800
2	O	-1.38700400	-0.16320200	10.26480000
3	O	0.35020500	1.77508900	10.12160500
4	O	-1.90929900	-2.64050100	10.65650100
5	Si	-2.31670000	-4.06080000	11.29600000
6	Si	-5.02660000	-5.18350000	10.35000000
7	O	-3.83590000	-4.30830000	10.92640000
8	O	-6.34110000	-4.27000000	10.39930000
9	Si	4.73290000	-0.80100500	7.13549900
10	Si	-7.29070000	2.20560000	5.67640000
11	Si	-4.57938700	3.32751800	6.62400700
12	Si	-1.94070000	7.20800000	6.08700000
13	Si	-4.59330000	6.04430000	5.10460000
14	O	-5.77090400	2.45289300	6.04722000
15	O	-3.26560400	2.41446300	6.57328900
16	O	-0.99450000	5.94280000	5.99240000
17	O	-3.27080000	6.91960000	5.26710000
18	O	-4.35770700	4.58889100	5.69438500
19	O	-7.46660000	2.24720000	4.09540000
20	O	-4.88400000	5.95910000	3.53970000
21	Si	-5.99570000	5.67090000	2.42990000
22	Si	-10.73910000	3.90040000	2.70070000
23	O	-11.73290000	2.70740000	2.34160000
24	Si	-12.07420000	1.15480000	2.31840000
25	O	-11.45520000	0.42330000	3.58130000
26	Si	-11.39460000	-4.15760000	7.24580000
27	Si	-13.29570000	-2.46030000	5.52120000
28	Si	-11.50890000	0.09760000	5.13610000
29	Si	-8.83680000	-0.22830000	6.67330000
30	O	-12.44950000	-3.64190000	6.15630000
31	O	-12.41530000	-1.16550000	5.38290000
32	O	-10.03410000	-0.20050000	5.63860000
33	O	-7.69650000	0.78430000	6.31660000
34	Si	-0.05970100	4.78730100	6.54670300
35	O	-10.24280000	-7.11800000	9.08650000
36	Si	-7.71660000	3.11370000	2.78820000
37	O	-6.95550000	4.50240000	2.92570000
38	O	-9.24950000	3.38730000	2.56950000
39	Si	-4.97250000	-7.60980000	-1.50390000
40	Si	-11.35590000	0.26280000	-0.54610000
41	O	-6.84510000	-7.72030000	2.70470000
42	O	-10.35620000	-0.94150000	-0.80140000
43	Si	-9.16490000	-9.40520000	0.52820000
44	Si	-9.33470000	-6.71560000	-0.96890000

1	Si	-11.54680000	-4.63200000	-1.45310000
2	Si	-9.77590000	-2.05450000	-1.77500000
3	O	-9.58580000	-8.00560000	-0.07990000
4	O	-10.67690000	-5.84320000	-0.91270000
5	O	-10.64710000	-3.36120000	-1.66840000
6	O	-8.28390000	-2.37400000	-1.34130000
7	O	-6.40440000	-3.94670000	-0.53100000
8	O	-8.15250000	-5.87130000	-0.34420000
9	O	-8.84920000	-9.23940000	2.07860000
10	O	-6.41640000	-5.42400000	1.54900000
11	O	-5.61290000	-6.41590000	-0.70840000
12	O	-5.77369900	-1.60340100	-1.35130800
13	Si	-6.81090000	-5.43360000	5.68340000
14	Si	-8.50460000	-8.00720000	6.05360000
15	O	-7.72180000	-6.63160000	6.20070000
16	Si	-10.95800000	-7.17850000	7.67890000
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18	O	-11.40780000	-5.74300000	7.18590000
19	O	-8.21960000	-1.69260000	6.70790000
20	O	-9.95660000	-3.63110000	6.85010000
21	O	-9.98360000	-7.83070000	6.60240000
22	O	-7.53000000	-4.04100000	5.99020000
23	O	-7.92320000	-3.54700000	8.50450000
24	Si	0.12370000	4.64450000	-2.14540000
25	Si	-2.82299300	3.84600000	-1.95510300
26	O	-3.94892100	0.19042500	-1.21845500
27	O	0.75580400	3.76930200	-0.98750300
28	O	-1.45550000	4.66540000	-1.97180000
29	O	-2.55360400	2.34859900	-1.49988900
30	O	-6.33219900	0.83849800	-0.42849800
31	O	-3.77030000	4.57610000	-0.90140000
32	Si	-5.28020000	4.78230000	-0.42350000
33	Si	-7.00390000	2.22870000	-0.05400000
34	Si	-9.63060000	2.52380000	-1.72000000
35	O	-6.07880000	3.41370000	-0.57020000
36	O	-8.42830000	2.36750000	-0.70540000
37	O	-10.83220000	1.58900000	-1.25000000
38	O	-5.20960000	5.26350000	1.09860000
39	O	-7.15699800	2.26929900	1.54270100
40	O	-11.46650000	0.47770000	1.01990000
41	O	-6.60040000	-5.49380000	4.09960000
42	O	-8.61720000	-8.44720000	4.51360000
43	O	-1.68267400	1.69084700	8.46851400
44	Si	-1.74892600	2.17157900	6.97412800

1	O	-0.91871600	3.49570800	6.81428400
2	Si	2.50949700	3.95248100	5.10418000
3	Si	2.56680400	1.37877300	6.82675400
4	Si	3.01121500	-3.35756100	7.49347300
5	Si	-0.01130400	-2.57106800	7.40598100
6	O	2.86459500	2.66323700	5.94595200
7	O	3.90011400	0.51782100	6.89190900
8	O	3.77240000	-1.96900000	7.63100000
9	O	1.47828600	-3.08405700	7.27486400
10	O	2.15450100	1.79121900	8.29129500
11	O	-0.24970400	-2.04665300	8.86408300
12	O	1.05379900	4.47370100	5.45679900
13	O	-1.00419000	-3.76440100	7.04720500
14	Si	0.52349700	-7.58779900	-0.03029200
15	Si	-2.45310000	-8.37930000	0.08690000
16	O	-1.02440000	-7.79970000	-0.28570000
17	O	-3.48040000	-7.82240000	-1.00870000
18	O	-2.05275900	-6.52239500	3.54848600
19	O	-4.53619500	-6.55018900	2.91500000
20	O	-2.87429600	-7.94910700	1.53380400
21	O	0.93450000	-7.98310000	1.44400000
22	O	0.37165600	-7.41293000	3.90386900
23	Si	0.95191400	-8.52588600	2.93029300
24	Si	-1.34640500	-5.31660200	7.02370600
25	Si	-4.32960000	-6.05610000	7.41270000
26	O	-2.92290100	-5.44189600	7.01849400
27	O	-5.41450000	-5.45960000	6.41750000
28	O	-4.71840000	-5.65910000	8.88780000
29	O	-1.36620000	-5.12610000	10.61890000
30	O	-0.72730000	-6.04810000	8.28660000
31	Si	-0.78110000	-6.37380000	9.84140000
32	Si	4.19159800	1.79580000	-2.03250100
33	Si	4.36131200	-0.89369800	-0.53531000
34	Si	1.79907800	-4.81758900	0.05479500
35	Si	1.68499100	-2.17148400	-1.47841100
36	Si	3.22788900	3.06048500	2.23970200
37	Si	5.44849000	-1.68950100	4.28209500
38	Si	3.72402200	-4.24269500	4.65118600
39	O	4.61249900	0.39619600	-1.42440600
40	O	1.43102100	-3.66270800	-0.97331400
41	O	3.17919700	-1.73800600	-1.16009000
42	O	4.64900600	-3.05760200	4.13510500
43	O	2.93690900	2.40530000	-1.28878700
44	O	2.15282000	3.10901300	1.07408900

1	O	2.54300400	3.62290900	3.55349800
2	O	5.51820100	-1.20778900	5.80379600
3	O	3.57088500	-4.20200700	6.24789800
4	O	-0.73789000	-5.99420600	5.72550200
5	H	-1.30770000	8.45280000	5.54490000
6	H	3.53900000	4.98890000	5.43620000
7	H	-5.91550000	5.84190000	-1.27060000
8	H	-6.78570000	6.92250000	2.19890000
9	H	-12.70540000	-0.03450000	-1.12450000
10	H	-13.56750000	1.03610000	2.31350000
11	H	-12.61360000	-4.36250000	-0.43650000
12	H	-12.17550000	-5.02190000	-2.75570000
13	H	-14.47190000	-2.17020000	6.40220000
14	H	-13.77040000	-2.92530000	4.17860000
15	H	6.86450100	-1.88259900	3.83330200
16	H	-2.15040000	-4.10050000	12.78420000
17	H	1.31010000	-8.39770000	-1.01480000
18	H	-12.21020000	-7.97290000	7.89080000
19	H	0.36340000	-1.65380000	11.27870000
20	H	0.62130000	6.05740000	-2.14750000
21	H	0.50140000	4.07440000	-3.47820000
22	H	-2.25700000	7.49990000	7.52180000
23	H	-5.73850000	6.73170000	5.78280000
24	H	-10.96700000	4.40130000	4.09400000
25	H	-11.01960000	5.00810000	1.73210000
26	H	-12.06290000	1.27880000	5.87220000
27	H	-10.59640000	-6.34750000	11.45320000
28	H	-8.66420000	-7.73420000	10.94950000
29	H	2.77450500	1.81970800	10.74639900
30	H	1.80019000	3.79900000	9.78439700
31	H	5.77540000	-0.53010000	8.17660000
32	H	3.24710000	-4.17500000	8.72650000
33	H	0.61160000	-6.65520000	10.31590000
34	H	-1.64370000	-7.57580000	10.07620000
35	H	0.12290000	-9.76940000	3.03170000
36	H	2.36090000	-8.82750000	3.33990000
37	H	-10.15040000	3.92860000	-1.73450000
38	H	-9.16390000	2.16210000	-3.09680000
39	H	3.89500000	1.63920000	-3.49250000
40	H	5.32300000	2.73990000	-1.76330000
41	H	4.42880000	3.88350200	1.88700200
42	H	5.61649900	-1.70970100	-0.58829900
43	H	4.35729700	-5.55350200	4.29820300
44	H	3.22919900	-5.21290300	-0.15129900

1	H	-5.23700000	-6.37850000	11.22840000
2	H	-7.76830000	-9.07120000	6.80850000
3	H	-6.95230000	-10.08460000	3.55430000
4	H	-10.29630000	-10.34930000	0.25900000
5	H	-2.42150000	-9.87450000	0.00040000
6	H	-3.42900900	-8.60989300	3.88980700
7	H	-4.28320000	-7.54880000	7.29620000
8	H	-3.45780000	3.89970000	-3.31080000
9	H	0.59910200	5.23699900	7.81469900
10	H	-9.79240000	-1.54060000	-3.18200000
11	H	-8.38790000	-2.95530000	10.89960000
12	H	-4.87448800	3.78241800	8.02039700
13	H	-2.02270000	2.13730000	10.92000000
14	H	-4.91220000	-7.27130000	-2.96190000
15	H	-8.98790000	-7.09310000	-2.37650000
16	H	1.45750400	-2.18460600	-2.95900100
17	H	-5.88650100	0.35320300	-2.87169900
18	H	-6.57060000	-3.25690000	-2.96870000
19	H	-11.74490000	-3.66940000	8.61800000
20	H	-9.32890000	0.16850000	8.03140000
21	H	-8.19140000	3.21540000	6.31880000
22	H	-5.78340000	-8.84910000	-1.27830000
23	H	-7.97590000	-9.98270000	-0.17660000
24	H	-2.11759100	0.35870000	-2.97419700
25	C	-2.48626039	-0.32734024	3.19344764
26	H	-2.84087973	0.26464268	4.03122163
27	H	-1.97958263	0.15295361	2.36307078
28	C	-2.66138369	-1.70533119	3.18330188
29	H	-2.24448164	-2.24228472	2.33541068
30	C	-3.20226201	-2.49639386	4.32214414
31	H	-2.32535621	-2.88462572	4.85242551
32	H	-3.77299802	-1.88687891	5.02328617
33	H	-3.79405100	-3.34608293	3.98207013
34	H	-3.55915475	-0.89275231	2.64601271
35				
36				
37	Z-CH2CH2CH3			
38	Si	-3.86075355	2.17612569	3.05937090
39	Si	-3.82939769	-0.74876304	-1.85033034
40	Si	-7.28800080	-0.35049296	1.61496256
41	Si	-3.46000839	-2.86914647	2.50797824
42	Al	-4.30201732	-0.18941437	1.05669685
43	O	-3.10022712	-1.37389891	1.81334877
44	O	-5.83053011	-0.93115236	1.26372474

1	O	-3.99877215	1.29900278	1.76837240
2	O	-3.74503791	0.05006144	-0.50414120
3	O	-2.44845983	2.94272694	3.06014142
4	O	-3.04527664	-2.15597603	-1.76792913
5	O	-5.35416517	-1.08703168	-2.29093456
6	O	-3.08866229	0.21432523	-2.88315006
7	O	-5.10006073	3.19267525	3.09071735
8	O	-7.78331698	0.93464601	0.79068863
9	O	-8.36072370	-1.49958521	1.29076284
10	O	-4.51446157	-3.81675326	1.76464174
11	O	-7.34696280	0.03340264	3.17710360
12	O	-3.97232043	-2.62111124	4.00009886
13	O	-3.90832114	1.29068772	4.40620450
14	O	-1.99757410	-3.51473928	2.45399815
15	C	-1.69635751	-0.79876450	1.97682153
16	H	-1.27699888	-1.27955145	2.85637503
17	H	-1.86332340	0.25423363	2.18257654
18	C	-0.84081583	-0.99658003	0.74563961
19	H	-1.29693177	-0.47687596	-0.09622420
20	H	-0.79040252	-2.05509488	0.48688896
21	C	0.56645194	-0.44188928	1.00655974
22	H	1.06963627	-0.97744960	1.81525942
23	H	1.18064941	-0.54202727	0.11015738
24	H	0.53635262	0.61860086	1.27037322
25	O	-2.44912762	-2.89130839	6.15194238
26	Si	1.27929234	4.53538210	3.29049902
27	Si	-1.78313384	4.31369872	3.57250937
28	Si	-6.37307734	3.90133996	2.41621542
29	Si	3.46633400	2.74162300	4.43426600
30	Si	4.30498600	-0.19963600	4.38378600
31	Si	-1.06234795	-4.80272379	2.26620567
32	Si	1.80174640	-4.39529284	3.37452798
33	Si	4.08535500	-2.53573600	2.44613200
34	Si	6.59134300	-4.27499300	3.01505000
35	Si	4.87050900	-3.78637500	-5.14187400
36	Si	7.38651500	-5.58701100	-4.58988500
37	O	6.12143600	-4.67645100	-4.80925800
38	Si	-6.40481046	-1.52529686	-6.10021715
39	Si	-2.60691855	-4.18979157	-5.21358821
40	Si	-3.30821592	-1.45816942	-6.40109974
41	O	-2.55790207	-2.80404173	-5.99031090
42	O	-4.87565081	-1.70665968	-6.45849756
43	O	-1.18077943	-4.83542064	-5.25528322
44	Si	-0.29239400	-6.17744400	-5.21147500

1	Si	2.64424100	-5.76609500	-4.37129800
2	O	1.21573500	-5.72113900	-5.05928700
3	O	3.54162700	-4.65127700	-5.09011700
4	Si	-8.02385450	-3.61324618	-1.85250159
5	Si	2.11832900	3.24931400	-4.25596600
6	Si	-0.81933901	2.83609090	-5.09687302
7	Si	-4.67538800	5.41856400	-5.97493500
8	Si	-1.77729100	5.79775500	-5.07335800
9	O	0.60970700	2.79205500	-4.40898100
10	O	-1.71624697	1.72237793	-4.37712109
11	O	-5.10237154	4.15716099	-5.11964937
12	O	-3.32692000	6.01231800	-5.38023500
13	O	-1.47595300	4.25470200	-4.85032600
14	O	2.27463900	4.13954100	-2.94627300
15	O	-1.46831100	6.61313100	-3.73905300
16	Si	-0.32236200	7.28695700	-2.85398100
17	Si	4.73910800	7.18555700	-3.13520200
18	O	6.09730700	6.71393700	-2.44766200
19	Si	6.97464200	5.58151100	-1.75810700
20	O	6.65468100	4.16118500	-2.38537800
21	Si	8.23026000	-1.40377500	-3.36805200
22	Si	9.40087400	1.42288200	-3.03800500
23	Si	6.81495300	3.12636100	-3.58112800
24	Si	4.43227800	1.26091200	-4.25364100
25	O	9.03378800	-0.11088500	-2.86950400
26	O	8.11409100	2.26383900	-3.36621400
27	O	5.54401500	2.17724400	-3.59844700
28	O	3.00557500	1.90563100	-4.21198900
29	Si	-5.56114463	2.65813575	-4.87733403
30	O	8.21280800	-5.07498300	-3.34130200
31	Si	2.20194500	5.57735200	-2.27581800
32	O	0.99141900	6.39059500	-2.90821800
33	O	3.53461900	6.38057600	-2.50226700
34	Si	3.52081000	-1.71752000	6.99732000
35	Si	6.63852800	6.09671000	1.26490100
36	O	5.28857300	-3.36624800	3.07458300
37	O	6.14044000	4.94941500	2.23985600
38	Si	8.06918300	-2.90274800	5.31308600
39	Si	7.26636200	0.07373100	5.30118800
40	Si	8.58246700	2.67731400	4.32218500
41	Si	6.00404000	4.36937800	3.71239300
42	O	7.96089100	-1.33824300	5.09763700
43	O	8.20435300	1.16050500	4.59067000
44	O	7.28666600	3.53210400	4.07524700

1	O	4.72506900	3.43267100	3.76766100
2	O	3.53391000	1.17706500	4.16247000
3	O	5.85668900	0.07192100	4.58459300
4	O	7.70793500	-3.65360700	3.95787100
5	O	4.06737400	-1.06385400	3.06581200
6	O	3.68497200	-0.96346800	5.62882300
7	O	2.10581300	3.28480800	3.88018300
8	Si	4.42013100	-3.04889900	-0.56518600
9	Si	6.92491000	-4.78611700	0.01553800
10	O	5.69881000	-3.99497000	-0.61490200
11	Si	8.90823100	-4.18886200	-2.23329200
12	Si	5.13339800	-1.46937600	-3.06644400
13	O	8.81345900	-2.64499900	-2.57024500
14	O	4.38331500	-0.12497000	-3.47695500
15	O	6.70094300	-1.22207600	-3.00777400
16	O	8.23876300	-4.46724000	-0.81625600
17	O	4.58842100	-1.86264000	-1.62113800
18	O	4.76606100	-2.62042800	-4.09389900
19	Si	-5.64171964	6.89932357	2.71291253
20	Si	-2.60568492	7.06754686	2.37694823
21	O	-0.24282504	4.09899578	3.25868201
22	O	-5.92076951	5.41237427	2.24655751
23	O	-4.17638300	7.31424200	2.25925500
24	O	-2.32020336	5.54859805	2.74207778
25	O	1.74381200	4.95322400	1.82794000
26	O	-1.98945100	7.41183600	0.94783000
27	Si	-0.65713800	7.80011900	0.15733600
28	Si	1.86843500	6.08858800	0.72362800
29	Si	4.22042400	7.98065700	1.53011400
30	O	0.58118200	7.01926700	0.78118100
31	O	3.15036200	6.96959100	0.95384900
32	O	5.67580200	7.35990100	1.34268500
33	O	-0.90310300	7.39289200	-1.36811300
34	O	1.98941700	5.35784700	-0.69972100
35	O	6.65726500	5.50871800	-0.20638600
36	O	4.25259200	-2.35815400	0.86700100
37	O	7.19531300	-4.32371800	1.52912600
38	O	-2.94116620	-0.30926299	-5.37331807
39	Si	-3.04571468	0.85673291	-4.32545532
40	O	-4.29606840	1.74753146	-4.65802379
41	Si	-7.65107914	1.92749261	-2.76135975
42	Si	-6.78619807	-1.03552331	-3.01934503
43	Si	-5.49903158	-5.32197820	-1.27456679
44	Si	-2.96177293	-3.71388823	-2.13393154

1	O	-7.52227221	0.35346283	-2.81209062
2	O	-7.72045395	-2.17202765	-2.42077274
3	O	-6.70960900	-4.50886500	-1.90690500
4	O	-4.16634055	-4.51879755	-1.50102942
5	O	-6.55648819	-1.32014775	-4.55295246
6	O	-2.93472968	-3.95877174	-3.68215560
7	O	-6.48220035	2.61617117	-3.58273480
8	O	-1.60433476	-4.18624180	-1.44625120
9	Si	-1.62141292	-4.14035384	6.74156866
10	Si	1.44001500	-3.92009900	6.45964900
11	O	-0.09984100	-3.70453600	6.77321700
12	O	2.20299200	-2.59946100	6.94914000
13	O	0.38252008	-4.30647939	2.67500716
14	O	2.71233900	-3.24249600	2.77113900
15	O	1.67158300	-4.17874200	4.93142100
16	O	-1.86928200	-5.33341600	5.73465200
17	O	-1.56061955	-5.95003282	3.24116721
18	Si	-1.69688044	-6.53006032	4.71368516
19	Si	-0.72626848	-5.31792886	-0.75681113
20	Si	2.32134700	-5.19177000	-1.29869900
21	O	0.78966100	-4.93062500	-0.98696000
22	O	3.12335500	-3.87249700	-0.92514200
23	O	2.53450800	-5.50141900	-2.82950800
24	O	-0.79269500	-6.98361700	-3.94792300
25	O	-1.04634700	-6.73827500	-1.38406500
26	Si	-0.88598200	-7.77306900	-2.57983400
27	Si	-8.41201459	3.29697023	4.71890606
28	Si	-7.60899857	0.32061304	4.73079871
29	Si	-3.80888079	-2.34728098	5.59773485
30	Si	-4.64765503	0.59525401	5.64787466
31	Si	-7.98762910	2.44293010	0.26152608
32	Si	-8.35878128	-3.10009727	1.15873589
33	Si	-5.83257828	-4.81080009	1.72502334
34	O	-8.30360321	1.73251567	4.93446573
35	O	-3.87666808	-0.78281268	5.86979742
36	O	-6.19944052	0.32252429	5.44747240
37	O	-7.11980608	-3.88011396	1.78242013
38	O	-7.46374672	3.79644071	3.55692952
39	O	-6.99582913	3.40405452	1.04230518
40	O	-7.55675875	2.43922637	-1.26364994
41	O	-8.60405940	-3.50641139	-0.36678091
42	O	-5.71166188	-5.54148764	0.30163263
43	O	-1.04429076	-5.39150086	0.79502989
44	H	-5.71152500	6.50046100	-5.97774200

1	H	-8.98615900	2.27588400	-3.34513200
2	H	-0.44194400	9.27839300	0.26839800
3	H	-0.03473600	8.65460300	-3.39321900
4	H	8.00720300	6.56668100	1.65212200
5	H	8.41059600	5.94834100	-1.97612400
6	H	9.47615400	2.70661300	3.12025600
7	H	9.31526900	3.21844200	5.51140100
8	H	10.38982900	1.57128200	-4.15322300
9	H	10.01720800	1.87646300	-1.75016400
10	H	-9.60832982	-3.46365157	1.90046200
11	H	-0.44001000	-7.01607600	-6.44390200
12	H	-2.05933000	-4.53449400	8.11882300
13	H	10.36145700	-4.55003900	-2.27408300
14	H	-3.65910071	-5.05718060	-5.83374526
15	H	-6.61418900	7.88397100	2.14033000
16	H	-5.78257400	7.00078800	4.20087200
17	H	-4.49185700	5.02247800	-7.40788100
18	H	-0.95933300	6.35924900	-6.19568900
19	H	4.76513000	6.95148700	-4.61461400
20	H	4.60652200	8.65495400	-2.87605400
21	H	6.90334800	3.87374200	-4.87635000
22	H	8.25465400	-5.54755000	-5.81008700
23	H	6.95334400	-7.00267400	-4.36120700
24	H	-7.15634592	-2.73448963	-6.56606746
25	H	-6.95537062	-0.35345780	-6.85349016
26	H	-9.09871400	-4.24483500	-2.68317000
27	H	-5.43051200	-6.67829000	-1.90691200
28	H	-2.08620600	-8.66925100	-2.59621500
29	H	0.35035500	-8.59382300	-2.37527100
30	H	-0.47636400	-7.32682600	5.05904100
31	H	-2.90476300	-7.41456200	4.76579800
32	H	4.19983800	9.27846400	0.78235900
33	H	3.92143300	8.24482000	2.97407900
34	H	-8.07217900	4.00351200	5.99557800
35	H	-9.80847000	3.57162900	4.25212500
36	H	-9.40236636	2.91413585	0.40053315
37	H	-8.48614529	-0.69562840	5.39567746
38	H	-5.95007080	-5.88138728	2.76616200
39	H	-4.99997317	-3.00116812	6.22858770
40	H	3.26665400	-7.10877900	-4.60299300
41	H	6.61748800	-6.25222900	0.00481100
42	H	6.23568400	-5.66697200	3.43910200
43	H	9.46576700	-3.17735400	5.77999300
44	H	1.94907300	-5.08903700	7.24612800

1	H	2.41624800	-5.73564900	3.11026800
2	H	2.81583300	-6.34802400	-0.48479600
3	H	-2.02662700	7.99445400	3.40130800
4	H	-6.34339725	2.17341574	-6.05937773
5	H	5.84085600	5.50222600	4.67885100
6	H	4.97578500	-3.21707100	-6.52342400
7	H	-0.71407100	2.58411500	-6.56976600
8	H	-2.79578100	-1.08978400	-7.75961700
9	H	3.34933400	-0.72356900	8.10485800
10	H	7.08506100	0.37773900	6.75680600
11	H	-4.42427431	1.40650341	6.88735215
12	H	1.51373700	5.66575100	4.24512100
13	H	3.45175900	3.02078000	5.90597000
14	H	8.37514400	-1.59965900	-4.84609800
15	H	4.74241800	1.04230700	-5.70280400
16	H	2.59230100	4.01310900	-5.45413200
17	H	4.72237900	-2.57953900	7.23705800
18	H	7.17092600	-3.37579500	6.41460000
19	H	-2.00408322	4.56157203	5.03320554
20				
21				
22	Z-CH3 methylation-TS			
23	Si	-0.04619859	-0.00583903	-0.01369929
24	Si	-0.06237300	-0.00051156	5.65480152
25	Si	3.72078699	-0.04882626	2.48711613
26	Si	1.03988035	-3.89763891	2.99492447
27	Al	0.75699937	-0.82776428	2.92022288
28	O	0.24210468	-2.50309663	3.04056100
29	O	2.45856663	-0.78665972	3.12074375
30	O	-0.00439543	-0.23353858	1.53023316
31	O	-0.11428939	0.04118131	4.08944474
32	O	-1.58967078	0.15684615	-0.44239565
33	O	-0.36588576	-1.46826185	6.28168160
34	O	1.36508773	0.47616846	6.25657576
35	O	-1.26905023	0.96850293	6.06858793
36	O	0.81821574	1.28396656	-0.43275125
37	O	3.68902117	1.55391895	2.53146930
38	O	5.01777870	-0.46504811	3.33654630
39	O	2.20264152	-4.07195693	4.10031877
40	O	3.90730109	-0.48334892	0.94573434
41	O	1.71163798	-4.22016238	1.56486101
42	O	0.54007414	-1.25021139	-0.84739679
43	O	-0.16065822	-4.93686587	3.31126353
44	C	-1.89212287	-2.35685198	3.08735880

1	H	-1.75282239	-1.53834586	2.40125253
2	H	-1.78502996	-2.18354999	4.14716209
3	H	-1.96910725	-3.37530272	2.74378361
4	C	-4.00508972	-1.76973336	3.75001831
5	H	-4.18584921	-2.41088745	4.60566990
6	H	-3.79630586	-0.72554508	3.95534978
7	C	-4.12685691	-2.23530227	2.48946888
8	H	-4.02048555	-1.58389020	1.62924831
9	H	-4.41272702	-3.26207269	2.29170072
10	O	0.80122100	-6.00641400	-0.15262000
11	Si	-5.49760600	-0.02107600	-1.47428500
12	Si	-2.51928400	0.76951600	-1.59090100
13	Si	1.67079800	2.63419300	-0.36391000
14	Si	-6.77250100	-2.79180000	-1.55910200
15	Si	-6.65860000	-5.43650000	-0.02630000
16	Si	-0.62804600	-6.20853200	4.15918600
17	Si	-3.21920800	-7.43500200	2.98451900
18	Si	-6.09540000	-6.32220000	2.83000000
19	Si	-7.79180000	-8.89230000	3.21140000
20	Si	-7.85690000	-4.02790000	9.99880000
21	Si	-9.54690000	-6.64300000	10.42590000
22	O	-8.68790000	-5.35140000	10.15840000
23	Si	1.78780500	2.30219000	9.72780400
24	Si	-0.76981200	-1.62740400	10.29929800
25	Si	-1.17799500	1.38378700	9.93889500
26	O	-1.38698700	-0.16319500	10.26480200
27	O	0.35019500	1.77511000	10.12159500
28	O	-1.90930600	-2.64049400	10.65649600
29	Si	-2.31670000	-4.06080000	11.29600000
30	Si	-5.02660000	-5.18350000	10.35000000
31	O	-3.83590000	-4.30830000	10.92640000
32	O	-6.34110000	-4.27000000	10.39930000
33	Si	4.73289900	-0.80104500	7.13549900
34	Si	-7.29070000	2.20560000	5.67640000
35	Si	-4.57939700	3.32750400	6.62399200
36	Si	-1.94070000	7.20800000	6.08700000
37	Si	-4.59330000	6.04430000	5.10460000
38	O	-5.77090000	2.45290000	6.04720000
39	O	-3.26549900	2.41430800	6.57330100
40	O	-0.99450100	5.94280100	5.99240400
41	O	-3.27080000	6.91960000	5.26710000
42	O	-4.35770000	4.58890000	5.69440000
43	O	-7.46660000	2.24719900	4.09540000
44	O	-4.88400000	5.95910000	3.53970000

1	Si	-5.99570000	5.67090000	2.42990000
2	Si	-10.73910000	3.90040000	2.70070000
3	O	-11.73290000	2.70740000	2.34160000
4	Si	-12.07420000	1.15480000	2.31840000
5	O	-11.45520000	0.42330000	3.58130000
6	Si	-11.39460000	-4.15760000	7.24580000
7	Si	-13.29570000	-2.46030000	5.52120000
8	Si	-11.50890000	0.09760000	5.13610000
9	Si	-8.83679800	-0.22830100	6.67329700
10	O	-12.44950000	-3.64190000	6.15630000
11	O	-12.41530000	-1.16550000	5.38290000
12	O	-10.03410000	-0.20050000	5.63859900
13	O	-7.69650000	0.78430200	6.31660100
14	Si	-0.05969600	4.78729800	6.54670400
15	O	-10.24280000	-7.11800000	9.08650000
16	Si	-7.71660000	3.11370000	2.78820000
17	O	-6.95550000	4.50240000	2.92570000
18	O	-9.24950000	3.38730000	2.56950000
19	Si	-4.97250000	-7.60980000	-1.50390000
20	Si	-11.35590000	0.26280000	-0.54610000
21	O	-6.84510000	-7.72030000	2.70470000
22	O	-10.35620000	-0.94150000	-0.80140000
23	Si	-9.16490000	-9.40520000	0.52820000
24	Si	-9.33470000	-6.71560000	-0.96890000
25	Si	-11.54680000	-4.63200000	-1.45310000
26	Si	-9.77590000	-2.05450000	-1.77500000
27	O	-9.58580000	-8.00560000	-0.07990000
28	O	-10.67690000	-5.84320000	-0.91270000
29	O	-10.64710000	-3.36120000	-1.66840000
30	O	-8.28390000	-2.37400000	-1.34130000
31	O	-6.40439900	-3.94669900	-0.53099900
32	O	-8.15250000	-5.87130000	-0.34420000
33	O	-8.84920000	-9.23940000	2.07860000
34	O	-6.41640000	-5.42400000	1.54900000
35	O	-5.61290000	-6.41590000	-0.70840000
36	O	-5.77370000	-1.60340000	-1.35129900
37	Si	-6.81090000	-5.43360000	5.68340000
38	Si	-8.50460000	-8.00720000	6.05360000
39	O	-7.72180000	-6.63160000	6.20070000
40	Si	-10.95800000	-7.17850000	7.67890000
41	Si	-8.42889900	-3.23820000	7.03330000
42	O	-11.40780000	-5.74300000	7.18590000
43	O	-8.21959700	-1.69259900	6.70789900
44	O	-9.95660000	-3.63110000	6.85010000

1	O	-9.98360000	-7.83070000	6.60240000
2	O	-7.53000000	-4.04100000	5.99020000
3	O	-7.92320000	-3.54700000	8.50450000
4	Si	0.12322800	4.64409000	-2.14545100
5	Si	-2.82306900	3.84599700	-1.95507000
6	O	-3.94896200	0.19035300	-1.21852800
7	O	0.75695300	3.77013800	-0.98767000
8	O	-1.45550000	4.66540000	-1.97180000
9	O	-2.55349200	2.34860600	-1.49996000
10	O	-6.33220000	0.83850000	-0.42850000
11	O	-3.77030000	4.57610000	-0.90140000
12	Si	-5.28020000	4.78230000	-0.42350000
13	Si	-7.00390000	2.22870000	-0.05400000
14	Si	-9.63060000	2.52380000	-1.72000000
15	O	-6.07880000	3.41370000	-0.57020000
16	O	-8.42830000	2.36750000	-0.70540000
17	O	-10.83220000	1.58900000	-1.25000000
18	O	-5.20960000	5.26350000	1.09860000
19	O	-7.15700000	2.26930000	1.54270000
20	O	-11.46650000	0.47770000	1.01990000
21	O	-6.60040000	-5.49380000	4.09960000
22	O	-8.61720000	-8.44720000	4.51360000
23	O	-1.68270300	1.69082600	8.46850900
24	Si	-1.74890600	2.17174000	6.97412700
25	O	-0.91868800	3.49569400	6.81431500
26	Si	2.50950500	3.95251700	5.10420800
27	Si	2.56677900	1.37896500	6.82674400
28	Si	3.01120300	-3.35761700	7.49351800
29	Si	-0.01122900	-2.57096500	7.40596500
30	O	2.86461900	2.66318300	5.94588200
31	O	3.90009600	0.51779700	6.89195000
32	O	3.77240000	-1.96900000	7.63100000
33	O	1.47830600	-3.08397400	7.27476900
34	O	2.15449900	1.79117300	8.29130700
35	O	-0.24972000	-2.04669800	8.86409600
36	O	1.05379600	4.47370200	5.45679600
37	O	-1.00420000	-3.76439500	7.04719000
38	Si	0.52349600	-7.58779800	-0.03028800
39	Si	-2.45310000	-8.37930000	0.08690000
40	O	-1.02440000	-7.79970000	-0.28570000
41	O	-3.48040000	-7.82240000	-1.00870000
42	O	-2.05278500	-6.52240100	3.54846500
43	O	-4.53620000	-6.55020000	2.91500000
44	O	-2.87430000	-7.94910000	1.53380000

1	O	0.93450000	-7.98310000	1.44400000
2	O	0.37168300	-7.41291600	3.90390900
3	Si	0.95190700	-8.52589400	2.93029700
4	Si	-1.34639200	-5.31658500	7.02371100
5	Si	-4.32960000	-6.05610000	7.41270000
6	O	-2.92290000	-5.44189700	7.01849700
7	O	-5.41450000	-5.45960000	6.41750000
8	O	-4.71840000	-5.65910000	8.88780000
9	O	-1.36620000	-5.12610000	10.61890000
10	O	-0.72730000	-6.04810000	8.28660000
11	Si	-0.78110000	-6.37380000	9.84140000
12	Si	4.19136000	1.79565900	-2.03280500
13	Si	4.36127700	-0.89372000	-0.53528000
14	Si	1.79916100	-4.81764600	0.05471200
15	Si	1.68560700	-2.17103900	-1.47839500
16	Si	3.22757900	3.05991400	2.23998500
17	Si	5.44840200	-1.68949100	4.28207100
18	Si	3.72401600	-4.24268000	4.65115500
19	O	4.61251500	0.39622100	-1.42436600
20	O	1.43068300	-3.66258800	-0.97316200
21	O	3.17927600	-1.73818900	-1.16016400
22	O	4.64905800	-3.05762900	4.13511500
23	O	2.93740600	2.40542800	-1.28813800
24	O	2.15409200	3.10993100	1.07333900
25	O	2.54298400	3.62284300	3.55351600
26	O	5.51822400	-1.20772500	5.80377500
27	O	3.57087200	-4.20201400	6.24789800
28	O	-0.73793800	-5.99422600	5.72550100
29	H	-1.30770000	8.45280000	5.54490000
30	H	3.53900000	4.98890000	5.43620000
31	H	-5.91550000	5.84190000	-1.27060000
32	H	-6.78570000	6.92250000	2.19890000
33	H	-12.70540000	-0.03450000	-1.12450000
34	H	-13.56750000	1.03610000	2.31350000
35	H	-12.61360000	-4.36250000	-0.43650000
36	H	-12.17550000	-5.02190000	-2.75570000
37	H	-14.47190000	-2.17020000	6.40220000
38	H	-13.77040000	-2.92530000	4.17860000
39	H	6.86450400	-1.88259800	3.83330900
40	H	-2.15040000	-4.10050000	12.78420000
41	H	1.31010000	-8.39770000	-1.01480000
42	H	-12.21020000	-7.97290000	7.89080000
43	H	0.36339800	-1.65381000	11.27870300
44	H	0.62130000	6.05740000	-2.14750000

1	H	0.50140000	4.07440000	-3.47820000
2	H	-2.25700000	7.49990000	7.52180000
3	H	-5.73850000	6.73170000	5.78280000
4	H	-10.96700000	4.40130000	4.09400000
5	H	-11.01960000	5.00810000	1.73210000
6	H	-12.06290000	1.27880000	5.87220000
7	H	-10.59640000	-6.34750000	11.45320000
8	H	-8.66420000	-7.73420000	10.94950000
9	H	2.77449700	1.81969500	10.74640100
10	H	1.80020600	3.79900000	9.78440200
11	H	5.77540000	-0.53010000	8.17660000
12	H	3.24710000	-4.17500000	8.72650000
13	H	0.61160000	-6.65520000	10.31590000
14	H	-1.64370000	-7.57580000	10.07620000
15	H	0.12290000	-9.76940000	3.03170000
16	H	2.36090000	-8.82750000	3.33990000
17	H	-10.15040000	3.92860000	-1.73450000
18	H	-9.16390000	2.16210000	-3.09680000
19	H	3.89500000	1.63920000	-3.49250000
20	H	5.32300000	2.73990000	-1.76330000
21	H	4.42879100	3.88353600	1.88705100
22	H	5.61650800	-1.70968700	-0.58830800
23	H	4.35728500	-5.55351200	4.29821600
24	H	3.22920000	-5.21290700	-0.15128900
25	H	-5.23700000	-6.37850000	11.22840000
26	H	-7.76830000	-9.07120000	6.80850000
27	H	-6.95230000	-10.08460000	3.55430000
28	H	-10.29630000	-10.34930000	0.25900000
29	H	-2.42150000	-9.87450000	0.00040000
30	H	-3.42900000	-8.60990000	3.88980000
31	H	-4.28320000	-7.54880000	7.29620000
32	H	-3.45780000	3.89970000	-3.31080000
33	H	0.59910200	5.23699800	7.81469900
34	H	-9.79240000	-1.54060000	-3.18200000
35	H	-8.38790000	-2.95530000	10.89960000
36	H	-4.87450000	3.78240000	8.02040000
37	H	-2.02270000	2.13730000	10.92000000
38	H	-4.91220000	-7.27130000	-2.96190000
39	H	-8.98790000	-7.09310000	-2.37650000
40	H	1.45738000	-2.18476500	-2.95898000
41	H	-5.88650000	0.35320000	-2.87170000
42	H	-6.57060000	-3.25690000	-2.96870000
43	H	-11.74490000	-3.66940000	8.61800000
44	H	-9.32890000	0.16850000	8.03140000

1	H	-8.19140000	3.21540000	6.31880000
2	H	-5.78340000	-8.84910000	-1.27830000
3	H	-7.97590000	-9.98270000	-0.17660000
4	H	-2.11765800	0.35871300	-2.97422000
5				
6				
7	Z-CH3			
8	Si	-0.04424669	-0.00370807	-0.03385487
9	Si	-0.05802245	-0.00194169	5.66630226
10	Si	3.70692351	-0.07345455	2.48712971
11	Si	1.05370941	-3.91691443	2.99255723
12	Al	0.77854854	-0.76835738	2.91278141
13	O	0.14737431	-2.49975564	3.04412213
14	O	2.47012452	-0.91359437	3.07826683
15	O	0.04741236	-0.24629086	1.50648970
16	O	-0.07172201	0.06068520	4.09734925
17	O	-1.58195243	0.17153356	-0.43959101
18	O	-0.33998557	-1.48062401	6.26375566
19	O	1.37865524	0.46217859	6.25629318
20	O	-1.25379472	0.96945849	6.07420066
21	O	0.83612930	1.27615198	-0.44352066
22	O	3.59846330	1.52433648	2.55805504
23	O	5.00131654	-0.45735453	3.35268040
24	O	2.20037237	-3.99173928	4.10111680
25	O	3.92475169	-0.47527206	0.94632918
26	O	1.69725350	-4.15650685	1.55182688
27	O	0.53147222	-1.25831861	-0.85827116
28	O	-0.12468750	-4.94478509	3.31297869
29	O	0.80133166	-6.00647601	-0.15279746
30	Si	-5.49760387	-0.02108440	-1.47428973
31	Si	-2.51910288	0.76907537	-1.59036439
32	Si	1.67286868	2.63505913	-0.36444097
33	Si	-6.77250000	-2.79180000	-1.55910000
34	Si	-6.65860000	-5.43650000	-0.02630000
35	Si	-0.62800661	-6.20816974	4.15919385
36	Si	-3.21923027	-7.43500711	2.98457484
37	Si	-6.09540000	-6.32220000	2.83000000
38	Si	-7.79180000	-8.89230000	3.21140000
39	Si	-7.85690000	-4.02790000	9.99880000
40	Si	-9.54690000	-6.64300000	10.42590000
41	O	-8.68790000	-5.35140000	10.15840000
42	Si	1.78781600	2.30218600	9.72780900
43	Si	-0.76980886	-1.62740248	10.29929895
44	Si	-1.17800792	1.38382247	9.93890713

1	O	-1.38699000	-0.16319600	10.26480100
2	O	0.35018900	1.77512200	10.12159000
3	O	-1.90930600	-2.64049400	10.65649700
4	Si	-2.31670000	-4.06080000	11.29600000
5	Si	-5.02660000	-5.18350000	10.35000000
6	O	-3.83590000	-4.30830000	10.92640000
7	O	-6.34110000	-4.27000000	10.39930000
8	Si	4.73289695	-0.80096186	7.13546985
9	Si	-7.29070000	2.20560000	5.67640000
10	Si	-4.57940648	3.32748983	6.62401754
11	Si	-1.94070000	7.20800000	6.08700000
12	Si	-4.59330000	6.04430000	5.10460000
13	O	-5.77090000	2.45290000	6.04720000
14	O	-3.26560187	2.41456855	6.57334741
15	O	-0.99449900	5.94279900	5.99239600
16	O	-3.27080000	6.91960000	5.26710000
17	O	-4.35770000	4.58890000	5.69440000
18	O	-7.46660000	2.24720000	4.09540000
19	O	-4.88400000	5.95910000	3.53970000
20	Si	-5.99570000	5.67090000	2.42990000
21	Si	-10.73910000	3.90040000	2.70070000
22	O	-11.73290000	2.70740000	2.34160000
23	Si	-12.07420000	1.15480000	2.31840000
24	O	-11.45520000	0.42330000	3.58130000
25	Si	-11.39460000	-4.15760000	7.24580000
26	Si	-13.29570000	-2.46030000	5.52120000
27	Si	-11.50890000	0.09760000	5.13610000
28	Si	-8.83680000	-0.22830000	6.67330000
29	O	-12.44950000	-3.64190000	6.15630000
30	O	-12.41530000	-1.16550000	5.38290000
31	O	-10.03410000	-0.20050000	5.63860000
32	O	-7.69650000	0.78430000	6.31660000
33	Si	-0.05969900	4.78730300	6.54672400
34	O	-10.24280000	-7.11800000	9.08650000
35	Si	-7.71660000	3.11370000	2.78820000
36	O	-6.95550000	4.50240000	2.92570000
37	O	-9.24950000	3.38730000	2.56950000
38	Si	-4.97250000	-7.60980000	-1.50390000
39	Si	-11.35590000	0.26280000	-0.54610000
40	O	-6.84510000	-7.72030000	2.70470000
41	O	-10.35620000	-0.94150000	-0.80140000
42	Si	-9.16490000	-9.40520000	0.52820000
43	Si	-9.33470000	-6.71560000	-0.96890000
44	Si	-11.54680000	-4.63200000	-1.45310000

1	Si	-9.77590000	-2.05450000	-1.77500000
2	O	-9.58580000	-8.00560000	-0.07990000
3	O	-10.67690000	-5.84320000	-0.91270000
4	O	-10.64710000	-3.36120000	-1.66840000
5	O	-8.28390000	-2.37400000	-1.34130000
6	O	-6.40440000	-3.94670000	-0.53100000
7	O	-8.15250000	-5.87130000	-0.34420000
8	O	-8.84920000	-9.23940000	2.07860000
9	O	-6.41640000	-5.42400000	1.54900000
10	O	-5.61290000	-6.41590000	-0.70840000
11	O	-5.77370000	-1.60340000	-1.35130000
12	Si	-6.81090000	-5.43360000	5.68340000
13	Si	-8.50460000	-8.00720000	6.05360000
14	O	-7.72180000	-6.63160000	6.20070000
15	Si	-10.95800000	-7.17850000	7.67890000
16	Si	-8.42890000	-3.23820000	7.03330000
17	O	-11.40780000	-5.74300000	7.18590000
18	O	-8.21960000	-1.69260000	6.70790000
19	O	-9.95660000	-3.63110000	6.85010000
20	O	-9.98360000	-7.83070000	6.60240000
21	O	-7.53000000	-4.04100000	5.99020000
22	O	-7.92320000	-3.54700000	8.50450000
23	Si	0.12365890	4.64446444	-2.14540445
24	Si	-2.82299182	3.84600020	-1.95510383
25	O	-3.94896099	0.19046586	-1.21863309
26	O	0.75595546	3.76941785	-0.98751563
27	O	-1.45550000	4.66540000	-1.97180000
28	O	-2.55362815	2.34860666	-1.50001881
29	O	-6.33220000	0.83850000	-0.42850000
30	O	-3.77030000	4.57610000	-0.90140000
31	Si	-5.28020000	4.78230000	-0.42350000
32	Si	-7.00390000	2.22870000	-0.05400000
33	Si	-9.63060000	2.52380000	-1.72000000
34	O	-6.07880000	3.41370000	-0.57020000
35	O	-8.42830000	2.36750000	-0.70540000
36	O	-10.83220000	1.58900000	-1.25000000
37	O	-5.20960000	5.26350000	1.09860000
38	O	-7.15700000	2.26930000	1.54270000
39	O	-11.46650000	0.47770000	1.01990000
40	O	-6.60040000	-5.49380000	4.09960000
41	O	-8.61720000	-8.44720000	4.51360000
42	O	-1.68268048	1.69081843	8.46850483
43	Si	-1.74882926	2.17136469	6.97378474
44	O	-0.91870989	3.49571693	6.81439201

1	Si	2.50951282	3.95256064	5.10425743
2	Si	2.56655417	1.37886580	6.82672486
3	Si	3.01134077	-3.35747144	7.49346513
4	Si	-0.01128611	-2.57102562	7.40589287
5	O	2.86464355	2.66311166	5.94588615
6	O	3.90010915	0.51781921	6.89195368
7	O	3.77240000	-1.96900000	7.63100000
8	O	1.47826890	-3.08412599	7.27493907
9	O	2.15456451	1.79119218	8.29132009
10	O	-0.24968124	-2.04670291	8.86410405
11	O	1.05379000	4.47370400	5.45678900
12	O	-1.00410079	-3.76441598	7.04698036
13	Si	0.52346610	-7.58778742	-0.03021190
14	Si	-2.45310000	-8.37930000	0.08690000
15	O	-1.02440000	-7.79970000	-0.28570000
16	O	-3.48040000	-7.82240000	-1.00870000
17	O	-2.05273932	-6.52245985	3.54838944
18	O	-4.53620000	-6.55020000	2.91500000
19	O	-2.87430000	-7.94910000	1.53380000
20	O	0.93450000	-7.98310000	1.44400000
21	O	0.37155749	-7.41294455	3.90394401
22	Si	0.95190704	-8.52589310	2.93029705
23	Si	-1.34644032	-5.31655731	7.02384669
24	Si	-4.32960000	-6.05610000	7.41270000
25	O	-2.92290000	-5.44190000	7.01850000
26	O	-5.41450000	-5.45960000	6.41750000
27	O	-4.71840000	-5.65910000	8.88780000
28	O	-1.36620000	-5.12610000	10.61890000
29	O	-0.72730000	-6.04810000	8.28660000
30	Si	-0.78110000	-6.37380000	9.84140000
31	Si	4.19162420	1.79582068	-2.03246252
32	Si	4.36135388	-0.89366047	-0.53537003
33	Si	1.79909434	-4.81750990	0.05493402
34	Si	1.68505205	-2.17070361	-1.47852397
35	Si	3.22794995	3.06039429	2.23972261
36	Si	5.44854670	-1.68946627	4.28208782
37	Si	3.72402432	-4.24257200	4.65111429
38	O	4.61235648	0.39619144	-1.42445362
39	O	1.43072563	-3.66259515	-0.97311170
40	O	3.17929640	-1.73845351	-1.15985154
41	O	4.64906147	-3.05763718	4.13514056
42	O	2.93691138	2.40525809	-1.28877488
43	O	2.15294098	3.10901471	1.07405743
44	O	2.54296416	3.62286179	3.55349750

1	O	5.51815108	-1.20788445	5.80382872
2	O	3.57065581	-4.20214726	6.24788070
3	O	-0.73794891	-5.99433094	5.72551465
4	H	-1.30770000	8.45280000	5.54490000
5	H	3.53900000	4.98890000	5.43620000
6	H	-5.91550000	5.84190000	-1.27060000
7	H	-6.78570000	6.92250000	2.19890000
8	H	-12.70540000	-0.03450000	-1.12450000
9	H	-13.56750000	1.03610000	2.31350000
10	H	-12.61360000	-4.36250000	-0.43650000
11	H	-12.17550000	-5.02190000	-2.75570000
12	H	-14.47190000	-2.17020000	6.40220000
13	H	-13.77040000	-2.92530000	4.17860000
14	H	6.86449487	-1.88259729	3.83328172
15	H	-2.15040000	-4.10050000	12.78420000
16	H	1.31010000	-8.39770000	-1.01480000
17	H	-12.21020000	-7.97290000	7.89080000
18	H	0.36339800	-1.65380700	11.27870200
19	H	0.62130000	6.05740000	-2.14750000
20	H	0.50140000	4.07440000	-3.47820000
21	H	-2.25700000	7.49990000	7.52180000
22	H	-5.73850000	6.73170000	5.78280000
23	H	-10.96700000	4.40130000	4.09400000
24	H	-11.01960000	5.00810000	1.73210000
25	H	-12.06290000	1.27880000	5.87220000
26	H	-10.59640000	-6.34750000	11.45320000
27	H	-8.66420000	-7.73420000	10.94950000
28	H	2.77449000	1.81968400	10.74640200
29	H	1.80021000	3.79900000	9.78440300
30	H	5.77540000	-0.53010000	8.17660000
31	H	3.24710000	-4.17500000	8.72650000
32	H	0.61160000	-6.65520000	10.31590000
33	H	-1.64370000	-7.57580000	10.07620000
34	H	0.12290000	-9.76940000	3.03170000
35	H	2.36090000	-8.82750000	3.33990000
36	H	-10.15040000	3.92860000	-1.73450000
37	H	-9.16390000	2.16210000	-3.09680000
38	H	3.89500000	1.63920000	-3.49250000
39	H	5.32300000	2.73990000	-1.76330000
40	H	4.42878710	3.88352288	1.88700905
41	H	5.61653017	-1.70965170	-0.58831746
42	H	4.35729674	-5.55350604	4.29821789
43	H	3.22919052	-5.21293850	-0.15129044
44	H	-5.23700000	-6.37850000	11.22840000

1	H	-7.76830000	-9.07120000	6.80850000
2	H	-6.95230000	-10.08460000	3.55430000
3	H	-10.29630000	-10.34930000	0.25900000
4	H	-2.42150000	-9.87450000	0.00040000
5	H	-3.42900000	-8.60990000	3.88980000
6	H	-4.28320000	-7.54880000	7.29620000
7	H	-3.45780000	3.89970000	-3.31080000
8	H	0.59911000	5.23699300	7.81469700
9	H	-9.79240000	-1.54060000	-3.18200000
10	H	-8.38790000	-2.95530000	10.89960000
11	H	-4.87450000	3.78240000	8.02040000
12	H	-2.02270000	2.13730000	10.92000000
13	H	-4.91220000	-7.27130000	-2.96190000
14	H	-8.98790000	-7.09310000	-2.37650000
15	H	1.45748304	-2.18476228	-2.95899601
16	H	-5.88650000	0.35320000	-2.87170000
17	H	-6.57060000	-3.25690000	-2.96870000
18	H	-11.74490000	-3.66940000	8.61800000
19	H	-9.32890000	0.16850000	8.03140000
20	H	-8.19140000	3.21540000	6.31880000
21	H	-5.78340000	-8.84910000	-1.27830000
22	H	-7.97590000	-9.98270000	-0.17660000
23	H	-2.11767040	0.35882454	-2.97425757
24	C	-1.34417911	-2.52941489	3.09901455
25	H	-1.63099529	-2.75480050	4.12157351
26	H	-1.67736680	-1.53830259	2.80956866
27	H	-1.70067918	-3.27872082	2.40078255
28				
29				
30	Z-CH3_C2H4(ads)			
31	Si	-0.04624557	-0.00696014	-0.03290316
32	Si	-0.05865101	-0.00062931	5.66596133
33	Si	3.70500930	-0.07430412	2.48734900
34	Si	1.05339688	-3.91771717	2.99281404
35	Al	0.77505056	-0.77416058	2.91540621
36	O	0.14807162	-2.50302897	3.05661102
37	O	2.46805514	-0.91383812	3.07779730
38	O	0.04440723	-0.26051484	1.50525513
39	O	-0.06798533	0.06803040	4.09700884
40	O	-1.58453133	0.17155176	-0.43803954
41	O	-0.33857454	-1.47948730	6.26405655
42	O	1.37605280	0.46443735	6.25962870
43	O	-1.25825664	0.96785716	6.07366536
44	O	0.83162701	1.27711061	-0.43632885

1	O	3.59696545	1.52369765	2.55817134
2	O	4.99986224	-0.45755466	3.35299092
3	O	2.20136548	-3.99508153	4.10027940
4	O	3.92435241	-0.47602112	0.94646659
5	O	1.69683963	-4.15436104	1.55076323
6	O	0.53050925	-1.25488239	-0.86618735
7	O	-0.12212103	-4.94987516	3.30870939
8	C	-1.34790424	-2.53223264	3.11806439
9	H	-1.68086734	-1.54008692	2.83694552
10	H	-1.63116272	-2.76270120	4.13979109
11	H	-1.70788557	-3.27598222	2.41654062
12	C	-4.90325504	-1.45917823	3.83026868
13	H	-5.49302063	-2.07585232	4.50058921
14	H	-4.38630418	-0.61549513	4.27659730
15	C	-4.83839957	-1.71159553	2.52628497
16	H	-4.26649364	-1.08296115	1.85096694
17	H	-5.36697068	-2.54677845	2.07851322
18	O	0.80122026	-6.00641341	-0.15261981
19	Si	-5.49760613	-0.02107544	-1.47428465
20	Si	-2.51928371	0.76951690	-1.59090105
21	Si	1.67079870	2.63420243	-0.36391346
22	Si	-6.77250100	-2.79180000	-1.55910200
23	Si	-6.65860000	-5.43650000	-0.02630000
24	Si	-0.62804694	-6.20853080	4.15918667
25	Si	-3.21920790	-7.43500198	2.98451876
26	Si	-6.09540000	-6.32220000	2.83000000
27	Si	-7.79180000	-8.89230000	3.21140000
28	Si	-7.85690000	-4.02790000	9.99880000
29	Si	-9.54690000	-6.64300000	10.42590000
30	O	-8.68790000	-5.35140000	10.15840000
31	Si	1.78780502	2.30219008	9.72780398
32	Si	-0.76981192	-1.62740398	10.29929801
33	Si	-1.17799487	1.38378666	9.93889488
34	O	-1.38698713	-0.16319505	10.26480198
35	O	0.35019510	1.77510979	10.12159509
36	O	-1.90930590	-2.64049409	10.65649606
37	Si	-2.31670000	-4.06080000	11.29600000
38	Si	-5.02660000	-5.18350000	10.35000000
39	O	-3.83590000	-4.30830000	10.92640000
40	O	-6.34110000	-4.27000000	10.39930000
41	Si	4.73289898	-0.80104318	7.13549856
42	Si	-7.29070000	2.20560000	5.67640000
43	Si	-4.57939681	3.32750431	6.62399145
44	Si	-1.94070000	7.20800000	6.08700000

1	Si	-4.59330000	6.04430000	5.10460000
2	O	-5.77090000	2.45290000	6.04720000
3	O	-3.26549912	2.41430821	6.57330159
4	O	-0.99450101	5.94280101	5.99240403
5	O	-3.27080000	6.91960000	5.26710000
6	O	-4.35770000	4.58890000	5.69440000
7	O	-7.46660000	2.24719900	4.09540000
8	O	-4.88400000	5.95910000	3.53970000
9	Si	-5.99570000	5.67090000	2.42990000
10	Si	-10.73910000	3.90040000	2.70070000
11	O	-11.73290000	2.70740000	2.34160000
12	Si	-12.07420000	1.15480000	2.31840000
13	O	-11.45520000	0.42330000	3.58130000
14	Si	-11.39460000	-4.15760000	7.24580000
15	Si	-13.29570000	-2.46030000	5.52120000
16	Si	-11.50890000	0.09760000	5.13610000
17	Si	-8.83679800	-0.22830100	6.67329700
18	O	-12.44950000	-3.64190000	6.15630000
19	O	-12.41530000	-1.16550000	5.38290000
20	O	-10.03410000	-0.20050000	5.63859900
21	O	-7.69650000	0.78430200	6.31660100
22	Si	-0.05969601	4.78729801	6.54670404
23	O	-10.24280000	-7.11800000	9.08650000
24	Si	-7.71660000	3.11370000	2.78820000
25	O	-6.95550000	4.50240000	2.92570000
26	O	-9.24950000	3.38730000	2.56950000
27	Si	-4.97250000	-7.60980000	-1.50390000
28	Si	-11.35590000	0.26280000	-0.54610000
29	O	-6.84510000	-7.72030000	2.70470000
30	O	-10.35620000	-0.94150000	-0.80140000
31	Si	-9.16490000	-9.40520000	0.52820000
32	Si	-9.33470000	-6.71560000	-0.96890000
33	Si	-11.54680000	-4.63200000	-1.45310000
34	Si	-9.77590000	-2.05450000	-1.77500000
35	O	-9.58580000	-8.00560000	-0.07990000
36	O	-10.67690000	-5.84320000	-0.91270000
37	O	-10.64710000	-3.36120000	-1.66840000
38	O	-8.28390000	-2.37400000	-1.34130000
39	O	-6.40439900	-3.94669900	-0.53099900
40	O	-8.15250000	-5.87130000	-0.34420000
41	O	-8.84920000	-9.23940000	2.07860000
42	O	-6.41640000	-5.42400000	1.54900000
43	O	-5.61290000	-6.41590000	-0.70840000
44	O	-5.77370000	-1.60340000	-1.35129900

1	Si	-6.81090000	-5.43360000	5.68340000
2	Si	-8.50460000	-8.00720000	6.05360000
3	O	-7.72180000	-6.63160000	6.20070000
4	Si	-10.95800000	-7.17850000	7.67890000
5	Si	-8.42889900	-3.23820000	7.03330000
6	O	-11.40780000	-5.74300000	7.18590000
7	O	-8.21959700	-1.69259900	6.70789900
8	O	-9.95660000	-3.63110000	6.85010000
9	O	-9.98360000	-7.83070000	6.60240000
10	O	-7.53000000	-4.04100000	5.99020000
11	O	-7.92320000	-3.54700000	8.50450000
12	Si	0.12322824	4.64409021	-2.14545098
13	Si	-2.82306893	3.84599700	-1.95507003
14	O	-3.94896193	0.19035255	-1.21852842
15	O	0.75695069	3.77013651	-0.98766933
16	O	-1.45550000	4.66540000	-1.97180000
17	O	-2.55349135	2.34860599	-1.49995964
18	O	-6.33220000	0.83850000	-0.42850000
19	O	-3.77030000	4.57610000	-0.90140000
20	Si	-5.28020000	4.78230000	-0.42350000
21	Si	-7.00390000	2.22870000	-0.05400000
22	Si	-9.63060000	2.52380000	-1.72000000
23	O	-6.07880000	3.41370000	-0.57020000
24	O	-8.42830000	2.36750000	-0.70540000
25	O	-10.83220000	1.58900000	-1.25000000
26	O	-5.20960000	5.26350000	1.09860000
27	O	-7.15700000	2.26930000	1.54270000
28	O	-11.46650000	0.47770000	1.01990000
29	O	-6.60040000	-5.49380000	4.09960000
30	O	-8.61720000	-8.44720000	4.51360000
31	O	-1.68270403	1.69082687	8.46850932
32	Si	-1.74890667	2.17174111	6.97412753
33	O	-0.91868702	3.49569341	6.81431520
34	Si	2.50950645	3.95252023	5.10420705
35	Si	2.56678128	1.37896630	6.82674689
36	Si	3.01120233	-3.35761724	7.49351784
37	Si	-0.01122870	-2.57096530	7.40596344
38	O	2.86461857	2.66318326	5.94588223
39	O	3.90009611	0.51779713	6.89194949
40	O	3.77240000	-1.96900000	7.63100000
41	O	1.47830614	-3.08397372	7.27476948
42	O	2.15450008	1.79117322	8.29130724
43	O	-0.24972045	-2.04669801	8.86409593
44	O	1.05379597	4.47370201	5.45679597

1	O	-1.00419953	-3.76439525	7.04718952
2	Si	0.52349602	-7.58779801	-0.03028805
3	Si	-2.45310000	-8.37930000	0.08690000
4	O	-1.02440000	-7.79970000	-0.28570000
5	O	-3.48040000	-7.82240000	-1.00870000
6	O	-2.05278541	-6.52240083	3.54846586
7	O	-4.53620000	-6.55020000	2.91500000
8	O	-2.87430000	-7.94910000	1.53380000
9	O	0.93450000	-7.98310000	1.44400000
10	O	0.37168320	-7.41291573	3.90390850
11	Si	0.95190694	-8.52589405	2.93029703
12	Si	-1.34639231	-5.31658526	7.02371113
13	Si	-4.32960000	-6.05610000	7.41270000
14	O	-2.92290000	-5.44189700	7.01849700
15	O	-5.41450000	-5.45960000	6.41750000
16	O	-4.71840000	-5.65910000	8.88780000
17	O	-1.36620000	-5.12610000	10.61890000
18	O	-0.72730000	-6.04810000	8.28660000
19	Si	-0.78110000	-6.37380000	9.84140000
20	Si	4.19136250	1.79566184	-2.03280016
21	Si	4.36128704	-0.89372779	-0.53529142
22	Si	1.79916023	-4.81764426	0.05471385
23	Si	1.68560790	-2.17103881	-1.47840031
24	Si	3.22759246	3.05992648	2.23996859
25	Si	5.44840452	-1.68948779	4.28207775
26	Si	3.72401480	-4.24267999	4.65115537
27	O	4.61252696	0.39621537	-1.42437079
28	O	1.43068467	-3.66258814	-0.97316238
29	O	3.17926842	-1.73817859	-1.16016428
30	O	4.64905874	-3.05763019	4.13511867
31	O	2.93740657	2.40543165	-1.28813812
32	O	2.15408080	3.10991555	1.07335016
33	O	2.54297526	3.62282040	3.55352113
34	O	5.51822543	-1.20772653	5.80377542
35	O	3.57087325	-4.20201287	6.24789809
36	O	-0.73793664	-5.99422590	5.72550108
37	H	-1.30770000	8.45280000	5.54490000
38	H	3.53900000	4.98890000	5.43620000
39	H	-5.91550000	5.84190000	-1.27060000
40	H	-6.78570000	6.92250000	2.19890000
41	H	-12.70540000	-0.03450000	-1.12450000
42	H	-13.56750000	1.03610000	2.31350000
43	H	-12.61360000	-4.36250000	-0.43650000
44	H	-12.17550000	-5.02190000	-2.75570000

1	H	-14.47190000	-2.17020000	6.40220000
2	H	-13.77040000	-2.92530000	4.17860000
3	H	6.86450365	-1.88260108	3.83330923
4	H	-2.15040000	-4.10050000	12.78420000
5	H	1.31010000	-8.39770000	-1.01480000
6	H	-12.21020000	-7.97290000	7.89080000
7	H	0.36339804	-1.65380985	11.27870296
8	H	0.62130000	6.05740000	-2.14750000
9	H	0.50140000	4.07440000	-3.47820000
10	H	-2.25700000	7.49990000	7.52180000
11	H	-5.73850000	6.73170000	5.78280000
12	H	-10.96700000	4.40130000	4.09400000
13	H	-11.01960000	5.00810000	1.73210000
14	H	-12.06290000	1.27880000	5.87220000
15	H	-10.59640000	-6.34750000	11.45320000
16	H	-8.66420000	-7.73420000	10.94950000
17	H	2.77449714	1.81969522	10.74640097
18	H	1.80020569	3.79900001	9.78440191
19	H	5.77540000	-0.53010000	8.17660000
20	H	3.24710000	-4.17500000	8.72650000
21	H	0.61160000	-6.65520000	10.31590000
22	H	-1.64370000	-7.57580000	10.07620000
23	H	0.12290000	-9.76940000	3.03170000
24	H	2.36090000	-8.82750000	3.33990000
25	H	-10.15040000	3.92860000	-1.73450000
26	H	-9.16390000	2.16210000	-3.09680000
27	H	3.89500000	1.63920000	-3.49250000
28	H	5.32300000	2.73990000	-1.76330000
29	H	4.42877998	3.88355454	1.88705677
30	H	5.61649787	-1.70970248	-0.58830954
31	H	4.35728584	-5.55351177	4.29821666
32	H	3.22919988	-5.21290764	-0.15128859
33	H	-5.23700000	-6.37850000	11.22840000
34	H	-7.76830000	-9.07120000	6.80850000
35	H	-6.95230000	-10.08460000	3.55430000
36	H	-10.29630000	-10.34930000	0.25900000
37	H	-2.42150000	-9.87450000	0.00040000
38	H	-3.42900000	-8.60990000	3.88980000
39	H	-4.28320000	-7.54880000	7.29620000
40	H	-3.45780000	3.89970000	-3.31080000
41	H	0.59910206	5.23699796	7.81469898
42	H	-9.79240000	-1.54060000	-3.18200000
43	H	-8.38790000	-2.95530000	10.89960000
44	H	-4.87450000	3.78240000	8.02040000

H -2.02270000 2.13730000 10.92000000
H -4.91220000 -7.27130000 -2.96190000
H -8.98790000 -7.09310000 -2.37650000
H 1.45738094 -2.18476560 -2.95898014
H -5.88650000 0.35320000 -2.87170000
H -6.57060000 -3.25690000 -2.96870000
H -11.74490000 -3.66940000 8.61800000
H -9.32890000 0.16850000 8.03140000
H -8.19140000 3.21540000 6.31880000
H -5.78340000 -8.84910000 -1.27830000
H -7.97590000 -9.98270000 -0.17660000
H -2.11765832 0.35871338 -2.97422021

Z-CH3_CH3OCH3(ads)-to-Z-(CH3)3O+-TS
Si -0.04513820 -0.00414975 -0.01546553
Si -0.06032614 -0.00012000 5.65669143
Si 3.71315366 -0.05605104 2.48728682
Si 1.04031007 -3.89513838 2.99360044
Al 0.75266634 -0.82700848 2.91571156
O 0.21006460 -2.50593708 3.05216772
O 2.45680565 -0.82342435 3.10315863
O 0.00406687 -0.22614364 1.52847999
O -0.09425848 0.05198482 4.09206585
O -1.58599901 0.16189039 -0.44489594
O -0.36665382 -1.47095971 6.27815458
O 1.36535351 0.47089944 6.26593240
O -1.26904588 0.96620487 6.07056623
O 0.82403115 1.28259041 -0.43723517
O 3.66478647 1.54675432 2.54053109
O 5.00942018 -0.46262697 3.34344476
O 2.20393931 -4.05200532 4.09817150
O 3.91584289 -0.47770817 0.94548882
O 1.70786684 -4.19968375 1.55988395
O 0.54033108 -1.25219732 -0.84515178
O -0.14381812 -4.94631732 3.30820540
O 0.80120000 -6.00640000 -0.15260000
Si -5.49760000 -0.02110000 -1.47430000
Si -2.51950000 0.76950000 -1.59090000
Si 1.67330000 2.63520000 -0.36440000
Si -6.77250000 -2.79180000 -1.55910000
Si -6.65860000 -5.43650000 -0.02630000
Si -0.62810000 -6.20850000 4.15930000
Si -3.21920000 -7.43500000 2.98450000

1	Si	-6.09540000	-6.32220000	2.83000000
2	Si	-7.79180000	-8.89230000	3.21140000
3	Si	-7.85690000	-4.02790000	9.99880000
4	Si	-9.54690000	-6.64300000	10.42590000
5	O	-8.68790000	-5.35140000	10.15840000
6	Si	1.78780000	2.30220000	9.72780000
7	Si	-0.76980000	-1.62740000	10.29930000
8	Si	-1.17800000	1.38380000	9.93890000
9	O	-1.38700000	-0.16320000	10.26480000
10	O	0.35020000	1.77510000	10.12160000
11	O	-1.90930000	-2.64050000	10.65650000
12	Si	-2.31670000	-4.06080000	11.29600000
13	Si	-5.02660000	-5.18350000	10.35000000
14	O	-3.83590000	-4.30830000	10.92640000
15	O	-6.34110000	-4.27000000	10.39930000
16	Si	4.73290000	-0.80100000	7.13550000
17	Si	-7.29070000	2.20560000	5.67640000
18	Si	-4.57940000	3.32750000	6.62400000
19	Si	-1.94070000	7.20800000	6.08700000
20	Si	-4.59330000	6.04430000	5.10460000
21	O	-5.77090000	2.45290000	6.04720000
22	O	-3.26560000	2.41450000	6.57330000
23	O	-0.99450000	5.94280000	5.99240000
24	O	-3.27080000	6.91960000	5.26710000
25	O	-4.35770000	4.58890000	5.69440000
26	O	-7.46660000	2.24720000	4.09540000
27	O	-4.88400000	5.95910000	3.53970000
28	Si	-5.99570000	5.67090000	2.42990000
29	Si	-10.73910000	3.90040000	2.70070000
30	O	-11.73290000	2.70740000	2.34160000
31	Si	-12.07420000	1.15480000	2.31840000
32	O	-11.45520000	0.42330000	3.58130000
33	Si	-11.39460000	-4.15760000	7.24580000
34	Si	-13.29570000	-2.46030000	5.52120000
35	Si	-11.50890000	0.09760000	5.13610000
36	Si	-8.83680000	-0.22830000	6.67330000
37	O	-12.44950000	-3.64190000	6.15630000
38	O	-12.41530000	-1.16550000	5.38290000
39	O	-10.03410000	-0.20050000	5.63860000
40	O	-7.69650000	0.78430000	6.31660000
41	Si	-0.05970000	4.78730000	6.54670000
42	O	-10.24280000	-7.11800000	9.08650000
43	Si	-7.71660000	3.11370000	2.78820000
44	O	-6.95550000	4.50240000	2.92570000

1	O	-9.24950000	3.38730000	2.56950000
2	Si	-4.97250000	-7.60980000	-1.50390000
3	Si	-11.35590000	0.26280000	-0.54610000
4	O	-6.84510000	-7.72030000	2.70470000
5	O	-10.35620000	-0.94150000	-0.80140000
6	Si	-9.16490000	-9.40520000	0.52820000
7	Si	-9.33470000	-6.71560000	-0.96890000
8	Si	-11.54680000	-4.63200000	-1.45310000
9	Si	-9.77590000	-2.05450000	-1.77500000
10	O	-9.58580000	-8.00560000	-0.07990000
11	O	-10.67690000	-5.84320000	-0.91270000
12	O	-10.64710000	-3.36120000	-1.66840000
13	O	-8.28390000	-2.37400000	-1.34130000
14	O	-6.40440000	-3.94670000	-0.53100000
15	O	-8.15250000	-5.87130000	-0.34420000
16	O	-8.84920000	-9.23940000	2.07860000
17	O	-6.41640000	-5.42400000	1.54900000
18	O	-5.61290000	-6.41590000	-0.70840000
19	O	-5.77370000	-1.60340000	-1.35130000
20	Si	-6.81090000	-5.43360000	5.68340000
21	Si	-8.50460000	-8.00720000	6.05360000
22	O	-7.72180000	-6.63160000	6.20070000
23	Si	-10.95800000	-7.17850000	7.67890000
24	Si	-8.42890000	-3.23820000	7.03330000
25	O	-11.40780000	-5.74300000	7.18590000
26	O	-8.21960000	-1.69260000	6.70790000
27	O	-9.95660000	-3.63110000	6.85010000
28	O	-9.98360000	-7.83070000	6.60240000
29	O	-7.53000000	-4.04100000	5.99020000
30	O	-7.92320000	-3.54700000	8.50450000
31	Si	0.12370000	4.64450000	-2.14540000
32	Si	-2.82300000	3.84600000	-1.95510000
33	O	-3.94890000	0.19040000	-1.21850000
34	O	0.75580000	3.76930000	-0.98750000
35	O	-1.45550000	4.66540000	-1.97180000
36	O	-2.55360000	2.34860000	-1.49990000
37	O	-6.33220000	0.83850000	-0.42850000
38	O	-3.77030000	4.57610000	-0.90140000
39	Si	-5.28020000	4.78230000	-0.42350000
40	Si	-7.00390000	2.22870000	-0.05400000
41	Si	-9.63060000	2.52380000	-1.72000000
42	O	-6.07880000	3.41370000	-0.57020000
43	O	-8.42830000	2.36750000	-0.70540000
44	O	-10.83220000	1.58900000	-1.25000000

1	O	-5.20960000	5.26350000	1.09860000
2	O	-7.15700000	2.26930000	1.54270000
3	O	-11.46650000	0.47770000	1.01990000
4	O	-6.60040000	-5.49380000	4.09960000
5	O	-8.61720000	-8.44720000	4.51360000
6	O	-1.68270000	1.69080000	8.46850000
7	Si	-1.74890000	2.17160000	6.97410000
8	O	-0.91870000	3.49570000	6.81430000
9	Si	2.50950000	3.95250000	5.10420000
10	Si	2.56680000	1.37880000	6.82680000
11	Si	3.01120000	-3.35760000	7.49350000
12	Si	-0.01130000	-2.57110000	7.40600000
13	O	2.86460000	2.66320000	5.94600000
14	O	3.90010000	0.51780000	6.89190000
15	O	3.77240000	-1.96900000	7.63100000
16	O	1.47830000	-3.08400000	7.27480000
17	O	2.15450000	1.79120000	8.29130000
18	O	-0.24970000	-2.04670000	8.86410000
19	O	1.05380000	4.47370000	5.45680000
20	O	-1.00420000	-3.76440000	7.04720000
21	Si	0.52350000	-7.58780000	-0.03030000
22	Si	-2.45310000	-8.37930000	0.08690000
23	O	-1.02440000	-7.79970000	-0.28570000
24	O	-3.48040000	-7.82240000	-1.00870000
25	O	-2.05280000	-6.52240000	3.54850000
26	O	-4.53620000	-6.55020000	2.91500000
27	O	-2.87430000	-7.94910000	1.53380000
28	O	0.93450000	-7.98310000	1.44400000
29	O	0.37160000	-7.41290000	3.90390000
30	Si	0.95190000	-8.52590000	2.93030000
31	Si	-1.34640000	-5.31660000	7.02370000
32	Si	-4.32960000	-6.05610000	7.41270000
33	O	-2.92290000	-5.44190000	7.01850000
34	O	-5.41450000	-5.45960000	6.41750000
35	O	-4.71840000	-5.65910000	8.88780000
36	O	-1.36620000	-5.12610000	10.61890000
37	O	-0.72730000	-6.04810000	8.28660000
38	Si	-0.78110000	-6.37380000	9.84140000
39	Si	4.19160000	1.79580000	-2.03250000
40	Si	4.36130000	-0.89370000	-0.53530000
41	Si	1.79910000	-4.81760000	0.05480000
42	Si	1.68500000	-2.17150000	-1.47840000
43	Si	3.22790000	3.06050000	2.23970000
44	Si	5.44850000	-1.68950000	4.28210000

1	Si	3.72400000	-4.24270000	4.65120000
2	O	4.61250000	0.39620000	-1.42440000
3	O	1.43100000	-3.66270000	-0.97330000
4	O	3.17920000	-1.73800000	-1.16010000
5	O	4.64900000	-3.05760000	4.13510000
6	O	2.93690000	2.40530000	-1.28880000
7	O	2.15280000	3.10900000	1.07410000
8	O	2.54300000	3.62290000	3.55350000
9	O	5.51820000	-1.20780000	5.80380000
10	O	3.57090000	-4.20200000	6.24790000
11	O	-0.73790000	-5.99420000	5.72550000
12	H	-1.30770000	8.45280000	5.54490000
13	H	3.53900000	4.98890000	5.43620000
14	H	-5.91550000	5.84190000	-1.27060000
15	H	-6.78570000	6.92250000	2.19890000
16	H	-12.70540000	-0.03450000	-1.12450000
17	H	-13.56750000	1.03610000	2.31350000
18	H	-12.61360000	-4.36250000	-0.43650000
19	H	-12.17550000	-5.02190000	-2.75570000
20	H	-14.47190000	-2.17020000	6.40220000
21	H	-13.77040000	-2.92530000	4.17860000
22	H	6.86450000	-1.88260000	3.83330000
23	H	-2.15040000	-4.10050000	12.78420000
24	H	1.31010000	-8.39770000	-1.01480000
25	H	-12.21020000	-7.97290000	7.89080000
26	H	0.36340000	-1.65380000	11.27870000
27	H	0.62130000	6.05740000	-2.14750000
28	H	0.50140000	4.07440000	-3.47820000
29	H	-2.25700000	7.49990000	7.52180000
30	H	-5.73850000	6.73170000	5.78280000
31	H	-10.96700000	4.40130000	4.09400000
32	H	-11.01960000	5.00810000	1.73210000
33	H	-12.06290000	1.27880000	5.87220000
34	H	-10.59640000	-6.34750000	11.45320000
35	H	-8.66420000	-7.73420000	10.94950000
36	H	2.77450000	1.81970000	10.74640000
37	H	1.80020000	3.79900000	9.78440000
38	H	5.77540000	-0.53010000	8.17660000
39	H	3.24710000	-4.17500000	8.72650000
40	H	0.61160000	-6.65520000	10.31590000
41	H	-1.64370000	-7.57580000	10.07620000
42	H	0.12290000	-9.76940000	3.03170000
43	H	2.36090000	-8.82750000	3.33990000
44	H	-10.15040000	3.92860000	-1.73450000

1	H	-9.16390000	2.16210000	-3.09680000
2	H	3.89500000	1.63920000	-3.49250000
3	H	5.32300000	2.73990000	-1.76330000
4	H	4.42880000	3.88350000	1.88700000
5	H	5.61650000	-1.70970000	-0.58830000
6	H	4.35730000	-5.55350000	4.29820000
7	H	3.22920000	-5.21290000	-0.15130000
8	H	-5.23700000	-6.37850000	11.22840000
9	H	-7.76830000	-9.07120000	6.80850000
10	H	-6.95230000	-10.08460000	3.55430000
11	H	-10.29630000	-10.34930000	0.25900000
12	H	-2.42150000	-9.87450000	0.00040000
13	H	-3.42900000	-8.60990000	3.88980000
14	H	-4.28320000	-7.54880000	7.29620000
15	H	-3.45780000	3.89970000	-3.31080000
16	H	0.59910000	5.23700000	7.81470000
17	H	-9.79240000	-1.54060000	-3.18200000
18	H	-8.38790000	-2.95530000	10.89960000
19	H	-4.87450000	3.78240000	8.02040000
20	H	-2.02270000	2.13730000	10.92000000
21	H	-4.91220000	-7.27130000	-2.96190000
22	H	-8.98790000	-7.09310000	-2.37650000
23	H	1.45750000	-2.18460000	-2.95900000
24	H	-5.88650000	0.35320000	-2.87170000
25	H	-6.57060000	-3.25690000	-2.96870000
26	H	-11.74490000	-3.66940000	8.61800000
27	H	-9.32890000	0.16850000	8.03140000
28	H	-8.19140000	3.21540000	6.31880000
29	H	-5.78340000	-8.84910000	-1.27830000
30	H	-7.97590000	-9.98270000	-0.17660000
31	H	-2.11760000	0.35870000	-2.97420000
32	C	-1.77200662	-2.45306258	3.24065456
33	H	-1.64605161	-2.38584156	4.30657358
34	H	-1.87751479	-3.41902458	2.78126243
35	H	-1.78874640	-1.55708611	2.64222941
36	O	-3.75045096	-2.36961590	3.48350555
37	C	-4.45042221	-2.12858432	2.24989841
38	H	-4.09968576	-2.86508483	1.53028594
39	H	-5.52062768	-2.26755925	2.41327845
40	H	-4.24930486	-1.11819170	1.88116784
41	C	-4.14914918	-1.47962751	4.54378166
42	H	-3.91313417	-0.44179451	4.29158111
43	H	-5.22075140	-1.59419800	4.72058042
44	H	-3.59914346	-1.77804601	5.43397445

1
2
3 Z-CH3_CH3OCH3(ads)
4 Si -0.04332469 -0.00124258 -0.03322936
5 Si -0.05889520 -0.00165152 5.66642531
6 Si 3.70253469 -0.07409504 2.48724254
7 Si 1.05412305 -3.91579648 2.99062442
8 Al 0.76927992 -0.77643434 2.91032837
9 O 0.14743345 -2.50371069 3.03782811
10 O 2.46398201 -0.91223845 3.07447364
11 O 0.04860740 -0.22446536 1.50923862
12 O -0.06743656 0.06305705 4.09906236
13 O -1.58138976 0.16964125 -0.44326113
14 O -0.34512842 -1.47739577 6.26925045
15 O 1.37477819 0.46386376 6.26275528
16 O -1.25851743 0.96887031 6.07302996
17 O 0.83421500 1.27791778 -0.45415628
18 O 3.59929365 1.52495610 2.55759257
19 O 4.99658400 -0.45767841 3.35483581
20 O 2.20187484 -3.99099548 4.10053811
21 O 3.92644472 -0.47441099 0.94642764
22 O 1.70383368 -4.15864774 1.55179155
23 O 0.53414259 -1.26032414 -0.85017002
24 O -0.11701985 -4.95149669 3.31006906
25 O 0.80120000 -6.00640000 -0.15260000
26 Si -5.49760000 -0.02110000 -1.47430000
27 Si -2.51950000 0.76950000 -1.59090000
28 Si 1.67330000 2.63520000 -0.36440000
29 Si -6.77250000 -2.79180000 -1.55910000
30 Si -6.65860000 -5.43650000 -0.02630000
31 Si -0.62810000 -6.20850000 4.15930000
32 Si -3.21920000 -7.43500000 2.98450000
33 Si -6.09540000 -6.32220000 2.83000000
34 Si -7.79180000 -8.89230000 3.21140000
35 Si -7.85690000 -4.02790000 9.99880000
36 Si -9.54690000 -6.64300000 10.42590000
37 O -8.68790000 -5.35140000 10.15840000
38 Si 1.78780000 2.30220000 9.72780000
39 Si -0.76980000 -1.62740000 10.29930000
40 Si -1.17800000 1.38380000 9.93890000
41 O -1.38700000 -0.16320000 10.26480000
42 O 0.35020000 1.77510000 10.12160000
43 O -1.90930000 -2.64050000 10.65650000
44 Si -2.31670000 -4.06080000 11.29600000

1	Si	-5.02660000	-5.18350000	10.35000000
2	O	-3.83590000	-4.30830000	10.92640000
3	O	-6.34110000	-4.27000000	10.39930000
4	Si	4.73290000	-0.80100000	7.13550000
5	Si	-7.29070000	2.20560000	5.67640000
6	Si	-4.57940000	3.32750000	6.62400000
7	Si	-1.94070000	7.20800000	6.08700000
8	Si	-4.59330000	6.04430000	5.10460000
9	O	-5.77090000	2.45290000	6.04720000
10	O	-3.26560000	2.41450000	6.57330000
11	O	-0.99450000	5.94280000	5.99240000
12	O	-3.27080000	6.91960000	5.26710000
13	O	-4.35770000	4.58890000	5.69440000
14	O	-7.46660000	2.24720000	4.09540000
15	O	-4.88400000	5.95910000	3.53970000
16	Si	-5.99570000	5.67090000	2.42990000
17	Si	-10.73910000	3.90040000	2.70070000
18	O	-11.73290000	2.70740000	2.34160000
19	Si	-12.07420000	1.15480000	2.31840000
20	O	-11.45520000	0.42330000	3.58130000
21	Si	-11.39460000	-4.15760000	7.24580000
22	Si	-13.29570000	-2.46030000	5.52120000
23	Si	-11.50890000	0.09760000	5.13610000
24	Si	-8.83680000	-0.22830000	6.67330000
25	O	-12.44950000	-3.64190000	6.15630000
26	O	-12.41530000	-1.16550000	5.38290000
27	O	-10.03410000	-0.20050000	5.63860000
28	O	-7.69650000	0.78430000	6.31660000
29	Si	-0.05970000	4.78730000	6.54670000
30	O	-10.24280000	-7.11800000	9.08650000
31	Si	-7.71660000	3.11370000	2.78820000
32	O	-6.95550000	4.50240000	2.92570000
33	O	-9.24950000	3.38730000	2.56950000
34	Si	-4.97250000	-7.60980000	-1.50390000
35	Si	-11.35590000	0.26280000	-0.54610000
36	O	-6.84510000	-7.72030000	2.70470000
37	O	-10.35620000	-0.94150000	-0.80140000
38	Si	-9.16490000	-9.40520000	0.52820000
39	Si	-9.33470000	-6.71560000	-0.96890000
40	Si	-11.54680000	-4.63200000	-1.45310000
41	Si	-9.77590000	-2.05450000	-1.77500000
42	O	-9.58580000	-8.00560000	-0.07990000
43	O	-10.67690000	-5.84320000	-0.91270000
44	O	-10.64710000	-3.36120000	-1.66840000

1	O	-8.28390000	-2.37400000	-1.34130000
2	O	-6.40440000	-3.94670000	-0.53100000
3	O	-8.15250000	-5.87130000	-0.34420000
4	O	-8.84920000	-9.23940000	2.07860000
5	O	-6.41640000	-5.42400000	1.54900000
6	O	-5.61290000	-6.41590000	-0.70840000
7	O	-5.77370000	-1.60340000	-1.35130000
8	Si	-6.81090000	-5.43360000	5.68340000
9	Si	-8.50460000	-8.00720000	6.05360000
10	O	-7.72180000	-6.63160000	6.20070000
11	Si	-10.95800000	-7.17850000	7.67890000
12	Si	-8.42890000	-3.23820000	7.03330000
13	O	-11.40780000	-5.74300000	7.18590000
14	O	-8.21960000	-1.69260000	6.70790000
15	O	-9.95660000	-3.63110000	6.85010000
16	O	-9.98360000	-7.83070000	6.60240000
17	O	-7.53000000	-4.04100000	5.99020000
18	O	-7.92320000	-3.54700000	8.50450000
19	Si	0.12370000	4.64450000	-2.14540000
20	Si	-2.82300000	3.84600000	-1.95510000
21	O	-3.94890000	0.19040000	-1.21850000
22	O	0.75580000	3.76930000	-0.98750000
23	O	-1.45550000	4.66540000	-1.97180000
24	O	-2.55360000	2.34860000	-1.49990000
25	O	-6.33220000	0.83850000	-0.42850000
26	O	-3.77030000	4.57610000	-0.90140000
27	Si	-5.28020000	4.78230000	-0.42350000
28	Si	-7.00390000	2.22870000	-0.05400000
29	Si	-9.63060000	2.52380000	-1.72000000
30	O	-6.07880000	3.41370000	-0.57020000
31	O	-8.42830000	2.36750000	-0.70540000
32	O	-10.83220000	1.58900000	-1.25000000
33	O	-5.20960000	5.26350000	1.09860000
34	O	-7.15700000	2.26930000	1.54270000
35	O	-11.46650000	0.47770000	1.01990000
36	O	-6.60040000	-5.49380000	4.09960000
37	O	-8.61720000	-8.44720000	4.51360000
38	O	-1.68270000	1.69080000	8.46850000
39	Si	-1.74890000	2.17160000	6.97410000
40	O	-0.91870000	3.49570000	6.81430000
41	Si	2.50950000	3.95250000	5.10420000
42	Si	2.56680000	1.37880000	6.82680000
43	Si	3.01120000	-3.35760000	7.49350000
44	Si	-0.01130000	-2.57110000	7.40600000

1	O	2.86460000	2.66320000	5.94600000
2	O	3.90010000	0.51780000	6.89190000
3	O	3.77240000	-1.96900000	7.63100000
4	O	1.47830000	-3.08400000	7.27480000
5	O	2.15450000	1.79120000	8.29130000
6	O	-0.24970000	-2.04670000	8.86410000
7	O	1.05380000	4.47370000	5.45680000
8	O	-1.00420000	-3.76440000	7.04720000
9	Si	0.52350000	-7.58780000	-0.03030000
10	Si	-2.45310000	-8.37930000	0.08690000
11	O	-1.02440000	-7.79970000	-0.28570000
12	O	-3.48040000	-7.82240000	-1.00870000
13	O	-2.05280000	-6.52240000	3.54850000
14	O	-4.53620000	-6.55020000	2.91500000
15	O	-2.87430000	-7.94910000	1.53380000
16	O	0.93450000	-7.98310000	1.44400000
17	O	0.37160000	-7.41290000	3.90390000
18	Si	0.95190000	-8.52590000	2.93030000
19	Si	-1.34640000	-5.31660000	7.02370000
20	Si	-4.32960000	-6.05610000	7.41270000
21	O	-2.92290000	-5.44190000	7.01850000
22	O	-5.41450000	-5.45960000	6.41750000
23	O	-4.71840000	-5.65910000	8.88780000
24	O	-1.36620000	-5.12610000	10.61890000
25	O	-0.72730000	-6.04810000	8.28660000
26	Si	-0.78110000	-6.37380000	9.84140000
27	Si	4.19160000	1.79580000	-2.03250000
28	Si	4.36130000	-0.89370000	-0.53530000
29	Si	1.79910000	-4.81760000	0.05480000
30	Si	1.68500000	-2.17150000	-1.47840000
31	Si	3.22790000	3.06050000	2.23970000
32	Si	5.44850000	-1.68950000	4.28210000
33	Si	3.72400000	-4.24270000	4.65120000
34	O	4.61250000	0.39620000	-1.42440000
35	O	1.43100000	-3.66270000	-0.97330000
36	O	3.17920000	-1.73800000	-1.16010000
37	O	4.64900000	-3.05760000	4.13510000
38	O	2.93690000	2.40530000	-1.28880000
39	O	2.15280000	3.10900000	1.07410000
40	O	2.54300000	3.62290000	3.55350000
41	O	5.51820000	-1.20780000	5.80380000
42	O	3.57090000	-4.20200000	6.24790000
43	O	-0.73790000	-5.99420000	5.72550000
44	H	-1.30770000	8.45280000	5.54490000

1	H	3.53900000	4.98890000	5.43620000
2	H	-5.91550000	5.84190000	-1.27060000
3	H	-6.78570000	6.92250000	2.19890000
4	H	-12.70540000	-0.03450000	-1.12450000
5	H	-13.56750000	1.03610000	2.31350000
6	H	-12.61360000	-4.36250000	-0.43650000
7	H	-12.17550000	-5.02190000	-2.75570000
8	H	-14.47190000	-2.17020000	6.40220000
9	H	-13.77040000	-2.92530000	4.17860000
10	H	6.86450000	-1.88260000	3.83330000
11	H	-2.15040000	-4.10050000	12.78420000
12	H	1.31010000	-8.39770000	-1.01480000
13	H	-12.21020000	-7.97290000	7.89080000
14	H	0.36340000	-1.65380000	11.27870000
15	H	0.62130000	6.05740000	-2.14750000
16	H	0.50140000	4.07440000	-3.47820000
17	H	-2.25700000	7.49990000	7.52180000
18	H	-5.73850000	6.73170000	5.78280000
19	H	-10.96700000	4.40130000	4.09400000
20	H	-11.01960000	5.00810000	1.73210000
21	H	-12.06290000	1.27880000	5.87220000
22	H	-10.59640000	-6.34750000	11.45320000
23	H	-8.66420000	-7.73420000	10.94950000
24	H	2.77450000	1.81970000	10.74640000
25	H	1.80020000	3.79900000	9.78440000
26	H	5.77540000	-0.53010000	8.17660000
27	H	3.24710000	-4.17500000	8.72650000
28	H	0.61160000	-6.65520000	10.31590000
29	H	-1.64370000	-7.57580000	10.07620000
30	H	0.12290000	-9.76940000	3.03170000
31	H	2.36090000	-8.82750000	3.33990000
32	H	-10.15040000	3.92860000	-1.73450000
33	H	-9.16390000	2.16210000	-3.09680000
34	H	3.89500000	1.63920000	-3.49250000
35	H	5.32300000	2.73990000	-1.76330000
36	H	4.42880000	3.88350000	1.88700000
37	H	5.61650000	-1.70970000	-0.58830000
38	H	4.35730000	-5.55350000	4.29820000
39	H	3.22920000	-5.21290000	-0.15130000
40	H	-5.23700000	-6.37850000	11.22840000
41	H	-7.76830000	-9.07120000	6.80850000
42	H	-6.95230000	-10.08460000	3.55430000
43	H	-10.29630000	-10.34930000	0.25900000
44	H	-2.42150000	-9.87450000	0.00040000

1	H	-3.42900000	-8.60990000	3.88980000
2	H	-4.28320000	-7.54880000	7.29620000
3	H	-3.45780000	3.89970000	-3.31080000
4	H	0.59910000	5.23700000	7.81470000
5	H	-9.79240000	-1.54060000	-3.18200000
6	H	-8.38790000	-2.95530000	10.89960000
7	H	-4.87450000	3.78240000	8.02040000
8	H	-2.02270000	2.13730000	10.92000000
9	H	-4.91220000	-7.27130000	-2.96190000
10	H	-8.98790000	-7.09310000	-2.37650000
11	H	1.45750000	-2.18460000	-2.95900000
12	H	-5.88650000	0.35320000	-2.87170000
13	H	-6.57060000	-3.25690000	-2.96870000
14	H	-11.74490000	-3.66940000	8.61800000
15	H	-9.32890000	0.16850000	8.03140000
16	H	-8.19140000	3.21540000	6.31880000
17	H	-5.78340000	-8.84910000	-1.27830000
18	H	-7.97590000	-9.98270000	-0.17660000
19	H	-2.11760000	0.35870000	-2.97420000
20	C	-1.35608465	-2.54064383	3.12072698
21	H	-1.62094868	-2.80852114	4.13529427
22	H	-1.72049853	-3.26327759	2.40086210
23	H	-1.69499773	-1.54075273	2.87995669
24	O	-4.21725940	-2.34087764	3.77794787
25	C	-5.19606674	-1.97911236	2.81576629
26	H	-5.01426727	-2.57312573	1.92059652
27	H	-6.20777255	-2.19471429	3.18290235
28	H	-5.13166270	-0.91216686	2.56165284
29	C	-4.37819168	-1.62844563	4.99560931
30	H	-4.24771105	-0.54781014	4.85019235
31	H	-5.36859746	-1.80970594	5.43187671
32	H	-3.61269487	-1.98578550	5.68539165
33				
34				
35	Z-CH3_H2O(ads)			
36	Si	-0.03867939	0.00682832	-0.03823537
37	Si	-0.06020533	-0.00368512	5.66474913
38	Si	3.70383683	-0.07401724	2.48785807
39	Si	1.05417557	-3.91339933	2.98870686
40	Al	0.77273596	-0.76854255	2.90658157
41	O	0.14895992	-2.49800329	2.99906103
42	O	2.46618374	-0.90953724	3.08048738
43	O	0.07777018	-0.17300141	1.50811528
44	O	-0.08167422	0.04729960	4.09711537

1	O	-1.58337012	0.15731842	-0.44476640
2	O	-0.34071809	-1.47728851	6.27064802
3	O	1.37686038	0.46675202	6.25255287
4	O	-1.25310270	0.97265754	6.07207613
5	O	0.82565438	1.28356500	-0.49070249
6	O	3.60195119	1.52536737	2.55527528
7	O	4.99983684	-0.45798268	3.35222007
8	O	2.20148527	-3.97964789	4.10066506
9	O	3.92329767	-0.47572020	0.94611639
10	O	1.71053140	-4.17094600	1.55556273
11	O	0.53515199	-1.26584261	-0.83682607
12	O	-0.11854151	-4.94254058	3.32214602
13	O	0.80133400	-6.00647700	-0.15280300
14	Si	-5.49760300	-0.02108800	-1.47429200
15	Si	-2.51910400	0.76907700	-1.59036400
16	Si	1.67287300	2.63506400	-0.36445800
17	Si	-6.77250000	-2.79180000	-1.55910000
18	Si	-6.65860000	-5.43650000	-0.02630000
19	Si	-0.62798600	-6.20818700	4.15920500
20	Si	-3.21923400	-7.43500800	2.98458400
21	Si	-6.09540000	-6.32220000	2.83000000
22	Si	-7.79180000	-8.89230000	3.21140000
23	Si	-7.85690000	-4.02790000	9.99880000
24	Si	-9.54690000	-6.64300000	10.42590000
25	O	-8.68790000	-5.35140000	10.15840000
26	Si	1.78781600	2.30218600	9.72780900
27	Si	-0.76980800	-1.62740500	10.29930000
28	Si	-1.17801000	1.38382800	9.93890900
29	O	-1.38699000	-0.16319600	10.26480100
30	O	0.35018900	1.77512200	10.12159000
31	O	-1.90930600	-2.64049400	10.65649700
32	Si	-2.31670000	-4.06080000	11.29600000
33	Si	-5.02660000	-5.18350000	10.35000000
34	O	-3.83590000	-4.30830000	10.92640000
35	O	-6.34110000	-4.27000000	10.39930000
36	Si	4.73289700	-0.80096600	7.13547100
37	Si	-7.29070000	2.20560000	5.67640000
38	Si	-4.57940700	3.32748900	6.62401900
39	Si	-1.94070000	7.20800000	6.08700000
40	Si	-4.59330000	6.04430000	5.10460000
41	O	-5.77090000	2.45290000	6.04720000
42	O	-3.26560100	2.41457000	6.57334500
43	O	-0.99449900	5.94279900	5.99239600
44	O	-3.27080000	6.91960000	5.26710000

1	O	-4.35770000	4.58890000	5.69440000
2	O	-7.46660000	2.24720000	4.09540000
3	O	-4.88400000	5.95910000	3.53970000
4	Si	-5.99570000	5.67090000	2.42990000
5	Si	-10.73910000	3.90040000	2.70070000
6	O	-11.73290000	2.70740000	2.34160000
7	Si	-12.07420000	1.15480000	2.31840000
8	O	-11.45520000	0.42330000	3.58130000
9	Si	-11.39460000	-4.15760000	7.24580000
10	Si	-13.29570000	-2.46030000	5.52120000
11	Si	-11.50890000	0.09760000	5.13610000
12	Si	-8.83680000	-0.22830000	6.67330000
13	O	-12.44950000	-3.64190000	6.15630000
14	O	-12.41530000	-1.16550000	5.38290000
15	O	-10.03410000	-0.20050000	5.63860000
16	O	-7.69650000	0.78430000	6.31660000
17	Si	-0.05969900	4.78730300	6.54672400
18	O	-10.24280000	-7.11800000	9.08650000
19	Si	-7.71660000	3.11370000	2.78820000
20	O	-6.95550000	4.50240000	2.92570000
21	O	-9.24950000	3.38730000	2.56950000
22	Si	-4.97250000	-7.60980000	-1.50390000
23	Si	-11.35590000	0.26280000	-0.54610000
24	O	-6.84510000	-7.72030000	2.70470000
25	O	-10.35620000	-0.94150000	-0.80140000
26	Si	-9.16490000	-9.40520000	0.52820000
27	Si	-9.33470000	-6.71560000	-0.96890000
28	Si	-11.54680000	-4.63200000	-1.45310000
29	Si	-9.77590000	-2.05450000	-1.77500000
30	O	-9.58580000	-8.00560000	-0.07990000
31	O	-10.67690000	-5.84320000	-0.91270000
32	O	-10.64710000	-3.36120000	-1.66840000
33	O	-8.28390000	-2.37400000	-1.34130000
34	O	-6.40440000	-3.94670000	-0.53100000
35	O	-8.15250000	-5.87130000	-0.34420000
36	O	-8.84920000	-9.23940000	2.07860000
37	O	-6.41640000	-5.42400000	1.54900000
38	O	-5.61290000	-6.41590000	-0.70840000
39	O	-5.77370000	-1.60340000	-1.35130000
40	Si	-6.81090000	-5.43360000	5.68340000
41	Si	-8.50460000	-8.00720000	6.05360000
42	O	-7.72180000	-6.63160000	6.20070000
43	Si	-10.95800000	-7.17850000	7.67890000
44	Si	-8.42890000	-3.23820000	7.03330000

1	O	-11.40780000	-5.74300000	7.18590000
2	O	-8.21960000	-1.69260000	6.70790000
3	O	-9.95660000	-3.63110000	6.85010000
4	O	-9.98360000	-7.83070000	6.60240000
5	O	-7.53000000	-4.04100000	5.99020000
6	O	-7.92320000	-3.54700000	8.50450000
7	Si	0.12366300	4.64446800	-2.14540400
8	Si	-2.82299600	3.84600000	-1.95510200
9	O	-3.94896200	0.19047100	-1.21862900
10	O	0.75594600	3.76941000	-0.98751600
11	O	-1.45550000	4.66540000	-1.97180000
12	O	-2.55362100	2.34860700	-1.50002200
13	O	-6.33220000	0.83850000	-0.42850000
14	O	-3.77030000	4.57610000	-0.90140000
15	Si	-5.28020000	4.78230000	-0.42350000
16	Si	-7.00390000	2.22870000	-0.05400000
17	Si	-9.63060000	2.52380000	-1.72000000
18	O	-6.07880000	3.41370000	-0.57020000
19	O	-8.42830000	2.36750000	-0.70540000
20	O	-10.83220000	1.58900000	-1.25000000
21	O	-5.20960000	5.26350000	1.09860000
22	O	-7.15700000	2.26930000	1.54270000
23	O	-11.46650000	0.47770000	1.01990000
24	O	-6.60040000	-5.49380000	4.09960000
25	O	-8.61720000	-8.44720000	4.51360000
26	O	-1.68267700	1.69080700	8.46850100
27	Si	-1.74883000	2.17137100	6.97378800
28	O	-0.91871000	3.49571700	6.81439200
29	Si	2.50951500	3.95256600	5.10425700
30	Si	2.56655600	1.37886700	6.82672600
31	Si	3.01133200	-3.35747800	7.49346600
32	Si	-0.01128600	-2.57102900	7.40589500
33	O	2.86464300	2.66311100	5.94588500
34	O	3.90010900	0.51781900	6.89195400
35	O	3.77240000	-1.96900000	7.63100000
36	O	1.47827000	-3.08412200	7.27493600
37	O	2.15456400	1.79119200	8.29132000
38	O	-0.24968300	-2.04669800	8.86410200
39	O	1.05379000	4.47370400	5.45678900
40	O	-1.00410100	-3.76441600	7.04698100
41	Si	0.52346500	-7.58778700	-0.03020900
42	Si	-2.45310000	-8.37930000	0.08690000
43	O	-1.02440000	-7.79970000	-0.28570000
44	O	-3.48040000	-7.82240000	-1.00870000

1	O	-2.05273400	-6.52245200	3.54837300
2	O	-4.53620000	-6.55020000	2.91500000
3	O	-2.87430000	-7.94910000	1.53380000
4	O	0.93450000	-7.98310000	1.44400000
5	O	0.37156100	-7.41294100	3.90394100
6	Si	0.95190500	-8.52589500	2.93029800
7	Si	-1.34643500	-5.31655200	7.02384600
8	Si	-4.32960000	-6.05610000	7.41270000
9	O	-2.92290000	-5.44190000	7.01850000
10	O	-5.41450000	-5.45960000	6.41750000
11	O	-4.71840000	-5.65910000	8.88780000
12	O	-1.36620000	-5.12610000	10.61890000
13	O	-0.72730000	-6.04810000	8.28660000
14	Si	-0.78110000	-6.37380000	9.84140000
15	Si	4.19161300	1.79581300	-2.03247800
16	Si	4.36134900	-0.89364500	-0.53540000
17	Si	1.79907000	-4.81750700	0.05494800
18	Si	1.68503400	-2.17067700	-1.47853500
19	Si	3.22795900	3.06040500	2.23972000
20	Si	5.44855100	-1.68947600	4.28209500
21	Si	3.72401800	-4.24258400	4.65111300
22	O	4.61236200	0.39619700	-1.42444400
23	O	1.43075500	-3.66260500	-0.97313200
24	O	3.17929700	-1.73848700	-1.15980900
25	O	4.64904700	-3.05762800	4.13513400
26	O	2.93692900	2.40526700	-1.28875300
27	O	2.15293300	3.10900600	1.07406300
28	O	2.54295900	3.62285200	3.55349900
29	O	5.51815200	-1.20787600	5.80382600
30	O	3.57067200	-4.20213700	6.24788200
31	O	-0.73796800	-5.99433600	5.72551400
32	H	-1.30770000	8.45280000	5.54490000
33	H	3.53900000	4.98890000	5.43620000
34	H	-5.91550000	5.84190000	-1.27060000
35	H	-6.78570000	6.92250000	2.19890000
36	H	-12.70540000	-0.03450000	-1.12450000
37	H	-13.56750000	1.03610000	2.31350000
38	H	-12.61360000	-4.36250000	-0.43650000
39	H	-12.17550000	-5.02190000	-2.75570000
40	H	-14.47190000	-2.17020000	6.40220000
41	H	-13.77040000	-2.92530000	4.17860000
42	H	6.86449500	-1.88259700	3.83328200
43	H	-2.15040000	-4.10050000	12.78420000
44	H	1.31010000	-8.39770000	-1.01480000

1	H	-12.21020000	-7.97290000	7.89080000
2	H	0.36339800	-1.65380700	11.27870200
3	H	0.62130000	6.05740000	-2.14750000
4	H	0.50140000	4.07440000	-3.47820000
5	H	-2.25700000	7.49990000	7.52180000
6	H	-5.73850000	6.73170000	5.78280000
7	H	-10.96700000	4.40130000	4.09400000
8	H	-11.01960000	5.00810000	1.73210000
9	H	-12.06290000	1.27880000	5.87220000
10	H	-10.59640000	-6.34750000	11.45320000
11	H	-8.66420000	-7.73420000	10.94950000
12	H	2.77449000	1.81968400	10.74640200
13	H	1.80021000	3.79900000	9.78440300
14	H	5.77540000	-0.53010000	8.17660000
15	H	3.24710000	-4.17500000	8.72650000
16	H	0.61160000	-6.65520000	10.31590000
17	H	-1.64370000	-7.57580000	10.07620000
18	H	0.12290000	-9.76940000	3.03170000
19	H	2.36090000	-8.82750000	3.33990000
20	H	-10.15040000	3.92860000	-1.73450000
21	H	-9.16390000	2.16210000	-3.09680000
22	H	3.89500000	1.63920000	-3.49250000
23	H	5.32300000	2.73990000	-1.76330000
24	H	4.42878700	3.88352300	1.88700900
25	H	5.61653000	-1.70965200	-0.58831700
26	H	4.35729800	-5.55350600	4.29822000
27	H	3.22919100	-5.21293700	-0.15129000
28	H	-5.23700000	-6.37850000	11.22840000
29	H	-7.76830000	-9.07120000	6.80850000
30	H	-6.95230000	-10.08460000	3.55430000
31	H	-10.29630000	-10.34930000	0.25900000
32	H	-2.42150000	-9.87450000	0.00040000
33	H	-3.42900000	-8.60990000	3.88980000
34	H	-4.28320000	-7.54880000	7.29620000
35	H	-3.45780000	3.89970000	-3.31080000
36	H	0.59911000	5.23699300	7.81469700
37	H	-9.79240000	-1.54060000	-3.18200000
38	H	-8.38790000	-2.95530000	10.89960000
39	H	-4.87450000	3.78240000	8.02040000
40	H	-2.02270000	2.13730000	10.92000000
41	H	-4.91220000	-7.27130000	-2.96190000
42	H	-8.98790000	-7.09310000	-2.37650000
43	H	1.45748300	-2.18476300	-2.95899600
44	H	-5.88650000	0.35320000	-2.87170000

1	H	-6.57060000	-3.25690000	-2.96870000
2	H	-11.74490000	-3.66940000	8.61800000
3	H	-9.32890000	0.16850000	8.03140000
4	H	-8.19140000	3.21540000	6.31880000
5	H	-5.78340000	-8.84910000	-1.27830000
6	H	-7.97590000	-9.98270000	-0.17660000
7	H	-2.11767000	0.35882300	-2.97425700
8	H	-4.73780416	-3.42353995	1.43315303
9	C	-1.35406270	-2.53564743	2.99349767
10	H	-1.67486817	-2.79018107	3.99862335
11	H	-1.67542241	-1.53555844	2.72454681
12	H	-1.69444077	-3.25318039	2.25729398
13	O	-3.83040156	-3.24676765	1.16196544
14	H	-3.93153479	-2.73738843	0.35039934
15				
16				
17	Z-CH3_H2O(ads)_CH3OH(ads)			
18	Si	-0.02039905	0.03731690	-0.04149275
19	Si	-0.06729709	-0.01098888	5.65427386
20	Si	3.68512234	-0.07200526	2.48889070
21	Si	1.06929939	-3.91613237	2.97678944
22	Al	0.73474135	-0.76290674	2.86963401
23	O	0.16385836	-2.50767431	2.81708724
24	O	2.42536290	-0.86015908	3.10318454
25	O	0.11975511	0.02743739	1.52218321
26	O	-0.22024800	-0.07875505	4.08511507
27	O	-1.56714133	0.15515938	-0.45352183
28	O	-0.33805409	-1.45459934	6.30563264
29	O	1.38389435	0.49436844	6.17495508
30	O	-1.23328098	1.00759020	6.03828706
31	O	0.83402772	1.28422315	-0.58432718
32	O	3.61897617	1.52995171	2.54377449
33	O	4.97815426	-0.46861271	3.35187280
34	O	2.19991095	-3.93722332	4.10869492
35	O	3.90185680	-0.49349148	0.94964376
36	O	1.76026912	-4.22938529	1.57299852
37	O	0.56280548	-1.29491831	-0.73527463
38	O	-0.10910107	-4.92745620	3.34477700
39	O	0.80133195	-6.00647567	-0.15280075
40	Si	-5.49760299	-0.02108804	-1.47429202
41	Si	-2.51910099	0.76907347	-1.59035924
42	Si	1.67287201	2.63506648	-0.36445986
43	Si	-6.77250000	-2.79180000	-1.55910000
44	Si	-6.65860000	-5.43650000	-0.02630000

1	Si	-0.62798711	-6.20818465	4.15920358
2	Si	-3.21923415	-7.43500804	2.98458437
3	Si	-6.09540000	-6.32220000	2.83000000
4	Si	-7.79180000	-8.89230000	3.21140000
5	Si	-7.85690000	-4.02790000	9.99880000
6	Si	-9.54690000	-6.64300000	10.42590000
7	O	-8.68790000	-5.35140000	10.15840000
8	Si	1.78781602	2.30218598	9.72780901
9	Si	-0.76980808	-1.62740499	10.29929998
10	Si	-1.17801007	1.38382818	9.93890906
11	O	-1.38698985	-0.16319594	10.26480102
12	O	0.35018894	1.77512212	10.12158995
13	O	-1.90930612	-2.64049389	10.65649693
14	Si	-2.31670000	-4.06080000	11.29600000
15	Si	-5.02660000	-5.18350000	10.35000000
16	O	-3.83590000	-4.30830000	10.92640000
17	O	-6.34110000	-4.27000000	10.39930000
18	Si	4.73289699	-0.80096582	7.13547088
19	Si	-7.29070000	2.20560000	5.67640000
20	Si	-4.57940717	3.32748872	6.62401949
21	Si	-1.94070000	7.20800000	6.08700000
22	Si	-4.59330000	6.04430000	5.10460000
23	O	-5.77090000	2.45290000	6.04720000
24	O	-3.26560070	2.41457040	6.57334411
25	O	-0.99449908	5.94279911	5.99239638
26	O	-3.27080000	6.91960000	5.26710000
27	O	-4.35770000	4.58890000	5.69440000
28	O	-7.46660000	2.24720000	4.09540000
29	O	-4.88400000	5.95910000	3.53970000
30	Si	-5.99570000	5.67090000	2.42990000
31	Si	-10.73910000	3.90040000	2.70070000
32	O	-11.73290000	2.70740000	2.34160000
33	Si	-12.07420000	1.15480000	2.31840000
34	O	-11.45520000	0.42330000	3.58130000
35	Si	-11.39460000	-4.15760000	7.24580000
36	Si	-13.29570000	-2.46030000	5.52120000
37	Si	-11.50890000	0.09760000	5.13610000
38	Si	-8.83680000	-0.22830000	6.67330000
39	O	-12.44950000	-3.64190000	6.15630000
40	O	-12.41530000	-1.16550000	5.38290000
41	O	-10.03410000	-0.20050000	5.63860000
42	O	-7.69650000	0.78430000	6.31660000
43	Si	-0.05969890	4.78730294	6.54672406
44	O	-10.24280000	-7.11800000	9.08650000

1	Si	-7.71660000	3.11370000	2.78820000
2	O	-6.95550000	4.50240000	2.92570000
3	O	-9.24950000	3.38730000	2.56950000
4	Si	-4.97250000	-7.60980000	-1.50390000
5	Si	-11.35590000	0.26280000	-0.54610000
6	O	-6.84510000	-7.72030000	2.70470000
7	O	-10.35620000	-0.94150000	-0.80140000
8	Si	-9.16490000	-9.40520000	0.52820000
9	Si	-9.33470000	-6.71560000	-0.96890000
10	Si	-11.54680000	-4.63200000	-1.45310000
11	Si	-9.77590000	-2.05450000	-1.77500000
12	O	-9.58580000	-8.00560000	-0.07990000
13	O	-10.67690000	-5.84320000	-0.91270000
14	O	-10.64710000	-3.36120000	-1.66840000
15	O	-8.28390000	-2.37400000	-1.34130000
16	O	-6.40440000	-3.94670000	-0.53100000
17	O	-8.15250000	-5.87130000	-0.34420000
18	O	-8.84920000	-9.23940000	2.07860000
19	O	-6.41640000	-5.42400000	1.54900000
20	O	-5.61290000	-6.41590000	-0.70840000
21	O	-5.77370000	-1.60340000	-1.35130000
22	Si	-6.81090000	-5.43360000	5.68340000
23	Si	-8.50460000	-8.00720000	6.05360000
24	O	-7.72180000	-6.63160000	6.20070000
25	Si	-10.95800000	-7.17850000	7.67890000
26	Si	-8.42890000	-3.23820000	7.03330000
27	O	-11.40780000	-5.74300000	7.18590000
28	O	-8.21960000	-1.69260000	6.70790000
29	O	-9.95660000	-3.63110000	6.85010000
30	O	-9.98360000	-7.83070000	6.60240000
31	O	-7.53000000	-4.04100000	5.99020000
32	O	-7.92320000	-3.54700000	8.50450000
33	Si	0.12366303	4.64446802	-2.14540400
34	Si	-2.82299603	3.84600000	-1.95510199
35	O	-3.94896180	0.19047077	-1.21862858
36	O	0.75594571	3.76941011	-0.98751538
37	O	-1.45550000	4.66540000	-1.97180000
38	O	-2.55362077	2.34860699	-1.50002179
39	O	-6.33220000	0.83850000	-0.42850000
40	O	-3.77030000	4.57610000	-0.90140000
41	Si	-5.28020000	4.78230000	-0.42350000
42	Si	-7.00390000	2.22870000	-0.05400000
43	Si	-9.63060000	2.52380000	-1.72000000
44	O	-6.07880000	3.41370000	-0.57020000

1	O	-8.42830000	2.36750000	-0.70540000
2	O	-10.83220000	1.58900000	-1.25000000
3	O	-5.20960000	5.26350000	1.09860000
4	O	-7.15700000	2.26930000	1.54270000
5	O	-11.46650000	0.47770000	1.01990000
6	O	-6.60040000	-5.49380000	4.09960000
7	O	-8.61720000	-8.44720000	4.51360000
8	O	-1.68267691	1.69080603	8.46850068
9	Si	-1.74883028	2.17136954	6.97378530
10	O	-0.91870999	3.49571701	6.81439219
11	Si	2.50951452	3.95256494	5.10425732
12	Si	2.56655584	1.37886799	6.82672531
13	Si	3.01133198	-3.35747815	7.49346612
14	Si	-0.01128509	-2.57102838	7.40589286
15	O	2.86464309	2.66311093	5.94588493
16	O	3.90010899	0.51781899	6.89195409
17	O	3.77240000	-1.96900000	7.63100000
18	O	1.47827015	-3.08412165	7.27493636
19	O	2.15456395	1.79119199	8.29131999
20	O	-0.24968355	-2.04669746	8.86410172
21	O	1.05378980	4.47370409	5.45678877
22	O	-1.00410025	-3.76441619	7.04697957
23	Si	0.52346577	-7.58778729	-0.03021104
24	Si	-2.45310000	-8.37930000	0.08690000
25	O	-1.02440000	-7.79970000	-0.28570000
26	O	-3.48040000	-7.82240000	-1.00870000
27	O	-2.05273372	-6.52245207	3.54837238
28	O	-4.53620000	-6.55020000	2.91500000
29	O	-2.87430000	-7.94910000	1.53380000
30	O	0.93450000	-7.98310000	1.44400000
31	O	0.37156178	-7.41294036	3.90394103
32	Si	0.95190469	-8.52589529	2.93029814
33	Si	-1.34643542	-5.31655201	7.02384675
34	Si	-4.32960000	-6.05610000	7.41270000
35	O	-2.92290000	-5.44190000	7.01850000
36	O	-5.41450000	-5.45960000	6.41750000
37	O	-4.71840000	-5.65910000	8.88780000
38	O	-1.36620000	-5.12610000	10.61890000
39	O	-0.72730000	-6.04810000	8.28660000
40	Si	-0.78110000	-6.37380000	9.84140000
41	Si	4.19161315	1.79581320	-2.03247768
42	Si	4.36135062	-0.89364687	-0.53540110
43	Si	1.79907238	-4.81750722	0.05494907
44	Si	1.68503481	-2.17067394	-1.47853456

1	Si	3.22796292	3.06040208	2.23971590
2	Si	5.44855088	-1.68947387	4.28209478
3	Si	3.72401578	-4.24258383	4.65111385
4	O	4.61236210	0.39619670	-1.42444441
5	O	1.43075341	-3.66260303	-0.97312877
6	O	3.17929789	-1.73848876	-1.15981100
7	O	4.64904661	-3.05762811	4.13513355
8	O	2.93692865	2.40526791	-1.28875370
9	O	2.15293065	3.10900371	1.07406622
10	O	2.54295917	3.62284914	3.55350031
11	O	5.51815147	-1.20787562	5.80382590
12	O	3.57067207	-4.20213643	6.24788199
13	O	-0.73796803	-5.99433527	5.72551390
14	H	-1.30770000	8.45280000	5.54490000
15	H	3.53900000	4.98890000	5.43620000
16	H	-5.91550000	5.84190000	-1.27060000
17	H	-6.78570000	6.92250000	2.19890000
18	H	-12.70540000	-0.03450000	-1.12450000
19	H	-13.56750000	1.03610000	2.31350000
20	H	-12.61360000	-4.36250000	-0.43650000
21	H	-12.17550000	-5.02190000	-2.75570000
22	H	-14.47190000	-2.17020000	6.40220000
23	H	-13.77040000	-2.92530000	4.17860000
24	H	6.86449516	-1.88259709	3.83328254
25	H	-2.15040000	-4.10050000	12.78420000
26	H	1.31010000	-8.39770000	-1.01480000
27	H	-12.21020000	-7.97290000	7.89080000
28	H	0.36339795	-1.65380721	11.27870206
29	H	0.62130000	6.05740000	-2.14750000
30	H	0.50140000	4.07440000	-3.47820000
31	H	-2.25700000	7.49990000	7.52180000
32	H	-5.73850000	6.73170000	5.78280000
33	H	-10.96700000	4.40130000	4.09400000
34	H	-11.01960000	5.00810000	1.73210000
35	H	-12.06290000	1.27880000	5.87220000
36	H	-10.59640000	-6.34750000	11.45320000
37	H	-8.66420000	-7.73420000	10.94950000
38	H	2.77448990	1.81968384	10.74640202
39	H	1.80021018	3.79900000	9.78440305
40	H	5.77540000	-0.53010000	8.17660000
41	H	3.24710000	-4.17500000	8.72650000
42	H	0.61160000	-6.65520000	10.31590000
43	H	-1.64370000	-7.57580000	10.07620000
44	H	0.12290000	-9.76940000	3.03170000

1	H	2.36090000	-8.82750000	3.33990000
2	H	-10.15040000	3.92860000	-1.73450000
3	H	-9.16390000	2.16210000	-3.09680000
4	H	3.89500000	1.63920000	-3.49250000
5	H	5.32300000	2.73990000	-1.76330000
6	H	4.42878608	3.88352522	1.88701105
7	H	5.61652972	-1.70965241	-0.58831745
8	H	4.35729790	-5.55350619	4.29822054
9	H	3.22919086	-5.21293683	-0.15129127
10	H	-5.23700000	-6.37850000	11.22840000
11	H	-7.76830000	-9.07120000	6.80850000
12	H	-6.95230000	-10.08460000	3.55430000
13	H	-10.29630000	-10.34930000	0.25900000
14	H	-2.42150000	-9.87450000	0.00040000
15	H	-3.42900000	-8.60990000	3.88980000
16	H	-4.28320000	-7.54880000	7.29620000
17	H	-3.45780000	3.89970000	-3.31080000
18	H	0.59911030	5.23699280	7.81469692
19	H	-9.79240000	-1.54060000	-3.18200000
20	H	-8.38790000	-2.95530000	10.89960000
21	H	-4.87450000	3.78240000	8.02040000
22	H	-2.02270000	2.13730000	10.92000000
23	H	-4.91220000	-7.27130000	-2.96190000
24	H	-8.98790000	-7.09310000	-2.37650000
25	H	1.45748080	-2.18476331	-2.95899566
26	H	-5.88650000	0.35320000	-2.87170000
27	H	-6.57060000	-3.25690000	-2.96870000
28	H	-11.74490000	-3.66940000	8.61800000
29	H	-9.32890000	0.16850000	8.03140000
30	H	-8.19140000	3.21540000	6.31880000
31	H	-5.78340000	-8.84910000	-1.27830000
32	H	-7.97590000	-9.98270000	-0.17660000
33	H	-2.11766959	0.35882249	-2.97425673
34	H	-2.15281383	0.24248345	3.61946898
35	C	-3.44210588	1.41211184	2.70711823
36	H	-3.45087517	2.20908298	3.45880569
37	H	-4.45499262	1.29093197	2.32083821
38	H	-2.78318048	1.70326144	1.88251065
39	O	-3.05569730	0.16537585	3.27468381
40	H	-3.94150419	-1.53134225	3.04761638
41	C	-1.33474826	-2.61286877	2.62460159
42	H	-1.77590787	-2.88623166	3.57315762
43	H	-1.66957010	-1.63608807	2.29996196
44	H	-1.52511416	-3.36086799	1.86419151

1	O	-4.10298802	-2.46587972	2.83022161
2	H	-4.86723293	-2.47001669	2.24715333
3				
4				
5	Z-(CH3)3O+ methylation-TS			
6	Si	-3.89790801	2.12360958	3.05885753
7	Si	-3.88846772	-0.75367290	-1.81429364
8	Si	-7.38412862	-0.30764753	1.61443943
9	Si	-3.55753373	-2.88646481	2.52333346
10	Al	-4.31217558	-0.26820463	1.10757863
11	O	-3.33864839	-1.46334628	1.86033365
12	O	-5.96070218	-0.78165482	1.09089356
13	O	-4.01683713	1.29685267	1.73494845
14	O	-3.71995155	0.04515510	-0.47075289
15	O	-2.47058092	2.90533797	3.04618199
16	O	-3.12825477	-2.17445754	-1.79736644
17	O	-5.41695525	-1.03584096	-2.28604590
18	O	-3.12934500	0.23073965	-2.84251857
19	O	-5.10406887	3.18952288	3.08591090
20	O	-7.98544387	0.97870478	0.85774412
21	O	-8.45387708	-1.47437103	1.33831973
22	O	-4.60144600	-3.91552997	1.82187337
23	O	-7.36765655	0.04850598	3.19423391
24	O	-4.07610300	-2.74684181	4.05038416
25	O	-3.96033132	1.28596745	4.42956355
26	O	-2.08370915	-3.55689838	2.45981545
27	C	-1.47786838	3.06675978	-1.25972624
28	H	-1.47363112	2.36347890	-2.08267397
29	H	-0.66521773	3.78302284	-1.21288981
30	C	-2.50589704	3.11560927	-0.38717323
31	H	-2.53904720	3.86575667	0.39392504
32	H	-3.33353840	2.41846615	-0.44262162
33	C	-0.96099928	1.55428925	0.31669065
34	H	-1.16811642	2.03350692	1.26122803
35	H	-1.64632027	0.81408864	-0.06607801
36	H	-0.00347392	1.72786300	-0.14616088
37	O	0.09567917	0.01491651	1.33934856
38	C	-0.20096097	-0.10782394	2.73998727
39	H	0.52328198	-0.78742188	3.19694690
40	H	-0.08954590	0.88289511	3.17683472
41	H	-1.21546909	-0.48494177	2.88539963
42	C	0.00096062	-1.23741840	0.63887121
43	H	-1.01316613	-1.63737522	0.70185301
44	H	0.27344712	-1.04462752	-0.39822046

1	H	0.71108611	-1.94514682	1.07306982
2	O	-2.55044800	-2.94123100	6.16653200
3	Si	1.26902600	4.44344900	3.31632200
4	Si	-1.79603400	4.25864600	3.59730900
5	Si	-6.38926000	3.90379900	2.43936800
6	Si	3.43373600	2.62149400	4.45818400
7	Si	4.23645100	-0.32970500	4.40378200
8	Si	-1.18616300	-4.86398800	2.27845600
9	Si	1.68246900	-4.49309600	3.38803500
10	Si	3.98883000	-2.66023900	2.46280300
11	Si	6.47326400	-4.43073700	3.02988300
12	Si	4.76061300	-3.90975100	-5.12676000
13	Si	7.25431900	-5.74172300	-4.57669400
14	O	6.00050000	-4.81548900	-4.79509200
15	Si	-6.48604100	-1.50993800	-6.08463200
16	Si	-2.72115400	-4.22180100	-5.20082900
17	Si	-3.38877300	-1.48015900	-6.38468900
18	O	-2.65505200	-2.83566600	-5.97559900
19	O	-4.95910800	-1.70942300	-6.44280300
20	O	-1.30299200	-4.88471600	-5.24308900
21	Si	-0.43106300	-6.23754600	-5.20094900
22	Si	2.51015700	-5.86323600	-4.35949300
23	O	1.08248300	-5.79989100	-5.04776100
24	O	3.42126300	-4.75844600	-5.07653400
25	Si	-8.13153300	-3.58393000	-1.84029500
26	Si	2.09425500	3.15774900	-4.23165100
27	Si	-0.84801300	2.78156500	-5.07384900
28	Si	-4.67204700	5.41213500	-5.94920500
29	Si	-1.76977100	5.75467500	-5.04640300
30	O	0.58020500	2.71914600	-4.38566700
31	O	-1.75864700	1.67790500	-4.35585400
32	O	-5.11461000	4.15484100	-5.09578400
33	O	-3.31658800	5.98855900	-5.35335000
34	O	-1.48733900	4.20774900	-4.82546100
35	O	2.26108000	4.04417000	-2.92067400
36	O	-1.45120800	6.56435300	-3.71088200
37	Si	-0.29734900	7.22290700	-2.82459300
38	Si	4.76257900	7.06015000	-3.10474300
39	O	6.11474600	6.57103100	-2.41754000
40	Si	6.97802200	5.42702200	-1.72936300
41	O	6.64091600	4.01158400	-2.35870000
42	Si	8.14872900	-1.57080700	-3.34879600
43	Si	9.35366000	1.24089200	-3.01450800
44	Si	6.78885600	2.97655500	-3.55586100

1	Si	4.38377000	1.14126000	-4.23155800
2	O	8.96784400	-0.28851600	-2.84824400
3	O	8.07731800	2.09794500	-3.34184500
4	O	5.50643700	2.04304200	-3.57481400
5	O	2.96502900	1.80328000	-4.18934500
6	Si	-5.59170300	2.66118200	-4.85569400
7	O	8.08647700	-5.24156200	-3.32719600
8	Si	2.20576200	5.48182200	-2.24822200
9	O	1.00541100	6.31065900	-2.87977100
10	O	3.54819600	6.26904200	-2.47322600
11	Si	3.43314200	-1.84156200	7.01499800
12	Si	6.64744300	5.94205500	1.29428300
13	O	5.18166400	-3.50624800	3.09037800
14	O	6.13514400	4.79956000	2.26751100
15	Si	7.96714700	-3.07984300	5.33019300
16	Si	7.20070600	-0.09377600	5.32227500
17	Si	8.54873200	2.49492100	4.34723800
18	Si	5.99129900	4.21917200	3.73920100
19	O	7.87800800	-1.51383200	5.11691200
20	O	8.15207000	0.98246500	4.61350600
21	O	7.26352000	3.36580400	4.10118700
22	O	4.70098000	3.29806400	3.79284900
23	O	3.48228700	1.05661000	4.18421100
24	O	5.79130000	-0.07738300	4.60534100
25	O	7.59711300	-3.82434100	3.97384100
26	O	3.98865000	-1.18911500	3.08454100
27	O	3.60684400	-1.08765500	5.64759900
28	O	2.08008600	3.18201400	3.90453700
29	Si	4.31809200	-3.17323600	-0.54915100
30	Si	6.80133900	-4.94169800	0.02973800
31	O	5.58514500	-4.13476900	-0.59988700
32	Si	8.79237700	-4.36554300	-2.21777900
33	Si	5.05121900	-1.59903800	-3.04802200
34	O	8.71653500	-2.82016900	-2.55259000
35	O	4.31770200	-0.24500600	-3.45682800
36	O	6.62165100	-1.37096500	-2.98863000
37	O	8.11919800	-4.63771300	-0.80129500
38	O	4.50111400	-1.98764400	-1.60339900
39	O	4.67012900	-2.74408300	-4.07717800
40	Si	-5.62217500	6.89233900	2.74055600
41	Si	-2.58453800	7.02405800	2.40548700
42	O	-0.25826400	4.02559400	3.28376800
43	O	-5.92016000	5.40983400	2.27189800
44	O	-4.15206200	7.29006400	2.28775400

1	O	-2.31765500	5.50125000	2.76855600
2	O	1.73899500	4.85759200	1.85454800
3	O	-1.96376600	7.36280100	0.97699100
4	Si	-0.62661100	7.73590400	0.18736000
5	Si	1.87774500	5.99289300	0.75185800
6	Si	4.25243700	7.85499300	1.56155800
7	O	0.60192900	6.93912900	0.81040700
8	O	3.17026700	6.85786600	0.98362000
9	O	5.70018200	7.21678900	1.37360800
10	O	-0.87713500	7.33384200	-1.33871600
11	O	1.99016700	5.26272300	-0.67248500
12	O	6.65938200	5.35593700	-0.17782100
13	O	4.15862700	-2.48250300	0.88396300
14	O	7.07697500	-4.48475000	1.54403700
15	O	-3.00799800	-0.33727300	-5.35518900
16	Si	-3.09861000	0.82844700	-4.30563500
17	O	-4.33788500	1.73489700	-4.63738100
18	Si	-7.69099700	1.95315800	-2.74142100
19	Si	-6.86214100	-1.01978100	-3.00349300
20	Si	-5.62787900	-5.32414100	-1.26409700
21	Si	-3.07102800	-3.74589400	-2.12057100
22	O	-7.58127700	0.37769900	-2.79375500
23	O	-7.81039700	-2.14565100	-2.40629300
24	O	-6.82828900	-4.49541400	-1.89558000
25	O	-4.28544600	-4.53692100	-1.48910100
26	O	-6.63561100	-1.30513700	-4.53711600
27	O	-3.04651900	-3.98894300	-3.66915300
28	O	-6.51353000	2.62865800	-3.56136500
29	O	-1.71956700	-4.23575500	-1.43327100
30	Si	-1.73819700	-4.20110800	6.75463000
31	Si	1.32576600	-4.01783400	6.47374200
32	O	-0.21142600	-3.78393600	6.78724300
33	O	2.10467400	-2.70728900	6.96526700
34	O	0.26459900	-4.38598000	2.68832400
35	O	2.60720900	-3.35064700	2.78649000
36	O	1.55455300	-4.27714400	4.94520800
37	O	-2.00034300	-5.38965100	5.74597200
38	O	-1.69855600	-6.00651300	3.25170200
39	Si	-1.84230800	-6.58687200	4.72337300
40	Si	-0.85558500	-5.37902200	-0.74519100
41	Si	2.19350600	-5.28931100	-1.28617000
42	O	0.66504100	-5.00993300	-0.97443200
43	O	3.01145500	-3.98044600	-0.91057200
44	O	2.40326600	-5.59939700	-2.81735900

1	O	-0.94148600	-7.03932200	-3.93864800
2	O	-1.19278500	-6.79448900	-1.37450900
3	Si	-1.04475000	-7.82948900	-2.57168900
4	Si	-8.43689600	3.32138900	4.74088400
5	Si	-7.67039700	0.33538300	4.74865000
6	Si	-3.90339100	-2.37991800	5.61287500
7	Si	-4.70640400	0.57267700	5.66692500
8	Si	-8.02166900	2.46816200	0.28224400
9	Si	-8.46092400	-3.07088200	1.17163000
10	Si	-5.95595400	-4.81312900	1.73613500
11	O	-8.34775600	1.75537900	4.95416500
12	O	-3.95194200	-0.81503400	5.88684800
13	O	-6.26108400	0.31901100	5.46568900
14	O	-7.23171200	-3.86683300	1.79453300
15	O	-7.48271700	3.81069200	3.57942800
16	O	-7.01933600	3.41671500	1.06479900
17	O	-7.59073700	2.46154700	-1.24278200
18	O	-8.71077600	-3.47207000	-0.35450500
19	O	-5.84356700	-5.54321900	0.31174500
20	O	-1.17480300	-5.45090100	0.80647600
21	H	-5.69490600	6.50659700	-5.95074300
22	H	-9.02151700	2.31861200	-3.32484100
23	H	-0.39342500	9.21128500	0.30054600
24	H	0.00708000	8.58769500	-3.36184400
25	H	8.02165100	6.39474900	1.68249100
26	H	8.41840000	5.77660800	-1.94652200
27	H	9.44301800	2.51499500	3.14556500
28	H	9.28777600	3.02540400	5.53738600
29	H	10.34463800	1.37877400	-4.12928000
30	H	9.97515300	1.68511700	-1.72588400
31	H	-9.71501200	-3.42024400	1.91255800
32	H	-0.58858400	-7.07259100	-6.43458500
33	H	-2.18124100	-4.59180400	8.13121500
34	H	10.24109800	-4.74436700	-2.25872800
35	H	-3.78368600	-5.07542300	-5.82245300
36	H	-6.58270400	7.88966200	2.16904400
37	H	-5.76245600	6.99351700	4.22854500
38	H	-4.49299600	5.01584300	-7.38266100
39	H	-0.94473500	6.30771500	-6.16775000
40	H	4.78612200	6.82785000	-4.58447500
41	H	4.64786500	8.53069100	-2.84356800
42	H	6.88669500	3.72461300	-4.85001400
43	H	8.12318800	-5.71115100	-5.79663100
44	H	6.80384900	-7.15231400	-4.35010400

1	H	-7.25214600	-2.70920700	-6.55235800
2	H	-7.02205700	-0.33040200	-6.83639500
3	H	-9.21379500	-4.20116700	-2.67204600
4	H	-5.57575700	-6.68028300	-1.89832200
5	H	-2.25581600	-8.71093600	-2.58961400
6	H	0.18142800	-8.66555200	-2.36798100
7	H	-0.63167800	-7.39896200	5.06790200
8	H	-3.06089100	-7.45665000	4.77395400
9	H	4.24788000	9.15400000	0.81561800
10	H	3.95632100	8.12076600	3.00582000
11	H	-8.08892200	4.02189400	6.01849900
12	H	-9.82990600	3.61366800	4.27402700
13	H	-9.43086600	2.95666200	0.42159800
14	H	-8.56003800	-0.67099300	5.41192900
15	H	-6.08674600	-5.88363400	2.77574400
16	H	-5.10247700	-3.02006500	6.24242100
17	H	3.11620000	-7.21308800	-4.59292000
18	H	6.47605400	-6.40393400	0.01688200
19	H	6.10053900	-5.81886500	3.45189800
20	H	9.36015700	-3.37212100	5.79705000
21	H	1.82032100	-5.19399400	7.25870400
22	H	2.28063300	-5.84047400	3.12205300
23	H	2.67363900	-6.45265000	-0.47376900
24	H	-1.99446000	7.94239700	3.43127400
25	H	-6.37950500	2.18770200	-6.03859500
26	H	5.84170100	5.35257400	4.70720600
27	H	4.87318100	-3.33984200	-6.50748600
28	H	-0.74545700	2.53039700	-6.54705900
29	H	-2.87153300	-1.11616100	-7.74255700
30	H	3.27352300	-0.84714200	8.12388700
31	H	7.02275500	0.21038600	6.77827400
32	H	-4.47315900	1.37928800	6.90752100
33	H	1.51701100	5.56949200	4.27267000
34	H	3.42219000	2.89875000	5.93027400
35	H	8.29159200	-1.76637700	-4.82708000
36	H	4.69159100	0.92091400	-5.68095200
37	H	2.57781800	3.91737900	-5.42863200
38	H	4.62404300	-2.71851200	7.25381600
39	H	7.06290300	-3.54343400	6.43082800
40	H	-2.01420000	4.50723900	5.05836300
41				
42				
43	Z-(CH3)3O+			
44	Si	-0.02831933	0.02537166	-0.01535336

1	Si	-0.07020106	-0.00665139	5.64525570
2	Si	3.70988198	-0.03660636	2.48791278
3	Si	1.04580835	-3.88958134	2.97632619
4	Al	0.72927410	-0.83675665	2.87955629
5	O	0.28091166	-2.50267478	2.85590797
6	O	2.42262834	-0.69049785	3.15254266
7	O	0.04229344	-0.02175966	1.54672901
8	O	-0.20177167	-0.06009154	4.08428654
9	O	-1.58975230	0.13878614	-0.44385764
10	O	-0.37426360	-1.44711288	6.31777459
11	O	1.35798298	0.50365641	6.21664330
12	O	-1.26908441	0.98853599	6.04138044
13	O	0.80728674	1.29511541	-0.54162439
14	O	3.73941228	1.56965247	2.50415284
15	O	5.00453187	-0.47538227	3.33147940
16	O	2.20271288	-4.03514782	4.10728118
17	O	3.88520799	-0.49732286	0.94763442
18	O	1.76402050	-4.30151148	1.58621573
19	O	0.55406398	-1.27305945	-0.77033396
20	O	-0.15025220	-4.92129706	3.34594883
21	O	0.80121873	-6.00641120	-0.15262591
22	Si	-5.49760218	-0.02109094	-1.47429429
23	Si	-2.51950482	0.76951711	-1.59089820
24	Si	1.67330837	2.63517044	-0.36439033
25	Si	-6.77250000	-2.79180000	-1.55910000
26	Si	-6.65860000	-5.43650000	-0.02630000
27	Si	-0.62808953	-6.20849802	4.15929276
28	Si	-3.21919592	-7.43499902	2.98448997
29	Si	-6.09540000	-6.32220000	2.83000000
30	Si	-7.79180000	-8.89230000	3.21140000
31	Si	-7.85690000	-4.02790000	9.99880000
32	Si	-9.54690000	-6.64300000	10.42590000
33	O	-8.68790000	-5.35140000	10.15840000
34	Si	1.78779969	2.30219987	9.72779996
35	Si	-0.76980094	-1.62739994	10.29929973
36	Si	-1.17800210	1.38380556	9.93890188
37	O	-1.38699812	-0.16319920	10.26480023
38	O	0.35020018	1.77509964	10.12160016
39	O	-1.90930154	-2.64049858	10.65649913
40	Si	-2.31670000	-4.06080000	11.29600000
41	Si	-5.02660000	-5.18350000	10.35000000
42	O	-3.83590000	-4.30830000	10.92640000
43	O	-6.34110000	-4.27000000	10.39930000
44	Si	4.73289997	-0.80100476	7.13550051

1	Si	-7.29070000	2.20560000	5.67640000
2	Si	-4.57939835	3.32750264	6.62399535
3	Si	-1.94070000	7.20800000	6.08700000
4	Si	-4.59330000	6.04430000	5.10460000
5	O	-5.77090000	2.45290000	6.04720000
6	O	-3.26560122	2.41449336	6.57330061
7	O	-0.99449873	5.94279822	5.99239414
8	O	-3.27080000	6.91960000	5.26710000
9	O	-4.35770000	4.58890000	5.69440000
10	O	-7.46660000	2.24720000	4.09540000
11	O	-4.88400000	5.95910000	3.53970000
12	Si	-5.99570000	5.67090000	2.42990000
13	Si	-10.73910000	3.90040000	2.70070000
14	O	-11.73290000	2.70740000	2.34160000
15	Si	-12.07420000	1.15480000	2.31840000
16	O	-11.45520000	0.42330000	3.58130000
17	Si	-11.39460000	-4.15760000	7.24580000
18	Si	-13.29570000	-2.46030000	5.52120000
19	Si	-11.50890000	0.09760000	5.13610000
20	Si	-8.83680000	-0.22830000	6.67330000
21	O	-12.44950000	-3.64190000	6.15630000
22	O	-12.41530000	-1.16550000	5.38290000
23	O	-10.03410000	-0.20050000	5.63860000
24	O	-7.69650000	0.78430000	6.31660000
25	Si	-0.05970132	4.78730047	6.54669767
26	O	-10.24280000	-7.11800000	9.08650000
27	Si	-7.71660000	3.11370000	2.78820000
28	O	-6.95550000	4.50240000	2.92570000
29	O	-9.24950000	3.38730000	2.56950000
30	Si	-4.97250000	-7.60980000	-1.50390000
31	Si	-11.35590000	0.26280000	-0.54610000
32	O	-6.84510000	-7.72030000	2.70470000
33	O	-10.35620000	-0.94150000	-0.80140000
34	Si	-9.16490000	-9.40520000	0.52820000
35	Si	-9.33470000	-6.71560000	-0.96890000
36	Si	-11.54680000	-4.63200000	-1.45310000
37	Si	-9.77590000	-2.05450000	-1.77500000
38	O	-9.58580000	-8.00560000	-0.07990000
39	O	-10.67690000	-5.84320000	-0.91270000
40	O	-10.64710000	-3.36120000	-1.66840000
41	O	-8.28390000	-2.37400000	-1.34130000
42	O	-6.40440000	-3.94670000	-0.53100000
43	O	-8.15250000	-5.87130000	-0.34420000
44	O	-8.84920000	-9.23940000	2.07860000

1	O	-6.41640000	-5.42400000	1.54900000
2	O	-5.61290000	-6.41590000	-0.70840000
3	O	-5.77370000	-1.60340000	-1.35130000
4	Si	-6.81090000	-5.43360000	5.68340000
5	Si	-8.50460000	-8.00720000	6.05360000
6	O	-7.72180000	-6.63160000	6.20070000
7	Si	-10.95800000	-7.17850000	7.67890000
8	Si	-8.42890000	-3.23820000	7.03330000
9	O	-11.40780000	-5.74300000	7.18590000
10	O	-8.21960000	-1.69260000	6.70790000
11	O	-9.95660000	-3.63110000	6.85010000
12	O	-9.98360000	-7.83070000	6.60240000
13	O	-7.53000000	-4.04100000	5.99020000
14	O	-7.92320000	-3.54700000	8.50450000
15	Si	0.12369998	4.64449999	-2.14540000
16	Si	-2.82300211	3.84599990	-1.95509908
17	O	-3.94889762	0.19038982	-1.21850670
18	O	0.75579590	3.76929549	-0.98750218
19	O	-1.45550000	4.66540000	-1.97180000
20	O	-2.55358569	2.34859999	-1.49989439
21	O	-6.33220000	0.83850000	-0.42850000
22	O	-3.77030000	4.57610000	-0.90140000
23	Si	-5.28020000	4.78230000	-0.42350000
24	Si	-7.00390000	2.22870000	-0.05400000
25	Si	-9.63060000	2.52380000	-1.72000000
26	O	-6.07880000	3.41370000	-0.57020000
27	O	-8.42830000	2.36750000	-0.70540000
28	O	-10.83220000	1.58900000	-1.25000000
29	O	-5.20960000	5.26350000	1.09860000
30	O	-7.15700000	2.26930000	1.54270000
31	O	-11.46650000	0.47770000	1.01990000
32	O	-6.60040000	-5.49380000	4.09960000
33	O	-8.61720000	-8.44720000	4.51360000
34	O	-1.68269906	1.69079835	8.46849943
35	Si	-1.74886520	2.17160056	6.97410138
36	O	-0.91869577	3.49569776	6.81430342
37	Si	2.50949823	3.95249626	5.10420156
38	Si	2.56679059	1.37878601	6.82679856
39	Si	3.01121763	-3.35759482	7.49350527
40	Si	-0.01129457	-2.57108632	7.40600275
41	O	2.86459815	2.66320288	5.94600357
42	O	3.90009910	0.51779874	6.89190165
43	O	3.77240000	-1.96900000	7.63100000
44	O	1.47830180	-3.08399243	7.27479079

1	O	2.15449961	1.79120139	8.29129950
2	O	-0.24969848	-2.04670148	8.86410078
3	O	1.05380354	4.47369838	5.45680408
4	O	-1.00420344	-3.76439781	7.04720222
5	Si	0.52349210	-7.58779700	-0.03027916
6	Si	-2.45310000	-8.37930000	0.08690000
7	O	-1.02440000	-7.79970000	-0.28570000
8	O	-3.48040000	-7.82240000	-1.00870000
9	O	-2.05280482	-6.52240600	3.54851433
10	O	-4.53620000	-6.55020000	2.91500000
11	O	-2.87430000	-7.94910000	1.53380000
12	O	0.93450000	-7.98310000	1.44400000
13	O	0.37160329	-7.41289668	3.90389723
14	Si	0.95190343	-8.52589681	2.93029840
15	Si	-1.34640697	-5.31660849	7.02369835
16	Si	-4.32960000	-6.05610000	7.41270000
17	O	-2.92290000	-5.44190000	7.01850000
18	O	-5.41450000	-5.45960000	6.41750000
19	O	-4.71840000	-5.65910000	8.88780000
20	O	-1.36620000	-5.12610000	10.61890000
21	O	-0.72730000	-6.04810000	8.28660000
22	Si	-0.78110000	-6.37380000	9.84140000
23	Si	4.19160223	1.79580091	-2.03249769
24	Si	4.36130451	-0.89369693	-0.53530613
25	Si	1.79906383	-4.81757228	0.05481964
26	Si	1.68501206	-2.17152457	-1.47841557
27	Si	3.22787145	3.06049769	2.23973279
28	Si	5.44849734	-1.68949011	4.28209538
29	Si	3.72401860	-4.24268586	4.65119177
30	O	4.61250071	0.39620052	-1.42439905
31	O	1.43100995	-3.66271051	-0.97331251
32	O	3.17920103	-1.73800551	-1.16009342
33	O	4.64899671	-3.05759627	4.13509726
34	O	2.93689473	2.40529837	-1.28880680
35	O	2.15279152	3.10900892	1.07409429
36	O	2.54300048	3.62292058	3.55349144
37	O	5.51819025	-1.20779404	5.80379856
38	O	3.57086443	-4.20202788	6.24789730
39	O	-0.73788601	-5.99419568	5.72550039
40	H	-1.30770000	8.45280000	5.54490000
41	H	3.53900000	4.98890000	5.43620000
42	H	-5.91550000	5.84190000	-1.27060000
43	H	-6.78570000	6.92250000	2.19890000
44	H	-12.70540000	-0.03450000	-1.12450000

1	H	-13.56750000	1.03610000	2.31350000
2	H	-12.61360000	-4.36250000	-0.43650000
3	H	-12.17550000	-5.02190000	-2.75570000
4	H	-14.47190000	-2.17020000	6.40220000
5	H	-13.77040000	-2.92530000	4.17860000
6	H	6.86450221	-1.88259058	3.83330293
7	H	-2.15040000	-4.10050000	12.78420000
8	H	1.31010000	-8.39770000	-1.01480000
9	H	-12.21020000	-7.97290000	7.89080000
10	H	0.36339936	-1.65380256	11.27870067
11	H	0.62130000	6.05740000	-2.14750000
12	H	0.50140000	4.07440000	-3.47820000
13	H	-2.25700000	7.49990000	7.52180000
14	H	-5.73850000	6.73170000	5.78280000
15	H	-10.96700000	4.40130000	4.09400000
16	H	-11.01960000	5.00810000	1.73210000
17	H	-12.06290000	1.27880000	5.87220000
18	H	-10.59640000	-6.34750000	11.45320000
19	H	-8.66420000	-7.73420000	10.94950000
20	H	2.77450041	1.81970063	10.74639991
21	H	1.80019959	3.79900001	9.78439989
22	H	5.77540000	-0.53010000	8.17660000
23	H	3.24710000	-4.17500000	8.72650000
24	H	0.61160000	-6.65520000	10.31590000
25	H	-1.64370000	-7.57580000	10.07620000
26	H	0.12290000	-9.76940000	3.03170000
27	H	2.36090000	-8.82750000	3.33990000
28	H	-10.15040000	3.92860000	-1.73450000
29	H	-9.16390000	2.16210000	-3.09680000
30	H	3.89500000	1.63920000	-3.49250000
31	H	5.32300000	2.73990000	-1.76330000
32	H	4.42881016	3.88348537	1.88700045
33	H	5.61650433	-1.70969332	-0.58830033
34	H	4.35728145	-5.55350596	4.29818886
35	H	3.22920214	-5.21290219	-0.15128092
36	H	-5.23700000	-6.37850000	11.22840000
37	H	-7.76830000	-9.07120000	6.80850000
38	H	-6.95230000	-10.08460000	3.55430000
39	H	-10.29630000	-10.34930000	0.25900000
40	H	-2.42150000	-9.87450000	0.00040000
41	H	-3.42900000	-8.60990000	3.88980000
42	H	-4.28320000	-7.54880000	7.29620000
43	H	-3.45780000	3.89970000	-3.31080000
44	H	0.59909435	5.23700391	7.81470155

1	H	-9.79240000	-1.54060000	-3.18200000
2	H	-8.38790000	-2.95530000	10.89960000
3	H	-4.87450000	3.78240000	8.02040000
4	H	-2.02270000	2.13730000	10.92000000
5	H	-4.91220000	-7.27130000	-2.96190000
6	H	-8.98790000	-7.09310000	-2.37650000
7	H	1.45750463	-2.18459910	-2.95900072
8	H	-5.88650000	0.35320000	-2.87170000
9	H	-6.57060000	-3.25690000	-2.96870000
10	H	-11.74490000	-3.66940000	8.61800000
11	H	-9.32890000	0.16850000	8.03140000
12	H	-8.19140000	3.21540000	6.31880000
13	H	-5.78340000	-8.84910000	-1.27830000
14	H	-7.97590000	-9.98270000	-0.17660000
15	H	-2.11761421	0.35870313	-2.97420506
16	C	-3.00149208	-2.13642984	4.20490102
17	H	-3.48612198	-1.55074136	4.98022408
18	H	-3.42346563	-3.13661176	4.14901847
19	H	-1.91985541	-2.14830956	4.31410510
20	O	-3.34676639	-1.48470518	2.92067633
21	C	-2.83443208	-2.22798576	1.73894923
22	H	-3.43134309	-3.13560214	1.69234128
23	H	-3.00871622	-1.59033173	0.87818798
24	H	-1.77532504	-2.42915994	1.89622505
25	C	-3.13526291	-0.00949085	2.89465617
26	H	-2.07377342	0.20060346	3.01395393
27	H	-3.52966530	0.31685135	1.93757214
28	H	-3.72698759	0.37665318	3.72043609
29				
30				
31	Z-(CH3)3O+_C2H4(ads)			
32	Si	-3.88274400	2.11680800	3.05485200
33	Si	-3.89641000	-0.75986800	-1.82267900
34	Si	-7.39419800	-0.31186100	1.61861300
35	Si	-3.55082500	-2.88580900	2.51243800
36	Al	-4.32986100	-0.28065100	1.09832200
37	O	-3.31550100	-1.48737700	1.79626100
38	O	-5.96848100	-0.80851600	1.12046300
39	O	-3.95185700	1.24730300	1.75666600
40	O	-3.76784100	0.04772300	-0.48317800
41	O	-2.45759800	2.89067700	3.07822700
42	O	-3.11421100	-2.17664000	-1.76980600
43	O	-5.41582200	-1.07007700	-2.29507700
44	O	-3.11954400	0.19504400	-2.85642400

1	O	-5.10610700	3.16227700	3.05367300
2	O	-7.97356900	0.97493300	0.85060900
3	O	-8.46634000	-1.47397600	1.33628400
4	O	-4.59493800	-3.92543300	1.83102200
5	O	-7.37957600	0.04809500	3.19477000
6	O	-4.06192600	-2.71081400	4.03789400
7	O	-3.96477300	1.28786400	4.43310900
8	O	-2.07273300	-3.55099500	2.46577300
9	C	-2.91790100	4.13454100	-1.51040300
10	H	-2.40352800	3.38903800	-2.10798900
11	H	-2.64275300	5.16905500	-1.67901900
12	C	-3.85986000	3.79328600	-0.63752800
13	H	-4.38837800	4.54596000	-0.06268500
14	H	-4.14042800	2.76071400	-0.46613000
15	C	-0.96921800	1.53502800	0.16786700
16	H	-0.79788000	2.35508000	0.85649600
17	H	-2.02278600	1.28156700	0.07735600
18	H	-0.49710900	1.71300200	-0.79432600
19	O	-0.23915000	0.36669000	0.74597100
20	C	-0.46097900	0.13270600	2.19556500
21	H	0.36973800	-0.49162300	2.51485900
22	H	-0.42749000	1.10967200	2.66698600
23	H	-1.42457500	-0.36024100	2.31920400
24	C	-0.34238600	-0.86972100	-0.06095500
25	H	-1.34575500	-1.27614300	0.04451600
26	H	-0.12391200	-0.58020800	-1.08449100
27	H	0.41967000	-1.54097500	0.32667600
28	O	-2.55048400	-2.94123900	6.16661200
29	Si	1.26900700	4.44353200	3.31616500
30	Si	-1.79568100	4.25863800	3.59789600
31	Si	-6.38926900	3.90384300	2.43921400
32	Si	3.43373600	2.62149400	4.45818400
33	Si	4.23645100	-0.32970500	4.40378200
34	Si	-1.18609600	-4.86394100	2.27847300
35	Si	1.68245900	-4.49308400	3.38805800
36	Si	3.98883000	-2.66023900	2.46280300
37	Si	6.47326400	-4.43073700	3.02988300
38	Si	4.76061300	-3.90975100	-5.12676000
39	Si	7.25431900	-5.74172300	-4.57669400
40	O	6.00050000	-4.81548900	-4.79509200
41	Si	-6.48602800	-1.50991600	-6.08463400
42	Si	-2.72115100	-4.22179900	-5.20082900
43	Si	-3.38877300	-1.48012100	-6.38473100
44	O	-2.65505000	-2.83566600	-5.97559900

1	O	-4.95911100	-1.70945900	-6.44279800
2	O	-1.30299600	-4.88472400	-5.24308800
3	Si	-0.43106300	-6.23754600	-5.20094900
4	Si	2.51015700	-5.86323600	-4.35949300
5	O	1.08248300	-5.79989100	-5.04776100
6	O	3.42126300	-4.75844600	-5.07653400
7	Si	-8.13153700	-3.58394600	-1.84032200
8	Si	2.09425500	3.15774900	-4.23165100
9	Si	-0.84800200	2.78154500	-5.07386300
10	Si	-4.67204700	5.41213500	-5.94920500
11	Si	-1.76977200	5.75467500	-5.04640100
12	O	0.58020500	2.71914600	-4.38566700
13	O	-1.75865600	1.67792400	-4.35577000
14	O	-5.11461100	4.15484400	-5.09577000
15	O	-3.31658800	5.98855900	-5.35335000
16	O	-1.48733700	4.20774900	-4.82546600
17	O	2.26108000	4.04417000	-2.92067400
18	O	-1.45120900	6.56435200	-3.71088000
19	Si	-0.29734800	7.22290800	-2.82459400
20	Si	4.76257900	7.06015000	-3.10474300
21	O	6.11474600	6.57103100	-2.41754000
22	Si	6.97802200	5.42702200	-1.72936300
23	O	6.64091600	4.01158400	-2.35870000
24	Si	8.14872900	-1.57080700	-3.34879600
25	Si	9.35366000	1.24089200	-3.01450800
26	Si	6.78885600	2.97655500	-3.55586100
27	Si	4.38377000	1.14126000	-4.23155800
28	O	8.96784400	-0.28851600	-2.84824400
29	O	8.07731800	2.09794500	-3.34184500
30	O	5.50643700	2.04304200	-3.57481400
31	O	2.96502900	1.80328000	-4.18934500
32	Si	-5.59169000	2.66120500	-4.85567500
33	O	8.08647700	-5.24156200	-3.32719600
34	Si	2.20576200	5.48182200	-2.24822200
35	O	1.00541100	6.31065900	-2.87977100
36	O	3.54819600	6.26904200	-2.47322600
37	Si	3.43314200	-1.84156200	7.01499800
38	Si	6.64744300	5.94205500	1.29428300
39	O	5.18166400	-3.50624800	3.09037800
40	O	6.13514400	4.79956000	2.26751100
41	Si	7.96714700	-3.07984300	5.33019300
42	Si	7.20070600	-0.09377600	5.32227500
43	Si	8.54873200	2.49492100	4.34723800
44	Si	5.99129900	4.21917200	3.73920100

1	O	7.87800800	-1.51383200	5.11691200
2	O	8.15207000	0.98246500	4.61350600
3	O	7.26352000	3.36580400	4.10118700
4	O	4.70098000	3.29806400	3.79284900
5	O	3.48228700	1.05661000	4.18421100
6	O	5.79130000	-0.07738300	4.60534100
7	O	7.59711300	-3.82434100	3.97384100
8	O	3.98865000	-1.18911500	3.08454100
9	O	3.60684400	-1.08765500	5.64759900
10	O	2.08008600	3.18201400	3.90453700
11	Si	4.31809200	-3.17323600	-0.54915100
12	Si	6.80133900	-4.94169800	0.02973800
13	O	5.58514500	-4.13476900	-0.59988700
14	Si	8.79237700	-4.36554300	-2.21777900
15	Si	5.05121900	-1.59903800	-3.04802200
16	O	8.71653500	-2.82016900	-2.55259000
17	O	4.31770200	-0.24500600	-3.45682800
18	O	6.62165100	-1.37096500	-2.98863000
19	O	8.11919800	-4.63771300	-0.80129500
20	O	4.50111400	-1.98764400	-1.60339900
21	O	4.67012900	-2.74408300	-4.07717800
22	Si	-5.62213100	6.89232600	2.74056800
23	Si	-2.58461100	7.02405500	2.40552800
24	O	-0.25825700	4.02547300	3.28389200
25	O	-5.92023900	5.40985900	2.27190000
26	O	-4.15206200	7.29006400	2.28775400
27	O	-2.31752700	5.50117000	2.76835700
28	O	1.73899500	4.85759200	1.85454800
29	O	-1.96376600	7.36280000	0.97699000
30	Si	-0.62661100	7.73590400	0.18736000
31	Si	1.87774500	5.99289300	0.75185800
32	Si	4.25243700	7.85499300	1.56155800
33	O	0.60192900	6.93912900	0.81040700
34	O	3.17026700	6.85786600	0.98362000
35	O	5.70018200	7.21678900	1.37360800
36	O	-0.87713500	7.33384300	-1.33871600
37	O	1.99016700	5.26272300	-0.67248500
38	O	6.65938200	5.35593700	-0.17782100
39	O	4.15862700	-2.48250300	0.88396300
40	O	7.07697500	-4.48475000	1.54403700
41	O	-3.00792400	-0.33735600	-5.35509000
42	Si	-3.09882900	0.82842000	-4.30588600
43	O	-4.33786200	1.73494000	-4.63734900
44	Si	-7.69099400	1.95315600	-2.74141600

1	Si	-6.86230900	-1.02008500	-3.00354300
2	Si	-5.62787600	-5.32416700	-1.26410300
3	Si	-3.07098100	-3.74587500	-2.12064900
4	O	-7.58120900	0.37774000	-2.79379700
5	O	-7.81040500	-2.14558900	-2.40619000
6	O	-6.82828900	-4.49541400	-1.89558000
7	O	-4.28547400	-4.53685500	-1.48907200
8	O	-6.63557000	-1.30508700	-4.53711900
9	O	-3.04650300	-3.98894400	-3.66915300
10	O	-6.51354700	2.62863100	-3.56137800
11	O	-1.71955400	-4.23577400	-1.43331100
12	Si	-1.73818500	-4.20111900	6.75458900
13	Si	1.32576600	-4.01783400	6.47374200
14	O	-0.21142600	-3.78393600	6.78724300
15	O	2.10467400	-2.70728900	6.96526700
16	O	0.26461800	-4.38601000	2.68829200
17	O	2.60720900	-3.35064700	2.78649000
18	O	1.55455300	-4.27714400	4.94520800
19	O	-2.00034300	-5.38965100	5.74597200
20	O	-1.69859900	-6.00650000	3.25169500
21	Si	-1.84228700	-6.58688400	4.72337000
22	Si	-0.85556300	-5.37902800	-0.74515400
23	Si	2.19350600	-5.28931100	-1.28617000
24	O	0.66504100	-5.00993300	-0.97443200
25	O	3.01145500	-3.98044600	-0.91057200
26	O	2.40326600	-5.59939700	-2.81735900
27	O	-0.94148600	-7.03932200	-3.93864800
28	O	-1.19278500	-6.79448900	-1.37450900
29	Si	-1.04475000	-7.82948900	-2.57168900
30	Si	-8.43688900	3.32139100	4.74089400
31	Si	-7.67034200	0.33533000	4.74862200
32	Si	-3.90336800	-2.37986700	5.61281900
33	Si	-4.70642500	0.57279300	5.66685400
34	Si	-8.02163500	2.46810000	0.28223000
35	Si	-8.46095500	-3.07096700	1.17164500
36	Si	-5.95592200	-4.81304800	1.73612600
37	O	-8.34775700	1.75538000	4.95415500
38	O	-3.95193700	-0.81503300	5.88684300
39	O	-6.26108600	0.31898800	5.46571300
40	O	-7.23172000	-3.86684500	1.79453200
41	O	-7.48269400	3.81067500	3.57944900
42	O	-7.01943400	3.41674700	1.06483100
43	O	-7.59073900	2.46156000	-1.24278300
44	O	-8.71078000	-3.47204700	-0.35451100

1	O	-5.84355300	-5.54324400	0.31175900
2	O	-1.17488400	-5.45089000	0.80647100
3	H	-5.69490600	6.50659700	-5.95074300
4	H	-9.02151700	2.31861200	-3.32484100
5	H	-0.39342500	9.21128500	0.30054600
6	H	0.00708000	8.58769500	-3.36184400
7	H	8.02165100	6.39474900	1.68249100
8	H	8.41840000	5.77660800	-1.94652200
9	H	9.44301800	2.51499500	3.14556500
10	H	9.28777600	3.02540400	5.53738600
11	H	10.34463800	1.37877400	-4.12928000
12	H	9.97515300	1.68511700	-1.72588400
13	H	-9.71501600	-3.42023200	1.91255700
14	H	-0.58858400	-7.07259100	-6.43458500
15	H	-2.18124100	-4.59180400	8.13121500
16	H	10.24109800	-4.74436700	-2.25872800
17	H	-3.78369000	-5.07541700	-5.82245400
18	H	-6.58270400	7.88966200	2.16904400
19	H	-5.76245600	6.99351700	4.22854500
20	H	-4.49299600	5.01584300	-7.38266100
21	H	-0.94473500	6.30771500	-6.16775000
22	H	4.78612200	6.82785000	-4.58447500
23	H	4.64786500	8.53069100	-2.84356800
24	H	6.88669500	3.72461300	-4.85001400
25	H	8.12318800	-5.71115100	-5.79663100
26	H	6.80384900	-7.15231400	-4.35010400
27	H	-7.25217200	-2.70918800	-6.55236400
28	H	-7.02203700	-0.33039200	-6.83639400
29	H	-9.21379500	-4.20116700	-2.67204600
30	H	-5.57575700	-6.68028300	-1.89832200
31	H	-2.25581600	-8.71093600	-2.58961400
32	H	0.18142800	-8.66555200	-2.36798100
33	H	-0.63167800	-7.39896200	5.06790200
34	H	-3.06089100	-7.45665000	4.77395400
35	H	4.24788000	9.15400000	0.81561800
36	H	3.95632100	8.12076600	3.00582000
37	H	-8.08892200	4.02189400	6.01849900
38	H	-9.82990600	3.61366800	4.27402700
39	H	-9.43086200	2.95667200	0.42160800
40	H	-8.56007700	-0.67095800	5.41193000
41	H	-6.08675900	-5.88364500	2.77573100
42	H	-5.10246900	-3.02007900	6.24242200
43	H	3.11620000	-7.21308800	-4.59292000
44	H	6.47605400	-6.40393400	0.01688200

1	H	6.10053900	-5.81886500	3.45189800
2	H	9.36015700	-3.37212100	5.79705000
3	H	1.82032100	-5.19399400	7.25870400
4	H	2.28063300	-5.84047400	3.12205300
5	H	2.67363900	-6.45265000	-0.47376900
6	H	-1.99446000	7.94239700	3.43127400
7	H	-6.37949200	2.18771500	-6.03860900
8	H	5.84170100	5.35257400	4.70720600
9	H	4.87318100	-3.33984200	-6.50748600
10	H	-0.74545700	2.53039700	-6.54705900
11	H	-2.87153300	-1.11616100	-7.74255700
12	H	3.27352300	-0.84714200	8.12388700
13	H	7.02275500	0.21038600	6.77827400
14	H	-4.47314000	1.37927100	6.90752900
15	H	1.51701100	5.56949200	4.27267000
16	H	3.42219000	2.89875000	5.93027400
17	H	8.29159200	-1.76637700	-4.82708000
18	H	4.69159100	0.92091400	-5.68095200
19	H	2.57781800	3.91737900	-5.42863200
20	H	4.62404300	-2.71851200	7.25381600
21	H	7.06290300	-3.54343400	6.43082800
22	H	-2.01439900	4.50736800	5.05831100
23				
24				
25	Z-(CH3)3O+_CH3OH(ads)			
26	Si	-0.04064156	0.01200307	0.00047656
27	Si	-0.06271358	-0.00594120	5.66103612
28	Si	3.70567504	-0.03622201	2.48439393
29	Si	1.03687955	-3.88194489	2.98688284
30	Al	0.70635083	-0.82800490	2.90137467
31	O	0.27264292	-2.49082541	2.96269735
32	O	2.40810328	-0.69080551	3.12206074
33	O	-0.03182912	-0.06308026	1.56453965
34	O	-0.14396171	0.07581232	4.09022342
35	O	-1.58717720	0.13706528	-0.45526715
36	O	-0.35789094	-1.47226547	6.27729007
37	O	1.36145477	0.48394697	6.25093890
38	O	-1.28439090	0.94068144	6.09115098
39	O	0.80906993	1.29153260	-0.48542727
40	O	3.73593018	1.57046501	2.50973190
41	O	4.99255509	-0.47525753	3.33857629
42	O	2.20727930	-4.05913358	4.09871281
43	O	3.89521875	-0.48794235	0.94528948
44	O	1.73157029	-4.25896349	1.57343597

1	O	0.56683306	-1.26630751	-0.76311008
2	O	-0.15213194	-4.92803436	3.33680793
3	O	0.80120000	-6.00640000	-0.15260000
4	Si	-5.49760000	-0.02110000	-1.47430000
5	Si	-2.51950000	0.76950000	-1.59090000
6	Si	1.67330000	2.63520000	-0.36440000
7	Si	-6.77250000	-2.79180000	-1.55910000
8	Si	-6.65860000	-5.43650000	-0.02630000
9	Si	-0.62810000	-6.20850000	4.15930000
10	Si	-3.21920000	-7.43500000	2.98450000
11	Si	-6.09540000	-6.32220000	2.83000000
12	Si	-7.79180000	-8.89230000	3.21140000
13	Si	-7.85690000	-4.02790000	9.99880000
14	Si	-9.54690000	-6.64300000	10.42590000
15	O	-8.68790000	-5.35140000	10.15840000
16	Si	1.78780000	2.30220000	9.72780000
17	Si	-0.76980000	-1.62740000	10.29930000
18	Si	-1.17800000	1.38380000	9.93890000
19	O	-1.38700000	-0.16320000	10.26480000
20	O	0.35020000	1.77510000	10.12160000
21	O	-1.90930000	-2.64050000	10.65650000
22	Si	-2.31670000	-4.06080000	11.29600000
23	Si	-5.02660000	-5.18350000	10.35000000
24	O	-3.83590000	-4.30830000	10.92640000
25	O	-6.34110000	-4.27000000	10.39930000
26	Si	4.73290000	-0.80100000	7.13550000
27	Si	-7.29070000	2.20560000	5.67640000
28	Si	-4.57940000	3.32750000	6.62400000
29	Si	-1.94070000	7.20800000	6.08700000
30	Si	-4.59330000	6.04430000	5.10460000
31	O	-5.77090000	2.45290000	6.04720000
32	O	-3.26560000	2.41450000	6.57330000
33	O	-0.99450000	5.94280000	5.99240000
34	O	-3.27080000	6.91960000	5.26710000
35	O	-4.35770000	4.58890000	5.69440000
36	O	-7.46660000	2.24720000	4.09540000
37	O	-4.88400000	5.95910000	3.53970000
38	Si	-5.99570000	5.67090000	2.42990000
39	Si	-10.73910000	3.90040000	2.70070000
40	O	-11.73290000	2.70740000	2.34160000
41	Si	-12.07420000	1.15480000	2.31840000
42	O	-11.45520000	0.42330000	3.58130000
43	Si	-11.39460000	-4.15760000	7.24580000
44	Si	-13.29570000	-2.46030000	5.52120000

1	Si	-11.50890000	0.09760000	5.13610000
2	Si	-8.83680000	-0.22830000	6.67330000
3	O	-12.44950000	-3.64190000	6.15630000
4	O	-12.41530000	-1.16550000	5.38290000
5	O	-10.03410000	-0.20050000	5.63860000
6	O	-7.69650000	0.78430000	6.31660000
7	Si	-0.05970000	4.78730000	6.54670000
8	O	-10.24280000	-7.11800000	9.08650000
9	Si	-7.71660000	3.11370000	2.78820000
10	O	-6.95550000	4.50240000	2.92570000
11	O	-9.24950000	3.38730000	2.56950000
12	Si	-4.97250000	-7.60980000	-1.50390000
13	Si	-11.35590000	0.26280000	-0.54610000
14	O	-6.84510000	-7.72030000	2.70470000
15	O	-10.35620000	-0.94150000	-0.80140000
16	Si	-9.16490000	-9.40520000	0.52820000
17	Si	-9.33470000	-6.71560000	-0.96890000
18	Si	-11.54680000	-4.63200000	-1.45310000
19	Si	-9.77590000	-2.05450000	-1.77500000
20	O	-9.58580000	-8.00560000	-0.07990000
21	O	-10.67690000	-5.84320000	-0.91270000
22	O	-10.64710000	-3.36120000	-1.66840000
23	O	-8.28390000	-2.37400000	-1.34130000
24	O	-6.40440000	-3.94670000	-0.53100000
25	O	-8.15250000	-5.87130000	-0.34420000
26	O	-8.84920000	-9.23940000	2.07860000
27	O	-6.41640000	-5.42400000	1.54900000
28	O	-5.61290000	-6.41590000	-0.70840000
29	O	-5.77370000	-1.60340000	-1.35130000
30	Si	-6.81090000	-5.43360000	5.68340000
31	Si	-8.50460000	-8.00720000	6.05360000
32	O	-7.72180000	-6.63160000	6.20070000
33	Si	-10.95800000	-7.17850000	7.67890000
34	Si	-8.42890000	-3.23820000	7.03330000
35	O	-11.40780000	-5.74300000	7.18590000
36	O	-8.21960000	-1.69260000	6.70790000
37	O	-9.95660000	-3.63110000	6.85010000
38	O	-9.98360000	-7.83070000	6.60240000
39	O	-7.53000000	-4.04100000	5.99020000
40	O	-7.92320000	-3.54700000	8.50450000
41	Si	0.12370000	4.64450000	-2.14540000
42	Si	-2.82300000	3.84600000	-1.95510000
43	O	-3.94890000	0.19040000	-1.21850000
44	O	0.75580000	3.76930000	-0.98750000

1	O	-1.45550000	4.66540000	-1.97180000
2	O	-2.55360000	2.34860000	-1.49990000
3	O	-6.33220000	0.83850000	-0.42850000
4	O	-3.77030000	4.57610000	-0.90140000
5	Si	-5.28020000	4.78230000	-0.42350000
6	Si	-7.00390000	2.22870000	-0.05400000
7	Si	-9.63060000	2.52380000	-1.72000000
8	O	-6.07880000	3.41370000	-0.57020000
9	O	-8.42830000	2.36750000	-0.70540000
10	O	-10.83220000	1.58900000	-1.25000000
11	O	-5.20960000	5.26350000	1.09860000
12	O	-7.15700000	2.26930000	1.54270000
13	O	-11.46650000	0.47770000	1.01990000
14	O	-6.60040000	-5.49380000	4.09960000
15	O	-8.61720000	-8.44720000	4.51360000
16	O	-1.68270000	1.69080000	8.46850000
17	Si	-1.74890000	2.17160000	6.97410000
18	O	-0.91870000	3.49570000	6.81430000
19	Si	2.50950000	3.95250000	5.10420000
20	Si	2.56680000	1.37880000	6.82680000
21	Si	3.01120000	-3.35760000	7.49350000
22	Si	-0.01130000	-2.57110000	7.40600000
23	O	2.86460000	2.66320000	5.94600000
24	O	3.90010000	0.51780000	6.89190000
25	O	3.77240000	-1.96900000	7.63100000
26	O	1.47830000	-3.08400000	7.27480000
27	O	2.15450000	1.79120000	8.29130000
28	O	-0.24970000	-2.04670000	8.86410000
29	O	1.05380000	4.47370000	5.45680000
30	O	-1.00420000	-3.76440000	7.04720000
31	Si	0.52350000	-7.58780000	-0.03030000
32	Si	-2.45310000	-8.37930000	0.08690000
33	O	-1.02440000	-7.79970000	-0.28570000
34	O	-3.48040000	-7.82240000	-1.00870000
35	O	-2.05280000	-6.52240000	3.54850000
36	O	-4.53620000	-6.55020000	2.91500000
37	O	-2.87430000	-7.94910000	1.53380000
38	O	0.93450000	-7.98310000	1.44400000
39	O	0.37160000	-7.41290000	3.90390000
40	Si	0.95190000	-8.52590000	2.93030000
41	Si	-1.34640000	-5.31660000	7.02370000
42	Si	-4.32960000	-6.05610000	7.41270000
43	O	-2.92290000	-5.44190000	7.01850000
44	O	-5.41450000	-5.45960000	6.41750000

1	O	-4.71840000	-5.65910000	8.88780000
2	O	-1.36620000	-5.12610000	10.61890000
3	O	-0.72730000	-6.04810000	8.28660000
4	Si	-0.78110000	-6.37380000	9.84140000
5	Si	4.19160000	1.79580000	-2.03250000
6	Si	4.36130000	-0.89370000	-0.53530000
7	Si	1.79910000	-4.81760000	0.05480000
8	Si	1.68500000	-2.17150000	-1.47840000
9	Si	3.22790000	3.06050000	2.23970000
10	Si	5.44850000	-1.68950000	4.28210000
11	Si	3.72400000	-4.24270000	4.65120000
12	O	4.61250000	0.39620000	-1.42440000
13	O	1.43100000	-3.66270000	-0.97330000
14	O	3.17920000	-1.73800000	-1.16010000
15	O	4.64900000	-3.05760000	4.13510000
16	O	2.93690000	2.40530000	-1.28880000
17	O	2.15280000	3.10900000	1.07410000
18	O	2.54300000	3.62290000	3.55350000
19	O	5.51820000	-1.20780000	5.80380000
20	O	3.57090000	-4.20200000	6.24790000
21	O	-0.73790000	-5.99420000	5.72550000
22	H	-1.30770000	8.45280000	5.54490000
23	H	3.53900000	4.98890000	5.43620000
24	H	-5.91550000	5.84190000	-1.27060000
25	H	-6.78570000	6.92250000	2.19890000
26	H	-12.70540000	-0.03450000	-1.12450000
27	H	-13.56750000	1.03610000	2.31350000
28	H	-12.61360000	-4.36250000	-0.43650000
29	H	-12.17550000	-5.02190000	-2.75570000
30	H	-14.47190000	-2.17020000	6.40220000
31	H	-13.77040000	-2.92530000	4.17860000
32	H	6.86450000	-1.88260000	3.83330000
33	H	-2.15040000	-4.10050000	12.78420000
34	H	1.31010000	-8.39770000	-1.01480000
35	H	-12.21020000	-7.97290000	7.89080000
36	H	0.36340000	-1.65380000	11.27870000
37	H	0.62130000	6.05740000	-2.14750000
38	H	0.50140000	4.07440000	-3.47820000
39	H	-2.25700000	7.49990000	7.52180000
40	H	-5.73850000	6.73170000	5.78280000
41	H	-10.96700000	4.40130000	4.09400000
42	H	-11.01960000	5.00810000	1.73210000
43	H	-12.06290000	1.27880000	5.87220000
44	H	-10.59640000	-6.34750000	11.45320000

1	H	-8.66420000	-7.73420000	10.94950000
2	H	2.77450000	1.81970000	10.74640000
3	H	1.80020000	3.79900000	9.78440000
4	H	5.77540000	-0.53010000	8.17660000
5	H	3.24710000	-4.17500000	8.72650000
6	H	0.61160000	-6.65520000	10.31590000
7	H	-1.64370000	-7.57580000	10.07620000
8	H	0.12290000	-9.76940000	3.03170000
9	H	2.36090000	-8.82750000	3.33990000
10	H	-10.15040000	3.92860000	-1.73450000
11	H	-9.16390000	2.16210000	-3.09680000
12	H	3.89500000	1.63920000	-3.49250000
13	H	5.32300000	2.73990000	-1.76330000
14	H	4.42880000	3.88350000	1.88700000
15	H	5.61650000	-1.70970000	-0.58830000
16	H	4.35730000	-5.55350000	4.29820000
17	H	3.22920000	-5.21290000	-0.15130000
18	H	-5.23700000	-6.37850000	11.22840000
19	H	-7.76830000	-9.07120000	6.80850000
20	H	-6.95230000	-10.08460000	3.55430000
21	H	-10.29630000	-10.34930000	0.25900000
22	H	-2.42150000	-9.87450000	0.00040000
23	H	-3.42900000	-8.60990000	3.88980000
24	H	-4.28320000	-7.54880000	7.29620000
25	H	-3.45780000	3.89970000	-3.31080000
26	H	0.59910000	5.23700000	7.81470000
27	H	-9.79240000	-1.54060000	-3.18200000
28	H	-8.38790000	-2.95530000	10.89960000
29	H	-4.87450000	3.78240000	8.02040000
30	H	-2.02270000	2.13730000	10.92000000
31	H	-4.91220000	-7.27130000	-2.96190000
32	H	-8.98790000	-7.09310000	-2.37650000
33	H	1.45750000	-2.18460000	-2.95900000
34	H	-5.88650000	0.35320000	-2.87170000
35	H	-6.57060000	-3.25690000	-2.96870000
36	H	-11.74490000	-3.66940000	8.61800000
37	H	-9.32890000	0.16850000	8.03140000
38	H	-8.19140000	3.21540000	6.31880000
39	H	-5.78340000	-8.84910000	-1.27830000
40	H	-7.97590000	-9.98270000	-0.17660000
41	H	-2.11760000	0.35870000	-2.97420000
42	C	-2.85030449	-2.36963712	3.88823054
43	H	-2.66592165	-1.93899634	4.86734660
44	H	-1.92232024	-2.48898901	3.32784573

1	H	-3.41503386	-3.29484617	3.96739720
2	O	-3.74493763	-1.41677108	3.18114011
3	C	-4.19960928	-1.88956681	1.86424146
4	H	-3.35865207	-1.88024643	1.17131273
5	H	-4.60484944	-2.88694848	2.00962126
6	H	-4.97988591	-1.20226840	1.55251293
7	C	-3.24551705	-0.00002976	3.15754738
8	H	-3.02214331	0.25997967	4.18554012
9	H	-2.36402878	0.03966035	2.52398112
10	H	-4.07329511	0.58565379	2.77074521
11	O	-1.73625851	2.40775545	3.38280482
12	H	-1.04482970	1.73026135	3.46135168
13	C	-1.38059920	3.34012527	2.36736998
14	H	-1.36236695	2.87726276	1.37337404
15	H	-0.40594822	3.80159964	2.55698931
16	H	-2.14134246	4.12243104	2.36400389
17				
18				
19	Z-(CH3)3O+_H2O(ads)			
20	Si	-3.81280277	2.05990966	3.05119275
21	Si	-3.82300178	-0.80113747	-1.83348373
22	Si	-7.29783729	-0.41285084	1.64394748
23	Si	-3.39834661	-2.91309603	2.49562332
24	Al	-4.22177454	-0.32254103	1.08440607
25	O	-3.19531324	-1.55776201	1.69287638
26	O	-5.85401220	-0.86212077	1.16229119
27	O	-3.78934949	1.18940444	1.74976829
28	O	-3.79857763	0.08779130	-0.53188669
29	O	-2.41935546	2.87973126	3.09096427
30	O	-3.00791915	-2.19375447	-1.73475829
31	O	-5.32506168	-1.16048925	-2.30783649
32	O	-3.02884405	0.13448761	-2.87094224
33	O	-5.07570750	3.05946801	3.01989015
34	O	-7.90646964	0.85839958	0.87129058
35	O	-8.34041848	-1.59829341	1.35305637
36	O	-4.43036753	-3.98874255	1.85068299
37	O	-7.30106340	-0.05238111	3.21741170
38	O	-3.89901478	-2.70151465	4.02196912
39	O	-3.90752421	1.23882928	4.43052792
40	O	-1.91352292	-3.55829969	2.46805367
41	O	-2.38391700	-2.96230100	6.15798800
42	Si	1.27668200	4.50149900	3.30517900
43	Si	-1.78281300	4.25635800	3.60176600
44	Si	-6.37374300	3.81553100	2.46721300

1	Si	3.48233800	2.71923900	4.43119100
2	Si	4.34182900	-0.21577300	4.36552500
3	Si	-1.00362400	-4.84906800	2.25784200
4	Si	1.86347000	-4.42556900	3.35329100
5	Si	4.12887400	-2.54611200	2.42052900
6	Si	6.65012400	-4.26958600	2.97004500
7	Si	4.88431800	-3.76317000	-5.17617100
8	Si	7.41591800	-5.54774300	-4.64366300
9	O	6.14325700	-4.64547500	-4.85322200
10	Si	-6.41164900	-1.57951800	-6.06889100
11	Si	-2.59027400	-4.21992500	-5.21146900
12	Si	-3.31716300	-1.48894800	-6.38532500
13	O	-2.55520800	-2.83100700	-5.98326800
14	O	-4.88304700	-1.74850000	-6.43560600
15	O	-1.15979000	-4.85510600	-5.26280900
16	Si	-0.26164000	-6.19092700	-5.22850300
17	Si	2.67622200	-5.76163400	-4.40170000
18	O	1.24394300	-5.72438400	-5.08226500
19	O	3.56193600	-4.63776400	-5.12090100
20	Si	-7.99405300	-3.69475000	-1.82102700
21	Si	2.08644100	3.24928500	-4.25010200
22	Si	-0.85239300	2.81803300	-5.07770100
23	Si	-4.73129000	5.37609300	-5.92650300
24	Si	-1.83142100	5.77272600	-5.03822600
25	O	0.58036700	2.78178700	-4.39716800
26	O	-1.73772500	1.69563400	-4.35758200
27	O	-5.14485800	4.10851000	-5.07375700
28	O	-3.38409000	5.97730200	-5.33644000
29	O	-1.51792200	4.23106000	-4.82247700
30	O	2.24305400	4.13577000	-2.93790900
31	O	-1.52148400	6.58536600	-3.70247500
32	Si	-0.37588600	7.26412000	-2.82072000
33	Si	4.68468100	7.20005600	-3.12797900
34	O	6.04970400	6.73565300	-2.44909700
35	Si	6.93862000	5.60701100	-1.76822600
36	O	6.62563200	4.18675200	-2.39915500
37	Si	8.23594100	-1.36310300	-3.41054100
38	Si	9.38797600	1.47063800	-3.07590100
39	Si	6.78720300	3.15752400	-3.59955200
40	Si	4.41453300	1.27753200	-4.26692200
41	O	9.03273200	-0.06633300	-2.91125800
42	O	8.09355600	2.30355200	-3.39444300
43	O	5.52301400	2.19938800	-3.61396200
44	O	2.98348700	1.91184500	-4.21563400

1	Si	-5.59170000	2.60537300	-4.83475800
2	O	8.24488100	-5.03441500	-3.39738600
3	Si	2.16349800	5.57053800	-2.26174100
4	O	0.94397900	6.37740900	-2.88495800
5	O	3.48922100	6.38412900	-2.49194900
6	Si	3.58175400	-1.74888300	6.97732700
7	Si	6.61424300	6.10862600	1.25834700
8	O	5.34134000	-3.37037400	3.03939300
9	O	6.12935000	4.95419800	2.23153300
10	Si	8.12984100	-2.89522200	5.26565500
11	Si	7.30570600	0.07543200	5.26891500
12	Si	8.59814600	2.69199600	4.29296900
13	Si	6.00460900	4.36776600	3.70257000
14	O	8.00926600	-1.33074900	5.05659100
15	O	8.23226300	1.17153500	4.55771300
16	O	7.29502300	3.53837900	4.05579200
17	O	4.73267000	3.42170900	3.76082800
18	O	3.55970400	1.15616800	4.15328200
19	O	5.89243800	0.06620200	4.55949800
20	O	7.76706900	-3.64364500	3.90950000
21	O	4.10340500	-1.07679700	3.04564400
22	O	3.73353100	-0.98857600	5.61086100
23	O	2.11510900	3.25458100	3.88607900
24	Si	4.45203900	-3.04583800	-0.59453800
25	Si	6.97207900	-4.76718300	-0.03300500
26	O	5.73715400	-3.98252700	-0.65426600
27	Si	8.93958800	-4.14742500	-2.28962200
28	Si	5.14120400	-1.45202200	-3.09348000
29	O	8.83206100	-2.60304900	-2.62033300
30	O	4.37944400	-0.11152300	-3.49516800
31	O	6.70722000	-1.19370500	-3.04183800
32	O	8.27936000	-4.43582500	-0.87025700
33	O	4.60642800	-1.85451500	-1.64690500
34	O	4.77687700	-2.60187800	-4.12334200
35	Si	-5.66343600	6.81769100	2.77170700
36	Si	-2.63099500	7.00903200	2.42092900
37	O	-0.24244000	4.05418200	3.27970300
38	O	-5.93570800	5.33091900	2.30102900
39	O	-4.20389000	7.24489600	2.31205900
40	O	-2.33250400	5.49092400	2.77888100
41	O	1.73074300	4.92794400	1.84191200
42	O	-2.02442500	7.36301000	0.98993500
43	Si	-0.69896900	7.76375100	0.19414800
44	Si	1.84163500	6.06830400	0.74125100

1	Si	4.18411000	7.97419200	1.54283800
2	O	0.54806700	6.98950200	0.80879100
3	O	3.11838400	6.95761100	0.96824000
4	O	5.64291700	7.36458500	1.34572000
5	O	-0.94978800	7.36040400	-1.33154100
6	O	1.96058500	5.34370000	-0.68541500
7	O	6.62968500	5.52621700	-0.21519700
8	O	4.28678900	-2.36160200	0.84103600
9	O	7.24687900	-4.30844600	1.48090500
10	O	-2.95308900	-0.34150900	-5.35484400
11	Si	-3.06061300	0.81993100	-4.30171800
12	O	-4.31902400	1.70296800	-4.62539900
13	Si	-7.66559500	1.85191700	-2.71132600
14	Si	-6.78044500	-1.10358600	-2.98505500
15	Si	-5.45420800	-5.38736100	-1.26209600
16	Si	-2.93316700	-3.75787700	-2.12813800
17	O	-7.52561900	0.27894100	-2.76740400
18	O	-7.70379700	-2.24903500	-2.38487700
19	O	-6.67369700	-4.58061400	-1.88523900
20	O	-4.12838300	-4.57384500	-1.49235000
21	O	-6.55702100	-1.38121900	-4.52013200
22	O	-2.91194500	-3.99694300	-3.67754200
23	O	-6.50567500	2.55187800	-3.53557300
24	O	-1.56866800	-4.22301400	-1.44904400
25	Si	-1.54424300	-4.20755500	6.73861000
26	Si	1.51404900	-3.96430800	6.44201800
27	O	-0.02569100	-3.76095100	6.76419200
28	O	2.27004600	-2.64004800	6.93255400
29	O	0.44006300	-4.34418300	2.66151900
30	O	2.76270200	-3.26404200	2.74963800
31	O	1.73967100	-4.21564600	4.91168300
32	O	-1.78870800	-5.39863300	5.72854900
33	O	-1.48805900	-6.00388800	3.23120500
34	Si	-1.61305900	-6.59018300	4.70228000
35	Si	-0.67896300	-5.35099800	-0.76868000
36	Si	2.36489500	-5.20098300	-1.32538500
37	O	0.83298900	-4.95198100	-1.00491200
38	O	3.15934100	-3.87738000	-0.95098500
39	O	2.57246000	-5.50344400	-2.85839800
40	O	-0.74971500	-7.00532500	-3.96544400
41	O	-0.99204400	-6.77127200	-1.39943600
42	Si	-0.83038000	-7.80046900	-2.59985200
43	Si	-8.39794300	3.18836200	4.77832400
44	Si	-7.57359900	0.21763800	4.77466800

1	Si	-3.75015500	-2.42597400	5.61241600
2	Si	-4.61018000	0.51036500	5.67789600
3	Si	-7.98975900	2.35308100	0.31571300
4	Si	-8.31711900	-3.19483500	1.19389800
5	Si	-5.77616900	-4.88966600	1.74110400
6	O	-8.27740900	1.62388600	4.98727100
7	O	-3.82777400	-0.86302300	5.89075700
8	O	-6.16064200	0.22700700	5.48457200
9	O	-7.06956900	-3.96842600	1.80843100
10	O	-7.45961700	3.69867000	3.61300000
11	O	-7.00246000	3.31972800	1.09507400
12	O	-7.56737300	2.35891000	-1.21184400
13	O	-8.56743000	-3.59745200	-0.33180000
14	O	-5.65693300	-5.61417900	0.31435300
15	O	-0.98832200	-5.43266900	0.78466700
16	H	-5.77513900	6.45053500	-5.92002300
17	H	-9.00601600	2.19291000	-3.28659600
18	H	-0.49379100	9.24311000	0.30962600
19	H	-0.10080200	8.63577500	-3.35630800
20	H	7.98147800	6.58696600	1.64037300
21	H	8.37078300	5.98493100	-1.99215300
22	H	9.48546200	2.73213900	3.08664100
23	H	9.33311100	3.23397300	5.48046200
24	H	10.37014600	1.63024200	-4.19555900
25	H	10.00760700	1.92387100	-1.78952000
26	H	-9.56035000	-3.57030600	1.94066800
27	H	-0.40953500	-7.02604200	-6.46328300
28	H	-1.97231000	-4.60989900	8.11661400
29	H	10.39513300	-4.49801900	-2.33912700
30	H	-3.63937000	-5.09259100	-5.82950400
31	H	-6.64628300	7.79756500	2.20762200
32	H	-5.79788000	6.91277000	4.26061400
33	H	-4.55223800	4.98662400	-7.36182800
34	H	-1.02323200	6.34420800	-6.16259000
35	H	4.70483400	6.97164100	-4.60836500
36	H	4.54291100	8.66749900	-2.86268700
37	H	6.86364700	3.91029500	-4.89241100
38	H	8.27752200	-5.49755500	-5.86809600
39	H	6.99405500	-6.96731100	-4.41806900
40	H	-7.15682000	-2.79233100	-6.53542300
41	H	-6.97440400	-0.40885900	-6.81499400
42	H	-9.06855500	-4.33086000	-2.64839000
43	H	-5.37913400	-6.74079700	-1.89981800
44	H	-2.02423200	-8.70516800	-2.61348600

1	H	0.41282300	-8.61308600	-2.40462100
2	H	-0.38503100	-7.37949700	5.03845800
3	H	-2.81420300	-7.48356000	4.75720800
4	H	4.15043200	9.27457000	0.80004000
5	H	3.89060200	8.23087400	2.98927600
6	H	-8.05681300	3.89254900	6.05572300
7	H	-9.79883500	3.45466400	4.31949900
8	H	-9.40768300	2.81431500	0.46342100
9	H	-8.44027200	-0.80712600	5.44044300
10	H	-5.88050700	-5.96488700	2.77877900
11	H	-4.93345200	-3.09073700	6.24701900
12	H	3.30703300	-7.09895600	-4.64155100
13	H	6.67509900	-6.23541200	-0.04763700
14	H	6.30663000	-5.66558700	3.39070300
15	H	9.53071500	-3.16152700	5.72444800
16	H	2.03545600	-5.13246000	7.22154400
17	H	2.48615700	-5.76043400	3.08097500
18	H	2.87178000	-6.35665800	-0.51831400
19	H	-2.05326100	7.93628700	3.44572400
20	H	-6.37647500	2.11942000	-6.01457700
21	H	5.83825500	5.49584000	4.67405900
22	H	4.97847600	-3.18803100	-6.55610600
23	H	-0.75288700	2.57233700	-6.55197300
24	H	-2.81430600	-1.11197900	-7.74493800
25	H	3.40881900	-0.76026200	8.08942700
26	H	7.12965400	0.37277300	6.72656400
27	H	-4.38586200	1.31844000	6.91932500
28	H	1.50793900	5.62993700	4.26288100
29	H	3.47325900	2.99282400	5.90401700
30	H	8.37468600	-1.55248700	-4.89002200
31	H	4.71883800	1.06650600	-5.71844300
32	H	2.54882400	4.02087600	-5.44780100
33	H	4.79066100	-2.60312300	7.20776500
34	H	7.24061700	-3.37876000	6.36993900
35	H	-1.99784600	4.49775800	5.06466400
36	C	-0.43780195	-0.73627415	0.09501440
37	H	-0.76920469	-0.88566543	-0.92695830
38	H	0.46282705	-1.30935410	0.29967503
39	H	-1.23650992	-0.93965608	0.80922340
40	O	-0.02679883	0.68855863	0.18924085
41	C	0.52427840	1.06835354	1.50062979
42	H	1.25682662	0.31077633	1.76444209
43	H	-0.28838792	1.13315782	2.22317347
44	H	1.00463673	2.03027859	1.35305754

1	C	-1.02560874	1.67497501	-0.33536187
2	H	-0.49383209	2.62108920	-0.37174825
3	H	-1.87946622	1.69456969	0.33661741
4	H	-1.29495551	1.33167468	-1.32813972
5	O	-3.61125666	2.84847433	-1.26805214
6	H	-3.82103884	1.95975166	-0.93298823
7	H	-4.38377665	3.38391771	-1.06412178
8				
9				
10	Z-C3H7+-to-Z-CH2CH2CH3-TS			
11	Si	-0.03540270	0.01412847	-0.01038639
12	Si	-0.07367284	-0.00518418	5.64607945
13	Si	3.71869986	-0.03036251	2.48516304
14	Si	1.04706355	-3.89518159	2.97890950
15	Al	0.73658582	-0.83922416	2.89693712
16	O	0.29380874	-2.50207664	2.88921582
17	O	2.42553638	-0.67086245	3.14899769
18	O	-0.01121848	-0.07553792	1.55477840
19	O	-0.19713205	-0.02668512	4.07957091
20	O	-1.59554018	0.14703698	-0.43499648
21	O	-0.36168172	-1.44635699	6.31379352
22	O	1.35733433	0.50804900	6.21325300
23	O	-1.27250157	0.98838578	6.04169748
24	O	0.81048900	1.28996718	-0.49883469
25	O	3.75352333	1.57443521	2.49852088
26	O	5.00896450	-0.47566574	3.32877056
27	O	2.20508791	-4.04805407	4.10548582
28	O	3.88264900	-0.49647574	0.94602609
29	O	1.76134605	-4.28977860	1.58176684
30	O	0.55173113	-1.26731721	-0.78198598
31	O	-0.14994251	-4.92694564	3.33593339
32	C	-2.69429576	-0.50922137	2.99070637
33	H	-3.46338078	0.18147529	3.32318218
34	H	-1.85023805	-0.11877959	2.42804025
35	C	-2.77742383	-1.87095234	3.31203114
36	H	-3.48495436	-2.18377081	4.07034768
37	H	-1.87290444	-2.46401026	3.21443501
38	C	-3.54948993	-1.77114763	1.84485946
39	H	-3.55407177	-0.81644726	1.28759516
40	H	-2.97505273	-2.43753728	1.20851781
41	H	-4.58342047	-2.05096170	2.01570408
42	O	0.80120000	-6.00640000	-0.15260000
43	Si	-5.49760000	-0.02110000	-1.47430000
44	Si	-2.51950000	0.76950000	-1.59080000

1	Si	1.67330000	2.63520000	-0.36440000
2	Si	-6.77250000	-2.79180000	-1.55910000
3	Si	-6.65860000	-5.43650000	-0.02630000
4	Si	-0.62810000	-6.20860000	4.15920000
5	Si	-3.21920000	-7.43500000	2.98450000
6	Si	-6.09540000	-6.32220000	2.83000000
7	Si	-7.79180000	-8.89230000	3.21140000
8	Si	-7.85690000	-4.02790000	9.99880000
9	Si	-9.54690000	-6.64300000	10.42590000
10	O	-8.68790000	-5.35140000	10.15840000
11	Si	1.78780000	2.30220000	9.72780000
12	Si	-0.76980000	-1.62740000	10.29930000
13	Si	-1.17800000	1.38380000	9.93890000
14	O	-1.38700000	-0.16320000	10.26480000
15	O	0.35020000	1.77510000	10.12160000
16	O	-1.90930000	-2.64050000	10.65650000
17	Si	-2.31670000	-4.06080000	11.29600000
18	Si	-5.02660000	-5.18350000	10.35000000
19	O	-3.83590000	-4.30830000	10.92640000
20	O	-6.34110000	-4.27000000	10.39930000
21	Si	4.73290000	-0.80100000	7.13550000
22	Si	-7.29070000	2.20560000	5.67640000
23	Si	-4.57940000	3.32750000	6.62400000
24	Si	-1.94070000	7.20800000	6.08700000
25	Si	-4.59330000	6.04430000	5.10460000
26	O	-5.77090000	2.45290000	6.04720000
27	O	-3.26550000	2.41430000	6.57330000
28	O	-0.99450000	5.94280000	5.99240000
29	O	-3.27080000	6.91960000	5.26710000
30	O	-4.35770000	4.58890000	5.69440000
31	O	-7.46660000	2.24720000	4.09540000
32	O	-4.88400000	5.95910000	3.53970000
33	Si	-5.99570000	5.67090000	2.42990000
34	Si	-10.73910000	3.90040000	2.70070000
35	O	-11.73290000	2.70740000	2.34160000
36	Si	-12.07420000	1.15480000	2.31840000
37	O	-11.45520000	0.42330000	3.58130000
38	Si	-11.39460000	-4.15760000	7.24580000
39	Si	-13.29570000	-2.46030000	5.52120000
40	Si	-11.50890000	0.09760000	5.13610000
41	Si	-8.83680000	-0.22830000	6.67330000
42	O	-12.44950000	-3.64190000	6.15630000
43	O	-12.41530000	-1.16550000	5.38290000
44	O	-10.03410000	-0.20050000	5.63860000

1	O	-7.69650000	0.78430000	6.31660000
2	Si	-0.05970000	4.78730000	6.54670000
3	O	-10.24280000	-7.11800000	9.08650000
4	Si	-7.71660000	3.11370000	2.78820000
5	O	-6.95550000	4.50240000	2.92570000
6	O	-9.24950000	3.38730000	2.56950000
7	Si	-4.97250000	-7.60980000	-1.50390000
8	Si	-11.35590000	0.26280000	-0.54610000
9	O	-6.84510000	-7.72030000	2.70470000
10	O	-10.35620000	-0.94150000	-0.80140000
11	Si	-9.16490000	-9.40520000	0.52820000
12	Si	-9.33470000	-6.71560000	-0.96890000
13	Si	-11.54680000	-4.63200000	-1.45310000
14	Si	-9.77590000	-2.05450000	-1.77500000
15	O	-9.58580000	-8.00560000	-0.07990000
16	O	-10.67690000	-5.84320000	-0.91270000
17	O	-10.64710000	-3.36120000	-1.66840000
18	O	-8.28390000	-2.37400000	-1.34130000
19	O	-6.40440000	-3.94670000	-0.53100000
20	O	-8.15250000	-5.87130000	-0.34420000
21	O	-8.84920000	-9.23940000	2.07860000
22	O	-6.41640000	-5.42400000	1.54900000
23	O	-5.61290000	-6.41590000	-0.70840000
24	O	-5.77370000	-1.60340000	-1.35130000
25	Si	-6.81090000	-5.43360000	5.68340000
26	Si	-8.50460000	-8.00720000	6.05360000
27	O	-7.72180000	-6.63160000	6.20070000
28	Si	-10.95800000	-7.17850000	7.67890000
29	Si	-8.42890000	-3.23820000	7.03330000
30	O	-11.40780000	-5.74300000	7.18590000
31	O	-8.21960000	-1.69260000	6.70790000
32	O	-9.95660000	-3.63110000	6.85010000
33	O	-9.98360000	-7.83070000	6.60240000
34	O	-7.53000000	-4.04100000	5.99020000
35	O	-7.92320000	-3.54700000	8.50450000
36	Si	0.12370000	4.64450000	-2.14540000
37	Si	-2.82300000	3.84600000	-1.95510000
38	O	-3.94900000	0.19040000	-1.21860000
39	O	0.75580000	3.76930000	-0.98750000
40	O	-1.45550000	4.66540000	-1.97180000
41	O	-2.55360000	2.34860000	-1.49990000
42	O	-6.33220000	0.83850000	-0.42850000
43	O	-3.77030000	4.57610000	-0.90140000
44	Si	-5.28020000	4.78230000	-0.42350000

1	Si	-7.00390000	2.22870000	-0.05400000
2	Si	-9.63060000	2.52380000	-1.72000000
3	O	-6.07880000	3.41370000	-0.57020000
4	O	-8.42830000	2.36750000	-0.70540000
5	O	-10.83220000	1.58900000	-1.25000000
6	O	-5.20960000	5.26350000	1.09860000
7	O	-7.15700000	2.26930000	1.54270000
8	O	-11.46650000	0.47770000	1.01990000
9	O	-6.60040000	-5.49380000	4.09960000
10	O	-8.61720000	-8.44720000	4.51360000
11	O	-1.68270000	1.69080000	8.46850000
12	Si	-1.74890000	2.17180000	6.97420000
13	O	-0.91870000	3.49570000	6.81430000
14	Si	2.50950000	3.95250000	5.10420000
15	Si	2.56680000	1.37890000	6.82680000
16	Si	3.01120000	-3.35760000	7.49350000
17	Si	-0.01130000	-2.57100000	7.40600000
18	O	2.86460000	2.66320000	5.94590000
19	O	3.90010000	0.51780000	6.89190000
20	O	3.77240000	-1.96900000	7.63100000
21	O	1.47830000	-3.08400000	7.27480000
22	O	2.15450000	1.79120000	8.29130000
23	O	-0.24970000	-2.04670000	8.86410000
24	O	1.05380000	4.47370000	5.45680000
25	O	-1.00420000	-3.76440000	7.04720000
26	Si	0.52350000	-7.58780000	-0.03030000
27	Si	-2.45310000	-8.37930000	0.08690000
28	O	-1.02440000	-7.79970000	-0.28570000
29	O	-3.48040000	-7.82240000	-1.00870000
30	O	-2.05280000	-6.52240000	3.54850000
31	O	-4.53620000	-6.55020000	2.91500000
32	O	-2.87430000	-7.94910000	1.53380000
33	O	0.93450000	-7.98310000	1.44400000
34	O	0.37170000	-7.41290000	3.90390000
35	Si	0.95190000	-8.52590000	2.93030000
36	Si	-1.34640000	-5.31660000	7.02370000
37	Si	-4.32960000	-6.05610000	7.41270000
38	O	-2.92290000	-5.44190000	7.01850000
39	O	-5.41450000	-5.45960000	6.41750000
40	O	-4.71840000	-5.65910000	8.88780000
41	O	-1.36620000	-5.12610000	10.61890000
42	O	-0.72730000	-6.04810000	8.28660000
43	Si	-0.78110000	-6.37380000	9.84140000
44	Si	4.19160000	1.79580000	-2.03250000

1	Si	4.36130000	-0.89370000	-0.53530000
2	Si	1.79910000	-4.81760000	0.05480000
3	Si	1.68500000	-2.17150000	-1.47840000
4	Si	3.22790000	3.06050000	2.23970000
5	Si	5.44850000	-1.68950000	4.28210000
6	Si	3.72400000	-4.24270000	4.65120000
7	O	4.61250000	0.39620000	-1.42440000
8	O	1.43100000	-3.66270000	-0.97330000
9	O	3.17920000	-1.73800000	-1.16010000
10	O	4.64900000	-3.05760000	4.13510000
11	O	2.93690000	2.40530000	-1.28880000
12	O	2.15280000	3.10900000	1.07410000
13	O	2.54300000	3.62290000	3.55350000
14	O	5.51820000	-1.20780000	5.80380000
15	O	3.57090000	-4.20200000	6.24790000
16	O	-0.73790000	-5.99420000	5.72550000
17	H	-1.30770000	8.45280000	5.54490000
18	H	3.53900000	4.98890000	5.43620000
19	H	-5.91550000	5.84190000	-1.27060000
20	H	-6.78570000	6.92250000	2.19890000
21	H	-12.70540000	-0.03450000	-1.12450000
22	H	-13.56750000	1.03610000	2.31350000
23	H	-12.61360000	-4.36250000	-0.43650000
24	H	-12.17550000	-5.02190000	-2.75570000
25	H	-14.47190000	-2.17020000	6.40220000
26	H	-13.77040000	-2.92530000	4.17860000
27	H	6.86450000	-1.88260000	3.83330000
28	H	-2.15040000	-4.10050000	12.78420000
29	H	1.31010000	-8.39770000	-1.01480000
30	H	-12.21020000	-7.97290000	7.89080000
31	H	0.36340000	-1.65380000	11.27870000
32	H	0.62130000	6.05740000	-2.14750000
33	H	0.50140000	4.07440000	-3.47820000
34	H	-2.25700000	7.49990000	7.52180000
35	H	-5.73850000	6.73170000	5.78280000
36	H	-10.96700000	4.40130000	4.09400000
37	H	-11.01960000	5.00810000	1.73210000
38	H	-12.06290000	1.27880000	5.87220000
39	H	-10.59640000	-6.34750000	11.45320000
40	H	-8.66420000	-7.73420000	10.94950000
41	H	2.77450000	1.81970000	10.74640000
42	H	1.80020000	3.79900000	9.78440000
43	H	5.77540000	-0.53010000	8.17660000
44	H	3.24710000	-4.17500000	8.72650000

1	H	0.61160000	-6.65520000	10.31590000
2	H	-1.64370000	-7.57580000	10.07620000
3	H	0.12290000	-9.76940000	3.03170000
4	H	2.36090000	-8.82750000	3.33990000
5	H	-10.15040000	3.92860000	-1.73450000
6	H	-9.16390000	2.16210000	-3.09680000
7	H	3.89500000	1.63920000	-3.49250000
8	H	5.32300000	2.73990000	-1.76330000
9	H	4.42880000	3.88350000	1.88700000
10	H	5.61650000	-1.70970000	-0.58830000
11	H	4.35730000	-5.55350000	4.29820000
12	H	3.22920000	-5.21290000	-0.15130000
13	H	-5.23700000	-6.37850000	11.22840000
14	H	-7.76830000	-9.07120000	6.80850000
15	H	-6.95230000	-10.08460000	3.55430000
16	H	-10.29630000	-10.34930000	0.25900000
17	H	-2.42150000	-9.87450000	0.00040000
18	H	-3.42900000	-8.60990000	3.88980000
19	H	-4.28320000	-7.54880000	7.29620000
20	H	-3.45780000	3.89970000	-3.31080000
21	H	0.59910000	5.23700000	7.81470000
22	H	-9.79240000	-1.54060000	-3.18200000
23	H	-8.38790000	-2.95530000	10.89960000
24	H	-4.87450000	3.78240000	8.02040000
25	H	-2.02270000	2.13730000	10.92000000
26	H	-4.91220000	-7.27130000	-2.96190000
27	H	-8.98790000	-7.09310000	-2.37650000
28	H	1.45750000	-2.18460000	-2.95900000
29	H	-5.88650000	0.35320000	-2.87170000
30	H	-6.57060000	-3.25690000	-2.96870000
31	H	-11.74490000	-3.66940000	8.61800000
32	H	-9.32890000	0.16850000	8.03140000
33	H	-8.19140000	3.21540000	6.31880000
34	H	-5.78340000	-8.84910000	-1.27830000
35	H	-7.97590000	-9.98270000	-0.17660000
36	H	-2.11760000	0.35870000	-2.97420000
37				
38				
39	Z-鈥□3H7+-to-ZH_cyclopropane(ads)-TS			
40	Si	-0.02041400	0.04028700	-0.01731600
41	Si	-0.07160300	-0.01201300	5.64175700
42	Si	3.69987100	-0.02019600	2.48843100
43	Si	1.05814600	-3.89973200	2.96293200
44	Al	0.72851400	-0.83244300	2.84218600

1	O	0.33870100	-2.49999500	2.75272500
2	O	2.38671800	-0.57396900	3.20682300
3	O	0.06944000	0.06679600	1.55366900
4	O	-0.34625800	-0.22173600	4.08098900
5	O	-1.57941200	0.15205400	-0.43903300
6	O	-0.38124400	-1.41521500	6.36041500
7	O	1.37170700	0.52101700	6.13170600
8	O	-1.24100200	1.02673500	6.00070300
9	O	0.81866600	1.29339500	-0.57413400
10	O	3.78587300	1.58341500	2.47886700
11	O	4.98426500	-0.48723500	3.32974900
12	O	2.20360400	-4.00559100	4.11368800
13	O	3.85257200	-0.52100800	0.95508400
14	O	1.80074700	-4.35621500	1.60261400
15	O	0.57251100	-1.27654500	-0.73026600
16	O	-0.14576400	-4.90445900	3.36819200
17	C	-3.98612100	-1.40740500	3.07733900
18	H	-4.33576700	-2.40747400	3.29682600
19	H	-4.74873300	-0.71486600	2.74592100
20	C	-3.00575500	-0.82728200	4.12709400
21	H	-3.22256100	0.19697500	4.40617400
22	H	-2.78907400	-1.52056400	4.93144300
23	C	-2.64587100	-1.24799400	2.55476600
24	H	-1.78277800	-0.60949900	3.80829800
25	H	-1.97530600	-2.09839300	2.49403600
26	H	-2.40242000	-0.40860000	1.91638500
27	O	0.80124600	-6.00642300	-0.15269600
28	Si	-5.49758200	-0.02118400	-1.47434500
29	Si	-2.51957000	0.76944600	-1.59083000
30	Si	1.67347600	2.63546900	-0.36490800
31	Si	-6.77250000	-2.79180000	-1.55910000
32	Si	-6.65860000	-5.43650000	-0.02630000
33	Si	-0.62792600	-6.20843400	4.15901300
34	Si	-3.21904700	-7.43494800	2.98402000
35	Si	-6.09539800	-6.32220400	2.82995300
36	Si	-7.79180000	-8.89230000	3.21140000
37	Si	-7.85690000	-4.02790000	9.99880000
38	Si	-9.54690000	-6.64300000	10.42590000
39	O	-8.68790000	-5.35140000	10.15840000
40	Si	1.78779900	2.30221100	9.72779700
41	Si	-0.76979700	-1.62740400	10.29930200
42	Si	-1.17781900	1.38331100	9.93873500
43	O	-1.38699700	-0.16319900	10.26480100
44	O	0.35020400	1.77509200	10.12160400

1	O	-1.90930400	-2.64049600	10.65649800
2	Si	-2.31670000	-4.06080000	11.29600000
3	Si	-5.02660000	-5.18350000	10.35000000
4	O	-3.83590000	-4.30830000	10.92640000
5	O	-6.34110000	-4.27000000	10.39930000
6	Si	4.73290900	-0.80094900	7.13557300
7	Si	-7.29070000	2.20560000	5.67640000
8	Si	-4.57937600	3.32753700	6.62397400
9	Si	-1.94070000	7.20800000	6.08700000
10	Si	-4.59330000	6.04430000	5.10460000
11	O	-5.77090400	2.45289300	6.04722000
12	O	-3.26562300	2.41443800	6.57334500
13	O	-0.99449700	5.94279600	5.99238700
14	O	-3.27080000	6.91960000	5.26710000
15	O	-4.35770700	4.58889100	5.69438500
16	O	-7.46660400	2.24719800	4.09540000
17	O	-4.88400000	5.95910000	3.53970000
18	Si	-5.99570000	5.67090000	2.42990000
19	Si	-10.73910000	3.90040000	2.70070000
20	O	-11.73290000	2.70740000	2.34160000
21	Si	-12.07420000	1.15480000	2.31840000
22	O	-11.45520000	0.42330000	3.58130000
23	Si	-11.39460000	-4.15760000	7.24580000
24	Si	-13.29570000	-2.46030000	5.52120000
25	Si	-11.50890000	0.09760000	5.13610000
26	Si	-8.83680000	-0.22830000	6.67330000
27	O	-12.44950000	-3.64190000	6.15630000
28	O	-12.41530000	-1.16550000	5.38290000
29	O	-10.03410000	-0.20050000	5.63860000
30	O	-7.69650000	0.78430000	6.31660000
31	Si	-0.05970700	4.78730400	6.54670000
32	O	-10.24280000	-7.11800000	9.08650000
33	Si	-7.71658800	3.11368700	2.78821400
34	O	-6.95550500	4.50240300	2.92569500
35	O	-9.24949900	3.38730300	2.56949800
36	Si	-4.97250000	-7.60980000	-1.50390000
37	Si	-11.35590000	0.26280000	-0.54610000
38	O	-6.84510100	-7.72030100	2.70471300
39	O	-10.35620000	-0.94150000	-0.80140000
40	Si	-9.16490000	-9.40520000	0.52820000
41	Si	-9.33470000	-6.71560000	-0.96890000
42	Si	-11.54680000	-4.63200000	-1.45310000
43	Si	-9.77590000	-2.05450000	-1.77500000
44	O	-9.58580000	-8.00560000	-0.07990000

1	O	-10.67690000	-5.84320000	-0.91270000
2	O	-10.64710000	-3.36120000	-1.66840000
3	O	-8.28390000	-2.37400000	-1.34130000
4	O	-6.40440000	-3.94670000	-0.53100000
5	O	-8.15250000	-5.87130000	-0.34420000
6	O	-8.84920000	-9.23940000	2.07860000
7	O	-6.41639900	-5.42399100	1.54900600
8	O	-5.61290000	-6.41590000	-0.70840000
9	O	-5.77369900	-1.60340100	-1.35130800
10	Si	-6.81090000	-5.43360000	5.68340000
11	Si	-8.50460000	-8.00720000	6.05360000
12	O	-7.72180000	-6.63160000	6.20070000
13	Si	-10.95800000	-7.17850000	7.67890000
14	Si	-8.42890000	-3.23820000	7.03330000
15	O	-11.40780000	-5.74300000	7.18590000
16	O	-8.21960000	-1.69260000	6.70790000
17	O	-9.95660000	-3.63110000	6.85010000
18	O	-9.98360000	-7.83070000	6.60240000
19	O	-7.53000000	-4.04100000	5.99020000
20	O	-7.92320000	-3.54700000	8.50450000
21	Si	0.12382600	4.64461000	-2.14538500
22	Si	-2.82302200	3.84599900	-1.95509000
23	O	-3.94895900	0.19055600	-1.21839600
24	O	0.75553200	3.76907500	-0.98751400
25	O	-1.45550000	4.66540000	-1.97180000
26	O	-2.55354400	2.34860100	-1.49991000
27	O	-6.33219400	0.83850000	-0.42849800
28	O	-3.77030000	4.57610000	-0.90140000
29	Si	-5.28020000	4.78230000	-0.42350000
30	Si	-7.00390800	2.22869100	-0.05400100
31	Si	-9.63060000	2.52380000	-1.72000000
32	O	-6.07880100	3.41370100	-0.57020000
33	O	-8.42830000	2.36750200	-0.70540000
34	O	-10.83220000	1.58900000	-1.25000000
35	O	-5.20960000	5.26350000	1.09860000
36	O	-7.15699800	2.26931200	1.54268600
37	O	-11.46650000	0.47770000	1.01990000
38	O	-6.60040100	-5.49380600	4.09960400
39	O	-8.61720000	-8.44720000	4.51360000
40	O	-1.68298500	1.69185100	8.46884900
41	Si	-1.74885600	2.17101600	6.97394000
42	O	-0.91872300	3.49571400	6.81429900
43	Si	2.50954000	3.95246600	5.10393500
44	Si	2.56686100	1.37860100	6.82659200

1	Si	3.01134200	-3.35731900	7.49333100
2	Si	-0.01124500	-2.57086900	7.40581700
3	O	2.86460300	2.66354900	5.94641100
4	O	3.90009400	0.51777700	6.89173200
5	O	3.77240000	-1.96900000	7.63100000
6	O	1.47817600	-3.08445000	7.27517100
7	O	2.15450900	1.79122700	8.29129500
8	O	-0.24969900	-2.04667400	8.86409100
9	O	1.05380700	4.47369700	5.45680800
10	O	-1.00418600	-3.76439500	7.04717500
11	Si	0.52348300	-7.58779400	-0.03025400
12	Si	-2.45310000	-8.37930000	0.08690000
13	O	-1.02440000	-7.79970000	-0.28570000
14	O	-3.48040000	-7.82240000	-1.00870000
15	O	-2.05303500	-6.52251100	3.54920400
16	O	-4.53620000	-6.55018600	2.91508700
17	O	-2.87429900	-7.94911100	1.53380500
18	O	0.93450000	-7.98310000	1.44400000
19	O	0.37158700	-7.41299700	3.90391300
20	Si	0.95194600	-8.52585600	2.93027800
21	Si	-1.34639800	-5.31658900	7.02371700
22	Si	-4.32960000	-6.05610000	7.41270000
23	O	-2.92290100	-5.44189600	7.01849400
24	O	-5.41450000	-5.45960000	6.41750000
25	O	-4.71840000	-5.65910000	8.88780000
26	O	-1.36620000	-5.12610000	10.61890000
27	O	-0.72730000	-6.04810000	8.28660000
28	Si	-0.78110000	-6.37380000	9.84140000
29	Si	4.19139100	1.79568600	-2.03275500
30	Si	4.36125900	-0.89338200	-0.53563600
31	Si	1.79903800	-4.81759500	0.05485500
32	Si	1.68494500	-2.17117400	-1.47873000
33	Si	3.22825700	3.06095400	2.23946300
34	Si	5.44838300	-1.68943900	4.28205700
35	Si	3.72403900	-4.24258700	4.65114000
36	O	4.61248100	0.39620600	-1.42439700
37	O	1.43104000	-3.66271200	-0.97332700
38	O	3.17923300	-1.73854500	-1.15942900
39	O	4.64917400	-3.05770400	4.13518900
40	O	2.93731900	2.40549400	-1.28827400
41	O	2.15237900	3.10847500	1.07443200
42	O	2.54286400	3.62263100	3.55354300
43	O	5.51820200	-1.20786100	5.80381900
44	O	3.57074700	-4.20209800	6.24788600

1	O	-0.73792800	-5.99422000	5.72550200
2	H	-1.30770000	8.45280000	5.54490000
3	H	3.53900000	4.98890000	5.43620000
4	H	-5.91550000	5.84190000	-1.27060000
5	H	-6.78570000	6.92250000	2.19890000
6	H	-12.70540000	-0.03450000	-1.12450000
7	H	-13.56750000	1.03610000	2.31350000
8	H	-12.61360000	-4.36250000	-0.43650000
9	H	-12.17550000	-5.02190000	-2.75570000
10	H	-14.47190000	-2.17020000	6.40220000
11	H	-13.77040000	-2.92530000	4.17860000
12	H	6.86450100	-1.88258900	3.83329500
13	H	-2.15040000	-4.10050000	12.78420000
14	H	1.31010000	-8.39770000	-1.01480000
15	H	-12.21020000	-7.97290000	7.89080000
16	H	0.36339800	-1.65380900	11.27870200
17	H	0.62130000	6.05740000	-2.14750000
18	H	0.50140000	4.07440000	-3.47820000
19	H	-2.25700000	7.49990000	7.52180000
20	H	-5.73850000	6.73170000	5.78280000
21	H	-10.96700000	4.40130000	4.09400000
22	H	-11.01960000	5.00810000	1.73210000
23	H	-12.06290000	1.27880000	5.87220000
24	H	-10.59640000	-6.34750000	11.45320000
25	H	-8.66420000	-7.73420000	10.94950000
26	H	2.77450100	1.81970100	10.74640000
27	H	1.80019500	3.79900000	9.78439800
28	H	5.77540000	-0.53010000	8.17660000
29	H	3.24710000	-4.17500000	8.72650000
30	H	0.61160000	-6.65520000	10.31590000
31	H	-1.64370000	-7.57580000	10.07620000
32	H	0.12290000	-9.76940000	3.03170000
33	H	2.36090000	-8.82750000	3.33990000
34	H	-10.15040000	3.92860000	-1.73450000
35	H	-9.16390000	2.16210000	-3.09680000
36	H	3.89500000	1.63920000	-3.49250000
37	H	5.32300000	2.73990000	-1.76330000
38	H	4.42881800	3.88348200	1.88701500
39	H	5.61649900	-1.70970100	-0.58830100
40	H	4.35729500	-5.55350300	4.29820300
41	H	3.22919800	-5.21290100	-0.15130700
42	H	-5.23700000	-6.37850000	11.22840000
43	H	-7.76830000	-9.07120000	6.80850000
44	H	-6.95230000	-10.08460000	3.55430000

1	H	-10.29630000	-10.34930000	0.25900000
2	H	-2.42150000	-9.87450000	0.00040000
3	H	-3.42900200	-8.60988100	3.88982400
4	H	-4.28320000	-7.54880000	7.29620000
5	H	-3.45780000	3.89970000	-3.31080000
6	H	0.59909300	5.23700500	7.81470200
7	H	-9.79240000	-1.54060000	-3.18200000
8	H	-8.38790000	-2.95530000	10.89960000
9	H	-4.87448800	3.78241800	8.02039700
10	H	-2.02270000	2.13730000	10.92000000
11	H	-4.91220000	-7.27130000	-2.96190000
12	H	-8.98790000	-7.09310000	-2.37650000
13	H	1.45750100	-2.18460600	-2.95900100
14	H	-5.88650100	0.35320300	-2.87169900
15	H	-6.57060000	-3.25690000	-2.96870000
16	H	-11.74490000	-3.66940000	8.61800000
17	H	-9.32890000	0.16850000	8.03140000
18	H	-8.19140000	3.21540000	6.31880000
19	H	-5.78340000	-8.84910000	-1.27830000
20	H	-7.97590000	-9.98270000	-0.17660000
21	H	-2.11757400	0.35871300	-2.97419600
22				
23				
24	Z-C3H7+			
25	Si	-0.04096300	0.00564200	-0.00852000
26	Si	-0.06722800	-0.00393000	5.65015600
27	Si	3.71959500	-0.04224400	2.48642400
28	Si	1.04295500	-3.89520000	2.98728100
29	Al	0.74794600	-0.83954700	2.90986100
30	O	0.25624900	-2.50703700	2.94268100
31	O	2.44539000	-0.74223800	3.13133900
32	O	-0.01286100	-0.15529300	1.54511400
33	O	-0.15100200	0.00552700	4.08286100
34	O	-1.59719700	0.13044700	-0.44334600
35	O	-0.35928500	-1.45482200	6.30177700
36	O	1.36468200	0.49196400	6.23044900
37	O	-1.26512000	0.98156600	6.05464100
38	O	0.80590200	1.28931500	-0.47233500
39	O	3.71449600	1.56170500	2.51711000
40	O	5.01570600	-0.47061200	3.33023500
41	O	2.20287200	-4.05377000	4.10379500
42	O	3.89380900	-0.48707900	0.94388800
43	O	1.73937400	-4.25651400	1.57307900
44	O	0.54223600	-1.26521100	-0.80734500

1	O	-0.15344200	-4.93660200	3.31663800
2	C	-2.46018400	-2.59190400	1.85721000
3	H	-2.07115700	-2.40848000	0.86044600
4	H	-1.49822700	-2.50404300	2.46913400
5	H	-2.84454000	-3.58075700	2.07610900
6	C	-2.79233000	-1.29615500	2.99607800
7	H	-2.91384600	-1.75149800	3.97211100
8	H	-2.03388100	-0.52360900	2.91566300
9	C	-3.72086600	-1.53576400	1.96769700
10	H	-3.72605700	-0.87756700	1.10904000
11	H	-4.63710700	-2.07306900	2.17531300
12	O	0.80122000	-6.00641400	-0.15261900
13	Si	-5.49760600	-0.02107600	-1.47428500
14	Si	-2.51928500	0.76951600	-1.59090100
15	Si	1.67079800	2.63419400	-0.36391200
16	Si	-6.77250100	-2.79180000	-1.55910200
17	Si	-6.65860000	-5.43650000	-0.02630000
18	Si	-0.62805400	-6.20853600	4.15918500
19	Si	-3.21920800	-7.43500200	2.98451800
20	Si	-6.09540000	-6.32220000	2.83000000
21	Si	-7.79180000	-8.89230000	3.21140000
22	Si	-7.85690000	-4.02790000	9.99880000
23	Si	-9.54690000	-6.64300000	10.42590000
24	O	-8.68790000	-5.35140000	10.15840000
25	Si	1.78780500	2.30219000	9.72780400
26	Si	-0.76981300	-1.62740000	10.29929600
27	Si	-1.17799400	1.38378400	9.93889400
28	O	-1.38698700	-0.16319500	10.26480200
29	O	0.35019500	1.77511000	10.12159500
30	O	-1.90930600	-2.64049400	10.65649600
31	Si	-2.31670000	-4.06080000	11.29600000
32	Si	-5.02660000	-5.18350000	10.35000000
33	O	-3.83590000	-4.30830000	10.92640000
34	O	-6.34110000	-4.27000000	10.39930000
35	Si	4.73289900	-0.80104400	7.13549900
36	Si	-7.29070000	2.20560000	5.67640000
37	Si	-4.57939700	3.32750400	6.62399200
38	Si	-1.94070000	7.20800000	6.08700000
39	Si	-4.59330000	6.04430000	5.10460000
40	O	-5.77090000	2.45290000	6.04720000
41	O	-3.26549900	2.41430800	6.57330100
42	O	-0.99450100	5.94280100	5.99240400
43	O	-3.27080000	6.91960000	5.26710000
44	O	-4.35770000	4.58890000	5.69440000

1	O	-7.46660000	2.24719900	4.09540000
2	O	-4.88400000	5.95910000	3.53970000
3	Si	-5.99570000	5.67090000	2.42990000
4	Si	-10.73910000	3.90040000	2.70070000
5	O	-11.73290000	2.70740000	2.34160000
6	Si	-12.07420000	1.15480000	2.31840000
7	O	-11.45520000	0.42330000	3.58130000
8	Si	-11.39460000	-4.15760000	7.24580000
9	Si	-13.29570000	-2.46030000	5.52120000
10	Si	-11.50890000	0.09760000	5.13610000
11	Si	-8.83679800	-0.22830100	6.67329700
12	O	-12.44950000	-3.64190000	6.15630000
13	O	-12.41530000	-1.16550000	5.38290000
14	O	-10.03410000	-0.20050000	5.63859900
15	O	-7.69650000	0.78430200	6.31660100
16	Si	-0.05969600	4.78729800	6.54670400
17	O	-10.24280000	-7.11800000	9.08650000
18	Si	-7.71660000	3.11370000	2.78820000
19	O	-6.95550000	4.50240000	2.92570000
20	O	-9.24950000	3.38730000	2.56950000
21	Si	-4.97250000	-7.60980000	-1.50390000
22	Si	-11.35590000	0.26280000	-0.54610000
23	O	-6.84510000	-7.72030000	2.70470000
24	O	-10.35620000	-0.94150000	-0.80140000
25	Si	-9.16490000	-9.40520000	0.52820000
26	Si	-9.33470000	-6.71560000	-0.96890000
27	Si	-11.54680000	-4.63200000	-1.45310000
28	Si	-9.77590000	-2.05450000	-1.77500000
29	O	-9.58580000	-8.00560000	-0.07990000
30	O	-10.67690000	-5.84320000	-0.91270000
31	O	-10.64710000	-3.36120000	-1.66840000
32	O	-8.28390000	-2.37400000	-1.34130000
33	O	-6.40439900	-3.94669900	-0.53099900
34	O	-8.15250000	-5.87130000	-0.34420000
35	O	-8.84920000	-9.23940000	2.07860000
36	O	-6.41640000	-5.42400000	1.54900000
37	O	-5.61290000	-6.41590000	-0.70840000
38	O	-5.77370000	-1.60340000	-1.35129900
39	Si	-6.81090000	-5.43360000	5.68340000
40	Si	-8.50460000	-8.00720000	6.05360000
41	O	-7.72180000	-6.63160000	6.20070000
42	Si	-10.95800000	-7.17850000	7.67890000
43	Si	-8.42889900	-3.23820000	7.03330000
44	O	-11.40780000	-5.74300000	7.18590000

1	O	-8.21959700	-1.69259900	6.70789900
2	O	-9.95660000	-3.63110000	6.85010000
3	O	-9.98360000	-7.83070000	6.60240000
4	O	-7.53000000	-4.04100000	5.99020000
5	O	-7.92320000	-3.54700000	8.50450000
6	Si	0.12322900	4.64409100	-2.14545100
7	Si	-2.82307000	3.84599700	-1.95507000
8	O	-3.94896200	0.19035300	-1.21852800
9	O	0.75695100	3.77013700	-0.98767000
10	O	-1.45550000	4.66540000	-1.97180000
11	O	-2.55349100	2.34860600	-1.49996000
12	O	-6.33220000	0.83850000	-0.42850000
13	O	-3.77030000	4.57610000	-0.90140000
14	Si	-5.28020000	4.78230000	-0.42350000
15	Si	-7.00390000	2.22870000	-0.05400000
16	Si	-9.63060000	2.52380000	-1.72000000
17	O	-6.07880000	3.41370000	-0.57020000
18	O	-8.42830000	2.36750000	-0.70540000
19	O	-10.83220000	1.58900000	-1.25000000
20	O	-5.20960000	5.26350000	1.09860000
21	O	-7.15700000	2.26930000	1.54270000
22	O	-11.46650000	0.47770000	1.01990000
23	O	-6.60040000	-5.49380000	4.09960000
24	O	-8.61720000	-8.44720000	4.51360000
25	O	-1.68270500	1.69083200	8.46851100
26	Si	-1.74890600	2.17173600	6.97412600
27	O	-0.91868800	3.49569400	6.81431500
28	Si	2.50950500	3.95251800	5.10420900
29	Si	2.56677800	1.37896500	6.82674500
30	Si	3.01119900	-3.35762900	7.49352600
31	Si	-0.01123200	-2.57097000	7.40597600
32	O	2.86461900	2.66318200	5.94588000
33	O	3.90009600	0.51779700	6.89195000
34	O	3.77240000	-1.96900000	7.63100000
35	O	1.47831200	-3.08395300	7.27475200
36	O	2.15449900	1.79117300	8.29130700
37	O	-0.24971700	-2.04670600	8.86409900
38	O	1.05379600	4.47370200	5.45679600
39	O	-1.00419900	-3.76439500	7.04718700
40	Si	0.52349600	-7.58779800	-0.03028900
41	Si	-2.45310000	-8.37930000	0.08690000
42	O	-1.02440000	-7.79970000	-0.28570000
43	O	-3.48040000	-7.82240000	-1.00870000
44	O	-2.05278600	-6.52240100	3.54846600

1	O	-4.53620000	-6.55020000	2.91500000
2	O	-2.87430000	-7.94910000	1.53380000
3	O	0.93450000	-7.98310000	1.44400000
4	O	0.37168600	-7.41291300	3.90390800
5	Si	0.95190600	-8.52589500	2.93029800
6	Si	-1.34639600	-5.31658800	7.02371300
7	Si	-4.32960000	-6.05610000	7.41270000
8	O	-2.92290000	-5.44189700	7.01849700
9	O	-5.41450000	-5.45960000	6.41750000
10	O	-4.71840000	-5.65910000	8.88780000
11	O	-1.36620000	-5.12610000	10.61890000
12	O	-0.72730000	-6.04810000	8.28660000
13	Si	-0.78110000	-6.37380000	9.84140000
14	Si	4.19135900	1.79565900	-2.03280600
15	Si	4.36127700	-0.89371900	-0.53528100
16	Si	1.79916400	-4.81764700	0.05471100
17	Si	1.68560800	-2.17103900	-1.47839700
18	Si	3.22757900	3.05991400	2.23998500
19	Si	5.44840000	-1.68948900	4.28206900
20	Si	3.72401500	-4.24268000	4.65115500
21	O	4.61251500	0.39622100	-1.42436600
22	O	1.43068100	-3.66258700	-0.97316100
23	O	3.17927600	-1.73819100	-1.16016100
24	O	4.64906200	-3.05763100	4.13511700
25	O	2.93740800	2.40542900	-1.28813600
26	O	2.15409200	3.10993100	1.07333900
27	O	2.54298400	3.62284300	3.55351600
28	O	5.51822400	-1.20772600	5.80377500
29	O	3.57087400	-4.20201300	6.24789800
30	O	-0.73793100	-5.99422000	5.72550100
31	H	-1.30770000	8.45280000	5.54490000
32	H	3.53900000	4.98890000	5.43620000
33	H	-5.91550000	5.84190000	-1.27060000
34	H	-6.78570000	6.92250000	2.19890000
35	H	-12.70540000	-0.03450000	-1.12450000
36	H	-13.56750000	1.03610000	2.31350000
37	H	-12.61360000	-4.36250000	-0.43650000
38	H	-12.17550000	-5.02190000	-2.75570000
39	H	-14.47190000	-2.17020000	6.40220000
40	H	-13.77040000	-2.92530000	4.17860000
41	H	6.86450400	-1.88259800	3.83330900
42	H	-2.15040000	-4.10050000	12.78420000
43	H	1.31010000	-8.39770000	-1.01480000
44	H	-12.21020000	-7.97290000	7.89080000

1	H	0.36339800	-1.65381000	11.27870300
2	H	0.62130000	6.05740000	-2.14750000
3	H	0.50140000	4.07440000	-3.47820000
4	H	-2.25700000	7.49990000	7.52180000
5	H	-5.73850000	6.73170000	5.78280000
6	H	-10.96700000	4.40130000	4.09400000
7	H	-11.01960000	5.00810000	1.73210000
8	H	-12.06290000	1.27880000	5.87220000
9	H	-10.59640000	-6.34750000	11.45320000
10	H	-8.66420000	-7.73420000	10.94950000
11	H	2.77449700	1.81969500	10.74640100
12	H	1.80020600	3.79900000	9.78440200
13	H	5.77540000	-0.53010000	8.17660000
14	H	3.24710000	-4.17500000	8.72650000
15	H	0.61160000	-6.65520000	10.31590000
16	H	-1.64370000	-7.57580000	10.07620000
17	H	0.12290000	-9.76940000	3.03170000
18	H	2.36090000	-8.82750000	3.33990000
19	H	-10.15040000	3.92860000	-1.73450000
20	H	-9.16390000	2.16210000	-3.09680000
21	H	3.89500000	1.63920000	-3.49250000
22	H	5.32300000	2.73990000	-1.76330000
23	H	4.42879100	3.88353600	1.88705100
24	H	5.61650800	-1.70968700	-0.58830800
25	H	4.35728500	-5.55351200	4.29821600
26	H	3.22920000	-5.21290700	-0.15128900
27	H	-5.23700000	-6.37850000	11.22840000
28	H	-7.76830000	-9.07120000	6.80850000
29	H	-6.95230000	-10.08460000	3.55430000
30	H	-10.29630000	-10.34930000	0.25900000
31	H	-2.42150000	-9.87450000	0.00040000
32	H	-3.42900000	-8.60990000	3.88980000
33	H	-4.28320000	-7.54880000	7.29620000
34	H	-3.45780000	3.89970000	-3.31080000
35	H	0.59910200	5.23699800	7.81469900
36	H	-9.79240000	-1.54060000	-3.18200000
37	H	-8.38790000	-2.95530000	10.89960000
38	H	-4.87450000	3.78240000	8.02040000
39	H	-2.02270000	2.13730000	10.92000000
40	H	-4.91220000	-7.27130000	-2.96190000
41	H	-8.98790000	-7.09310000	-2.37650000
42	H	1.45738000	-2.18476500	-2.95898000
43	H	-5.88650000	0.35320000	-2.87170000
44	H	-6.57060000	-3.25690000	-2.96870000

1	H	-11.74490000	-3.66940000	8.61800000
2	H	-9.32890000	0.16850000	8.03140000
3	H	-8.19140000	3.21540000	6.31880000
4	H	-5.78340000	-8.84910000	-1.27830000
5	H	-7.97590000	-9.98270000	-0.17660000
6	H	-2.11765800	0.35871300	-2.97422000
7				
8				
9	Z-C3H7+_CH3OCH3(ads)			
10	Si	-3.90186540	2.12360805	3.05938414
11	Si	-3.88899815	-0.75228819	-1.81271736
12	Si	-7.38863826	-0.30555770	1.61424847
13	Si	-3.55524203	-2.88167184	2.52103319
14	Al	-4.31629313	-0.26452465	1.10409991
15	O	-3.34681608	-1.46042891	1.85058555
16	O	-5.96608385	-0.77005866	1.08205605
17	O	-4.01469908	1.30896972	1.72425728
18	O	-3.73713631	0.06816303	-0.47901583
19	O	-2.47283087	2.90976149	3.02560202
20	O	-3.13382947	-2.17369715	-1.79126232
21	O	-5.41327070	-1.02954040	-2.29537601
22	O	-3.11340297	0.22701385	-2.84129052
23	O	-5.10548470	3.19029533	3.08874541
24	O	-7.99473368	0.98055237	0.86062030
25	O	-8.45557874	-1.47418484	1.33930756
26	O	-4.60476475	-3.91150047	1.82306609
27	O	-7.36575443	0.05068932	3.19379131
28	O	-4.07796326	-2.73729496	4.04801256
29	O	-3.96115761	1.28792225	4.42777435
30	O	-2.08779063	-3.56066837	2.46270579
31	C	-1.16883394	2.31490584	-1.16744944
32	H	-1.39440887	1.52538403	-1.87122483
33	H	-0.27797722	2.90173101	-1.34927725
34	C	-2.18418855	2.81212480	-0.35428175
35	H	-2.08073040	3.76145133	0.15674418
36	H	-3.14636839	2.31090137	-0.31453359
37	C	-1.09490876	1.60007817	0.36579973
38	H	-1.55064739	2.03976312	1.27354982
39	H	-1.48865949	0.60261188	0.24103613
40	H	-0.02388930	1.67619865	0.54688695
41	O	0.83751355	-0.30675959	1.33399442
42	C	0.27693595	-0.51784959	2.62560802
43	H	0.75991957	-1.36255534	3.12713210
44	H	0.46092855	0.38806348	3.20358945

1	H	-0.80012097	-0.71608045	2.56606539
2	C	0.61624008	-1.40314572	0.45651903
3	H	-0.45540458	-1.59323670	0.31034924
4	H	1.07692100	-1.14899280	-0.49882910
5	H	1.07954229	-2.31606095	0.84059599
6	O	-2.55044254	-2.94123078	6.16651889
7	Si	1.26901134	4.44351171	3.31620348
8	Si	-1.79591955	4.25884756	3.59756370
9	Si	-6.38931062	3.90381668	2.43934405
10	Si	3.43373600	2.62149400	4.45818400
11	Si	4.23645100	-0.32970500	4.40378200
12	Si	-1.18617353	-4.86400460	2.27845523
13	Si	1.68247086	-4.49309813	3.38803091
14	Si	3.98883000	-2.66023900	2.46280300
15	Si	6.47326400	-4.43073700	3.02988300
16	Si	4.76061300	-3.90975100	-5.12676000
17	Si	7.25431900	-5.74172300	-4.57669400
18	O	6.00050000	-4.81548900	-4.79509200
19	Si	-6.48604456	-1.50993770	-6.08463248
20	Si	-2.72115760	-4.22179689	-5.20083004
21	Si	-3.38877300	-1.48017897	-6.38466683
22	O	-2.65505208	-2.83566600	-5.97559901
23	O	-4.95910781	-1.70942098	-6.44280330
24	O	-1.30299111	-4.88471408	-5.24308920
25	Si	-0.43106300	-6.23754600	-5.20094900
26	Si	2.51015700	-5.86323600	-4.35949300
27	O	1.08248300	-5.79989100	-5.04776100
28	O	3.42126300	-4.75844600	-5.07653400
29	Si	-8.13153769	-3.58393188	-1.84031151
30	Si	2.09425500	3.15774900	-4.23165100
31	Si	-0.84814701	2.78169271	-5.07382255
32	Si	-4.67204700	5.41213500	-5.94920500
33	Si	-1.76977100	5.75467500	-5.04640300
34	O	0.58020865	2.71913757	-4.38567534
35	O	-1.75853191	1.67773557	-4.35626418
36	O	-5.11461059	4.15484232	-5.09577695
37	O	-3.31658800	5.98855900	-5.35335000
38	O	-1.48730735	4.20775467	-4.82541212
39	O	2.26108000	4.04417000	-2.92067400
40	O	-1.45120800	6.56435300	-3.71088200
41	Si	-0.29734900	7.22290700	-2.82459300
42	Si	4.76257900	7.06015000	-3.10474300
43	O	6.11474600	6.57103100	-2.41754000
44	Si	6.97802200	5.42702200	-1.72936300

1	O	6.64091600	4.01158400	-2.35870000
2	Si	8.14872900	-1.57080700	-3.34879600
3	Si	9.35366000	1.24089200	-3.01450800
4	Si	6.78885600	2.97655500	-3.55586100
5	Si	4.38377000	1.14126000	-4.23155800
6	O	8.96784400	-0.28851600	-2.84824400
7	O	8.07731800	2.09794500	-3.34184500
8	O	5.50643700	2.04304200	-3.57481400
9	O	2.96502900	1.80328000	-4.18934500
10	Si	-5.59170078	2.66118679	-4.85568810
11	O	8.08647700	-5.24156200	-3.32719600
12	Si	2.20576200	5.48182200	-2.24822200
13	O	1.00541100	6.31065900	-2.87977100
14	O	3.54819600	6.26904200	-2.47322600
15	Si	3.43314200	-1.84156200	7.01499800
16	Si	6.64744300	5.94205500	1.29428300
17	O	5.18166400	-3.50624800	3.09037800
18	O	6.13514400	4.79956000	2.26751100
19	Si	7.96714700	-3.07984300	5.33019300
20	Si	7.20070600	-0.09377600	5.32227500
21	Si	8.54873200	2.49492100	4.34723800
22	Si	5.99129900	4.21917200	3.73920100
23	O	7.87800800	-1.51383200	5.11691200
24	O	8.15207000	0.98246500	4.61350600
25	O	7.26352000	3.36580400	4.10118700
26	O	4.70098000	3.29806400	3.79284900
27	O	3.48228700	1.05661000	4.18421100
28	O	5.79130000	-0.07738300	4.60534100
29	O	7.59711300	-3.82434100	3.97384100
30	O	3.98865000	-1.18911500	3.08454100
31	O	3.60684400	-1.08765500	5.64759900
32	O	2.08008600	3.18201400	3.90453700
33	Si	4.31809200	-3.17323600	-0.54915100
34	Si	6.80133900	-4.94169800	0.02973800
35	O	5.58514500	-4.13476900	-0.59988700
36	Si	8.79237700	-4.36554300	-2.21777900
37	Si	5.05121900	-1.59903800	-3.04802200
38	O	8.71653500	-2.82016900	-2.55259000
39	O	4.31770200	-0.24500600	-3.45682800
40	O	6.62165100	-1.37096500	-2.98863000
41	O	8.11919800	-4.63771300	-0.80129500
42	O	4.50111400	-1.98764400	-1.60339900
43	O	4.67012900	-2.74408300	-4.07717800
44	Si	-5.62218888	6.89234293	2.74055241

1	Si	-2.58446306	7.02406092	2.40544420
2	O	-0.25825500	4.02544203	3.28392521
3	O	-5.92012326	5.40982347	2.27190623
4	O	-4.15206200	7.29006400	2.28775400
5	O	-2.31777073	5.50119681	2.76854913
6	O	1.73899500	4.85759200	1.85454800
7	O	-1.96376600	7.36280100	0.97699100
8	Si	-0.62661100	7.73590400	0.18736000
9	Si	1.87774500	5.99289300	0.75185800
10	Si	4.25243700	7.85499300	1.56155800
11	O	0.60192900	6.93912900	0.81040700
12	O	3.17026700	6.85786600	0.98362000
13	O	5.70018200	7.21678900	1.37360800
14	O	-0.87713500	7.33384200	-1.33871600
15	O	1.99016700	5.26272300	-0.67248500
16	O	6.65938200	5.35593700	-0.17782100
17	O	4.15862700	-2.48250300	0.88396300
18	O	7.07697500	-4.48475000	1.54403700
19	O	-3.00802489	-0.33720827	-5.35526318
20	Si	-3.09852948	0.82835079	-4.30551912
21	O	-4.33789209	1.73490752	-4.63732576
22	Si	-7.69099857	1.95315594	-2.74143463
23	Si	-6.86212493	-1.01980683	-3.00358044
24	Si	-5.62787182	-5.32414552	-1.26409714
25	Si	-3.07103056	-3.74593446	-2.12058358
26	O	-7.58129085	0.37768353	-2.79369943
27	O	-7.81039939	-2.14562869	-2.40625476
28	O	-6.82828900	-4.49541400	-1.89558000
29	O	-4.28545176	-4.53690453	-1.48909145
30	O	-6.63562071	-1.30510810	-4.53712281
31	O	-3.04652694	-3.98893048	-3.66915509
32	O	-6.51353523	2.62864971	-3.56136893
33	O	-1.71956336	-4.23574232	-1.43326912
34	Si	-1.73819940	-4.20110574	6.75463815
35	Si	1.32576600	-4.01783400	6.47374200
36	O	-0.21142600	-3.78393600	6.78724300
37	O	2.10467400	-2.70728900	6.96526700
38	O	0.26459441	-4.38596998	2.68832854
39	O	2.60720900	-3.35064700	2.78649000
40	O	1.55455300	-4.27714400	4.94520800
41	O	-2.00034300	-5.38965100	5.74597200
42	O	-1.69855073	-6.00651315	3.25170459
43	Si	-1.84231094	-6.58687038	4.72337335
44	Si	-0.85559350	-5.37901762	-0.74518725

1	Si	2.19350600	-5.28931100	-1.28617000
2	O	0.66504100	-5.00993300	-0.97443200
3	O	3.01145500	-3.98044600	-0.91057200
4	O	2.40326600	-5.59939700	-2.81735900
5	O	-0.94148600	-7.03932200	-3.93864800
6	O	-1.19278500	-6.79448900	-1.37450900
7	Si	-1.04475000	-7.82948900	-2.57168900
8	Si	-8.43689136	3.32139141	4.74088677
9	Si	-7.67040223	0.33536958	4.74865210
10	Si	-3.90338812	-2.37992030	5.61285823
11	Si	-4.70644730	0.57272406	5.66704472
12	Si	-8.02168298	2.46817188	0.28224870
13	Si	-8.46093443	-3.07087385	1.17162978
14	Si	-5.95595909	-4.81315190	1.73613777
15	O	-8.34774324	1.75538351	4.95417590
16	O	-3.95194209	-0.81503814	5.88682621
17	O	-6.26106438	0.31895628	5.46563288
18	O	-7.23170935	-3.86682790	1.79453463
19	O	-7.48272378	3.81068477	3.57942091
20	O	-7.01932041	3.41669707	1.06479778
21	O	-7.59074294	2.46155046	-1.24278369
22	O	-8.71077345	-3.47207698	-0.35450358
23	O	-5.84357647	-5.54321248	0.31174091
24	O	-1.17479022	-5.45090063	0.80647595
25	H	-5.69490600	6.50659700	-5.95074300
26	H	-9.02151700	2.31861200	-3.32484100
27	H	-0.39342500	9.21128500	0.30054600
28	H	0.00708000	8.58769500	-3.36184400
29	H	8.02165100	6.39474900	1.68249100
30	H	8.41840000	5.77660800	-1.94652200
31	H	9.44301800	2.51499500	3.14556500
32	H	9.28777600	3.02540400	5.53738600
33	H	10.34463800	1.37877400	-4.12928000
34	H	9.97515300	1.68511700	-1.72588400
35	H	-9.71501046	-3.42024724	1.91255907
36	H	-0.58858400	-7.07259100	-6.43458500
37	H	-2.18124100	-4.59180400	8.13121500
38	H	10.24109800	-4.74436700	-2.25872800
39	H	-3.78368254	-5.07542817	-5.82245181
40	H	-6.58270400	7.88966200	2.16904400
41	H	-5.76245600	6.99351700	4.22854500
42	H	-4.49299600	5.01584300	-7.38266100
43	H	-0.94473500	6.30771500	-6.16775000
44	H	4.78612200	6.82785000	-4.58447500

1	H	4.64786500	8.53069100	-2.84356800
2	H	6.88669500	3.72461300	-4.85001400
3	H	8.12318800	-5.71115100	-5.79663100
4	H	6.80384900	-7.15231400	-4.35010400
5	H	-7.25214217	-2.70920980	-6.55235709
6	H	-7.02205810	-0.33040253	-6.83639505
7	H	-9.21379500	-4.20116700	-2.67204600
8	H	-5.57575700	-6.68028300	-1.89832200
9	H	-2.25581600	-8.71093600	-2.58961400
10	H	0.18142800	-8.66555200	-2.36798100
11	H	-0.63167800	-7.39896200	5.06790200
12	H	-3.06089100	-7.45665000	4.77395400
13	H	4.24788000	9.15400000	0.81561800
14	H	3.95632100	8.12076600	3.00582000
15	H	-8.08892200	4.02189400	6.01849900
16	H	-9.82990600	3.61366800	4.27402700
17	H	-9.43086538	2.95666341	0.42159933
18	H	-8.56004892	-0.67098052	5.41193329
19	H	-6.08674581	-5.88363140	2.77574670
20	H	-5.10247882	-3.02006086	6.24242174
21	H	3.11620000	-7.21308800	-4.59292000
22	H	6.47605400	-6.40393400	0.01688200
23	H	6.10053900	-5.81886500	3.45189800
24	H	9.36015700	-3.37212100	5.79705000
25	H	1.82032100	-5.19399400	7.25870400
26	H	2.28063300	-5.84047400	3.12205300
27	H	2.67363900	-6.45265000	-0.47376900
28	H	-1.99446000	7.94239700	3.43127400
29	H	-6.37949883	2.18770839	-6.03860166
30	H	5.84170100	5.35257400	4.70720600
31	H	4.87318100	-3.33984200	-6.50748600
32	H	-0.74545213	2.53039358	-6.54705808
33	H	-2.87153300	-1.11616100	-7.74255700
34	H	3.27352300	-0.84714200	8.12388700
35	H	7.02275500	0.21038600	6.77827400
36	H	-4.47314247	1.37929110	6.90751587
37	H	1.51701100	5.56949200	4.27267000
38	H	3.42219000	2.89875000	5.93027400
39	H	8.29159200	-1.76637700	-4.82708000
40	H	4.69159100	0.92091400	-5.68095200
41	H	2.57781800	3.91737900	-5.42863200
42	H	4.62404300	-2.71851200	7.25381600
43	H	7.06290300	-3.54343400	6.43082800
44	H	-2.01425193	4.50727010	5.05834995

1
2
3 Z-C3H7+_H2O(ads)
4 Si -0.02783453 0.03396833 -0.01224595
5 Si -0.07272097 -0.01489452 5.63820149
6 Si 3.70417837 -0.02990577 2.48516554
7 Si 1.05741573 -3.89666260 2.96410510
8 Al 0.71926711 -0.83451113 2.84628399
9 O 0.30852893 -2.50746276 2.75779003
10 O 2.39770465 -0.64455815 3.15506614
11 O 0.02046795 0.07334679 1.56572061
12 O -0.26836554 -0.16739120 4.08296777
13 O -1.58036443 0.12315173 -0.45472706
14 O -0.39684152 -1.42455739 6.35301833
15 O 1.36497357 0.50546966 6.17787110
16 O -1.24219946 1.03762117 5.98664921
17 O 0.81653819 1.28790833 -0.55768644
18 O 3.75576589 1.57400484 2.49670226
19 O 4.98865504 -0.48157406 3.33443030
20 O 2.20067408 -4.00985914 4.11250310
21 O 3.87411339 -0.50760075 0.94988509
22 O 1.79168147 -4.35255095 1.60164885
23 O 0.58602817 -1.28477412 -0.70041611
24 O -0.15712014 -4.89565585 3.37270709
25 H -1.75983217 1.86275494 3.73786370
26 C -3.10466644 -0.81444008 2.73561570
27 H -3.83155326 -0.12628782 3.14852234
28 H -2.16488393 -0.58923036 3.31591339
29 H -2.78391998 -0.64743096 1.71163491
30 O -1.97594220 1.93617037 2.80196419
31 C -2.66635401 -2.30445011 3.61519695
32 H -2.77729367 -2.10932546 4.67581862
33 H -1.68108218 -2.62311467 3.27697372
34 C -3.78362480 -2.31711570 2.76352423
35 H -3.70364604 -2.78551157 1.79138476
36 H -4.78016094 -2.27445681 3.18368759
37 H -1.23908434 1.46589495 2.38249624
38 O 0.80119695 -6.00639837 -0.15259467
39 Si -5.49759701 -0.02111243 -1.47430784
40 Si -2.51927490 0.76945826 -1.59080843
41 Si 1.67075783 2.63420898 -0.36381484
42 Si -6.77250000 -2.79180000 -1.55910000
43 Si -6.65860000 -5.43650000 -0.02630000
44 Si -0.62798627 -6.20850755 4.15919131

1	Si	-3.21920146	-7.43500035	2.98450358
2	Si	-6.09540000	-6.32220000	2.83000000
3	Si	-7.79180000	-8.89230000	3.21140000
4	Si	-7.85690000	-4.02790000	9.99880000
5	Si	-9.54690000	-6.64300000	10.42590000
6	O	-8.68790000	-5.35140000	10.15840000
7	Si	1.78780042	2.30219870	9.72780053
8	Si	-0.76979922	-1.62739898	10.29929987
9	Si	-1.17800017	1.38380046	9.93890016
10	O	-1.38700159	-0.16320067	10.26479980
11	O	0.35019825	1.77510357	10.12159839
12	O	-1.90929863	-2.64050127	10.65650077
13	Si	-2.31670000	-4.06080000	11.29600000
14	Si	-5.02660000	-5.18350000	10.35000000
15	O	-3.83590000	-4.30830000	10.92640000
16	O	-6.34110000	-4.27000000	10.39930000
17	Si	4.73289903	-0.80100630	7.13549247
18	Si	-7.29070000	2.20560000	5.67640000
19	Si	-4.57940635	3.32748987	6.62401789
20	Si	-1.94070000	7.20800000	6.08700000
21	Si	-4.59330000	6.04430000	5.10460000
22	O	-5.77090000	2.45290000	6.04720000
23	O	-3.26548938	2.41431737	6.57327032
24	O	-0.99450185	5.94280259	5.99240851
25	O	-3.27080000	6.91960000	5.26710000
26	O	-4.35770000	4.58890000	5.69440000
27	O	-7.46660000	2.24720000	4.09540000
28	O	-4.88400000	5.95910000	3.53970000
29	Si	-5.99570000	5.67090000	2.42990000
30	Si	-10.73910000	3.90040000	2.70070000
31	O	-11.73290000	2.70740000	2.34160000
32	Si	-12.07420000	1.15480000	2.31840000
33	O	-11.45520000	0.42330000	3.58130000
34	Si	-11.39460000	-4.15760000	7.24580000
35	Si	-13.29570000	-2.46030000	5.52120000
36	Si	-11.50890000	0.09760000	5.13610000
37	Si	-8.83680000	-0.22830000	6.67330000
38	O	-12.44950000	-3.64190000	6.15630000
39	O	-12.41530000	-1.16550000	5.38290000
40	O	-10.03410000	-0.20050000	5.63860000
41	O	-7.69650000	0.78430000	6.31660000
42	Si	-0.05969771	4.78729878	6.54670158
43	O	-10.24280000	-7.11800000	9.08650000
44	Si	-7.71660000	3.11370000	2.78820000

1	O	-6.95550000	4.50240000	2.92570000
2	O	-9.24950000	3.38730000	2.56950000
3	Si	-4.97250000	-7.60980000	-1.50390000
4	Si	-11.35590000	0.26280000	-0.54610000
5	O	-6.84510000	-7.72030000	2.70470000
6	O	-10.35620000	-0.94150000	-0.80140000
7	Si	-9.16490000	-9.40520000	0.52820000
8	Si	-9.33470000	-6.71560000	-0.96890000
9	Si	-11.54680000	-4.63200000	-1.45310000
10	Si	-9.77590000	-2.05450000	-1.77500000
11	O	-9.58580000	-8.00560000	-0.07990000
12	O	-10.67690000	-5.84320000	-0.91270000
13	O	-10.64710000	-3.36120000	-1.66840000
14	O	-8.28390000	-2.37400000	-1.34130000
15	O	-6.40440000	-3.94670000	-0.53100000
16	O	-8.15250000	-5.87130000	-0.34420000
17	O	-8.84920000	-9.23940000	2.07860000
18	O	-6.41640000	-5.42400000	1.54900000
19	O	-5.61290000	-6.41590000	-0.70840000
20	O	-5.77370000	-1.60340000	-1.35130000
21	Si	-6.81090000	-5.43360000	5.68340000
22	Si	-8.50460000	-8.00720000	6.05360000
23	O	-7.72180000	-6.63160000	6.20070000
24	Si	-10.95800000	-7.17850000	7.67890000
25	Si	-8.42890000	-3.23820000	7.03330000
26	O	-11.40780000	-5.74300000	7.18590000
27	O	-8.21960000	-1.69260000	6.70790000
28	O	-9.95660000	-3.63110000	6.85010000
29	O	-9.98360000	-7.83070000	6.60240000
30	O	-7.53000000	-4.04100000	5.99020000
31	O	-7.92320000	-3.54700000	8.50450000
32	Si	0.12318136	4.64408396	-2.14550190
33	Si	-2.82308184	3.84600085	-1.95510796
34	O	-3.94900720	0.19041794	-1.21849976
35	O	0.75702729	3.77012132	-0.98770116
36	O	-1.45550000	4.66540000	-1.97180000
37	O	-2.55353369	2.34859839	-1.49998463
38	O	-6.33220000	0.83850000	-0.42850000
39	O	-3.77030000	4.57610000	-0.90140000
40	Si	-5.28020000	4.78230000	-0.42350000
41	Si	-7.00390000	2.22870000	-0.05400000
42	Si	-9.63060000	2.52380000	-1.72000000
43	O	-6.07880000	3.41370000	-0.57020000
44	O	-8.42830000	2.36750000	-0.70540000

1	O	-10.83220000	1.58900000	-1.25000000
2	O	-5.20960000	5.26350000	1.09860000
3	O	-7.15700000	2.26930000	1.54270000
4	O	-11.46650000	0.47770000	1.01990000
5	O	-6.60040000	-5.49380000	4.09960000
6	O	-8.61720000	-8.44720000	4.51360000
7	O	-1.68269632	1.69078933	8.46849640
8	Si	-1.74886896	2.17172693	6.97400267
9	O	-0.91870172	3.49570154	6.81430381
10	Si	2.50949946	3.95249936	5.10420149
11	Si	2.56679830	1.37898150	6.82659682
12	Si	3.01119705	-3.35760648	7.49350403
13	Si	-0.01120219	-2.57096650	7.40589516
14	O	2.86459957	2.66320934	5.94591347
15	O	3.90010601	0.51781008	6.89191031
16	O	3.77240000	-1.96900000	7.63100000
17	O	1.47830105	-3.08399410	7.27478885
18	O	2.15448719	1.79117113	8.29130452
19	O	-0.24969679	-2.04668534	8.86409525
20	O	1.05379524	4.47370218	5.45679451
21	O	-1.00419005	-3.76440035	7.04717364
22	Si	0.52350118	-7.58780045	-0.03030311
23	Si	-2.45310000	-8.37930000	0.08690000
24	O	-1.02440000	-7.79970000	-0.28570000
25	O	-3.48040000	-7.82240000	-1.00870000
26	O	-2.05279684	-6.52239743	3.54849132
27	O	-4.53620000	-6.55020000	2.91500000
28	O	-2.87430000	-7.94910000	1.53380000
29	O	0.93450000	-7.98310000	1.44400000
30	O	0.37169722	-7.41290281	3.90390238
31	Si	0.95190035	-8.52589967	2.93029984
32	Si	-1.34640558	-5.31659500	7.02371864
33	Si	-4.32960000	-6.05610000	7.41270000
34	O	-2.92290000	-5.44190000	7.01850000
35	O	-5.41450000	-5.45960000	6.41750000
36	O	-4.71840000	-5.65910000	8.88780000
37	O	-1.36620000	-5.12610000	10.61890000
38	O	-0.72730000	-6.04810000	8.28660000
39	Si	-0.78110000	-6.37380000	9.84140000
40	Si	4.19140156	1.79569991	-2.03279920
41	Si	4.36127655	-0.89370415	-0.53526935
42	Si	1.79922878	-4.81761234	0.05468921
43	Si	1.68560904	-2.17096698	-1.47831767
44	Si	3.22759308	3.05988619	2.24000733

1	Si	5.44838538	-1.68951555	4.28212109
2	Si	3.72400806	-4.24271369	4.65120635
3	O	4.61249864	0.39620710	-1.42439009
4	O	1.43067264	-3.66258842	-0.97318346
5	O	3.17930510	-1.73821302	-1.16020040
6	O	4.64910106	-3.05760075	4.13510400
7	O	2.93738581	2.40538379	-1.28811544
8	O	2.15409920	3.10990442	1.07329968
9	O	2.54300316	3.62280724	3.55349854
10	O	5.51820433	-1.20769300	5.80379759
11	O	3.57090290	-4.20199873	6.24790025
12	O	-0.73790874	-5.99420412	5.72549995
13	H	-1.30770000	8.45280000	5.54490000
14	H	3.53900000	4.98890000	5.43620000
15	H	-5.91550000	5.84190000	-1.27060000
16	H	-6.78570000	6.92250000	2.19890000
17	H	-12.70540000	-0.03450000	-1.12450000
18	H	-13.56750000	1.03610000	2.31350000
19	H	-12.61360000	-4.36250000	-0.43650000
20	H	-12.17550000	-5.02190000	-2.75570000
21	H	-14.47190000	-2.17020000	6.40220000
22	H	-13.77040000	-2.92530000	4.17860000
23	H	6.86449869	-1.88259818	3.83329508
24	H	-2.15040000	-4.10050000	12.78420000
25	H	1.31010000	-8.39770000	-1.01480000
26	H	-12.21020000	-7.97290000	7.89080000
27	H	0.36340031	-1.65379874	11.27869967
28	H	0.62130000	6.05740000	-2.14750000
29	H	0.50140000	4.07440000	-3.47820000
30	H	-2.25700000	7.49990000	7.52180000
31	H	-5.73850000	6.73170000	5.78280000
32	H	-10.96700000	4.40130000	4.09400000
33	H	-11.01960000	5.00810000	1.73210000
34	H	-12.06290000	1.27880000	5.87220000
35	H	-10.59640000	-6.34750000	11.45320000
36	H	-8.66420000	-7.73420000	10.94950000
37	H	2.77449740	1.81969594	10.74640059
38	H	1.80020489	3.79899991	9.78440134
39	H	5.77540000	-0.53010000	8.17660000
40	H	3.24710000	-4.17500000	8.72650000
41	H	0.61160000	-6.65520000	10.31590000
42	H	-1.64370000	-7.57580000	10.07620000
43	H	0.12290000	-9.76940000	3.03170000
44	H	2.36090000	-8.82750000	3.33990000

1	H	-10.15040000	3.92860000	-1.73450000
2	H	-9.16390000	2.16210000	-3.09680000
3	H	3.89500000	1.63920000	-3.49250000
4	H	5.32300000	2.73990000	-1.76330000
5	H	4.42880346	3.88349441	1.88709875
6	H	5.61650273	-1.70969580	-0.58830007
7	H	4.35730158	-5.55349945	4.29820078
8	H	3.22919890	-5.21290116	-0.15130539
9	H	-5.23700000	-6.37850000	11.22840000
10	H	-7.76830000	-9.07120000	6.80850000
11	H	-6.95230000	-10.08460000	3.55430000
12	H	-10.29630000	-10.34930000	0.25900000
13	H	-2.42150000	-9.87450000	0.00040000
14	H	-3.42900000	-8.60990000	3.88980000
15	H	-4.28320000	-7.54880000	7.29620000
16	H	-3.45780000	3.89970000	-3.31080000
17	H	0.59910695	5.23699520	7.81469809
18	H	-9.79240000	-1.54060000	-3.18200000
19	H	-8.38790000	-2.95530000	10.89960000
20	H	-4.87450000	3.78240000	8.02040000
21	H	-2.02270000	2.13730000	10.92000000
22	H	-4.91220000	-7.27130000	-2.96190000
23	H	-8.98790000	-7.09310000	-2.37650000
24	H	1.45738854	-2.18478582	-2.95899837
25	H	-5.88650000	0.35320000	-2.87170000
26	H	-6.57060000	-3.25690000	-2.96870000
27	H	-11.74490000	-3.66940000	8.61800000
28	H	-9.32890000	0.16850000	8.03140000
29	H	-8.19140000	3.21540000	6.31880000
30	H	-5.78340000	-8.84910000	-1.27830000
31	H	-7.97590000	-9.98270000	-0.17660000
32	H	-2.11767806	0.35869745	-2.97419287
33				
34				
35	Z-CH+(CH3)2			
36	Si	-3.85394071	2.11068228	3.02096886
37	Si	-3.82194566	-0.74584053	-1.80801244
38	Si	-7.27810787	-0.35993182	1.60210059
39	Si	-3.45120691	-2.85621107	2.49999912
40	Al	-4.26465249	-0.27436170	1.08834505
41	O	-3.23818256	-1.41513158	1.87076167
42	O	-5.87965386	-0.86653084	1.04835131
43	O	-3.93083094	1.29814479	1.68584839
44	O	-3.63669090	0.04122927	-0.46613399

1	O	-2.44122407	2.90751228	3.05274108
2	O	-3.03534606	-2.15355558	-1.79755156
3	O	-5.34687977	-1.07789359	-2.26404947
4	O	-3.10681207	0.23884590	-2.85140838
5	O	-5.09661534	3.12884869	3.09220361
6	O	-7.91043327	0.91832025	0.85401393
7	O	-8.36658759	-1.51732558	1.36471621
8	O	-4.46546451	-3.90926016	1.77937563
9	O	-7.24741565	0.03890200	3.17346666
10	O	-4.00235320	-2.75584922	4.02459305
11	O	-3.90113952	1.26611682	4.39224362
12	O	-1.96640928	-3.51178547	2.44613687
13	O	-2.43615000	-2.92104000	6.14978300
14	Si	1.28268100	4.51488800	3.29974000
15	Si	-1.77936500	4.28963400	3.58410400
16	Si	-6.36856000	3.87476500	2.43094300
17	Si	3.47244400	2.72089500	4.43808400
18	Si	4.31383600	-0.21946000	4.38101800
19	Si	-1.05112300	-4.82337300	2.25889400
20	Si	1.81368600	-4.41548600	3.36562200
21	Si	4.09470200	-2.55191500	2.43892000
22	Si	6.60283800	-4.28991900	3.00216600
23	Si	4.87431700	-3.78673200	-5.15224700
24	Si	7.39251500	-5.58607300	-4.60606200
25	O	6.12638100	-4.67628000	-4.82250600
26	Si	-6.40399900	-1.53451100	-6.09612100
27	Si	-2.60274200	-4.19709400	-5.21814900
28	Si	-3.30772200	-1.46376800	-6.39964000
29	O	-2.55582400	-2.80976600	-5.99216900
30	O	-4.87496500	-1.71358500	-6.45613000
31	O	-1.17605600	-4.84125700	-5.26239500
32	Si	-0.28637900	-6.18255600	-5.22203600
33	Si	2.65060800	-5.77009100	-4.38363900
34	O	1.22145200	-5.72512400	-5.07027500
35	O	3.54630100	-4.65299600	-5.10103400
36	Si	-8.01726200	-3.63240900	-1.85110000
37	Si	2.11626100	3.24456800	-4.24992600
38	Si	-0.82178100	2.83026600	-5.08902700
39	Si	-4.68102800	5.41078100	-5.95857600
40	Si	-1.78249400	5.79093000	-5.05880900
41	O	0.60793700	2.78618200	-4.40251600
42	O	-1.71692600	1.71438400	-4.37090600
43	O	-5.10606100	4.14728200	-5.10539400
44	O	-3.33259700	6.00463200	-5.36388900

1	O	-1.47949700	4.24772400	-4.83911000
2	O	2.27288800	4.13234000	-2.93860500
3	O	-1.47310500	6.60394700	-3.72315900
4	Si	-0.32701100	7.27710000	-2.83776400
5	Si	4.73430200	7.18106200	-3.12366000
6	O	6.09355500	6.70936600	-2.43825900
7	Si	6.97257300	5.57640600	-1.75173200
8	O	6.65340200	4.15702600	-2.38154100
9	Si	8.23338000	-1.40447300	-3.37666500
10	Si	9.40160800	1.42263100	-3.04203600
11	Si	6.81359500	3.12473200	-3.57948700
12	Si	4.43209300	1.25836300	-4.25359800
13	O	9.03612400	-0.11181500	-2.87625900
14	O	8.11373900	2.26301700	-3.36743500
15	O	5.54354200	2.17444600	-3.59756700
16	O	3.00481700	1.90164300	-4.20940500
17	Si	-5.56319100	2.64734700	-4.86568300
18	O	8.21942900	-5.07574200	-3.35719400
19	Si	2.19942600	5.56874600	-2.26523100
20	O	0.98757000	6.38209600	-2.89494300
21	O	3.53113700	6.37368400	-2.49126100
22	Si	3.53341300	-1.74327700	6.99222300
23	Si	6.63865000	6.08528000	1.27259000
24	O	5.29926200	-3.38253100	3.06465600
25	O	6.14251300	4.93557800	2.24570300
26	Si	8.08141300	-2.92084000	5.30161600
27	Si	7.27576300	0.05489300	5.29634300
28	Si	8.58853400	2.66166400	4.32135300
29	Si	6.00796600	4.35248800	3.71720500
30	O	7.97144800	-1.35601300	5.08937300
31	O	8.21209400	1.14396600	4.58715800
32	O	7.29170500	3.51571300	4.07726000
33	O	4.72993300	3.41446000	3.77174100
34	O	3.54126100	1.15694500	4.16312000
35	O	5.86545800	0.05316900	4.58099200
36	O	7.71967600	-3.66934800	3.94523100
37	O	4.07587600	-1.08128400	3.06154000
38	O	3.69564900	-0.98635200	5.62508200
39	O	2.11091800	3.26388900	3.88628500
40	Si	4.42729600	-3.05877600	-0.57370600
41	Si	6.93423200	-4.79476700	0.00135000
42	O	5.70682500	-4.00353300	-0.62643200
43	Si	8.91499400	-4.19116400	-2.24804200
44	Si	5.13684900	-1.47361200	-3.07245000

1	O	8.81846100	-2.64672600	-2.58184100
2	O	4.38513100	-0.12910500	-3.47962500
3	O	6.70421200	-1.22494200	-3.01467400
4	O	8.24704500	-4.47299100	-0.83097000
5	O	4.59352600	-1.87026400	-1.62744700
6	O	4.76969300	-2.62296800	-4.10186600
7	Si	-5.64075900	6.87327900	2.73312900
8	Si	-2.60552700	7.04513200	2.39475700
9	O	-0.23911200	4.07693800	3.26855800
10	O	-5.91977100	5.38726200	2.26389500
11	O	-4.17652500	7.29057100	2.27892100
12	O	-2.31817700	5.52576600	2.75659700
13	O	1.74551900	4.93603400	1.83768300
14	O	-1.99084900	7.39284500	0.96576000
15	Si	-0.65960500	7.78396200	0.17486200
16	Si	1.86808900	6.07370600	0.73551900
17	Si	4.21899700	7.96640100	1.54368300
18	O	0.58000600	7.00304800	0.79605900
19	O	3.14938400	6.95546600	0.96635700
20	O	5.67479700	7.34740000	1.35373600
21	O	-0.90653500	7.37953200	-1.35117500
22	O	1.98850200	5.34591000	-0.68938600
23	O	6.65664000	5.50023000	-0.19987900
24	O	4.26037100	-2.37103800	0.85999800
25	O	7.20553700	-4.33511900	1.51561400
26	O	-2.94083200	-0.31660600	-5.36984700
27	Si	-3.04562100	0.84697300	-4.31920500
28	O	-4.29705700	1.73749800	-4.64934200
29	Si	-7.65042100	1.91030800	-2.74948800
30	Si	-6.78284600	-1.05087200	-3.01415200
31	Si	-5.49031300	-5.33988800	-1.27884100
32	Si	-2.95559000	-3.72772800	-2.13725000
33	O	-7.52028800	0.33659500	-2.80288600
34	O	-7.71575800	-2.18978600	-2.41690500
35	O	-6.70224100	-4.52663500	-1.90848500
36	O	-4.15860900	-4.53492800	-1.50484500
37	O	-6.55450200	-1.33259200	-4.54831500
38	O	-2.92942200	-3.96943100	-3.68597500
39	O	-6.48307600	2.60191300	-3.57036000
40	O	-1.59690200	-4.20001600	-1.45159000
41	Si	-1.60673900	-4.17047400	6.73621000
42	Si	1.45423000	-3.94675700	6.45201500
43	O	-0.08555100	-3.73327800	6.76737200
44	O	2.21638900	-2.62637000	6.94345500

1	O	0.39373600	-4.32660200	2.66757300
2	O	2.72264300	-3.26062100	2.76373500
3	O	1.68468900	-4.20214300	4.92307200
4	O	-1.85436700	-5.36177100	5.72713600
5	O	-1.54721400	-5.97311700	3.23214400
6	Si	-1.68175000	-6.55621300	4.70364400
7	Si	-0.71711700	-5.33231500	-0.76537200
8	Si	2.32989300	-5.20217700	-1.30962100
9	O	0.79823700	-4.94310600	-0.99601000
10	O	3.13098100	-3.88288800	-0.93415200
11	O	2.54199100	-5.50858300	-2.84122900
12	O	-0.78479600	-6.99171200	-3.95964700
13	O	-1.03640900	-6.75170400	-1.39508300
14	Si	-0.87612400	-7.78396800	-2.59304700
15	Si	-8.40601300	3.26446100	4.73450600
16	Si	-7.60012400	0.28899600	4.73924900
17	Si	-3.79696300	-2.37724600	5.59796200
18	Si	-4.63868200	0.56457200	5.65463400
19	Si	-7.98393100	2.41859300	0.27467000
20	Si	-8.34996800	-3.12541800	1.16156200
21	Si	-5.82178800	-4.83504500	1.72209400
22	O	-8.29619900	1.69958000	4.94663200
23	O	-3.86581900	-0.81330500	5.87296000
24	O	-6.19014300	0.29023400	5.45510500
25	O	-7.10968200	-3.90548000	1.78245200
26	O	-7.45963900	3.76700100	3.57227600
27	O	-6.99467600	3.38112700	1.05702400
28	O	-7.55584200	2.41983800	-1.25079900
29	O	-8.59634200	-3.52895400	-0.36471000
30	O	-5.70134200	-5.56267300	0.29710400
31	O	-1.03364200	-5.40926800	0.78668500
32	H	-5.71819200	6.49169800	-5.95831600
33	H	-8.98649000	2.25879400	-3.33121300
34	H	-0.44571300	9.26221600	0.28867200
35	H	-0.04115900	8.64608800	-3.37453700
36	H	8.00722100	6.55577900	1.65953500
37	H	8.40798500	5.94503100	-1.97028900
38	H	9.48112700	2.69419800	3.11869500
39	H	9.32187600	3.20112400	5.51099400
40	H	10.38943300	1.57418600	-4.15783100
41	H	10.01865300	1.87423800	-1.75384100
42	H	-9.59858200	-3.49178900	1.90347600
43	H	-0.43429200	-7.01887900	-6.45599600
44	H	-2.04306000	-4.56776700	8.11305700

1	H	10.36852400	-4.55088000	-2.29083400
2	H	-3.65467000	-5.06429000	-5.83909400
3	H	-6.61497400	7.85822200	2.16328400
4	H	-5.78069800	6.97173700	4.22133100
5	H	-4.49839200	5.01771600	-7.39246800
6	H	-0.96606300	6.35542800	-6.18074500
7	H	4.75923500	6.94995700	-4.60355600
8	H	4.60055400	8.64981500	-2.86147500
9	H	6.90013400	3.87476800	-4.87329900
10	H	8.25953600	-5.54336400	-5.82695000
11	H	6.96088900	-7.00259800	-4.37981500
12	H	-7.15474400	-2.74346300	-6.56370600
13	H	-6.95635700	-0.36166300	-6.84658500
14	H	-9.09228200	-4.26333100	-2.68211100
15	H	-5.42109100	-6.69484200	-1.91393400
16	H	-2.07551200	-8.68125400	-2.61014800
17	H	0.36117100	-8.60395300	-2.39120900
18	H	-0.46016200	-7.35251200	5.04633400
19	H	-2.88873400	-7.44196900	4.75506400
20	H	4.19652100	9.26567100	0.79852800
21	H	3.92103600	8.22741100	2.98843500
22	H	-8.06587200	3.96873100	6.01210000
23	H	-9.80329700	3.53866500	4.26932800
24	H	-9.39997100	2.88920900	0.41620200
25	H	-8.47599900	-0.72950700	5.40326500
26	H	-5.93725700	-5.90772800	2.76116000
27	H	-4.98683500	-3.03347200	6.22847000
28	H	3.27408700	-7.11172000	-4.61855200
29	H	6.62819000	-6.26114600	-0.01201900
30	H	6.24887400	-5.68307500	3.42376500
31	H	9.47867000	-3.19504700	5.76674200
32	H	1.96509100	-5.11677100	7.23571900
33	H	2.42921500	-5.75472300	3.09817100
34	H	2.82619500	-6.35957600	-0.49845400
35	H	-2.02640400	7.97055300	3.42042300
36	H	-6.34602500	2.16423800	-6.04800400
37	H	5.84456500	5.48325800	4.68605600
38	H	4.97783000	-3.21458500	-6.53275600
39	H	-0.71755700	2.58127900	-6.56253900
40	H	-2.79684000	-1.09222300	-7.75784800
41	H	3.36197700	-0.75169100	8.10188400
42	H	7.09546400	0.35583700	6.75272200
43	H	-4.41468700	1.37338700	6.89550000
44	H	1.51691100	5.64353900	4.25647700

1	H	3.45890800	2.99711400	5.91035300
2	H	8.37714000	-1.59728400	-4.85522400
3	H	4.74115600	1.04293100	-5.70346600
4	H	2.58844700	4.01119100	-5.44699100
5	H	4.73601000	-2.60462900	7.22918500
6	H	7.18458100	-3.39692600	6.40298100
7	H	-1.99915200	4.53449200	5.04547200
8	C	-0.95878958	1.75269712	0.15150174
9	H	-0.86018413	1.58978915	-0.92771607
10	H	-0.39858845	2.59629988	0.55255886
11	C	-0.87316046	0.54545607	0.91440257
12	H	-2.05767633	1.94218122	0.26636643
13	H	-1.30454511	-0.35638059	0.47264481
14	C	-0.32637615	0.42158887	2.24563131
15	H	0.06725526	1.34268600	2.67331733
16	H	-1.08886823	-0.05494663	2.88306098
17	H	0.45470919	-0.35928049	2.18506311
18				
19				
20	ZH			
21	Si	-0.04140160	0.02787556	0.01071408
22	Si	-0.07134417	-0.00188415	5.70666429
23	Si	3.71813907	-0.01607258	2.48334157
24	Si	1.04698046	-3.91039549	2.98250279
25	Al	0.76494606	-0.89078104	2.77789562
26	O	0.31576087	-2.50039691	2.96884790
27	O	2.39743832	-0.59170159	3.17491537
28	O	-0.02217554	0.04279433	1.59767212
29	O	-0.18706351	0.00117366	4.05573266
30	O	-1.56283751	0.14144284	-0.47145572
31	O	-0.35083683	-1.44677936	6.28843495
32	O	1.37072465	0.50436212	6.16682420
33	O	-1.25055153	1.02945459	5.97581687
34	O	0.83343874	1.28010168	-0.49390376
35	O	3.77941123	1.58492046	2.49869256
36	O	4.99020020	-0.47803942	3.33832217
37	O	2.21132026	-4.05073159	4.10540355
38	O	3.86311056	-0.50866836	0.95348138
39	O	1.76091226	-4.24966025	1.57269238
40	O	0.61673201	-1.28179163	-0.65549725
41	O	-0.12957330	-4.94669702	3.32473265
42	H	-0.88406613	0.53574113	3.65042366
43	O	0.80123457	-6.00643381	-0.15257577
44	Si	-5.49760220	-0.02109116	-1.47429447

1	Si	-2.51946596	0.76943571	-1.59072182
2	Si	1.67327488	2.63520604	-0.36433943
3	Si	-6.77250000	-2.79180000	-1.55910000
4	Si	-6.65860000	-5.43650000	-0.02630000
5	Si	-0.62825644	-6.20865902	4.15917618
6	Si	-3.21918841	-7.43499686	2.98447055
7	Si	-6.09540000	-6.32220000	2.83000000
8	Si	-7.79180000	-8.89230000	3.21140000
9	Si	-7.85690000	-4.02790000	9.99880000
10	Si	-9.54690000	-6.64300000	10.42590000
11	O	-8.68790000	-5.35140000	10.15840000
12	Si	1.78780261	2.30219803	9.72780147
13	Si	-0.76981198	-1.62740697	10.29929900
14	Si	-1.17799468	1.38378614	9.93889571
15	O	-1.38699498	-0.16319799	10.26480100
16	O	0.35019755	1.77510596	10.12159767
17	O	-1.90929605	-2.64050395	10.65650197
18	Si	-2.31670000	-4.06080000	11.29600000
19	Si	-5.02660000	-5.18350000	10.35000000
20	O	-3.83590000	-4.30830000	10.92640000
21	O	-6.34110000	-4.27000000	10.39930000
22	Si	4.73290072	-0.80097379	7.13549920
23	Si	-7.29070000	2.20560000	5.67640000
24	Si	-4.57939761	3.32750303	6.62399472
25	Si	-1.94070000	7.20800000	6.08700000
26	Si	-4.59330000	6.04430000	5.10460000
27	O	-5.77090000	2.45290000	6.04720000
28	O	-3.26550272	2.41430185	6.57330946
29	O	-0.99450036	5.94280050	5.99240165
30	O	-3.27080000	6.91960000	5.26710000
31	O	-4.35770000	4.58890000	5.69440000
32	O	-7.46660000	2.24720000	4.09540000
33	O	-4.88400000	5.95910000	3.53970000
34	Si	-5.99570000	5.67090000	2.42990000
35	Si	-10.73910000	3.90040000	2.70070000
36	O	-11.73290000	2.70740000	2.34160000
37	Si	-12.07420000	1.15480000	2.31840000
38	O	-11.45520000	0.42330000	3.58130000
39	Si	-11.39460000	-4.15760000	7.24580000
40	Si	-13.29570000	-2.46030000	5.52120000
41	Si	-11.50890000	0.09760000	5.13610000
42	Si	-8.83680000	-0.22830000	6.67330000
43	O	-12.44950000	-3.64190000	6.15630000
44	O	-12.41530000	-1.16550000	5.38290000

1	O	-10.03410000	-0.20050000	5.63860000
2	O	-7.69650000	0.78430000	6.31660000
3	Si	-0.05970266	4.78730087	6.54669653
4	O	-10.24280000	-7.11800000	9.08650000
5	Si	-7.71660000	3.11370000	2.78820000
6	O	-6.95550000	4.50240000	2.92570000
7	O	-9.24950000	3.38730000	2.56950000
8	Si	-4.97250000	-7.60980000	-1.50390000
9	Si	-11.35590000	0.26280000	-0.54610000
10	O	-6.84510000	-7.72030000	2.70470000
11	O	-10.35620000	-0.94150000	-0.80140000
12	Si	-9.16490000	-9.40520000	0.52820000
13	Si	-9.33470000	-6.71560000	-0.96890000
14	Si	-11.54680000	-4.63200000	-1.45310000
15	Si	-9.77590000	-2.05450000	-1.77500000
16	O	-9.58580000	-8.00560000	-0.07990000
17	O	-10.67690000	-5.84320000	-0.91270000
18	O	-10.64710000	-3.36120000	-1.66840000
19	O	-8.28390000	-2.37400000	-1.34130000
20	O	-6.40440000	-3.94670000	-0.53100000
21	O	-8.15250000	-5.87130000	-0.34420000
22	O	-8.84920000	-9.23940000	2.07860000
23	O	-6.41640000	-5.42400000	1.54900000
24	O	-5.61290000	-6.41590000	-0.70840000
25	O	-5.77370000	-1.60340000	-1.35130000
26	Si	-6.81090000	-5.43360000	5.68340000
27	Si	-8.50460000	-8.00720000	6.05360000
28	O	-7.72180000	-6.63160000	6.20070000
29	Si	-10.95800000	-7.17850000	7.67890000
30	Si	-8.42890000	-3.23820000	7.03330000
31	O	-11.40780000	-5.74300000	7.18590000
32	O	-8.21960000	-1.69260000	6.70790000
33	O	-9.95660000	-3.63110000	6.85010000
34	O	-9.98360000	-7.83070000	6.60240000
35	O	-7.53000000	-4.04100000	5.99020000
36	O	-7.92320000	-3.54700000	8.50450000
37	Si	0.12369376	4.64449466	-2.14540091
38	Si	-2.82302608	3.84599900	-1.95508797
39	O	-3.94900428	0.19039944	-1.21861677
40	O	0.75579952	3.76931106	-0.98748062
41	O	-1.45550000	4.66540000	-1.97180000
42	O	-2.55354534	2.34860190	-1.49990632
43	O	-6.33220000	0.83850000	-0.42850000
44	O	-3.77030000	4.57610000	-0.90140000

1	Si	-5.28020000	4.78230000	-0.42350000
2	Si	-7.00390000	2.22870000	-0.05400000
3	Si	-9.63060000	2.52380000	-1.72000000
4	O	-6.07880000	3.41370000	-0.57020000
5	O	-8.42830000	2.36750000	-0.70540000
6	O	-10.83220000	1.58900000	-1.25000000
7	O	-5.20960000	5.26350000	1.09860000
8	O	-7.15700000	2.26930000	1.54270000
9	O	-11.46650000	0.47770000	1.01990000
10	O	-6.60040000	-5.49380000	4.09960000
11	O	-8.61720000	-8.44720000	4.51360000
12	O	-1.68270145	1.69081930	8.46850603
13	Si	-1.74889616	2.17177453	6.97417245
14	O	-0.91870869	3.49570495	6.81429304
15	Si	2.50951474	3.95253761	5.10419541
16	Si	2.56674842	1.37890371	6.82680361
17	Si	3.01121209	-3.35757174	7.49348214
18	Si	-0.01125152	-2.57093068	7.40595798
19	O	2.86462092	2.66319048	5.94589402
20	O	3.90010179	0.51780118	6.89188572
21	O	3.77240000	-1.96900000	7.63100000
22	O	1.47828685	-3.08404420	7.27482312
23	O	2.15450557	1.79121111	8.29129857
24	O	-0.24971537	-2.04673183	8.86410920
25	O	1.05380199	4.47369946	5.45680183
26	O	-1.00421587	-3.76439443	7.04722751
27	Si	0.52350207	-7.58780089	-0.03030526
28	Si	-2.45310000	-8.37930000	0.08690000
29	O	-1.02440000	-7.79970000	-0.28570000
30	O	-3.48040000	-7.82240000	-1.00870000
31	O	-2.05281360	-6.52241164	3.54853820
32	O	-4.53620000	-6.55020000	2.91500000
33	O	-2.87430000	-7.94910000	1.53380000
34	O	0.93450000	-7.98310000	1.44400000
35	O	0.37175818	-7.41285046	3.90389876
36	Si	0.95187194	-8.52592712	2.93031356
37	Si	-1.34641329	-5.31662835	7.02367792
38	Si	-4.32960000	-6.05610000	7.41270000
39	O	-2.92290000	-5.44190000	7.01850000
40	O	-5.41450000	-5.45960000	6.41750000
41	O	-4.71840000	-5.65910000	8.88780000
42	O	-1.36620000	-5.12610000	10.61890000
43	O	-0.72730000	-6.04810000	8.28660000
44	Si	-0.78110000	-6.37380000	9.84140000

1	Si	4.19170302	1.79587029	-2.03235993
2	Si	4.36128654	-0.89370553	-0.53509116
3	Si	1.79910402	-4.81756095	0.05478195
4	Si	1.68500513	-2.17150622	-1.47833308
5	Si	3.22788949	3.06050372	2.23969065
6	Si	5.44846282	-1.68945909	4.28198911
7	Si	3.72401852	-4.24269366	4.65120200
8	O	4.61250276	0.39614153	-1.42448359
9	O	1.43093971	-3.66270179	-0.97330466
10	O	3.17921389	-1.73792958	-1.16026156
11	O	4.64904343	-3.05762911	4.13514639
12	O	2.93678558	2.40516320	-1.28892218
13	O	2.15286259	3.10905165	1.07405381
14	O	2.54297696	3.62281828	3.55352205
15	O	5.51819624	-1.20782141	5.80380662
16	O	3.57088763	-4.20199965	6.24789920
17	O	-0.73782542	-5.99414376	5.72549714
18	H	-1.30770000	8.45280000	5.54490000
19	H	3.53900000	4.98890000	5.43620000
20	H	-5.91550000	5.84190000	-1.27060000
21	H	-6.78570000	6.92250000	2.19890000
22	H	-12.70540000	-0.03450000	-1.12450000
23	H	-13.56750000	1.03610000	2.31350000
24	H	-12.61360000	-4.36250000	-0.43650000
25	H	-12.17550000	-5.02190000	-2.75570000
26	H	-14.47190000	-2.17020000	6.40220000
27	H	-13.77040000	-2.92530000	4.17860000
28	H	6.86451254	-1.88258750	3.83333317
29	H	-2.15040000	-4.10050000	12.78420000
30	H	1.31010000	-8.39770000	-1.01480000
31	H	-12.21020000	-7.97290000	7.89080000
32	H	0.36340198	-1.65379209	11.27869802
33	H	0.62130000	6.05740000	-2.14750000
34	H	0.50140000	4.07440000	-3.47820000
35	H	-2.25700000	7.49990000	7.52180000
36	H	-5.73850000	6.73170000	5.78280000
37	H	-10.96700000	4.40130000	4.09400000
38	H	-11.01960000	5.00810000	1.73210000
39	H	-12.06290000	1.27880000	5.87220000
40	H	-10.59640000	-6.34750000	11.45320000
41	H	-8.66420000	-7.73420000	10.94950000
42	H	2.77449577	1.81969352	10.74640051
43	H	1.80020492	3.79899993	9.78440108
44	H	5.77540000	-0.53010000	8.17660000

1	H	3.24710000	-4.17500000	8.72650000
2	H	0.61160000	-6.65520000	10.31590000
3	H	-1.64370000	-7.57580000	10.07620000
4	H	0.12290000	-9.76940000	3.03170000
5	H	2.36090000	-8.82750000	3.33990000
6	H	-10.15040000	3.92860000	-1.73450000
7	H	-9.16390000	2.16210000	-3.09680000
8	H	3.89500000	1.63920000	-3.49250000
9	H	5.32300000	2.73990000	-1.76330000
10	H	4.42880655	3.88349369	1.88700681
11	H	5.61649876	-1.70969851	-0.58834391
12	H	4.35731364	-5.55349320	4.29820027
13	H	3.22919544	-5.21291271	-0.15130488
14	H	-5.23700000	-6.37850000	11.22840000
15	H	-7.76830000	-9.07120000	6.80850000
16	H	-6.95230000	-10.08460000	3.55430000
17	H	-10.29630000	-10.34930000	0.25900000
18	H	-2.42150000	-9.87450000	0.00040000
19	H	-3.42900000	-8.60990000	3.88980000
20	H	-4.28320000	-7.54880000	7.29620000
21	H	-3.45780000	3.89970000	-3.31080000
22	H	0.59910155	5.23699893	7.81469957
23	H	-9.79240000	-1.54060000	-3.18200000
24	H	-8.38790000	-2.95530000	10.89960000
25	H	-4.87450000	3.78240000	8.02040000
26	H	-2.02270000	2.13730000	10.92000000
27	H	-4.91220000	-7.27130000	-2.96190000
28	H	-8.98790000	-7.09310000	-2.37650000
29	H	1.45750451	-2.18458080	-2.95900091
30	H	-5.88650000	0.35320000	-2.87170000
31	H	-6.57060000	-3.25690000	-2.96870000
32	H	-11.74490000	-3.66940000	8.61800000
33	H	-9.32890000	0.16850000	8.03140000
34	H	-8.19140000	3.21540000	6.31880000
35	H	-5.78340000	-8.84910000	-1.27830000
36	H	-7.97590000	-9.98270000	-0.17660000
37	H	-2.11761104	0.35875022	-2.97421837
38				
39				
40	ZH_2CH3OCH3(ads)			
41	Si	-0.03372409	0.02239683	-0.00686834
42	Si	-0.06763823	-0.00808205	5.68449675
43	Si	3.70292655	-0.02602474	2.48720349
44	Si	1.03866156	-3.89385199	2.98758284

1	Al	0.72559235	-0.85762640	2.84470911
2	O	0.30493174	-2.48628635	3.00753989
3	O	2.39002618	-0.60575050	3.18085372
4	O	0.03909358	0.01645807	1.56542501
5	O	-0.19727083	0.08977067	4.05833627
6	O	-1.57384335	0.16760809	-0.44606512
7	O	-0.32599810	-1.46853425	6.26143102
8	O	1.37097868	0.50293446	6.18172675
9	O	-1.25810330	0.97414984	6.05964653
10	O	0.81667807	1.29324749	-0.51615416
11	O	3.76444451	1.58009397	2.49642162
12	O	4.98516829	-0.47979598	3.33660386
13	O	2.21383298	-4.06009249	4.09741870
14	O	3.86421424	-0.50687982	0.95229928
15	O	1.73854798	-4.23245542	1.56656839
16	O	0.57851693	-1.27238814	-0.73131630
17	O	-0.13105714	-4.94647892	3.32353335
18	O	0.80120500	-6.00640200	-0.15260800
19	Si	-5.49760000	-0.02110100	-1.47430100
20	Si	-2.51949700	0.76949700	-1.59089800
21	Si	1.67330000	2.63519900	-0.36439800
22	Si	-6.77250000	-2.79180000	-1.55910000
23	Si	-6.65860000	-5.43650000	-0.02630000
24	Si	-0.62808200	-6.20848200	4.15929800
25	Si	-3.21919900	-7.43500000	2.98449700
26	Si	-6.09540000	-6.32220000	2.83000000
27	Si	-7.79180000	-8.89230000	3.21140000
28	Si	-7.85690000	-4.02790000	9.99880000
29	Si	-9.54690000	-6.64300000	10.42590000
30	O	-8.68790000	-5.35140000	10.15840000
31	Si	1.78780000	2.30220100	9.72780000
32	Si	-0.76980000	-1.62740000	10.29930000
33	Si	-1.17800000	1.38380000	9.93890000
34	O	-1.38700000	-0.16320000	10.26480000
35	O	0.35020000	1.77510000	10.12160000
36	O	-1.90930000	-2.64050000	10.65650000
37	Si	-2.31670000	-4.06080000	11.29600000
38	Si	-5.02660000	-5.18350000	10.35000000
39	O	-3.83590000	-4.30830000	10.92640000
40	O	-6.34110000	-4.27000000	10.39930000
41	Si	4.73290100	-0.80099500	7.13550500
42	Si	-7.29070000	2.20560000	5.67640000
43	Si	-4.57939900	3.32750100	6.62399900
44	Si	-1.94070000	7.20800000	6.08700000

1	Si	-4.59330000	6.04430000	5.10460000
2	O	-5.77090000	2.45290000	6.04720000
3	O	-3.26560100	2.41450000	6.57330300
4	O	-0.99450000	5.94280000	5.99240000
5	O	-3.27080000	6.91960000	5.26710000
6	O	-4.35770000	4.58890000	5.69440000
7	O	-7.46660000	2.24720000	4.09540000
8	O	-4.88400000	5.95910000	3.53970000
9	Si	-5.99570000	5.67090000	2.42990000
10	Si	-10.73910000	3.90040000	2.70070000
11	O	-11.73290000	2.70740000	2.34160000
12	Si	-12.07420000	1.15480000	2.31840000
13	O	-11.45520000	0.42330000	3.58130000
14	Si	-11.39460000	-4.15760000	7.24580000
15	Si	-13.29570000	-2.46030000	5.52120000
16	Si	-11.50890000	0.09760000	5.13610000
17	Si	-8.83680000	-0.22830000	6.67330000
18	O	-12.44950000	-3.64190000	6.15630000
19	O	-12.41530000	-1.16550000	5.38290000
20	O	-10.03410000	-0.20050000	5.63860000
21	O	-7.69650000	0.78430000	6.31660000
22	Si	-0.05970000	4.78730000	6.54670000
23	O	-10.24280000	-7.11800000	9.08650000
24	Si	-7.71660000	3.11370000	2.78820000
25	O	-6.95550000	4.50240000	2.92570000
26	O	-9.24950000	3.38730000	2.56950000
27	Si	-4.97250000	-7.60980000	-1.50390000
28	Si	-11.35590000	0.26280000	-0.54610000
29	O	-6.84510000	-7.72030000	2.70470000
30	O	-10.35620000	-0.94150000	-0.80140000
31	Si	-9.16490000	-9.40520000	0.52820000
32	Si	-9.33470000	-6.71560000	-0.96890000
33	Si	-11.54680000	-4.63200000	-1.45310000
34	Si	-9.77590000	-2.05450000	-1.77500000
35	O	-9.58580000	-8.00560000	-0.07990000
36	O	-10.67690000	-5.84320000	-0.91270000
37	O	-10.64710000	-3.36120000	-1.66840000
38	O	-8.28390000	-2.37400000	-1.34130000
39	O	-6.40440000	-3.94670000	-0.53100000
40	O	-8.15250000	-5.87130000	-0.34420000
41	O	-8.84920000	-9.23940000	2.07860000
42	O	-6.41640000	-5.42400000	1.54900000
43	O	-5.61290000	-6.41590000	-0.70840000
44	O	-5.77370000	-1.60340000	-1.35130000

1	Si	-6.81090000	-5.43360000	5.68340000
2	Si	-8.50460000	-8.00720000	6.05360000
3	O	-7.72180000	-6.63160000	6.20070000
4	Si	-10.95800000	-7.17850000	7.67890000
5	Si	-8.42890000	-3.23820000	7.03330000
6	O	-11.40780000	-5.74300000	7.18590000
7	O	-8.21960000	-1.69260000	6.70790000
8	O	-9.95660000	-3.63110000	6.85010000
9	O	-9.98360000	-7.83070000	6.60240000
10	O	-7.53000000	-4.04100000	5.99020000
11	O	-7.92320000	-3.54700000	8.50450000
12	Si	0.12369900	4.64449900	-2.14540000
13	Si	-2.82300000	3.84600000	-1.95510000
14	O	-3.94890100	0.19040300	-1.21849900
15	O	0.75580300	3.76930300	-0.98750000
16	O	-1.45550000	4.66540000	-1.97180000
17	O	-2.55360100	2.34860000	-1.49990000
18	O	-6.33220000	0.83850000	-0.42850000
19	O	-3.77030000	4.57610000	-0.90140000
20	Si	-5.28020000	4.78230000	-0.42350000
21	Si	-7.00390000	2.22870000	-0.05400000
22	Si	-9.63060000	2.52380000	-1.72000000
23	O	-6.07880000	3.41370000	-0.57020000
24	O	-8.42830000	2.36750000	-0.70540000
25	O	-10.83220000	1.58900000	-1.25000000
26	O	-5.20960000	5.26350000	1.09860000
27	O	-7.15700000	2.26930000	1.54270000
28	O	-11.46650000	0.47770000	1.01990000
29	O	-6.60040000	-5.49380000	4.09960000
30	O	-8.61720000	-8.44720000	4.51360000
31	O	-1.68270000	1.69080100	8.46850000
32	Si	-1.74889900	2.17159600	6.97409500
33	O	-0.91870000	3.49570000	6.81430100
34	Si	2.50950100	3.95250000	5.10419500
35	Si	2.56679600	1.37879200	6.82680300
36	Si	3.01120700	-3.35759000	7.49349500
37	Si	-0.01129500	-2.57109400	7.40599300
38	O	2.86460100	2.66320600	5.94601000
39	O	3.90009900	0.51779800	6.89188700
40	O	3.77240000	-1.96900000	7.63100000
41	O	1.47829600	-3.08401400	7.27481200
42	O	2.15450200	1.79120200	8.29130000
43	O	-0.24970000	-2.04670000	8.86410000
44	O	1.05380000	4.47370000	5.45680000

1	O	-1.00420100	-3.76439900	7.04720000
2	Si	0.52349800	-7.58779900	-0.03029600
3	Si	-2.45310000	-8.37930000	0.08690000
4	O	-1.02440000	-7.79970000	-0.28570000
5	O	-3.48040000	-7.82240000	-1.00870000
6	O	-2.05280100	-6.52240400	3.54850500
7	O	-4.53620000	-6.55020000	2.91500000
8	O	-2.87430000	-7.94910000	1.53380000
9	O	0.93450000	-7.98310000	1.44400000
10	O	0.37158600	-7.41291200	3.90390400
11	Si	0.95190700	-8.52589400	2.93029700
12	Si	-1.34639500	-5.31659400	7.02370000
13	Si	-4.32960000	-6.05610000	7.41270000
14	O	-2.92290000	-5.44190000	7.01850000
15	O	-5.41450000	-5.45960000	6.41750000
16	O	-4.71840000	-5.65910000	8.88780000
17	O	-1.36620000	-5.12610000	10.61890000
18	O	-0.72730000	-6.04810000	8.28660000
19	Si	-0.78110000	-6.37380000	9.84140000
20	Si	4.19160200	1.79580100	-2.03249800
21	Si	4.36130400	-0.89369700	-0.53530000
22	Si	1.79909100	-4.81759800	0.05480500
23	Si	1.68500000	-2.17150100	-1.47839900
24	Si	3.22790500	3.06050600	2.23969900
25	Si	5.44850300	-1.68949400	4.28209700
26	Si	3.72400000	-4.24269400	4.65120100
27	O	4.61249900	0.39620000	-1.42440000
28	O	1.43100400	-3.66270100	-0.97330300
29	O	3.17920000	-1.73799800	-1.16010200
30	O	4.64899900	-3.05760000	4.13510000
31	O	2.93689700	2.40529900	-1.28880400
32	O	2.15279700	3.10899700	1.07410200
33	O	2.54299600	3.62289300	3.55350100
34	O	5.51819900	-1.20780700	5.80380200
35	O	3.57089100	-4.20200700	6.24789900
36	O	-0.73791200	-5.99421200	5.72550100
37	H	-1.30770000	8.45280000	5.54490000
38	H	3.53900000	4.98890000	5.43620000
39	H	-5.91550000	5.84190000	-1.27060000
40	H	-6.78570000	6.92250000	2.19890000
41	H	-12.70540000	-0.03450000	-1.12450000
42	H	-13.56750000	1.03610000	2.31350000
43	H	-12.61360000	-4.36250000	-0.43650000
44	H	-12.17550000	-5.02190000	-2.75570000

1	H	-14.47190000	-2.17020000	6.40220000
2	H	-13.77040000	-2.92530000	4.17860000
3	H	6.86450000	-1.88260100	3.83330000
4	H	-2.15040000	-4.10050000	12.78420000
5	H	1.31010000	-8.39770000	-1.01480000
6	H	-12.21020000	-7.97290000	7.89080000
7	H	0.36340000	-1.65380100	11.27870000
8	H	0.62130000	6.05740000	-2.14750000
9	H	0.50140000	4.07440000	-3.47820000
10	H	-2.25700000	7.49990000	7.52180000
11	H	-5.73850000	6.73170000	5.78280000
12	H	-10.96700000	4.40130000	4.09400000
13	H	-11.01960000	5.00810000	1.73210000
14	H	-12.06290000	1.27880000	5.87220000
15	H	-10.59640000	-6.34750000	11.45320000
16	H	-8.66420000	-7.73420000	10.94950000
17	H	2.77450000	1.81970000	10.74640000
18	H	1.80020000	3.79900000	9.78440000
19	H	5.77540000	-0.53010000	8.17660000
20	H	3.24710000	-4.17500000	8.72650000
21	H	0.61160000	-6.65520000	10.31590000
22	H	-1.64370000	-7.57580000	10.07620000
23	H	0.12290000	-9.76940000	3.03170000
24	H	2.36090000	-8.82750000	3.33990000
25	H	-10.15040000	3.92860000	-1.73450000
26	H	-9.16390000	2.16210000	-3.09680000
27	H	3.89500000	1.63920000	-3.49250000
28	H	5.32300000	2.73990000	-1.76330000
29	H	4.42880000	3.88350000	1.88700000
30	H	5.61649800	-1.70970400	-0.58829900
31	H	4.35730100	-5.55350000	4.29820000
32	H	3.22920000	-5.21290000	-0.15130000
33	H	-5.23700000	-6.37850000	11.22840000
34	H	-7.76830000	-9.07120000	6.80850000
35	H	-6.95230000	-10.08460000	3.55430000
36	H	-10.29630000	-10.34930000	0.25900000
37	H	-2.42150000	-9.87450000	0.00040000
38	H	-3.42900000	-8.60990000	3.88980000
39	H	-4.28320000	-7.54880000	7.29620000
40	H	-3.45780000	3.89970000	-3.31080000
41	H	0.59910000	5.23700000	7.81470000
42	H	-9.79240000	-1.54060000	-3.18200000
43	H	-8.38790000	-2.95530000	10.89960000
44	H	-4.87450000	3.78240000	8.02040000

1	H	-2.02270000	2.13730000	10.92000000
2	H	-4.91220000	-7.27130000	-2.96190000
3	H	-8.98790000	-7.09310000	-2.37650000
4	H	1.45749900	-2.18460000	-2.95900000
5	H	-5.88650000	0.35320000	-2.87170000
6	H	-6.57060000	-3.25690000	-2.96870000
7	H	-11.74490000	-3.66940000	8.61800000
8	H	-9.32890000	0.16850000	8.03140000
9	H	-8.19140000	3.21540000	6.31880000
10	H	-5.78340000	-8.84910000	-1.27830000
11	H	-7.97590000	-9.98270000	-0.17660000
12	H	-2.11760100	0.35870100	-2.97420000
13	C	-4.49667158	-1.40330511	5.56172667
14	H	-4.03055644	-0.63111840	6.17365896
15	H	-3.76207579	-2.19421315	5.35626953
16	H	-5.34173486	-1.83670757	6.10996994
17	O	-4.93296982	-0.77778933	4.36714594
18	C	-5.56079089	-1.68661839	3.47600396
19	H	-4.86475702	-2.46931703	3.14522384
20	H	-6.42985179	-2.16495129	3.94365859
21	H	-5.89036300	-1.11248956	2.60950384
22	C	-3.03537395	1.38579422	2.80900796
23	H	-3.39291231	0.62476915	3.49945151
24	H	-2.94419821	0.97455555	1.80092203
25	H	-3.73022185	2.22933308	2.81429322
26	O	-1.74775689	1.84217094	3.26943687
27	H	-0.86926375	0.83010154	3.67011616
28	C	-1.22691241	2.93979677	2.50833508
29	H	-1.17563379	2.68027320	1.44914876
30	H	-0.23040536	3.16125173	2.88497795
31	H	-1.87502466	3.80979663	2.64325417
32				
33				
34	ZH_2CH3OCH3-to-Z-(CH3)3O+_H2O(ads)-TS			
35	Si	-0.03907800	0.00965300	0.00674000
36	Si	-0.05781100	-0.00685900	5.66371200
37	Si	3.70391600	-0.03529000	2.48372100
38	Si	1.03490600	-3.88218500	2.98596000
39	Al	0.70105400	-0.83666800	2.89826700
40	O	0.27237800	-2.49118100	2.97121300
41	O	2.40157500	-0.68260400	3.11719000
42	O	-0.04439700	-0.04723900	1.57444700
43	O	-0.12444200	0.10768300	4.08750400
44	O	-1.58213300	0.15650600	-0.45032000

1	O	-0.35258000	-1.46637400	6.27814600
2	O	1.36293700	0.48442000	6.25280500
3	O	-1.27519000	0.95872900	6.07220200
4	O	0.81107100	1.29139400	-0.47534600
5	O	3.73776600	1.57217500	2.50987800
6	O	4.98842800	-0.47513200	3.34026600
7	O	2.20982200	-4.05595100	4.09647600
8	O	3.89458700	-0.48433500	0.94422100
9	O	1.73465100	-4.24871900	1.57000800
10	O	0.57087700	-1.26617700	-0.75286600
11	O	-0.14120900	-4.93926400	3.32810000
12	O	0.80120000	-6.00640000	-0.15260000
13	Si	-5.49760000	-0.02110000	-1.47430000
14	Si	-2.51950000	0.76950000	-1.59090000
15	Si	1.67330000	2.63520000	-0.36440000
16	Si	-6.77250000	-2.79180000	-1.55910000
17	Si	-6.65860000	-5.43650000	-0.02630000
18	Si	-0.62810000	-6.20850000	4.15930000
19	Si	-3.21920000	-7.43500000	2.98450000
20	Si	-6.09540000	-6.32220000	2.83000000
21	Si	-7.79180000	-8.89230000	3.21140000
22	Si	-7.85690000	-4.02790000	9.99880000
23	Si	-9.54690000	-6.64300000	10.42590000
24	O	-8.68790000	-5.35140000	10.15840000
25	Si	1.78780000	2.30220000	9.72780000
26	Si	-0.76980000	-1.62740000	10.29930000
27	Si	-1.17800000	1.38380000	9.93890000
28	O	-1.38700000	-0.16320000	10.26480000
29	O	0.35020000	1.77510000	10.12160000
30	O	-1.90930000	-2.64050000	10.65650000
31	Si	-2.31670000	-4.06080000	11.29600000
32	Si	-5.02660000	-5.18350000	10.35000000
33	O	-3.83590000	-4.30830000	10.92640000
34	O	-6.34110000	-4.27000000	10.39930000
35	Si	4.73290000	-0.80100000	7.13550000
36	Si	-7.29070000	2.20560000	5.67640000
37	Si	-4.57940000	3.32750000	6.62400000
38	Si	-1.94070000	7.20800000	6.08700000
39	Si	-4.59330000	6.04430000	5.10460000
40	O	-5.77090000	2.45290000	6.04720000
41	O	-3.26560000	2.41450000	6.57330000
42	O	-0.99450000	5.94280000	5.99240000
43	O	-3.27080000	6.91960000	5.26710000
44	O	-4.35770000	4.58890000	5.69440000

1	O	-7.46660000	2.24720000	4.09540000
2	O	-4.88400000	5.95910000	3.53970000
3	Si	-5.99570000	5.67090000	2.42990000
4	Si	-10.73910000	3.90040000	2.70070000
5	O	-11.73290000	2.70740000	2.34160000
6	Si	-12.07420000	1.15480000	2.31840000
7	O	-11.45520000	0.42330000	3.58130000
8	Si	-11.39460000	-4.15760000	7.24580000
9	Si	-13.29570000	-2.46030000	5.52120000
10	Si	-11.50890000	0.09760000	5.13610000
11	Si	-8.83680000	-0.22830000	6.67330000
12	O	-12.44950000	-3.64190000	6.15630000
13	O	-12.41530000	-1.16550000	5.38290000
14	O	-10.03410000	-0.20050000	5.63860000
15	O	-7.69650000	0.78430000	6.31660000
16	Si	-0.05970000	4.78730000	6.54670000
17	O	-10.24280000	-7.11800000	9.08650000
18	Si	-7.71660000	3.11370000	2.78820000
19	O	-6.95550000	4.50240000	2.92570000
20	O	-9.24950000	3.38730000	2.56950000
21	Si	-4.97250000	-7.60980000	-1.50390000
22	Si	-11.35590000	0.26280000	-0.54610000
23	O	-6.84510000	-7.72030000	2.70470000
24	O	-10.35620000	-0.94150000	-0.80140000
25	Si	-9.16490000	-9.40520000	0.52820000
26	Si	-9.33470000	-6.71560000	-0.96890000
27	Si	-11.54680000	-4.63200000	-1.45310000
28	Si	-9.77590000	-2.05450000	-1.77500000
29	O	-9.58580000	-8.00560000	-0.07990000
30	O	-10.67690000	-5.84320000	-0.91270000
31	O	-10.64710000	-3.36120000	-1.66840000
32	O	-8.28390000	-2.37400000	-1.34130000
33	O	-6.40440000	-3.94670000	-0.53100000
34	O	-8.15250000	-5.87130000	-0.34420000
35	O	-8.84920000	-9.23940000	2.07860000
36	O	-6.41640000	-5.42400000	1.54900000
37	O	-5.61290000	-6.41590000	-0.70840000
38	O	-5.77370000	-1.60340000	-1.35130000
39	Si	-6.81090000	-5.43360000	5.68340000
40	Si	-8.50460000	-8.00720000	6.05360000
41	O	-7.72180000	-6.63160000	6.20070000
42	Si	-10.95800000	-7.17850000	7.67890000
43	Si	-8.42890000	-3.23820000	7.03330000
44	O	-11.40780000	-5.74300000	7.18590000

1	O	-8.21960000	-1.69260000	6.70790000
2	O	-9.95660000	-3.63110000	6.85010000
3	O	-9.98360000	-7.83070000	6.60240000
4	O	-7.53000000	-4.04100000	5.99020000
5	O	-7.92320000	-3.54700000	8.50450000
6	Si	0.12370000	4.64450000	-2.14540000
7	Si	-2.82300000	3.84600000	-1.95510000
8	O	-3.94890000	0.19040000	-1.21850000
9	O	0.75580000	3.76930000	-0.98750000
10	O	-1.45550000	4.66540000	-1.97180000
11	O	-2.55360000	2.34860000	-1.49990000
12	O	-6.33220000	0.83850000	-0.42850000
13	O	-3.77030000	4.57610000	-0.90140000
14	Si	-5.28020000	4.78230000	-0.42350000
15	Si	-7.00390000	2.22870000	-0.05400000
16	Si	-9.63060000	2.52380000	-1.72000000
17	O	-6.07880000	3.41370000	-0.57020000
18	O	-8.42830000	2.36750000	-0.70540000
19	O	-10.83220000	1.58900000	-1.25000000
20	O	-5.20960000	5.26350000	1.09860000
21	O	-7.15700000	2.26930000	1.54270000
22	O	-11.46650000	0.47770000	1.01990000
23	O	-6.60040000	-5.49380000	4.09960000
24	O	-8.61720000	-8.44720000	4.51360000
25	O	-1.68270000	1.69080000	8.46850000
26	Si	-1.74890000	2.17160000	6.97410000
27	O	-0.91870000	3.49570000	6.81430000
28	Si	2.50950000	3.95250000	5.10420000
29	Si	2.56680000	1.37880000	6.82680000
30	Si	3.01120000	-3.35760000	7.49350000
31	Si	-0.01130000	-2.57110000	7.40600000
32	O	2.86460000	2.66320000	5.94600000
33	O	3.90010000	0.51780000	6.89190000
34	O	3.77240000	-1.96900000	7.63100000
35	O	1.47830000	-3.08400000	7.27480000
36	O	2.15450000	1.79120000	8.29130000
37	O	-0.24970000	-2.04670000	8.86410000
38	O	1.05380000	4.47370000	5.45680000
39	O	-1.00420000	-3.76440000	7.04720000
40	Si	0.52350000	-7.58780000	-0.03030000
41	Si	-2.45310000	-8.37930000	0.08690000
42	O	-1.02440000	-7.79970000	-0.28570000
43	O	-3.48040000	-7.82240000	-1.00870000
44	O	-2.05280000	-6.52240000	3.54850000

1	O	-4.53620000	-6.55020000	2.91500000
2	O	-2.87430000	-7.94910000	1.53380000
3	O	0.93450000	-7.98310000	1.44400000
4	O	0.37160000	-7.41290000	3.90390000
5	Si	0.95190000	-8.52590000	2.93030000
6	Si	-1.34640000	-5.31660000	7.02370000
7	Si	-4.32960000	-6.05610000	7.41270000
8	O	-2.92290000	-5.44190000	7.01850000
9	O	-5.41450000	-5.45960000	6.41750000
10	O	-4.71840000	-5.65910000	8.88780000
11	O	-1.36620000	-5.12610000	10.61890000
12	O	-0.72730000	-6.04810000	8.28660000
13	Si	-0.78110000	-6.37380000	9.84140000
14	Si	4.19160000	1.79580000	-2.03250000
15	Si	4.36130000	-0.89370000	-0.53530000
16	Si	1.79910000	-4.81760000	0.05480000
17	Si	1.68500000	-2.17150000	-1.47840000
18	Si	3.22790000	3.06050000	2.23970000
19	Si	5.44850000	-1.68950000	4.28210000
20	Si	3.72400000	-4.24270000	4.65120000
21	O	4.61250000	0.39620000	-1.42440000
22	O	1.43100000	-3.66270000	-0.97330000
23	O	3.17920000	-1.73800000	-1.16010000
24	O	4.64900000	-3.05760000	4.13510000
25	O	2.93690000	2.40530000	-1.28880000
26	O	2.15280000	3.10900000	1.07410000
27	O	2.54300000	3.62290000	3.55350000
28	O	5.51820000	-1.20780000	5.80380000
29	O	3.57090000	-4.20200000	6.24790000
30	O	-0.73790000	-5.99420000	5.72550000
31	H	-1.30770000	8.45280000	5.54490000
32	H	3.53900000	4.98890000	5.43620000
33	H	-5.91550000	5.84190000	-1.27060000
34	H	-6.78570000	6.92250000	2.19890000
35	H	-12.70540000	-0.03450000	-1.12450000
36	H	-13.56750000	1.03610000	2.31350000
37	H	-12.61360000	-4.36250000	-0.43650000
38	H	-12.17550000	-5.02190000	-2.75570000
39	H	-14.47190000	-2.17020000	6.40220000
40	H	-13.77040000	-2.92530000	4.17860000
41	H	6.86450000	-1.88260000	3.83330000
42	H	-2.15040000	-4.10050000	12.78420000
43	H	1.31010000	-8.39770000	-1.01480000
44	H	-12.21020000	-7.97290000	7.89080000

1	H	0.36340000	-1.65380000	11.27870000
2	H	0.62130000	6.05740000	-2.14750000
3	H	0.50140000	4.07440000	-3.47820000
4	H	-2.25700000	7.49990000	7.52180000
5	H	-5.73850000	6.73170000	5.78280000
6	H	-10.96700000	4.40130000	4.09400000
7	H	-11.01960000	5.00810000	1.73210000
8	H	-12.06290000	1.27880000	5.87220000
9	H	-10.59640000	-6.34750000	11.45320000
10	H	-8.66420000	-7.73420000	10.94950000
11	H	2.77450000	1.81970000	10.74640000
12	H	1.80020000	3.79900000	9.78440000
13	H	5.77540000	-0.53010000	8.17660000
14	H	3.24710000	-4.17500000	8.72650000
15	H	0.61160000	-6.65520000	10.31590000
16	H	-1.64370000	-7.57580000	10.07620000
17	H	0.12290000	-9.76940000	3.03170000
18	H	2.36090000	-8.82750000	3.33990000
19	H	-10.15040000	3.92860000	-1.73450000
20	H	-9.16390000	2.16210000	-3.09680000
21	H	3.89500000	1.63920000	-3.49250000
22	H	5.32300000	2.73990000	-1.76330000
23	H	4.42880000	3.88350000	1.88700000
24	H	5.61650000	-1.70970000	-0.58830000
25	H	4.35730000	-5.55350000	4.29820000
26	H	3.22920000	-5.21290000	-0.15130000
27	H	-5.23700000	-6.37850000	11.22840000
28	H	-7.76830000	-9.07120000	6.80850000
29	H	-6.95230000	-10.08460000	3.55430000
30	H	-10.29630000	-10.34930000	0.25900000
31	H	-2.42150000	-9.87450000	0.00040000
32	H	-3.42900000	-8.60990000	3.88980000
33	H	-4.28320000	-7.54880000	7.29620000
34	H	-3.45780000	3.89970000	-3.31080000
35	H	0.59910000	5.23700000	7.81470000
36	H	-9.79240000	-1.54060000	-3.18200000
37	H	-8.38790000	-2.95530000	10.89960000
38	H	-4.87450000	3.78240000	8.02040000
39	H	-2.02270000	2.13730000	10.92000000
40	H	-4.91220000	-7.27130000	-2.96190000
41	H	-8.98790000	-7.09310000	-2.37650000
42	H	1.45750000	-2.18460000	-2.95900000
43	H	-5.88650000	0.35320000	-2.87170000
44	H	-6.57060000	-3.25690000	-2.96870000

1	H	-11.74490000	-3.66940000	8.61800000
2	H	-9.32890000	0.16850000	8.03140000
3	H	-8.19140000	3.21540000	6.31880000
4	H	-5.78340000	-8.84910000	-1.27830000
5	H	-7.97590000	-9.98270000	-0.17660000
6	H	-2.11760000	0.35870000	-2.97420000
7	C	-3.18749600	-2.49304600	3.68326900
8	H	-2.84546300	-2.20415900	4.67494900
9	H	-2.32711700	-2.62852900	3.02314800
10	H	-3.77218700	-3.41171400	3.74878900
11	O	-4.05187800	-1.43361600	3.20589300
12	C	-4.68105700	-1.74268600	1.94834300
13	H	-3.93684100	-1.83247100	1.15239500
14	H	-5.23904500	-2.67503700	2.04710000
15	H	-5.36998500	-0.92810500	1.73209200
16	C	-3.09845900	0.24776400	3.17846100
17	H	-2.90992000	0.15503100	4.23264600
18	H	-2.39432800	-0.12135300	2.45072600
19	H	-3.96866100	0.79910600	2.86081600
20	O	-1.97615500	1.90287800	3.31307000
21	H	-1.13896400	1.40665400	3.48290100
22	C	-1.83998400	2.79041700	2.19373800
23	H	-1.78474900	2.24107100	1.25324100
24	H	-0.93850700	3.39438600	2.31652300
25	H	-2.70857600	3.44864800	2.18981900
26				
27				
28	ZH_2CH3OH(ads)-to-Z-CH3_H2O(ads)_CH3OH(ads)-TS			
29	Si	-0.03118606	0.01817021	-0.02546586
30	Si	-0.06529868	-0.00689275	5.65021973
31	Si	3.70407876	-0.05436886	2.48945924
32	Si	1.05080826	-3.90144361	2.98158419
33	Al	0.74177541	-0.81700270	2.89462033
34	O	0.21692480	-2.50922251	2.91571583
35	O	2.43614639	-0.78023928	3.13909625
36	O	0.05804174	-0.07983598	1.53478387
37	O	-0.20918813	-0.03209505	4.07761120
38	O	-1.57986905	0.15566739	-0.44477179
39	O	-0.34763391	-1.45779420	6.29496337
40	O	1.37757497	0.49167684	6.19344890
41	O	-1.24166987	0.99983515	6.04499232
42	O	0.82292329	1.28651086	-0.51817739
43	O	3.67676254	1.54913777	2.52751473
44	O	5.00129993	-0.47033492	3.33769008

1	O	2.20086516	-4.00963898	4.10551161
2	O	3.89119623	-0.49513057	0.94857124
3	O	1.74714884	-4.24051885	1.57259350
4	O	0.54908101	-1.27555207	-0.78544672
5	O	-0.13756712	-4.93539463	3.32227834
6	O	0.80133390	-6.00647702	-0.15280270
7	Si	-5.49760292	-0.02108787	-1.47429234
8	Si	-2.51910450	0.76907727	-1.59036424
9	Si	1.67287314	2.63506358	-0.36445842
10	Si	-6.77250000	-2.79180000	-1.55910000
11	Si	-6.65860000	-5.43650000	-0.02630000
12	Si	-0.62798628	-6.20818709	4.15920517
13	Si	-3.21923424	-7.43500819	2.98458408
14	Si	-6.09540000	-6.32220000	2.83000000
15	Si	-7.79180000	-8.89230000	3.21140000
16	Si	-7.85690000	-4.02790000	9.99880000
17	Si	-9.54690000	-6.64300000	10.42590000
18	O	-8.68790000	-5.35140000	10.15840000
19	Si	1.78781638	2.30218565	9.72780896
20	Si	-0.76980786	-1.62740488	10.29929953
21	Si	-1.17801048	1.38382775	9.93890939
22	O	-1.38698994	-0.16319573	10.26480124
23	O	0.35018938	1.77512169	10.12159024
24	O	-1.90930614	-2.64049432	10.65649654
25	Si	-2.31670000	-4.06080000	11.29600000
26	Si	-5.02660000	-5.18350000	10.35000000
27	O	-3.83590000	-4.30830000	10.92640000
28	O	-6.34110000	-4.27000000	10.39930000
29	Si	4.73289732	-0.80096571	7.13547088
30	Si	-7.29070000	2.20560000	5.67640000
31	Si	-4.57940666	3.32748937	6.62401878
32	Si	-1.94070000	7.20800000	6.08700000
33	Si	-4.59330000	6.04430000	5.10460000
34	O	-5.77090000	2.45290000	6.04720000
35	O	-3.26560066	2.41456986	6.57334484
36	O	-0.99449904	5.94279866	5.99239558
37	O	-3.27080000	6.91960000	5.26710000
38	O	-4.35770000	4.58890000	5.69440000
39	O	-7.46660000	2.24720000	4.09540000
40	O	-4.88400000	5.95910000	3.53970000
41	Si	-5.99570000	5.67090000	2.42990000
42	Si	-10.73910000	3.90040000	2.70070000
43	O	-11.73290000	2.70740000	2.34160000
44	Si	-12.07420000	1.15480000	2.31840000

1	O	-11.45520000	0.42330000	3.58130000
2	Si	-11.39460000	-4.15760000	7.24580000
3	Si	-13.29570000	-2.46030000	5.52120000
4	Si	-11.50890000	0.09760000	5.13610000
5	Si	-8.83680000	-0.22830000	6.67330000
6	O	-12.44950000	-3.64190000	6.15630000
7	O	-12.41530000	-1.16550000	5.38290000
8	O	-10.03410000	-0.20050000	5.63860000
9	O	-7.69650000	0.78430000	6.31660000
10	Si	-0.05969924	4.78730349	6.54672435
11	O	-10.24280000	-7.11800000	9.08650000
12	Si	-7.71660000	3.11370000	2.78820000
13	O	-6.95550000	4.50240000	2.92570000
14	O	-9.24950000	3.38730000	2.56950000
15	Si	-4.97250000	-7.60980000	-1.50390000
16	Si	-11.35590000	0.26280000	-0.54610000
17	O	-6.84510000	-7.72030000	2.70470000
18	O	-10.35620000	-0.94150000	-0.80140000
19	Si	-9.16490000	-9.40520000	0.52820000
20	Si	-9.33470000	-6.71560000	-0.96890000
21	Si	-11.54680000	-4.63200000	-1.45310000
22	Si	-9.77590000	-2.05450000	-1.77500000
23	O	-9.58580000	-8.00560000	-0.07990000
24	O	-10.67690000	-5.84320000	-0.91270000
25	O	-10.64710000	-3.36120000	-1.66840000
26	O	-8.28390000	-2.37400000	-1.34130000
27	O	-6.40440000	-3.94670000	-0.53100000
28	O	-8.15250000	-5.87130000	-0.34420000
29	O	-8.84920000	-9.23940000	2.07860000
30	O	-6.41640000	-5.42400000	1.54900000
31	O	-5.61290000	-6.41590000	-0.70840000
32	O	-5.77370000	-1.60340000	-1.35130000
33	Si	-6.81090000	-5.43360000	5.68340000
34	Si	-8.50460000	-8.00720000	6.05360000
35	O	-7.72180000	-6.63160000	6.20070000
36	Si	-10.95800000	-7.17850000	7.67890000
37	Si	-8.42890000	-3.23820000	7.03330000
38	O	-11.40780000	-5.74300000	7.18590000
39	O	-8.21960000	-1.69260000	6.70790000
40	O	-9.95660000	-3.63110000	6.85010000
41	O	-9.98360000	-7.83070000	6.60240000
42	O	-7.53000000	-4.04100000	5.99020000
43	O	-7.92320000	-3.54700000	8.50450000
44	Si	0.12366306	4.64446783	-2.14540415

1	Si	-2.82299575	3.84600020	-1.95510186
2	O	-3.94896247	0.19047143	-1.21862876
3	O	0.75594640	3.76940972	-0.98751587
4	O	-1.45550000	4.66540000	-1.97180000
5	O	-2.55362117	2.34860654	-1.50002162
6	O	-6.33220000	0.83850000	-0.42850000
7	O	-3.77030000	4.57610000	-0.90140000
8	Si	-5.28020000	4.78230000	-0.42350000
9	Si	-7.00390000	2.22870000	-0.05400000
10	Si	-9.63060000	2.52380000	-1.72000000
11	O	-6.07880000	3.41370000	-0.57020000
12	O	-8.42830000	2.36750000	-0.70540000
13	O	-10.83220000	1.58900000	-1.25000000
14	O	-5.20960000	5.26350000	1.09860000
15	O	-7.15700000	2.26930000	1.54270000
16	O	-11.46650000	0.47770000	1.01990000
17	O	-6.60040000	-5.49380000	4.09960000
18	O	-8.61720000	-8.44720000	4.51360000
19	O	-1.68267730	1.69080725	8.46850133
20	Si	-1.74883044	2.17137104	6.97378772
21	O	-0.91871019	3.49571749	6.81439200
22	Si	2.50951458	3.95256580	5.10425651
23	Si	2.56655592	1.37886717	6.82672643
24	Si	3.01133211	-3.35747762	7.49346638
25	Si	-0.01128590	-2.57102871	7.40589510
26	O	2.86464258	2.66311143	5.94588526
27	O	3.90010935	0.51781858	6.89195423
28	O	3.77240000	-1.96900000	7.63100000
29	O	1.47826999	-3.08412200	7.27493628
30	O	2.15456386	1.79119227	8.29132015
31	O	-0.24968324	-2.04669790	8.86410199
32	O	1.05379033	4.47370442	5.45678885
33	O	-1.00410122	-3.76441639	7.04698120
34	Si	0.52346541	-7.58778687	-0.03020881
35	Si	-2.45310000	-8.37930000	0.08690000
36	O	-1.02440000	-7.79970000	-0.28570000
37	O	-3.48040000	-7.82240000	-1.00870000
38	O	-2.05273395	-6.52245223	3.54837277
39	O	-4.53620000	-6.55020000	2.91500000
40	O	-2.87430000	-7.94910000	1.53380000
41	O	0.93450000	-7.98310000	1.44400000
42	O	0.37156122	-7.41294088	3.90394098
43	Si	0.95190506	-8.52589530	2.93029764
44	Si	-1.34643518	-5.31655187	7.02384557

1	Si	-4.32960000	-6.05610000	7.41270000
2	O	-2.92290000	-5.44190000	7.01850000
3	O	-5.41450000	-5.45960000	6.41750000
4	O	-4.71840000	-5.65910000	8.88780000
5	O	-1.36620000	-5.12610000	10.61890000
6	O	-0.72730000	-6.04810000	8.28660000
7	Si	-0.78110000	-6.37380000	9.84140000
8	Si	4.19161287	1.79581262	-2.03247757
9	Si	4.36134852	-0.89364534	-0.53540007
10	Si	1.79907032	-4.81750694	0.05494751
11	Si	1.68503367	-2.17067677	-1.47853481
12	Si	3.22795947	3.06040544	2.23972033
13	Si	5.44855074	-1.68947638	4.28209485
14	Si	3.72401757	-4.24258365	4.65111298
15	O	4.61236202	0.39619661	-1.42444390
16	O	1.43075546	-3.66260515	-0.97313233
17	O	3.17929717	-1.73848743	-1.15980907
18	O	4.64904662	-3.05762798	4.13513432
19	O	2.93692860	2.40526689	-1.28875267
20	O	2.15293308	3.10900586	1.07406303
21	O	2.54295885	3.62285186	3.55349916
22	O	5.51815194	-1.20787604	5.80382627
23	O	3.57067150	-4.20213682	6.24788158
24	O	-0.73796757	-5.99433584	5.72551385
25	H	-1.30770000	8.45280000	5.54490000
26	H	3.53900000	4.98890000	5.43620000
27	H	-5.91550000	5.84190000	-1.27060000
28	H	-6.78570000	6.92250000	2.19890000
29	H	-12.70540000	-0.03450000	-1.12450000
30	H	-13.56750000	1.03610000	2.31350000
31	H	-12.61360000	-4.36250000	-0.43650000
32	H	-12.17550000	-5.02190000	-2.75570000
33	H	-14.47190000	-2.17020000	6.40220000
34	H	-13.77040000	-2.92530000	4.17860000
35	H	6.86449486	-1.88259679	3.83328240
36	H	-2.15040000	-4.10050000	12.78420000
37	H	1.31010000	-8.39770000	-1.01480000
38	H	-12.21020000	-7.97290000	7.89080000
39	H	0.36339825	-1.65380704	11.27870184
40	H	0.62130000	6.05740000	-2.14750000
41	H	0.50140000	4.07440000	-3.47820000
42	H	-2.25700000	7.49990000	7.52180000
43	H	-5.73850000	6.73170000	5.78280000
44	H	-10.96700000	4.40130000	4.09400000

1	H	-11.01960000	5.00810000	1.73210000
2	H	-12.06290000	1.27880000	5.87220000
3	H	-10.59640000	-6.34750000	11.45320000
4	H	-8.66420000	-7.73420000	10.94950000
5	H	2.77448985	1.81968414	10.74640232
6	H	1.80021035	3.79899981	9.78440284
7	H	5.77540000	-0.53010000	8.17660000
8	H	3.24710000	-4.17500000	8.72650000
9	H	0.61160000	-6.65520000	10.31590000
10	H	-1.64370000	-7.57580000	10.07620000
11	H	0.12290000	-9.76940000	3.03170000
12	H	2.36090000	-8.82750000	3.33990000
13	H	-10.15040000	3.92860000	-1.73450000
14	H	-9.16390000	2.16210000	-3.09680000
15	H	3.89500000	1.63920000	-3.49250000
16	H	5.32300000	2.73990000	-1.76330000
17	H	4.42878723	3.88352255	1.88700915
18	H	5.61653049	-1.70965200	-0.58831700
19	H	4.35729836	-5.55350609	4.29821966
20	H	3.22919121	-5.21293694	-0.15129013
21	H	-5.23700000	-6.37850000	11.22840000
22	H	-7.76830000	-9.07120000	6.80850000
23	H	-6.95230000	-10.08460000	3.55430000
24	H	-10.29630000	-10.34930000	0.25900000
25	H	-2.42150000	-9.87450000	0.00040000
26	H	-3.42900000	-8.60990000	3.88980000
27	H	-4.28320000	-7.54880000	7.29620000
28	H	-3.45780000	3.89970000	-3.31080000
29	H	0.59911016	5.23699298	7.81469721
30	H	-9.79240000	-1.54060000	-3.18200000
31	H	-8.38790000	-2.95530000	10.89960000
32	H	-4.87450000	3.78240000	8.02040000
33	H	-2.02270000	2.13730000	10.92000000
34	H	-4.91220000	-7.27130000	-2.96190000
35	H	-8.98790000	-7.09310000	-2.37650000
36	H	1.45748340	-2.18476270	-2.95899596
37	H	-5.88650000	0.35320000	-2.87170000
38	H	-6.57060000	-3.25690000	-2.96870000
39	H	-11.74490000	-3.66940000	8.61800000
40	H	-9.32890000	0.16850000	8.03140000
41	H	-8.19140000	3.21540000	6.31880000
42	H	-5.78340000	-8.84910000	-1.27830000
43	H	-7.97590000	-9.98270000	-0.17660000
44	H	-2.11767019	0.35882324	-2.97425698

H -2.01679414 0.41441952 3.52699483
C -3.34864021 1.65575686 2.74264637
H -3.25424294 2.43230283 3.50730054
H -4.39776324 1.57619349 2.45562074
H -2.75941508 1.93623150 1.86444727
O -2.95128891 0.38426627 3.25197843
H -3.67783180 -1.15914554 3.06346145
C -1.72975891 -2.46807773 2.87276037
H -1.75812747 -2.26710452 3.92775938
H -1.68274120 -1.66074084 2.16624536
H -1.84969397 -3.48318817 2.53760287
O -3.75601877 -2.13770034 2.92264847
H -4.16960802 -2.25715349 2.05876387

ZH_2CH3OH(ads)-to-ZH_CH3OCH3(ads)_H2O(ads)-TS
Si -0.01560455 0.02287958 -0.02970608
Si -0.06489900 -0.00309670 5.64435316
Si 3.70394871 -0.04493620 2.48959940
Si 1.03986966 -3.88376885 2.98308890
Al 0.73095224 -0.84454525 2.88886545
O 0.25054932 -2.50262383 2.90349646
O 2.42507642 -0.72101251 3.15651896
O 0.07812211 -0.02942406 1.53549117
O -0.19389875 0.01274596 4.06624249
O -1.59022042 0.20283929 -0.39264595
O -0.35150483 -1.45684159 6.29018197
O 1.36931992 0.49513403 6.20547531
O -1.25745341 0.98786708 6.04663822
O 0.82467380 1.28658912 -0.55088127
O 3.71472267 1.56087443 2.50920471
O 5.00209473 -0.47534088 3.33130610
O 2.19957798 -4.04616312 4.10510202
O 3.87877194 -0.50106259 0.94789254
O 1.74100334 -4.28165875 1.58285946
O 0.53131404 -1.27700055 -0.79583251
O -0.17870900 -4.90147754 3.35010423
O 0.80119850 -6.00639879 -0.15259970
Si -5.49759937 -0.02110261 -1.47430164
Si -2.51949310 0.76949471 -1.59088156
Si 1.67329219 2.63519594 -0.36439086
Si -6.77250000 -2.79180000 -1.55910000
Si -6.65860000 -5.43650000 -0.02630000
Si -0.62808999 -6.20848008 4.15928616

1	Si	-3.21919644	-7.43499915	2.98449126
2	Si	-6.09540000	-6.32220000	2.83000000
3	Si	-7.79180000	-8.89230000	3.21140000
4	Si	-7.85690000	-4.02790000	9.99880000
5	Si	-9.54690000	-6.64300000	10.42590000
6	O	-8.68790000	-5.35140000	10.15840000
7	Si	1.78780000	2.30220000	9.72780000
8	Si	-0.76979783	-1.62740640	10.29930266
9	Si	-1.17800006	1.38380017	9.93890006
10	O	-1.38700000	-0.16320000	10.26480000
11	O	0.35020000	1.77510000	10.12160000
12	O	-1.90930000	-2.64050000	10.65650000
13	Si	-2.31670000	-4.06080000	11.29600000
14	Si	-5.02660000	-5.18350000	10.35000000
15	O	-3.83590000	-4.30830000	10.92640000
16	O	-6.34110000	-4.27000000	10.39930000
17	Si	4.73289875	-0.80100242	7.13548942
18	Si	-7.29070000	2.20560000	5.67640000
19	Si	-4.57940091	3.32749855	6.62400256
20	Si	-1.94070000	7.20800000	6.08700000
21	Si	-4.59330000	6.04430000	5.10460000
22	O	-5.77090000	2.45290000	6.04720000
23	O	-3.26559930	2.41450227	6.57329872
24	O	-0.99450000	5.94280000	5.99240000
25	O	-3.27080000	6.91960000	5.26710000
26	O	-4.35770000	4.58890000	5.69440000
27	O	-7.46660000	2.24720000	4.09540000
28	O	-4.88400000	5.95910000	3.53970000
29	Si	-5.99570000	5.67090000	2.42990000
30	Si	-10.73910000	3.90040000	2.70070000
31	O	-11.73290000	2.70740000	2.34160000
32	Si	-12.07420000	1.15480000	2.31840000
33	O	-11.45520000	0.42330000	3.58130000
34	Si	-11.39460000	-4.15760000	7.24580000
35	Si	-13.29570000	-2.46030000	5.52120000
36	Si	-11.50890000	0.09760000	5.13610000
37	Si	-8.83680000	-0.22830000	6.67330000
38	O	-12.44950000	-3.64190000	6.15630000
39	O	-12.41530000	-1.16550000	5.38290000
40	O	-10.03410000	-0.20050000	5.63860000
41	O	-7.69650000	0.78430000	6.31660000
42	Si	-0.05970000	4.78730000	6.54670000
43	O	-10.24280000	-7.11800000	9.08650000
44	Si	-7.71660000	3.11370000	2.78820000

1	O	-6.95550000	4.50240000	2.92570000
2	O	-9.24950000	3.38730000	2.56950000
3	Si	-4.97250000	-7.60980000	-1.50390000
4	Si	-11.35590000	0.26280000	-0.54610000
5	O	-6.84510000	-7.72030000	2.70470000
6	O	-10.35620000	-0.94150000	-0.80140000
7	Si	-9.16490000	-9.40520000	0.52820000
8	Si	-9.33470000	-6.71560000	-0.96890000
9	Si	-11.54680000	-4.63200000	-1.45310000
10	Si	-9.77590000	-2.05450000	-1.77500000
11	O	-9.58580000	-8.00560000	-0.07990000
12	O	-10.67690000	-5.84320000	-0.91270000
13	O	-10.64710000	-3.36120000	-1.66840000
14	O	-8.28390000	-2.37400000	-1.34130000
15	O	-6.40440000	-3.94670000	-0.53100000
16	O	-8.15250000	-5.87130000	-0.34420000
17	O	-8.84920000	-9.23940000	2.07860000
18	O	-6.41640000	-5.42400000	1.54900000
19	O	-5.61290000	-6.41590000	-0.70840000
20	O	-5.77370000	-1.60340000	-1.35130000
21	Si	-6.81090000	-5.43360000	5.68340000
22	Si	-8.50460000	-8.00720000	6.05360000
23	O	-7.72180000	-6.63160000	6.20070000
24	Si	-10.95800000	-7.17850000	7.67890000
25	Si	-8.42890000	-3.23820000	7.03330000
26	O	-11.40780000	-5.74300000	7.18590000
27	O	-8.21960000	-1.69260000	6.70790000
28	O	-9.95660000	-3.63110000	6.85010000
29	O	-9.98360000	-7.83070000	6.60240000
30	O	-7.53000000	-4.04100000	5.99020000
31	O	-7.92320000	-3.54700000	8.50450000
32	Si	0.12369552	4.64449610	-2.14540050
33	Si	-2.82299252	3.84600035	-1.95510327
34	O	-3.94890204	0.19040402	-1.21850159
35	O	0.75581047	3.76930798	-0.98750089
36	O	-1.45550000	4.66540000	-1.97180000
37	O	-2.55361319	2.34859964	-1.49989862
38	O	-6.33220000	0.83850000	-0.42850000
39	O	-3.77030000	4.57610000	-0.90140000
40	Si	-5.28020000	4.78230000	-0.42350000
41	Si	-7.00390000	2.22870000	-0.05400000
42	Si	-9.63060000	2.52380000	-1.72000000
43	O	-6.07880000	3.41370000	-0.57020000
44	O	-8.42830000	2.36750000	-0.70540000

1	O	-10.83220000	1.58900000	-1.25000000
2	O	-5.20960000	5.26350000	1.09860000
3	O	-7.15700000	2.26930000	1.54270000
4	O	-11.46650000	0.47770000	1.01990000
5	O	-6.60040000	-5.49380000	4.09960000
6	O	-8.61720000	-8.44720000	4.51360000
7	O	-1.68270034	1.69080076	8.46850026
8	Si	-1.74889403	2.17159685	6.97408955
9	O	-0.91870177	3.49570153	6.81430345
10	Si	2.50949967	3.95249458	5.10419095
11	Si	2.56679322	1.37877775	6.82676379
12	Si	3.01120529	-3.35758628	7.49349093
13	Si	-0.01130655	-2.57109359	7.40598143
14	O	2.86460099	2.66321443	5.94602138
15	O	3.90010365	0.51780751	6.89192455
16	O	3.77240000	-1.96900000	7.63100000
17	O	1.47829402	-3.08402308	7.27482237
18	O	2.15450121	1.79120176	8.29129984
19	O	-0.24970038	-2.04668743	8.86409542
20	O	1.05380000	4.47370000	5.45680000
21	O	-1.00419812	-3.76440172	7.04720051
22	Si	0.52350061	-7.58780023	-0.03030162
23	Si	-2.45310000	-8.37930000	0.08690000
24	O	-1.02440000	-7.79970000	-0.28570000
25	O	-3.48040000	-7.82240000	-1.00870000
26	O	-2.05280780	-6.52240219	3.54851933
27	O	-4.53620000	-6.55020000	2.91500000
28	O	-2.87430000	-7.94910000	1.53380000
29	O	0.93450000	-7.98310000	1.44400000
30	O	0.37158535	-7.41291241	3.90390117
31	Si	0.95190571	-8.52589470	2.93029734
32	Si	-1.34640002	-5.31659953	7.02370083
33	Si	-4.32960000	-6.05610000	7.41270000
34	O	-2.92290000	-5.44190000	7.01850000
35	O	-5.41450000	-5.45960000	6.41750000
36	O	-4.71840000	-5.65910000	8.88780000
37	O	-1.36620000	-5.12610000	10.61890000
38	O	-0.72730000	-6.04810000	8.28660000
39	Si	-0.78110000	-6.37380000	9.84140000
40	Si	4.19160470	1.79580311	-2.03249365
41	Si	4.36130152	-0.89369841	-0.53529941
42	Si	1.79910189	-4.81759798	0.05481120
43	Si	1.68499950	-2.17149717	-1.47840096
44	Si	3.22789893	3.06049928	2.23969923

1	Si	5.44850367	-1.68950357	4.28210336
2	Si	3.72402613	-4.24270477	4.65121667
3	O	4.61249832	0.39619810	-1.42440323
4	O	1.43099957	-3.66270169	-0.97330188
5	O	3.17920052	-1.73800241	-1.16009874
6	O	4.64898266	-3.05759022	4.13508996
7	O	2.93689240	2.40529580	-1.28880935
8	O	2.15280341	3.10900249	1.07409815
9	O	2.54299964	3.62289849	3.55350046
10	O	5.51820031	-1.20780053	5.80380015
11	O	3.57089415	-4.20200170	6.24789948
12	O	-0.73789753	-5.99420340	5.72550064
13	H	-1.30770000	8.45280000	5.54490000
14	H	3.53900000	4.98890000	5.43620000
15	H	-5.91550000	5.84190000	-1.27060000
16	H	-6.78570000	6.92250000	2.19890000
17	H	-12.70540000	-0.03450000	-1.12450000
18	H	-13.56750000	1.03610000	2.31350000
19	H	-12.61360000	-4.36250000	-0.43650000
20	H	-12.17550000	-5.02190000	-2.75570000
21	H	-14.47190000	-2.17020000	6.40220000
22	H	-13.77040000	-2.92530000	4.17860000
23	H	6.86449999	-1.88260020	3.83330004
24	H	-2.15040000	-4.10050000	12.78420000
25	H	1.31010000	-8.39770000	-1.01480000
26	H	-12.21020000	-7.97290000	7.89080000
27	H	0.36340000	-1.65380000	11.27870000
28	H	0.62130000	6.05740000	-2.14750000
29	H	0.50140000	4.07440000	-3.47820000
30	H	-2.25700000	7.49990000	7.52180000
31	H	-5.73850000	6.73170000	5.78280000
32	H	-10.96700000	4.40130000	4.09400000
33	H	-11.01960000	5.00810000	1.73210000
34	H	-12.06290000	1.27880000	5.87220000
35	H	-10.59640000	-6.34750000	11.45320000
36	H	-8.66420000	-7.73420000	10.94950000
37	H	2.77450000	1.81970000	10.74640000
38	H	1.80020000	3.79900000	9.78440000
39	H	5.77540000	-0.53010000	8.17660000
40	H	3.24710000	-4.17500000	8.72650000
41	H	0.61160000	-6.65520000	10.31590000
42	H	-1.64370000	-7.57580000	10.07620000
43	H	0.12290000	-9.76940000	3.03170000
44	H	2.36090000	-8.82750000	3.33990000

1	H	-10.15040000	3.92860000	-1.73450000
2	H	-9.16390000	2.16210000	-3.09680000
3	H	3.89500000	1.63920000	-3.49250000
4	H	5.32300000	2.73990000	-1.76330000
5	H	4.42880033	3.88349976	1.88700059
6	H	5.61650001	-1.70969998	-0.58830013
7	H	4.35729698	-5.55350059	4.29819677
8	H	3.22919940	-5.21290091	-0.15130244
9	H	-5.23700000	-6.37850000	11.22840000
10	H	-7.76830000	-9.07120000	6.80850000
11	H	-6.95230000	-10.08460000	3.55430000
12	H	-10.29630000	-10.34930000	0.25900000
13	H	-2.42150000	-9.87450000	0.00040000
14	H	-3.42900000	-8.60990000	3.88980000
15	H	-4.28320000	-7.54880000	7.29620000
16	H	-3.45780000	3.89970000	-3.31080000
17	H	0.59910000	5.23700000	7.81470000
18	H	-9.79240000	-1.54060000	-3.18200000
19	H	-8.38790000	-2.95530000	10.89960000
20	H	-4.87450000	3.78240000	8.02040000
21	H	-2.02270000	2.13730000	10.92000000
22	H	-4.91220000	-7.27130000	-2.96190000
23	H	-8.98790000	-7.09310000	-2.37650000
24	H	1.45750090	-2.18460057	-2.95900013
25	H	-5.88650000	0.35320000	-2.87170000
26	H	-6.57060000	-3.25690000	-2.96870000
27	H	-11.74490000	-3.66940000	8.61800000
28	H	-9.32890000	0.16850000	8.03140000
29	H	-8.19140000	3.21540000	6.31880000
30	H	-5.78340000	-8.84910000	-1.27830000
31	H	-7.97590000	-9.98270000	-0.17660000
32	H	-2.11759878	0.35870275	-2.97420046
33	H	-1.62615190	0.82254111	3.16834505
34	C	-2.75291064	-1.15099025	2.75899516
35	H	-3.82432246	-1.04248624	2.73560878
36	H	-2.21851962	-1.29691697	1.83871353
37	H	-2.22301180	-1.10274634	3.68985702
38	O	-2.45864082	0.80402491	2.64291071
39	H	-2.15772888	0.92568770	1.72948376
40	C	-3.45638258	-3.43852835	4.23097729
41	H	-4.47530234	-3.05619085	4.20233623
42	H	-2.91142511	-2.99424900	5.06705173
43	H	-3.48417872	-4.51991923	4.32654900
44	O	-2.84675249	-3.09060908	2.97003567

H -1.90906172 -3.36053469 2.97774523

ZH_2CH3OH(ads)
Si -0.03500264 0.01278087 -0.01172926
Si -0.07062066 -0.00642287 5.67012561
Si 3.69809560 -0.02775120 2.47992253
Si 1.04594946 -3.89523300 2.98002383
Al 0.69443486 -0.84580416 2.86883791
O 0.27419160 -2.50138243 2.92825035
O 2.37456548 -0.63772109 3.11857792
O -0.07552994 -0.01180634 1.57161922
O -0.20395004 0.03303619 4.07927035
O -1.57664420 0.18324520 -0.43643766
O -0.34410050 -1.45170255 6.29677068
O 1.36305158 0.50505989 6.20045787
O -1.26961821 0.99621022 6.02617280
O 0.84232537 1.27127891 -0.48307922
O 3.75442275 1.57560900 2.50012283
O 4.96903569 -0.48242468 3.34389495
O 2.20900747 -4.03153446 4.10229771
O 3.87832998 -0.49945031 0.94685209
O 1.75615889 -4.25857516 1.57492140
O 0.57512773 -1.28502939 -0.71770275
O -0.13725509 -4.93240022 3.33579160
O 0.80119871 -6.00639885 -0.15259947
Si -5.49759946 -0.02110111 -1.47430081
Si -2.51948538 0.76949824 -1.59088456
Si 1.67328427 2.63518902 -0.36438543
Si -6.77250000 -2.79180000 -1.55910000
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Si -0.62808867 -6.20848078 4.15928706
Si -3.21919642 -7.43499910 2.98449203
Si -6.09540000 -6.32220000 2.83000000
Si -7.79180000 -8.89230000 3.21140000
Si -7.85690000 -4.02790000 9.99880000
Si -9.54690000 -6.64300000 10.42590000
O -8.68790000 -5.35140000 10.15840000
Si 1.78780000 2.30220000 9.72780000
Si -0.76979724 -1.62740825 10.29930393
Si -1.17800108 1.38380287 9.93890097
O -1.38700000 -0.16320000 10.26480000
O 0.35020000 1.77510000 10.12160000
O -1.90930000 -2.64050000 10.65650000

1	Si	-2.31670000	-4.06080000	11.29600000
2	Si	-5.02660000	-5.18350000	10.35000000
3	O	-3.83590000	-4.30830000	10.92640000
4	O	-6.34110000	-4.27000000	10.39930000
5	Si	4.73289879	-0.80100238	7.13548725
6	Si	-7.29070000	2.20560000	5.67640000
7	Si	-4.57940103	3.32749896	6.62400307
8	Si	-1.94070000	7.20800000	6.08700000
9	Si	-4.59330000	6.04430000	5.10460000
10	O	-5.77090000	2.45290000	6.04720000
11	O	-3.26559897	2.41450213	6.57329895
12	O	-0.99450000	5.94280000	5.99240000
13	O	-3.27080000	6.91960000	5.26710000
14	O	-4.35770000	4.58890000	5.69440000
15	O	-7.46660000	2.24720000	4.09540000
16	O	-4.88400000	5.95910000	3.53970000
17	Si	-5.99570000	5.67090000	2.42990000
18	Si	-10.73910000	3.90040000	2.70070000
19	O	-11.73290000	2.70740000	2.34160000
20	Si	-12.07420000	1.15480000	2.31840000
21	O	-11.45520000	0.42330000	3.58130000
22	Si	-11.39460000	-4.15760000	7.24580000
23	Si	-13.29570000	-2.46030000	5.52120000
24	Si	-11.50890000	0.09760000	5.13610000
25	Si	-8.83680000	-0.22830000	6.67330000
26	O	-12.44950000	-3.64190000	6.15630000
27	O	-12.41530000	-1.16550000	5.38290000
28	O	-10.03410000	-0.20050000	5.63860000
29	O	-7.69650000	0.78430000	6.31660000
30	Si	-0.05970000	4.78730000	6.54670000
31	O	-10.24280000	-7.11800000	9.08650000
32	Si	-7.71660000	3.11370000	2.78820000
33	O	-6.95550000	4.50240000	2.92570000
34	O	-9.24950000	3.38730000	2.56950000
35	Si	-4.97250000	-7.60980000	-1.50390000
36	Si	-11.35590000	0.26280000	-0.54610000
37	O	-6.84510000	-7.72030000	2.70470000
38	O	-10.35620000	-0.94150000	-0.80140000
39	Si	-9.16490000	-9.40520000	0.52820000
40	Si	-9.33470000	-6.71560000	-0.96890000
41	Si	-11.54680000	-4.63200000	-1.45310000
42	Si	-9.77590000	-2.05450000	-1.77500000
43	O	-9.58580000	-8.00560000	-0.07990000
44	O	-10.67690000	-5.84320000	-0.91270000

1	O	-10.64710000	-3.36120000	-1.66840000
2	O	-8.28390000	-2.37400000	-1.34130000
3	O	-6.40440000	-3.94670000	-0.53100000
4	O	-8.15250000	-5.87130000	-0.34420000
5	O	-8.84920000	-9.23940000	2.07860000
6	O	-6.41640000	-5.42400000	1.54900000
7	O	-5.61290000	-6.41590000	-0.70840000
8	O	-5.77370000	-1.60340000	-1.35130000
9	Si	-6.81090000	-5.43360000	5.68340000
10	Si	-8.50460000	-8.00720000	6.05360000
11	O	-7.72180000	-6.63160000	6.20070000
12	Si	-10.95800000	-7.17850000	7.67890000
13	Si	-8.42890000	-3.23820000	7.03330000
14	O	-11.40780000	-5.74300000	7.18590000
15	O	-8.21960000	-1.69260000	6.70790000
16	O	-9.95660000	-3.63110000	6.85010000
17	O	-9.98360000	-7.83070000	6.60240000
18	O	-7.53000000	-4.04100000	5.99020000
19	O	-7.92320000	-3.54700000	8.50450000
20	Si	0.12369271	4.64449314	-2.14540137
21	Si	-2.82298587	3.84600033	-1.95510612
22	O	-3.94890094	0.19040009	-1.21850400
23	O	0.75581700	3.76931376	-0.98750082
24	O	-1.45550000	4.66540000	-1.97180000
25	O	-2.55362753	2.34859933	-1.49989274
26	O	-6.33220000	0.83850000	-0.42850000
27	O	-3.77030000	4.57610000	-0.90140000
28	Si	-5.28020000	4.78230000	-0.42350000
29	Si	-7.00390000	2.22870000	-0.05400000
30	Si	-9.63060000	2.52380000	-1.72000000
31	O	-6.07880000	3.41370000	-0.57020000
32	O	-8.42830000	2.36750000	-0.70540000
33	O	-10.83220000	1.58900000	-1.25000000
34	O	-5.20960000	5.26350000	1.09860000
35	O	-7.15700000	2.26930000	1.54270000
36	O	-11.46650000	0.47770000	1.01990000
37	O	-6.60040000	-5.49380000	4.09960000
38	O	-8.61720000	-8.44720000	4.51360000
39	O	-1.68269804	1.69079505	8.46849800
40	Si	-1.74889455	2.17160036	6.97409090
41	O	-0.91870190	3.49570194	6.81430303
42	Si	2.50949970	3.95249399	5.10419055
43	Si	2.56679260	1.37877714	6.82676059
44	Si	3.01120375	-3.35758962	7.49349347

1	Si	-0.01130732	-2.57109916	7.40598503
2	O	2.86460116	2.66321485	5.94602230
3	O	3.90010431	0.51780876	6.89192873
4	O	3.77240000	-1.96900000	7.63100000
5	O	1.47829584	-3.08401632	7.27481679
6	O	2.15450109	1.79120197	8.29130003
7	O	-0.24970142	-2.04668235	8.86409310
8	O	1.05380000	4.47370000	5.45680000
9	O	-1.00419792	-3.76440203	7.04720089
10	Si	0.52350110	-7.58780004	-0.03030226
11	Si	-2.45310000	-8.37930000	0.08690000
12	O	-1.02440000	-7.79970000	-0.28570000
13	O	-3.48040000	-7.82240000	-1.00870000
14	O	-2.05280741	-6.52240119	3.54851707
15	O	-4.53619988	-6.55019974	2.91500006
16	O	-2.87430000	-7.94910000	1.53380000
17	O	0.93450000	-7.98310000	1.44400000
18	O	0.37158461	-7.41291233	3.90390103
19	Si	0.95190617	-8.52589484	2.93029692
20	Si	-1.34639967	-5.31659963	7.02370103
21	Si	-4.32960000	-6.05610000	7.41270000
22	O	-2.92290000	-5.44190000	7.01850000
23	O	-5.41450000	-5.45960000	6.41750000
24	O	-4.71840000	-5.65910000	8.88780000
25	O	-1.36620000	-5.12610000	10.61890000
26	O	-0.72730000	-6.04810000	8.28660000
27	Si	-0.78110000	-6.37380000	9.84140000
28	Si	4.19160620	1.79580366	-2.03249254
29	Si	4.36130251	-0.89370005	-0.53529695
30	Si	1.79910253	-4.81759815	0.05481035
31	Si	1.68500005	-2.17149968	-1.47839926
32	Si	3.22789441	3.06049298	2.23970283
33	Si	5.44850448	-1.68950374	4.28210274
34	Si	3.72402547	-4.24270520	4.65121699
35	O	4.61249807	0.39619801	-1.42440297
36	O	1.43099945	-3.66270175	-0.97330151
37	O	3.17920083	-1.73799820	-1.16010381
38	O	4.64898275	-3.05758987	4.13508987
39	O	2.93688970	2.40529517	-1.28881194
40	O	2.15281026	3.10901104	1.07409228
41	O	2.54300071	3.62289936	3.55349979
42	O	5.51819997	-1.20780112	5.80380004
43	O	3.57089453	-4.20200163	6.24789904
44	O	-0.73789901	-5.99420343	5.72550099

1	H	-1.30770000	8.45280000	5.54490000
2	H	3.53900000	4.98890000	5.43620000
3	H	-5.91550000	5.84190000	-1.27060000
4	H	-6.78570000	6.92250000	2.19890000
5	H	-12.70540000	-0.03450000	-1.12450000
6	H	-13.56750000	1.03610000	2.31350000
7	H	-12.61360000	-4.36250000	-0.43650000
8	H	-12.17550000	-5.02190000	-2.75570000
9	H	-14.47190000	-2.17020000	6.40220000
10	H	-13.77040000	-2.92530000	4.17860000
11	H	6.86450001	-1.88260012	3.83330008
12	H	-2.15040000	-4.10050000	12.78420000
13	H	1.31010000	-8.39770000	-1.01480000
14	H	-12.21020000	-7.97290000	7.89080000
15	H	0.36340000	-1.65380000	11.27870000
16	H	0.62130000	6.05740000	-2.14750000
17	H	0.50140000	4.07440000	-3.47820000
18	H	-2.25700000	7.49990000	7.52180000
19	H	-5.73850000	6.73170000	5.78280000
20	H	-10.96700000	4.40130000	4.09400000
21	H	-11.01960000	5.00810000	1.73210000
22	H	-12.06290000	1.27880000	5.87220000
23	H	-10.59640000	-6.34750000	11.45320000
24	H	-8.66420000	-7.73420000	10.94950000
25	H	2.77450000	1.81970000	10.74640000
26	H	1.80020000	3.79900000	9.78440000
27	H	5.77540000	-0.53010000	8.17660000
28	H	3.24710000	-4.17500000	8.72650000
29	H	0.61160000	-6.65520000	10.31590000
30	H	-1.64370000	-7.57580000	10.07620000
31	H	0.12290000	-9.76940000	3.03170000
32	H	2.36090000	-8.82750000	3.33990000
33	H	-10.15040000	3.92860000	-1.73450000
34	H	-9.16390000	2.16210000	-3.09680000
35	H	3.89500000	1.63920000	-3.49250000
36	H	5.32300000	2.73990000	-1.76330000
37	H	4.42879981	3.88350020	1.88700080
38	H	5.61649996	-1.70970006	-0.58830003
39	H	4.35729694	-5.55350103	4.29819700
40	H	3.22919901	-5.21290102	-0.15130191
41	H	-5.23700000	-6.37850000	11.22840000
42	H	-7.76830000	-9.07120000	6.80850000
43	H	-6.95230000	-10.08460000	3.55430000
44	H	-10.29630000	-10.34930000	0.25900000

1	H	-2.42150000	-9.87450000	0.00040000
2	H	-3.42900000	-8.60990000	3.88980000
3	H	-4.28320000	-7.54880000	7.29620000
4	H	-3.45780000	3.89970000	-3.31080000
5	H	0.59910000	5.23700000	7.81470000
6	H	-9.79240000	-1.54060000	-3.18200000
7	H	-8.38790000	-2.95530000	10.89960000
8	H	-4.87450000	3.78240000	8.02040000
9	H	-2.02270000	2.13730000	10.92000000
10	H	-4.91220000	-7.27130000	-2.96190000
11	H	-8.98790000	-7.09310000	-2.37650000
12	H	1.45750100	-2.18460108	-2.95900000
13	H	-5.88650000	0.35320000	-2.87170000
14	H	-6.57060000	-3.25690000	-2.96870000
15	H	-11.74490000	-3.66940000	8.61800000
16	H	-9.32890000	0.16850000	8.03140000
17	H	-8.19140000	3.21540000	6.31880000
18	H	-5.78340000	-8.84910000	-1.27830000
19	H	-7.97590000	-9.98270000	-0.17660000
20	H	-2.11759977	0.35870246	-2.97420006
21	H	-1.30258201	0.70050860	3.55839592
22	C	-3.41081526	0.77415535	3.09557844
23	H	-3.99793459	1.31557881	2.35788041
24	H	-3.50017050	-0.30434017	2.99198738
25	H	-3.65375753	1.10623811	4.10109351
26	O	-2.00454359	1.14868218	2.87774492
27	H	-1.62932521	0.77052429	2.04364636
28	C	-3.35050023	-3.09524866	3.94077554
29	H	-4.35830771	-2.68122298	4.01333102
30	H	-2.94886408	-3.19833184	4.95499943
31	H	-3.42156134	-4.08418593	3.47928676
32	O	-2.57693551	-2.19834114	3.15115397
33	H	-1.67127120	-2.53642040	3.07353969
34				
35				
36	ZH_CH2CHCH3(ads)-oniom			
37	Si	-0.01924218	0.04028283	0.00974120
38	Si	-0.05961508	-0.00870067	5.67747663
39	Si	3.66652060	-0.04417906	2.49918180
40	Si	1.04248994	-3.87500909	2.97690556
41	Al	0.75252272	-0.85553970	2.79782424
42	O	0.29585987	-2.47560491	2.91310125
43	O	2.39010874	-0.63264931	3.25665308
44	O	0.10183722	0.12353315	1.58142234

1	O	-0.23369155	0.03160010	4.03857110
2	O	-1.55116604	0.14490937	-0.45206775
3	O	-0.32445569	-1.45712761	6.26018986
4	O	1.38658913	0.48485323	6.15029092
5	O	-1.22020193	1.01266785	6.01111593
6	O	0.84896357	1.26433917	-0.57739655
7	O	3.75334555	1.56182386	2.50102816
8	O	4.98066445	-0.48606665	3.30645889
9	O	2.19134133	-4.02213154	4.12625357
10	O	3.80787197	-0.49805307	0.94975319
11	O	1.79997336	-4.25373510	1.59149122
12	O	0.59357475	-1.28120170	-0.67379312
13	O	-0.12211880	-4.92842607	3.33114128
14	C	-2.21452564	2.13971590	2.89507618
15	H	-1.67616246	2.81207147	3.56048460
16	H	-1.91659315	2.14364488	1.84937701
17	C	-3.26723687	1.42871998	3.32480415
18	H	-0.98523494	0.57237719	3.67468680
19	H	-3.54030606	1.49615971	4.37693026
20	C	-4.15633589	0.57777486	2.47307567
21	H	-4.24711995	-0.43274192	2.88510130
22	H	-5.16778637	0.99919928	2.46258801
23	H	-3.81380190	0.50376317	1.43897552
24	O	0.80119400	-6.00639700	-0.15258800
25	Si	-5.49759900	-0.02110400	-1.47430200
26	Si	-2.51946600	0.76949200	-1.59084300
27	Si	1.67331300	2.63519500	-0.36438200
28	Si	-6.77250000	-2.79180000	-1.55910000
29	Si	-6.65860000	-5.43650000	-0.02630000
30	Si	-0.62810700	-6.20847000	4.15931600
31	Si	-3.21919400	-7.43499800	2.98448500
32	Si	-6.09540000	-6.32220000	2.83000000
33	Si	-7.79180000	-8.89230000	3.21140000
34	Si	-7.85690000	-4.02790000	9.99880000
35	Si	-9.54690000	-6.64300000	10.42590000
36	O	-8.68790000	-5.35140000	10.15840000
37	Si	1.78780100	2.30219700	9.72780100
38	Si	-0.76980000	-1.62739800	10.29929900
39	Si	-1.17800200	1.38380500	9.93890200
40	O	-1.38699800	-0.16319900	10.26480000
41	O	0.35019600	1.77510800	10.12159700
42	O	-1.90930200	-2.64049800	10.65649900
43	Si	-2.31670000	-4.06080000	11.29600000
44	Si	-5.02660000	-5.18350000	10.35000000

1	O	-3.83590000	-4.30830000	10.92640000
2	O	-6.34110000	-4.27000000	10.39930000
3	Si	4.73289800	-0.80101300	7.13548700
4	Si	-7.29070000	2.20560000	5.67640000
5	Si	-4.57941000	3.32748400	6.62402800
6	Si	-1.94070000	7.20800000	6.08700000
7	Si	-4.59330000	6.04430000	5.10460000
8	O	-5.77090000	2.45290000	6.04720000
9	O	-3.26558900	2.41451100	6.57326400
10	O	-0.99450300	5.94280400	5.99241400
11	O	-3.27080000	6.91960000	5.26710000
12	O	-4.35770000	4.58890000	5.69440000
13	O	-7.46660000	2.24720000	4.09540000
14	O	-4.88400000	5.95910000	3.53970000
15	Si	-5.99570000	5.67090000	2.42990000
16	Si	-10.73910000	3.90040000	2.70070000
17	O	-11.73290000	2.70740000	2.34160000
18	Si	-12.07420000	1.15480000	2.31840000
19	O	-11.45520000	0.42330000	3.58130000
20	Si	-11.39460000	-4.15760000	7.24580000
21	Si	-13.29570000	-2.46030000	5.52120000
22	Si	-11.50890000	0.09760000	5.13610000
23	Si	-8.83680000	-0.22830000	6.67330000
24	O	-12.44950000	-3.64190000	6.15630000
25	O	-12.41530000	-1.16550000	5.38290000
26	O	-10.03410000	-0.20050000	5.63860000
27	O	-7.69650000	0.78430000	6.31660000
28	Si	-0.05969600	4.78729800	6.54670400
29	O	-10.24280000	-7.11800000	9.08650000
30	Si	-7.71660000	3.11370000	2.78820000
31	O	-6.95550000	4.50240000	2.92570000
32	O	-9.24950000	3.38730000	2.56950000
33	Si	-4.97250000	-7.60980000	-1.50390000
34	Si	-11.35590000	0.26280000	-0.54610000
35	O	-6.84510000	-7.72030000	2.70470000
36	O	-10.35620000	-0.94150000	-0.80140000
37	Si	-9.16490000	-9.40520000	0.52820000
38	Si	-9.33470000	-6.71560000	-0.96890000
39	Si	-11.54680000	-4.63200000	-1.45310000
40	Si	-9.77590000	-2.05450000	-1.77500000
41	O	-9.58580000	-8.00560000	-0.07990000
42	O	-10.67690000	-5.84320000	-0.91270000
43	O	-10.64710000	-3.36120000	-1.66840000
44	O	-8.28390000	-2.37400000	-1.34130000

1	O	-6.40440000	-3.94670000	-0.53100000
2	O	-8.15250000	-5.87130000	-0.34420000
3	O	-8.84920000	-9.23940000	2.07860000
4	O	-6.41640000	-5.42400000	1.54900000
5	O	-5.61290000	-6.41590000	-0.70840000
6	O	-5.77370000	-1.60340000	-1.35130000
7	Si	-6.81090000	-5.43360000	5.68340000
8	Si	-8.50460000	-8.00720000	6.05360000
9	O	-7.72180000	-6.63160000	6.20070000
10	Si	-10.95800000	-7.17850000	7.67890000
11	Si	-8.42890000	-3.23820000	7.03330000
12	O	-11.40780000	-5.74300000	7.18590000
13	O	-8.21960000	-1.69260000	6.70790000
14	O	-9.95660000	-3.63110000	6.85010000
15	O	-9.98360000	-7.83070000	6.60240000
16	O	-7.53000000	-4.04100000	5.99020000
17	O	-7.92320000	-3.54700000	8.50450000
18	Si	0.12369400	4.64449500	-2.14540100
19	Si	-2.82300000	3.84600000	-1.95510000
20	O	-3.94890100	0.19040700	-1.21849100
21	O	0.75580500	3.76930600	-0.98749600
22	O	-1.45550000	4.66540000	-1.97180000
23	O	-2.55359900	2.34860000	-1.49990000
24	O	-6.33220000	0.83850000	-0.42850000
25	O	-3.77030000	4.57610000	-0.90140000
26	Si	-5.28020000	4.78230000	-0.42350000
27	Si	-7.00390000	2.22870000	-0.05400000
28	Si	-9.63060000	2.52380000	-1.72000000
29	O	-6.07880000	3.41370000	-0.57020000
30	O	-8.42830000	2.36750000	-0.70540000
31	O	-10.83220000	1.58900000	-1.25000000
32	O	-5.20960000	5.26350000	1.09860000
33	O	-7.15700000	2.26930000	1.54270000
34	O	-11.46650000	0.47770000	1.01990000
35	O	-6.60040000	-5.49380000	4.09960000
36	O	-8.61720000	-8.44720000	4.51360000
37	O	-1.68268500	1.69077000	8.46849000
38	Si	-1.74890700	2.17158200	6.97406500
39	O	-0.91871600	3.49571100	6.81431100
40	Si	2.50950000	3.95250200	5.10420600
41	Si	2.56680300	1.37878300	6.82666500
42	Si	3.01119900	-3.35762100	7.49351800
43	Si	-0.01119000	-2.57107000	7.40579800
44	O	2.86459200	2.66321500	5.94602000

1	O	3.90011200	0.51782000	6.89191000
2	O	3.77240000	-1.96900000	7.63100000
3	O	1.47830600	-3.08396900	7.27474600
4	O	2.15447800	1.79115500	8.29130600
5	O	-0.24968200	-2.04668500	8.86409800
6	O	1.05379200	4.47370400	5.45679000
7	O	-1.00418800	-3.76439500	7.04715000
8	Si	0.52350300	-7.58780100	-0.03030900
9	Si	-2.45310000	-8.37930000	0.08690000
10	O	-1.02440000	-7.79970000	-0.28570000
11	O	-3.48040000	-7.82240000	-1.00870000
12	O	-2.05280900	-6.52240200	3.54852100
13	O	-4.53620000	-6.55020000	2.91500000
14	O	-2.87430000	-7.94910000	1.53380000
15	O	0.93450000	-7.98310000	1.44400000
16	O	0.37159500	-7.41290400	3.90390000
17	Si	0.95190700	-8.52589300	2.93029700
18	Si	-1.34641900	-5.31660400	7.02372700
19	Si	-4.32960000	-6.05610000	7.41270000
20	O	-2.92290000	-5.44190000	7.01850000
21	O	-5.41450000	-5.45960000	6.41750000
22	O	-4.71840000	-5.65910000	8.88780000
23	O	-1.36620000	-5.12610000	10.61890000
24	O	-0.72730000	-6.04810000	8.28660000
25	Si	-0.78110000	-6.37380000	9.84140000
26	Si	4.19159800	1.79579800	-2.03250300
27	Si	4.36126500	-0.89371900	-0.53523900
28	Si	1.79909000	-4.81757300	0.05487800
29	Si	1.68499800	-2.17149200	-1.47837600
30	Si	3.22786700	3.06046200	2.23971600
31	Si	5.44846500	-1.68951300	4.28214400
32	Si	3.72399100	-4.24269200	4.65124000
33	O	4.61250000	0.39621200	-1.42438300
34	O	1.43098600	-3.66268800	-0.97328000
35	O	3.17920400	-1.73801000	-1.16009400
36	O	4.64897900	-3.05759000	4.13509700
37	O	2.93689600	2.40530100	-1.28880500
38	O	2.15279600	3.10899800	1.07410400
39	O	2.54300400	3.62290800	3.55349900
40	O	5.51820600	-1.20778600	5.80379500
41	O	3.57090200	-4.20200800	6.24790000
42	O	-0.73789400	-5.99420300	5.72550100
43	H	-1.30770000	8.45280000	5.54490000
44	H	3.53900000	4.98890000	5.43620000

1	H	-5.91550000	5.84190000	-1.27060000
2	H	-6.78570000	6.92250000	2.19890000
3	H	-12.70540000	-0.03450000	-1.12450000
4	H	-13.56750000	1.03610000	2.31350000
5	H	-12.61360000	-4.36250000	-0.43650000
6	H	-12.17550000	-5.02190000	-2.75570000
7	H	-14.47190000	-2.17020000	6.40220000
8	H	-13.77040000	-2.92530000	4.17860000
9	H	6.86449900	-1.88259200	3.83329400
10	H	-2.15040000	-4.10050000	12.78420000
11	H	1.31010000	-8.39770000	-1.01480000
12	H	-12.21020000	-7.97290000	7.89080000
13	H	0.36339900	-1.65380500	11.27870100
14	H	0.62130000	6.05740000	-2.14750000
15	H	0.50140000	4.07440000	-3.47820000
16	H	-2.25700000	7.49990000	7.52180000
17	H	-5.73850000	6.73170000	5.78280000
18	H	-10.96700000	4.40130000	4.09400000
19	H	-11.01960000	5.00810000	1.73210000
20	H	-12.06290000	1.27880000	5.87220000
21	H	-10.59640000	-6.34750000	11.45320000
22	H	-8.66420000	-7.73420000	10.94950000
23	H	2.77449400	1.81969100	10.74640100
24	H	1.80021000	3.79900000	9.78440300
25	H	5.77540000	-0.53010000	8.17660000
26	H	3.24710000	-4.17500000	8.72650000
27	H	0.61160000	-6.65520000	10.31590000
28	H	-1.64370000	-7.57580000	10.07620000
29	H	0.12290000	-9.76940000	3.03170000
30	H	2.36090000	-8.82750000	3.33990000
31	H	-10.15040000	3.92860000	-1.73450000
32	H	-9.16390000	2.16210000	-3.09680000
33	H	3.89500000	1.63920000	-3.49250000
34	H	5.32300000	2.73990000	-1.76330000
35	H	4.42880800	3.88348800	1.88700000
36	H	5.61650100	-1.70969900	-0.58829900
37	H	4.35729400	-5.55350100	4.29819400
38	H	3.22920300	-5.21289400	-0.15129000
39	H	-5.23700000	-6.37850000	11.22840000
40	H	-7.76830000	-9.07120000	6.80850000
41	H	-6.95230000	-10.08460000	3.55430000
42	H	-10.29630000	-10.34930000	0.25900000
43	H	-2.42150000	-9.87450000	0.00040000
44	H	-3.42900000	-8.60990000	3.88980000

1	H	-4.28320000	-7.54880000	7.29620000
2	H	-3.45780000	3.89970000	-3.31080000
3	H	0.59911200	5.23699200	7.81469700
4	H	-9.79240000	-1.54060000	-3.18200000
5	H	-8.38790000	-2.95530000	10.89960000
6	H	-4.87450000	3.78240000	8.02040000
7	H	-2.02270000	2.13730000	10.92000000
8	H	-4.91220000	-7.27130000	-2.96190000
9	H	-8.98790000	-7.09310000	-2.37650000
10	H	1.45749000	-2.18459900	-2.95899900
11	H	-5.88650000	0.35320000	-2.87170000
12	H	-6.57060000	-3.25690000	-2.96870000
13	H	-11.74490000	-3.66940000	8.61800000
14	H	-9.32890000	0.16850000	8.03140000
15	H	-8.19140000	3.21540000	6.31880000
16	H	-5.78340000	-8.84910000	-1.27830000
17	H	-7.97590000	-9.98270000	-0.17660000
18	H	-2.11759500	0.35869400	-2.97419700
19				
20				
21	ZH_CH2CHCH3(ads)			
22	Si	-0.03311633	0.02887638	-0.00798769
23	Si	-0.06876781	-0.00413883	5.69597143
24	Si	3.71340557	-0.01701708	2.48660191
25	Si	1.04505891	-3.90307094	2.98374594
26	Al	0.76063513	-0.86859604	2.80424330
27	O	0.31889802	-2.49068978	2.96429208
28	O	2.39781919	-0.57929075	3.20061161
29	O	0.03098444	0.02768504	1.56938324
30	O	-0.22987248	-0.00085948	4.05512041
31	O	-1.57241561	0.15608553	-0.45071390
32	O	-0.34398254	-1.44970969	6.28885539
33	O	1.37490026	0.50744540	6.15166879
34	O	-1.25241972	1.00828014	6.00973288
35	O	0.82766797	1.28502501	-0.52498003
36	O	3.78410229	1.58452331	2.48822992
37	O	4.99125607	-0.48051524	3.33440801
38	O	2.21087316	-4.04977328	4.10485063
39	O	3.85495152	-0.51827737	0.95614142
40	O	1.75541539	-4.25462972	1.57432182
41	O	0.58702360	-1.27906580	-0.70766740
42	O	-0.13523207	-4.93799691	3.33181980
43	C	-2.88206308	1.14271402	2.94998458
44	H	-2.91351976	2.00568210	3.60579107

1	H	-2.54481845	1.29838565	1.93148572
2	C	-3.30232192	-0.05800851	3.36662123
3	H	-1.10210224	0.33150405	3.70625456
4	H	-3.64855688	-0.15367735	4.39462847
5	C	-3.34868248	-1.29914600	2.52912412
6	H	-2.69971575	-2.07765349	2.94472628
7	H	-4.36384601	-1.70897164	2.52072537
8	H	-3.04131119	-1.10307358	1.50163925
9	O	0.80119449	-6.00639739	-0.15258849
10	Si	-5.49759907	-0.02110387	-1.47430244
11	Si	-2.51946598	0.76949168	-1.59084283
12	Si	1.67331295	2.63519498	-0.36438223
13	Si	-6.77250000	-2.79180000	-1.55910000
14	Si	-6.65860000	-5.43650000	-0.02630000
15	Si	-0.62810691	-6.20847028	4.15931590
16	Si	-3.21919371	-7.43499849	2.98448456
17	Si	-6.09540000	-6.32220000	2.83000000
18	Si	-7.79180000	-8.89230000	3.21140000
19	Si	-7.85690000	-4.02790000	9.99880000
20	Si	-9.54690000	-6.64300000	10.42590000
21	O	-8.68790000	-5.35140000	10.15840000
22	Si	1.78780113	2.30219706	9.72780124
23	Si	-0.76980048	-1.62739801	10.29929922
24	Si	-1.17800176	1.38380466	9.93890158
25	O	-1.38699751	-0.16319894	10.26480031
26	O	0.35019631	1.77510754	10.12159661
27	O	-1.90930248	-2.64049770	10.65649860
28	Si	-2.31670000	-4.06080000	11.29600000
29	Si	-5.02660000	-5.18350000	10.35000000
30	O	-3.83590000	-4.30830000	10.92640000
31	O	-6.34110000	-4.27000000	10.39930000
32	Si	4.73289826	-0.80101294	7.13548688
33	Si	-7.29070000	2.20560000	5.67640000
34	Si	-4.57940978	3.32748440	6.62402755
35	Si	-1.94070000	7.20800000	6.08700000
36	Si	-4.59330000	6.04430000	5.10460000
37	O	-5.77090000	2.45290000	6.04720000
38	O	-3.26558882	2.41451122	6.57326448
39	O	-0.99450301	5.94280421	5.99241385
40	O	-3.27080000	6.91960000	5.26710000
41	O	-4.35770000	4.58890000	5.69440000
42	O	-7.46660000	2.24720000	4.09540000
43	O	-4.88400000	5.95910000	3.53970000
44	Si	-5.99570000	5.67090000	2.42990000

1	Si	-10.73910000	3.90040000	2.70070000
2	O	-11.73290000	2.70740000	2.34160000
3	Si	-12.07420000	1.15480000	2.31840000
4	O	-11.45520000	0.42330000	3.58130000
5	Si	-11.39460000	-4.15760000	7.24580000
6	Si	-13.29570000	-2.46030000	5.52120000
7	Si	-11.50890000	0.09760000	5.13610000
8	Si	-8.83680000	-0.22830000	6.67330000
9	O	-12.44950000	-3.64190000	6.15630000
10	O	-12.41530000	-1.16550000	5.38290000
11	O	-10.03410000	-0.20050000	5.63860000
12	O	-7.69650000	0.78430000	6.31660000
13	Si	-0.05969631	4.78729827	6.54670398
14	O	-10.24280000	-7.11800000	9.08650000
15	Si	-7.71660000	3.11370000	2.78820000
16	O	-6.95550000	4.50240000	2.92570000
17	O	-9.24950000	3.38730000	2.56950000
18	Si	-4.97250000	-7.60980000	-1.50390000
19	Si	-11.35590000	0.26280000	-0.54610000
20	O	-6.84510000	-7.72030000	2.70470000
21	O	-10.35620000	-0.94150000	-0.80140000
22	Si	-9.16490000	-9.40520000	0.52820000
23	Si	-9.33470000	-6.71560000	-0.96890000
24	Si	-11.54680000	-4.63200000	-1.45310000
25	Si	-9.77590000	-2.05450000	-1.77500000
26	O	-9.58580000	-8.00560000	-0.07990000
27	O	-10.67690000	-5.84320000	-0.91270000
28	O	-10.64710000	-3.36120000	-1.66840000
29	O	-8.28390000	-2.37400000	-1.34130000
30	O	-6.40440000	-3.94670000	-0.53100000
31	O	-8.15250000	-5.87130000	-0.34420000
32	O	-8.84920000	-9.23940000	2.07860000
33	O	-6.41640000	-5.42400000	1.54900000
34	O	-5.61290000	-6.41590000	-0.70840000
35	O	-5.77370000	-1.60340000	-1.35130000
36	Si	-6.81090000	-5.43360000	5.68340000
37	Si	-8.50460000	-8.00720000	6.05360000
38	O	-7.72180000	-6.63160000	6.20070000
39	Si	-10.95800000	-7.17850000	7.67890000
40	Si	-8.42890000	-3.23820000	7.03330000
41	O	-11.40780000	-5.74300000	7.18590000
42	O	-8.21960000	-1.69260000	6.70790000
43	O	-9.95660000	-3.63110000	6.85010000
44	O	-9.98360000	-7.83070000	6.60240000

1	O	-7.53000000	-4.04100000	5.99020000
2	O	-7.92320000	-3.54700000	8.50450000
3	Si	0.12369419	4.64449494	-2.14540065
4	Si	-2.82300008	3.84600000	-1.95509997
5	O	-3.94890051	0.19040676	-1.21849146
6	O	0.75580532	3.76930628	-0.98749641
7	O	-1.45550000	4.66540000	-1.97180000
8	O	-2.55359896	2.34860000	-1.49989953
9	O	-6.33220000	0.83850000	-0.42850000
10	O	-3.77030000	4.57610000	-0.90140000
11	Si	-5.28020000	4.78230000	-0.42350000
12	Si	-7.00390000	2.22870000	-0.05400000
13	Si	-9.63060000	2.52380000	-1.72000000
14	O	-6.07880000	3.41370000	-0.57020000
15	O	-8.42830000	2.36750000	-0.70540000
16	O	-10.83220000	1.58900000	-1.25000000
17	O	-5.20960000	5.26350000	1.09860000
18	O	-7.15700000	2.26930000	1.54270000
19	O	-11.46650000	0.47770000	1.01990000
20	O	-6.60040000	-5.49380000	4.09960000
21	O	-8.61720000	-8.44720000	4.51360000
22	O	-1.68268496	1.69077038	8.46848980
23	Si	-1.74890677	2.17158171	6.97406473
24	O	-0.91871574	3.49571114	6.81431059
25	Si	2.50949962	3.95250210	5.10420606
26	Si	2.56680299	1.37878294	6.82666483
27	Si	3.01119899	-3.35762115	7.49351795
28	Si	-0.01118963	-2.57106981	7.40579805
29	O	2.86459239	2.66321547	5.94601999
30	O	3.90011226	0.51781976	6.89191019
31	O	3.77240000	-1.96900000	7.63100000
32	O	1.47830597	-3.08396881	7.27474588
33	O	2.15447797	1.79115531	8.29130638
34	O	-0.24968192	-2.04668531	8.86409767
35	O	1.05379174	4.47370378	5.45679047
36	O	-1.00418752	-3.76439536	7.04715002
37	Si	0.52350326	-7.58780124	-0.03030860
38	Si	-2.45310000	-8.37930000	0.08690000
39	O	-1.02440000	-7.79970000	-0.28570000
40	O	-3.48040000	-7.82240000	-1.00870000
41	O	-2.05280863	-6.52240194	3.54852112
42	O	-4.53620000	-6.55020000	2.91500000
43	O	-2.87430000	-7.94910000	1.53380000
44	O	0.93450000	-7.98310000	1.44400000

1	O	0.37159547	-7.41290375	3.90389995
2	Si	0.95190714	-8.52589337	2.93029667
3	Si	-1.34641890	-5.31660432	7.02372715
4	Si	-4.32960000	-6.05610000	7.41270000
5	O	-2.92290000	-5.44190000	7.01850000
6	O	-5.41450000	-5.45960000	6.41750000
7	O	-4.71840000	-5.65910000	8.88780000
8	O	-1.36620000	-5.12610000	10.61890000
9	O	-0.72730000	-6.04810000	8.28660000
10	Si	-0.78110000	-6.37380000	9.84140000
11	Si	4.19159842	1.79579825	-2.03250299
12	Si	4.36126516	-0.89371924	-0.53523906
13	Si	1.79909010	-4.81757342	0.05487792
14	Si	1.68499793	-2.17149238	-1.47837555
15	Si	3.22786700	3.06046217	2.23971620
16	Si	5.44846515	-1.68951342	4.28214365
17	Si	3.72399114	-4.24269235	4.65123983
18	O	4.61249985	0.39621196	-1.42438269
19	O	1.43098589	-3.66268782	-0.97328013
20	O	3.17920354	-1.73801032	-1.16009356
21	O	4.64897896	-3.05758970	4.13509676
22	O	2.93689610	2.40530054	-1.28880546
23	O	2.15279557	3.10899850	1.07410446
24	O	2.54300384	3.62290780	3.55349867
25	O	5.51820606	-1.20778574	5.80379521
26	O	3.57090230	-4.20200841	6.24790043
27	O	-0.73789421	-5.99420260	5.72550076
28	H	-1.30770000	8.45280000	5.54490000
29	H	3.53900000	4.98890000	5.43620000
30	H	-5.91550000	5.84190000	-1.27060000
31	H	-6.78570000	6.92250000	2.19890000
32	H	-12.70540000	-0.03450000	-1.12450000
33	H	-13.56750000	1.03610000	2.31350000
34	H	-12.61360000	-4.36250000	-0.43650000
35	H	-12.17550000	-5.02190000	-2.75570000
36	H	-14.47190000	-2.17020000	6.40220000
37	H	-13.77040000	-2.92530000	4.17860000
38	H	6.86449905	-1.88259232	3.83329370
39	H	-2.15040000	-4.10050000	12.78420000
40	H	1.31010000	-8.39770000	-1.01480000
41	H	-12.21020000	-7.97290000	7.89080000
42	H	0.36339864	-1.65380547	11.27870143
43	H	0.62130000	6.05740000	-2.14750000
44	H	0.50140000	4.07440000	-3.47820000

1	H	-2.25700000	7.49990000	7.52180000
2	H	-5.73850000	6.73170000	5.78280000
3	H	-10.96700000	4.40130000	4.09400000
4	H	-11.01960000	5.00810000	1.73210000
5	H	-12.06290000	1.27880000	5.87220000
6	H	-10.59640000	-6.34750000	11.45320000
7	H	-8.66420000	-7.73420000	10.94950000
8	H	2.77449447	1.81969135	10.74640127
9	H	1.80021025	3.79899981	9.78440281
10	H	5.77540000	-0.53010000	8.17660000
11	H	3.24710000	-4.17500000	8.72650000
12	H	0.61160000	-6.65520000	10.31590000
13	H	-1.64370000	-7.57580000	10.07620000
14	H	0.12290000	-9.76940000	3.03170000
15	H	2.36090000	-8.82750000	3.33990000
16	H	-10.15040000	3.92860000	-1.73450000
17	H	-9.16390000	2.16210000	-3.09680000
18	H	3.89500000	1.63920000	-3.49250000
19	H	5.32300000	2.73990000	-1.76330000
20	H	4.42880789	3.88348835	1.88699965
21	H	5.61650101	-1.70969853	-0.58829856
22	H	4.35729450	-5.55350115	4.29819440
23	H	3.22920301	-5.21289424	-0.15129012
24	H	-5.23700000	-6.37850000	11.22840000
25	H	-7.76830000	-9.07120000	6.80850000
26	H	-6.95230000	-10.08460000	3.55430000
27	H	-10.29630000	-10.34930000	0.25900000
28	H	-2.42150000	-9.87450000	0.00040000
29	H	-3.42900000	-8.60990000	3.88980000
30	H	-4.28320000	-7.54880000	7.29620000
31	H	-3.45780000	3.89970000	-3.31080000
32	H	0.59911206	5.23699167	7.81469669
33	H	-9.79240000	-1.54060000	-3.18200000
34	H	-8.38790000	-2.95530000	10.89960000
35	H	-4.87450000	3.78240000	8.02040000
36	H	-2.02270000	2.13730000	10.92000000
37	H	-4.91220000	-7.27130000	-2.96190000
38	H	-8.98790000	-7.09310000	-2.37650000
39	H	1.45749042	-2.18459924	-2.95899853
40	H	-5.88650000	0.35320000	-2.87170000
41	H	-6.57060000	-3.25690000	-2.96870000
42	H	-11.74490000	-3.66940000	8.61800000
43	H	-9.32890000	0.16850000	8.03140000
44	H	-8.19140000	3.21540000	6.31880000

H -5.78340000 -8.84910000 -1.27830000
H -7.97590000 -9.98270000 -0.17660000
H -2.11759515 0.35869412 -2.97419684

ZH_CH3OCH3 methylation-TS
Si -0.01407207 0.03611438 -0.02388139
Si -0.06783088 -0.01010250 5.64327609
Si 3.70023438 -0.03940842 2.48991033
Si 1.04648903 -3.88520287 2.97126487
Al 0.72160554 -0.83138132 2.87263446
O 0.28765579 -2.49975110 2.80086381
O 2.41174228 -0.67788422 3.17066465
O 0.09476714 0.03098679 1.53646430
O -0.24183425 -0.06825986 4.07359144
O -1.58370954 0.13403012 -0.44336461
O -0.34740708 -1.44061469 6.32210354
O 1.37445867 0.50536980 6.17856788
O -1.23665736 1.01344181 6.03270621
O 0.80938297 1.29355214 -0.59000389
O 3.73915504 1.56708862 2.49387452
O 4.99847900 -0.48122591 3.32638284
O 2.19950982 -4.02855461 4.10610856
O 3.86950957 -0.50885277 0.94834889
O 1.77078095 -4.31531769 1.58821350
O 0.53919885 -1.29199689 -0.75843089
O -0.15643756 -4.92051133 3.33131445
H -1.90551440 0.21020821 3.60760454
C -2.85031979 -1.65038703 2.08151774
H -2.01724697 -1.95029499 2.69683797
H -2.65472373 -0.99153199 1.24729049
H -3.86397294 -1.75077302 2.43002260
O -2.84918582 0.15274633 3.33410070
C -2.67131097 -3.02142206 0.38230875
H -1.64906150 -2.82279216 0.08074453
H -3.46014071 -2.66543734 -0.27072594
C -2.95128513 -3.76232366 1.47904272
H -3.97240388 -4.02830499 1.72457381
H -2.16319621 -4.18211680 2.09409528
C -3.25729022 1.40203264 2.77860764
H -2.64680503 1.68088091 1.91431954
H -4.29990340 1.30255264 2.47231797
H -3.19002137 2.18784918 3.53610966
O 0.80120000 -6.00640000 -0.15260000

1	Si	-5.49760000	-0.02110000	-1.47430000
2	Si	-2.51930000	0.76950000	-1.59090000
3	Si	1.67080000	2.63420000	-0.36390000
4	Si	-6.77250000	-2.79180000	-1.55910000
5	Si	-6.65860000	-5.43650000	-0.02630000
6	Si	-0.62800000	-6.20850000	4.15920000
7	Si	-3.21920000	-7.43500000	2.98450000
8	Si	-6.09540000	-6.32220000	2.83000000
9	Si	-7.79180000	-8.89230000	3.21140000
10	Si	-7.85690000	-4.02790000	9.99880000
11	Si	-9.54690000	-6.64300000	10.42590000
12	O	-8.68790000	-5.35140000	10.15840000
13	Si	1.78780000	2.30220000	9.72780000
14	Si	-0.76980000	-1.62740000	10.29930000
15	Si	-1.17800000	1.38380000	9.93890000
16	O	-1.38700000	-0.16320000	10.26480000
17	O	0.35020000	1.77510000	10.12160000
18	O	-1.90930000	-2.64050000	10.65650000
19	Si	-2.31670000	-4.06080000	11.29600000
20	Si	-5.02660000	-5.18350000	10.35000000
21	O	-3.83590000	-4.30830000	10.92640000
22	O	-6.34110000	-4.27000000	10.39930000
23	Si	4.73290000	-0.80100000	7.13550000
24	Si	-7.29070000	2.20560000	5.67640000
25	Si	-4.57940000	3.32750000	6.62400000
26	Si	-1.94070000	7.20800000	6.08700000
27	Si	-4.59330000	6.04430000	5.10460000
28	O	-5.77090000	2.45290000	6.04720000
29	O	-3.26550000	2.41430000	6.57330000
30	O	-0.99450000	5.94280000	5.99240000
31	O	-3.27080000	6.91960000	5.26710000
32	O	-4.35770000	4.58890000	5.69440000
33	O	-7.46660000	2.24720000	4.09540000
34	O	-4.88400000	5.95910000	3.53970000
35	Si	-5.99570000	5.67090000	2.42990000
36	Si	-10.73910000	3.90040000	2.70070000
37	O	-11.73290000	2.70740000	2.34160000
38	Si	-12.07420000	1.15480000	2.31840000
39	O	-11.45520000	0.42330000	3.58130000
40	Si	-11.39460000	-4.15760000	7.24580000
41	Si	-13.29570000	-2.46030000	5.52120000
42	Si	-11.50890000	0.09760000	5.13610000
43	Si	-8.83680000	-0.22830000	6.67330000
44	O	-12.44950000	-3.64190000	6.15630000

1	O	-12.41530000	-1.16550000	5.38290000
2	O	-10.03410000	-0.20050000	5.63860000
3	O	-7.69650000	0.78430000	6.31660000
4	Si	-0.05970000	4.78730000	6.54670000
5	O	-10.24280000	-7.11800000	9.08650000
6	Si	-7.71660000	3.11370000	2.78820000
7	O	-6.95550000	4.50240000	2.92570000
8	O	-9.24950000	3.38730000	2.56950000
9	Si	-4.97250000	-7.60980000	-1.50390000
10	Si	-11.35590000	0.26280000	-0.54610000
11	O	-6.84510000	-7.72030000	2.70470000
12	O	-10.35620000	-0.94150000	-0.80140000
13	Si	-9.16490000	-9.40520000	0.52820000
14	Si	-9.33470000	-6.71560000	-0.96890000
15	Si	-11.54680000	-4.63200000	-1.45310000
16	Si	-9.77590000	-2.05450000	-1.77500000
17	O	-9.58580000	-8.00560000	-0.07990000
18	O	-10.67690000	-5.84320000	-0.91270000
19	O	-10.64710000	-3.36120000	-1.66840000
20	O	-8.28390000	-2.37400000	-1.34130000
21	O	-6.40440000	-3.94670000	-0.53100000
22	O	-8.15250000	-5.87130000	-0.34420000
23	O	-8.84920000	-9.23940000	2.07860000
24	O	-6.41640000	-5.42400000	1.54900000
25	O	-5.61290000	-6.41590000	-0.70840000
26	O	-5.77370000	-1.60340000	-1.35130000
27	Si	-6.81090000	-5.43360000	5.68340000
28	Si	-8.50460000	-8.00720000	6.05360000
29	O	-7.72180000	-6.63160000	6.20070000
30	Si	-10.95800000	-7.17850000	7.67890000
31	Si	-8.42890000	-3.23820000	7.03330000
32	O	-11.40780000	-5.74300000	7.18590000
33	O	-8.21960000	-1.69260000	6.70790000
34	O	-9.95660000	-3.63110000	6.85010000
35	O	-9.98360000	-7.83070000	6.60240000
36	O	-7.53000000	-4.04100000	5.99020000
37	O	-7.92320000	-3.54700000	8.50450000
38	Si	0.12320000	4.64410000	-2.14550000
39	Si	-2.82310000	3.84600000	-1.95510000
40	O	-3.94900000	0.19040000	-1.21850000
41	O	0.75700000	3.77010000	-0.98770000
42	O	-1.45550000	4.66540000	-1.97180000
43	O	-2.55350000	2.34860000	-1.50000000
44	O	-6.33220000	0.83850000	-0.42850000

1	O	-3.77030000	4.57610000	-0.90140000
2	Si	-5.28020000	4.78230000	-0.42350000
3	Si	-7.00390000	2.22870000	-0.05400000
4	Si	-9.63060000	2.52380000	-1.72000000
5	O	-6.07880000	3.41370000	-0.57020000
6	O	-8.42830000	2.36750000	-0.70540000
7	O	-10.83220000	1.58900000	-1.25000000
8	O	-5.20960000	5.26350000	1.09860000
9	O	-7.15700000	2.26930000	1.54270000
10	O	-11.46650000	0.47770000	1.01990000
11	O	-6.60040000	-5.49380000	4.09960000
12	O	-8.61720000	-8.44720000	4.51360000
13	O	-1.68270000	1.69080000	8.46850000
14	Si	-1.74890000	2.17170000	6.97410000
15	O	-0.91870000	3.49570000	6.81430000
16	Si	2.50950000	3.95250000	5.10420000
17	Si	2.56680000	1.37900000	6.82670000
18	Si	3.01120000	-3.35760000	7.49350000
19	Si	-0.01120000	-2.57100000	7.40600000
20	O	2.86460000	2.66320000	5.94590000
21	O	3.90010000	0.51780000	6.89190000
22	O	3.77240000	-1.96900000	7.63100000
23	O	1.47830000	-3.08400000	7.27480000
24	O	2.15450000	1.79120000	8.29130000
25	O	-0.24970000	-2.04670000	8.86410000
26	O	1.05380000	4.47370000	5.45680000
27	O	-1.00420000	-3.76440000	7.04720000
28	Si	0.52350000	-7.58780000	-0.03030000
29	Si	-2.45310000	-8.37930000	0.08690000
30	O	-1.02440000	-7.79970000	-0.28570000
31	O	-3.48040000	-7.82240000	-1.00870000
32	O	-2.05280000	-6.52240000	3.54850000
33	O	-4.53620000	-6.55020000	2.91500000
34	O	-2.87430000	-7.94910000	1.53380000
35	O	0.93450000	-7.98310000	1.44400000
36	O	0.37170000	-7.41290000	3.90390000
37	Si	0.95190000	-8.52590000	2.93030000
38	Si	-1.34640000	-5.31660000	7.02370000
39	Si	-4.32960000	-6.05610000	7.41270000
40	O	-2.92290000	-5.44190000	7.01850000
41	O	-5.41450000	-5.45960000	6.41750000
42	O	-4.71840000	-5.65910000	8.88780000
43	O	-1.36620000	-5.12610000	10.61890000
44	O	-0.72730000	-6.04810000	8.28660000

1	Si	-0.78110000	-6.37380000	9.84140000
2	Si	4.19140000	1.79570000	-2.03280000
3	Si	4.36130000	-0.89370000	-0.53530000
4	Si	1.79920000	-4.81760000	0.05470000
5	Si	1.68560000	-2.17100000	-1.47840000
6	Si	3.22760000	3.05990000	2.24000000
7	Si	5.44840000	-1.68950000	4.28210000
8	Si	3.72400000	-4.24270000	4.65120000
9	O	4.61250000	0.39620000	-1.42440000
10	O	1.43070000	-3.66260000	-0.97320000
11	O	3.17930000	-1.73820000	-1.16020000
12	O	4.64910000	-3.05760000	4.13510000
13	O	2.93740000	2.40540000	-1.28810000
14	O	2.15410000	3.10990000	1.07330000
15	O	2.54300000	3.62280000	3.55350000
16	O	5.51820000	-1.20770000	5.80380000
17	O	3.57090000	-4.20200000	6.24790000
18	O	-0.73790000	-5.99420000	5.72550000
19	H	-1.30770000	8.45280000	5.54490000
20	H	3.53900000	4.98890000	5.43620000
21	H	-5.91550000	5.84190000	-1.27060000
22	H	-6.78570000	6.92250000	2.19890000
23	H	-12.70540000	-0.03450000	-1.12450000
24	H	-13.56750000	1.03610000	2.31350000
25	H	-12.61360000	-4.36250000	-0.43650000
26	H	-12.17550000	-5.02190000	-2.75570000
27	H	-14.47190000	-2.17020000	6.40220000
28	H	-13.77040000	-2.92530000	4.17860000
29	H	6.86450000	-1.88260000	3.83330000
30	H	-2.15040000	-4.10050000	12.78420000
31	H	1.31010000	-8.39770000	-1.01480000
32	H	-12.21020000	-7.97290000	7.89080000
33	H	0.36340000	-1.65380000	11.27870000
34	H	0.62130000	6.05740000	-2.14750000
35	H	0.50140000	4.07440000	-3.47820000
36	H	-2.25700000	7.49990000	7.52180000
37	H	-5.73850000	6.73170000	5.78280000
38	H	-10.96700000	4.40130000	4.09400000
39	H	-11.01960000	5.00810000	1.73210000
40	H	-12.06290000	1.27880000	5.87220000
41	H	-10.59640000	-6.34750000	11.45320000
42	H	-8.66420000	-7.73420000	10.94950000
43	H	2.77450000	1.81970000	10.74640000
44	H	1.80020000	3.79900000	9.78440000

H 5.77540000 -0.53010000 8.17660000
H 3.24710000 -4.17500000 8.72650000
H 0.61160000 -6.65520000 10.31590000
H -1.64370000 -7.57580000 10.07620000
H 0.12290000 -9.76940000 3.03170000
H 2.36090000 -8.82750000 3.33990000
H -10.15040000 3.92860000 -1.73450000
H -9.16390000 2.16210000 -3.09680000
H 3.89500000 1.63920000 -3.49250000
H 5.32300000 2.73990000 -1.76330000
H 4.42880000 3.88350000 1.88710000
H 5.61650000 -1.70970000 -0.58830000
H 4.35730000 -5.55350000 4.29820000
H 3.22920000 -5.21290000 -0.15130000
H -5.23700000 -6.37850000 11.22840000
H -7.76830000 -9.07120000 6.80850000
H -6.95230000 -10.08460000 3.55430000
H -10.29630000 -10.34930000 0.25900000
H -2.42150000 -9.87450000 0.00040000
H -3.42900000 -8.60990000 3.88980000
H -4.28320000 -7.54880000 7.29620000
H -3.45780000 3.89970000 -3.31080000
H 0.59910000 5.23700000 7.81470000
H -9.79240000 -1.54060000 -3.18200000
H -8.38790000 -2.95530000 10.89960000
H -4.87450000 3.78240000 8.02040000
H -2.02270000 2.13730000 10.92000000
H -4.91220000 -7.27130000 -2.96190000
H -8.98790000 -7.09310000 -2.37650000
H 1.45740000 -2.18480000 -2.95900000
H -5.88650000 0.35320000 -2.87170000
H -6.57060000 -3.25690000 -2.96870000
H -11.74490000 -3.66940000 8.61800000
H -9.32890000 0.16850000 8.03140000
H -8.19140000 3.21540000 6.31880000
H -5.78340000 -8.84910000 -1.27830000
H -7.97590000 -9.98270000 -0.17660000
H -2.11770000 0.35870000 -2.97420000

ZH_CH3OCH3(ads)
Si -0.02613785 0.01581561 -0.03129730
Si -0.06223619 -0.00554697 5.65291859
Si 3.69507587 -0.06273632 2.48955992

1	Si	1.04723944	-3.89704611	2.98567722
2	Al	0.73357958	-0.83087658	2.89580465
3	O	0.18547908	-2.51571632	2.95353826
4	O	2.43431963	-0.82025158	3.11688072
5	O	0.07403490	-0.09222176	1.52597703
6	O	-0.16775113	-0.00406776	4.08056087
7	O	-1.58661111	0.17892134	-0.41935509
8	O	-0.35338882	-1.46628060	6.28594546
9	O	1.37781520	0.47985001	6.21418274
10	O	-1.24807119	0.98205502	6.06129769
11	O	0.82838839	1.28174653	-0.52591033
12	O	3.65318475	1.54119632	2.53317169
13	O	4.99323061	-0.46852098	3.34331273
14	O	2.20342060	-4.01003200	4.10120830
15	O	3.89798436	-0.49224235	0.94739567
16	O	1.72972018	-4.21696090	1.56481102
17	O	0.52887643	-1.28060046	-0.80594558
18	O	-0.13259466	-4.93795827	3.32636393
19	O	0.80121744	-6.00640771	-0.15263481
20	Si	-5.49759808	-0.02110766	-1.47430478
21	Si	-2.51946341	0.76949321	-1.59089789
22	Si	1.67328251	2.63518983	-0.36439390
23	Si	-6.77250000	-2.79180000	-1.55910000
24	Si	-6.65860000	-5.43650000	-0.02630000
25	Si	-0.62812891	-6.20850638	4.15930299
26	Si	-3.21920499	-7.43500076	2.98451252
27	Si	-6.09540000	-6.32220000	2.83000000
28	Si	-7.79180000	-8.89230000	3.21140000
29	Si	-7.85690000	-4.02790000	9.99880000
30	Si	-9.54690000	-6.64300000	10.42590000
31	O	-8.68790000	-5.35140000	10.15840000
32	Si	1.78780000	2.30220000	9.72780000
33	Si	-0.76979190	-1.62742340	10.29930968
34	Si	-1.17799903	1.38379779	9.93889924
35	O	-1.38700000	-0.16320000	10.26480000
36	O	0.35020000	1.77510000	10.12160000
37	O	-1.90930000	-2.64050000	10.65650000
38	Si	-2.31670000	-4.06080000	11.29600000
39	Si	-5.02660000	-5.18350000	10.35000000
40	O	-3.83590000	-4.30830000	10.92640000
41	O	-6.34110000	-4.27000000	10.39930000
42	Si	4.73289898	-0.80101067	7.13548774
43	Si	-7.29070000	2.20560000	5.67640000
44	Si	-4.57939981	3.32750131	6.62399946

1	Si	-1.94070000	7.20800000	6.08700000
2	Si	-4.59330000	6.04430000	5.10460000
3	O	-5.77090000	2.45290000	6.04720000
4	O	-3.26560134	2.41449848	6.57330596
5	O	-0.99450000	5.94280000	5.99240000
6	O	-3.27080000	6.91960000	5.26710000
7	O	-4.35770000	4.58890000	5.69440000
8	O	-7.46660000	2.24720000	4.09540000
9	O	-4.88400000	5.95910000	3.53970000
10	Si	-5.99570000	5.67090000	2.42990000
11	Si	-10.73910000	3.90040000	2.70070000
12	O	-11.73290000	2.70740000	2.34160000
13	Si	-12.07420000	1.15480000	2.31840000
14	O	-11.45520000	0.42330000	3.58130000
15	Si	-11.39460000	-4.15760000	7.24580000
16	Si	-13.29570000	-2.46030000	5.52120000
17	Si	-11.50890000	0.09760000	5.13610000
18	Si	-8.83680000	-0.22830000	6.67330000
19	O	-12.44950000	-3.64190000	6.15630000
20	O	-12.41530000	-1.16550000	5.38290000
21	O	-10.03410000	-0.20050000	5.63860000
22	O	-7.69650000	0.78430000	6.31660000
23	Si	-0.05970000	4.78730000	6.54670000
24	O	-10.24280000	-7.11800000	9.08650000
25	Si	-7.71660000	3.11370000	2.78820000
26	O	-6.95550000	4.50240000	2.92570000
27	O	-9.24950000	3.38730000	2.56950000
28	Si	-4.97250000	-7.60980000	-1.50390000
29	Si	-11.35590000	0.26280000	-0.54610000
30	O	-6.84510000	-7.72030000	2.70470000
31	O	-10.35620000	-0.94150000	-0.80140000
32	Si	-9.16490000	-9.40520000	0.52820000
33	Si	-9.33470000	-6.71560000	-0.96890000
34	Si	-11.54680000	-4.63200000	-1.45310000
35	Si	-9.77590000	-2.05450000	-1.77500000
36	O	-9.58580000	-8.00560000	-0.07990000
37	O	-10.67690000	-5.84320000	-0.91270000
38	O	-10.64710000	-3.36120000	-1.66840000
39	O	-8.28390000	-2.37400000	-1.34130000
40	O	-6.40440000	-3.94670000	-0.53100000
41	O	-8.15250000	-5.87130000	-0.34420000
42	O	-8.84920000	-9.23940000	2.07860000
43	O	-6.41640000	-5.42400000	1.54900000
44	O	-5.61290000	-6.41590000	-0.70840000

1	O	-5.77370000	-1.60340000	-1.35130000
2	Si	-6.81090000	-5.43360000	5.68340000
3	Si	-8.50460000	-8.00720000	6.05360000
4	O	-7.72180000	-6.63160000	6.20070000
5	Si	-10.95800000	-7.17850000	7.67890000
6	Si	-8.42890000	-3.23820000	7.03330000
7	O	-11.40780000	-5.74300000	7.18590000
8	O	-8.21960000	-1.69260000	6.70790000
9	O	-9.95660000	-3.63110000	6.85010000
10	O	-9.98360000	-7.83070000	6.60240000
11	O	-7.53000000	-4.04100000	5.99020000
12	O	-7.92320000	-3.54700000	8.50450000
13	Si	0.12369555	4.64449574	-2.14540116
14	Si	-2.82297698	3.84600105	-1.95511044
15	O	-3.94890385	0.19041340	-1.21849238
16	O	0.75581115	3.76930865	-0.98750082
17	O	-1.45550000	4.66540000	-1.97180000
18	O	-2.55364910	2.34859792	-1.49988042
19	O	-6.33220000	0.83850000	-0.42850000
20	O	-3.77030000	4.57610000	-0.90140000
21	Si	-5.28020000	4.78230000	-0.42350000
22	Si	-7.00390000	2.22870000	-0.05400000
23	Si	-9.63060000	2.52380000	-1.72000000
24	O	-6.07880000	3.41370000	-0.57020000
25	O	-8.42830000	2.36750000	-0.70540000
26	O	-10.83220000	1.58900000	-1.25000000
27	O	-5.20960000	5.26350000	1.09860000
28	O	-7.15700000	2.26930000	1.54270000
29	O	-11.46650000	0.47770000	1.01990000
30	O	-6.60040000	-5.49380000	4.09960000
31	O	-8.61720000	-8.44720000	4.51360000
32	O	-1.68270166	1.69080574	8.46850162
33	Si	-1.74889231	2.17159531	6.97408584
34	O	-0.91870219	3.49570217	6.81430339
35	Si	2.50949686	3.95248597	5.10418662
36	Si	2.56679414	1.37877320	6.82675340
37	Si	3.01120371	-3.35757811	7.49348449
38	Si	-0.01130049	-2.57110531	7.40598159
39	O	2.86460191	2.66322165	5.94603271
40	O	3.90010513	0.51780923	6.89193227
41	O	3.77240000	-1.96900000	7.63100000
42	O	1.47828926	-3.08404095	7.27483691
43	O	2.15450189	1.79120276	8.29130004
44	O	-0.24971037	-2.04665225	8.86408064

1	O	1.05380000	4.47370000	5.45680000
2	O	-1.00419702	-3.76440134	7.04719667
3	Si	0.52349343	-7.58779679	-0.03028251
4	Si	-2.45310000	-8.37930000	0.08690000
5	O	-1.02440000	-7.79970000	-0.28570000
6	O	-3.48040000	-7.82240000	-1.00870000
7	O	-2.05278990	-6.52240056	3.54847372
8	O	-4.53619700	-6.55019500	2.91500300
9	O	-2.87430000	-7.94910000	1.53380000
10	O	0.93450000	-7.98310000	1.44400000
11	O	0.37159989	-7.41289829	3.90389614
12	Si	0.95189857	-8.52590140	2.93030020
13	Si	-1.34641393	-5.31661365	7.02370355
14	Si	-4.32960000	-6.05610000	7.41270000
15	O	-2.92290000	-5.44190000	7.01850000
16	O	-5.41450000	-5.45960000	6.41750000
17	O	-4.71840000	-5.65910000	8.88780000
18	O	-1.36620000	-5.12610000	10.61890000
19	O	-0.72730000	-6.04810000	8.28660000
20	Si	-0.78110000	-6.37380000	9.84140000
21	Si	4.19159548	1.79579498	-2.03250969
22	Si	4.36129451	-0.89370411	-0.53530982
23	Si	1.79904667	-4.81756964	0.05486585
24	Si	1.68496301	-2.17148445	-1.47837325
25	Si	3.22789074	3.06048787	2.23970548
26	Si	5.44849347	-1.68950661	4.28210089
27	Si	3.72401569	-4.24269921	4.65120945
28	O	4.61250892	0.39620888	-1.42438420
29	O	1.43106507	-3.66272893	-0.97335371
30	O	3.17920091	-1.73800066	-1.16010492
31	O	4.64901124	-3.05760638	4.13510306
32	O	2.93690210	2.40530163	-1.28879759
33	O	2.15281245	3.10901298	1.07409009
34	O	2.54300501	3.62291013	3.55349761
35	O	5.51820082	-1.20778476	5.80379525
36	O	3.57090126	-4.20199916	6.24789986
37	O	-0.73786595	-5.99417742	5.72549979
38	H	-1.30770000	8.45280000	5.54490000
39	H	3.53900000	4.98890000	5.43620000
40	H	-5.91550000	5.84190000	-1.27060000
41	H	-6.78570000	6.92250000	2.19890000
42	H	-12.70540000	-0.03450000	-1.12450000
43	H	-13.56750000	1.03610000	2.31350000
44	H	-12.61360000	-4.36250000	-0.43650000

1	H	-12.17550000	-5.02190000	-2.75570000
2	H	-14.47190000	-2.17020000	6.40220000
3	H	-13.77040000	-2.92530000	4.17860000
4	H	6.86450001	-1.88260006	3.83330105
5	H	-2.15040000	-4.10050000	12.78420000
6	H	1.31010000	-8.39770000	-1.01480000
7	H	-12.21020000	-7.97290000	7.89080000
8	H	0.36340000	-1.65380000	11.27870000
9	H	0.62130000	6.05740000	-2.14750000
10	H	0.50140000	4.07440000	-3.47820000
11	H	-2.25700000	7.49990000	7.52180000
12	H	-5.73850000	6.73170000	5.78280000
13	H	-10.96700000	4.40130000	4.09400000
14	H	-11.01960000	5.00810000	1.73210000
15	H	-12.06290000	1.27880000	5.87220000
16	H	-10.59640000	-6.34750000	11.45320000
17	H	-8.66420000	-7.73420000	10.94950000
18	H	2.77450000	1.81970000	10.74640000
19	H	1.80020000	3.79900000	9.78440000
20	H	5.77540000	-0.53010000	8.17660000
21	H	3.24710000	-4.17500000	8.72650000
22	H	0.61160000	-6.65520000	10.31590000
23	H	-1.64370000	-7.57580000	10.07620000
24	H	0.12290000	-9.76940000	3.03170000
25	H	2.36090000	-8.82750000	3.33990000
26	H	-10.15040000	3.92860000	-1.73450000
27	H	-9.16390000	2.16210000	-3.09680000
28	H	3.89500000	1.63920000	-3.49250000
29	H	5.32300000	2.73990000	-1.76330000
30	H	4.42879892	3.88350109	1.88699992
31	H	5.61650000	-1.70969999	-0.58830005
32	H	4.35729794	-5.55350105	4.29819807
33	H	3.22919791	-5.21290319	-0.15130628
34	H	-5.23700000	-6.37850000	11.22840000
35	H	-7.76830000	-9.07120000	6.80850000
36	H	-6.95230000	-10.08460000	3.55430000
37	H	-10.29630000	-10.34930000	0.25900000
38	H	-2.42150000	-9.87450000	0.00040000
39	H	-3.42900000	-8.60990000	3.88980000
40	H	-4.28320000	-7.54880000	7.29620000
41	H	-3.45780000	3.89970000	-3.31080000
42	H	0.59910000	5.23700000	7.81470000
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 4  H   -8.98790000   -7.09310000   -2.37650000
 5  H   1.45750003    -2.18460215   -2.95900000
 6  H   -5.88650000   0.35320000    -2.87170000
 7  H   -6.57060000   -3.25690000   -2.96870000
 8  H   -11.74490000 -3.66940000   8.61800000
 9  H   -9.32890000   0.16850000    8.03140000
10  H   -8.19140000   3.21540000    6.31880000
11  H   -5.78340000   -8.84910000   -1.27830000
12  H   -7.97590000   -9.98270000   -0.17660000
13  H   -2.11760336   0.35870104    -2.97420012
14  H   -1.80210658   0.69421197    3.24038248
15  C   -2.83563147   -2.48407208   1.64999286
16  H   -3.80580803   -2.97617874   1.61127314
17  H   -2.16090201   -2.91505659   0.91467044
18  H   -2.92218575   -1.40662397   1.53042810
19  O   -2.64732886   0.73299899    2.76239243
20  H   -2.37920551   0.89598351    1.85190185
21  C   -2.98560136   -2.22288928   4.10510087
22  H   -3.90123186   -2.80438555   4.19957016
23  H   -3.18543742   -1.16851074   3.91873442
24  H   -2.34436342   -2.36560655   4.97057778
25  O   -2.25278068   -2.77160356   2.95858465
26  H   -1.17131069   -2.64341479   2.98707247
27
28
29  ZH_CH3OCH3(ads)_C2H4(ads)
30  Si -0.03078495   0.02742851    -0.00865315
31  Si -0.06811990   -0.00537736   5.67749864
32  Si 3.71157761    -0.01854642   2.48711380
33  Si 1.04803504    -3.90066058   2.98002122
34  Al 0.75231754    -0.85384260   2.82922828
35  O   0.32285063    -2.49143182   2.92448538
36  O   2.39933994    -0.57887541   3.20429058
37  O   0.04222104    0.02627017    1.56471079
38  O   -0.26339365   -0.04623170   4.06054008
39  O   -1.57637974   0.16498807    -0.44254203
40  O   -0.34546205   -1.44058443   6.30746403
41  O   1.37842469    0.51074769    6.14273407
42  O   -1.23860415   1.02091325    6.01097671
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4	O	1.76469070	-4.27187113	1.57814836
5	O	0.57597510	-1.27745180	-0.72682129
6	O	-0.13879633	-4.93464056	3.32987686
7	H	-1.27627931	0.12860082	3.70706040
8	C	-3.08372802	-0.93966469	2.62311666
9	H	-2.56645488	-1.80711620	3.02740894
10	H	-2.87980994	-0.85320713	1.55560624
11	H	-4.15690144	-1.02179074	2.80879691
12	O	-2.57520619	0.21356745	3.32782102
13	C	-2.51609995	-3.69056569	-0.45232328
14	H	-1.48304098	-3.80046845	-0.76217431
15	H	-3.21915934	-3.34860385	-1.20428249
16	C	-2.90821896	-3.95533320	0.78931479
17	H	-3.94542474	-3.84673589	1.08795051
18	H	-2.21145060	-4.28782259	1.55137643
19	C	-3.04231424	1.46758191	2.81637081
20	H	-2.70467983	1.60829646	1.78730398
21	H	-4.13377837	1.48969971	2.86438680
22	H	-2.63380951	2.24551981	3.45826218
23	O	0.80120000	-6.00640000	-0.15260000
24	Si	-5.49760000	-0.02110000	-1.47430000
25	Si	-2.51930000	0.76950000	-1.59090000
26	Si	1.67080000	2.63420000	-0.36390000
27	Si	-6.77250000	-2.79180000	-1.55910000
28	Si	-6.65860000	-5.43650000	-0.02630000
29	Si	-0.62800000	-6.20850000	4.15920000
30	Si	-3.21920000	-7.43500000	2.98450000
31	Si	-6.09540000	-6.32220000	2.83000000
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35	O	-8.68790000	-5.35140000	10.15840000
36	Si	1.78780000	2.30220000	9.72780000
37	Si	-0.76980000	-1.62740000	10.29930000
38	Si	-1.17800000	1.38380000	9.93890000
39	O	-1.38700000	-0.16320000	10.26480000
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41	O	-1.90930000	-2.64050000	10.65650000
42	Si	-2.31670000	-4.06080000	11.29600000
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44	O	-3.83590000	-4.30830000	10.92640000

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4	Si	-4.57940000	3.32750000	6.62400000
5	Si	-1.94070000	7.20800000	6.08700000
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7	O	-5.77090000	2.45290000	6.04720000
8	O	-3.26550000	2.41430000	6.57330000
9	O	-0.99450000	5.94280000	5.99240000
10	O	-3.27080000	6.91960000	5.26710000
11	O	-4.35770000	4.58890000	5.69440000
12	O	-7.46660000	2.24720000	4.09540000
13	O	-4.88400000	5.95910000	3.53970000
14	Si	-5.99570000	5.67090000	2.42990000
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16	O	-11.73290000	2.70740000	2.34160000
17	Si	-12.07420000	1.15480000	2.31840000
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19	Si	-11.39460000	-4.15760000	7.24580000
20	Si	-13.29570000	-2.46030000	5.52120000
21	Si	-11.50890000	0.09760000	5.13610000
22	Si	-8.83680000	-0.22830000	6.67330000
23	O	-12.44950000	-3.64190000	6.15630000
24	O	-12.41530000	-1.16550000	5.38290000
25	O	-10.03410000	-0.20050000	5.63860000
26	O	-7.69650000	0.78430000	6.31660000
27	Si	-0.05970000	4.78730000	6.54670000
28	O	-10.24280000	-7.11800000	9.08650000
29	Si	-7.71660000	3.11370000	2.78820000
30	O	-6.95550000	4.50240000	2.92570000
31	O	-9.24950000	3.38730000	2.56950000
32	Si	-4.97250000	-7.60980000	-1.50390000
33	Si	-11.35590000	0.26280000	-0.54610000
34	O	-6.84510000	-7.72030000	2.70470000
35	O	-10.35620000	-0.94150000	-0.80140000
36	Si	-9.16490000	-9.40520000	0.52820000
37	Si	-9.33470000	-6.71560000	-0.96890000
38	Si	-11.54680000	-4.63200000	-1.45310000
39	Si	-9.77590000	-2.05450000	-1.77500000
40	O	-9.58580000	-8.00560000	-0.07990000
41	O	-10.67690000	-5.84320000	-0.91270000
42	O	-10.64710000	-3.36120000	-1.66840000
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1	O	-8.15250000	-5.87130000	-0.34420000
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3	O	-6.41640000	-5.42400000	1.54900000
4	O	-5.61290000	-6.41590000	-0.70840000
5	O	-5.77370000	-1.60340000	-1.35130000
6	Si	-6.81090000	-5.43360000	5.68340000
7	Si	-8.50460000	-8.00720000	6.05360000
8	O	-7.72180000	-6.63160000	6.20070000
9	Si	-10.95800000	-7.17850000	7.67890000
10	Si	-8.42890000	-3.23820000	7.03330000
11	O	-11.40780000	-5.74300000	7.18590000
12	O	-8.21960000	-1.69260000	6.70790000
13	O	-9.95660000	-3.63110000	6.85010000
14	O	-9.98360000	-7.83070000	6.60240000
15	O	-7.53000000	-4.04100000	5.99020000
16	O	-7.92320000	-3.54700000	8.50450000
17	Si	0.12320000	4.64410000	-2.14550000
18	Si	-2.82310000	3.84600000	-1.95510000
19	O	-3.94900000	0.19040000	-1.21850000
20	O	0.75700000	3.77010000	-0.98770000
21	O	-1.45550000	4.66540000	-1.97180000
22	O	-2.55350000	2.34860000	-1.50000000
23	O	-6.33220000	0.83850000	-0.42850000
24	O	-3.77030000	4.57610000	-0.90140000
25	Si	-5.28020000	4.78230000	-0.42350000
26	Si	-7.00390000	2.22870000	-0.05400000
27	Si	-9.63060000	2.52380000	-1.72000000
28	O	-6.07880000	3.41370000	-0.57020000
29	O	-8.42830000	2.36750000	-0.70540000
30	O	-10.83220000	1.58900000	-1.25000000
31	O	-5.20960000	5.26350000	1.09860000
32	O	-7.15700000	2.26930000	1.54270000
33	O	-11.46650000	0.47770000	1.01990000
34	O	-6.60040000	-5.49380000	4.09960000
35	O	-8.61720000	-8.44720000	4.51360000
36	O	-1.68270000	1.69080000	8.46850000
37	Si	-1.74890000	2.17170000	6.97410000
38	O	-0.91870000	3.49570000	6.81430000
39	Si	2.50950000	3.95250000	5.10420000
40	Si	2.56680000	1.37900000	6.82670000
41	Si	3.01120000	-3.35760000	7.49350000
42	Si	-0.01120000	-2.57100000	7.40600000
43	O	2.86460000	2.66320000	5.94590000
44	O	3.90010000	0.51780000	6.89190000

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4	O	-0.24970000	-2.04670000	8.86410000
5	O	1.05380000	4.47370000	5.45680000
6	O	-1.00420000	-3.76440000	7.04720000
7	Si	0.52350000	-7.58780000	-0.03030000
8	Si	-2.45310000	-8.37930000	0.08690000
9	O	-1.02440000	-7.79970000	-0.28570000
10	O	-3.48040000	-7.82240000	-1.00870000
11	O	-2.05280000	-6.52240000	3.54850000
12	O	-4.53620000	-6.55020000	2.91500000
13	O	-2.87430000	-7.94910000	1.53380000
14	O	0.93450000	-7.98310000	1.44400000
15	O	0.37170000	-7.41290000	3.90390000
16	Si	0.95190000	-8.52590000	2.93030000
17	Si	-1.34640000	-5.31660000	7.02370000
18	Si	-4.32960000	-6.05610000	7.41270000
19	O	-2.92290000	-5.44190000	7.01850000
20	O	-5.41450000	-5.45960000	6.41750000
21	O	-4.71840000	-5.65910000	8.88780000
22	O	-1.36620000	-5.12610000	10.61890000
23	O	-0.72730000	-6.04810000	8.28660000
24	Si	-0.78110000	-6.37380000	9.84140000
25	Si	4.19140000	1.79570000	-2.03280000
26	Si	4.36130000	-0.89370000	-0.53530000
27	Si	1.79920000	-4.81760000	0.05470000
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31	Si	3.72400000	-4.24270000	4.65120000
32	O	4.61250000	0.39620000	-1.42440000
33	O	1.43070000	-3.66260000	-0.97320000
34	O	3.17930000	-1.73820000	-1.16020000
35	O	4.64910000	-3.05760000	4.13510000
36	O	2.93740000	2.40540000	-1.28810000
37	O	2.15410000	3.10990000	1.07330000
38	O	2.54300000	3.62280000	3.55350000
39	O	5.51820000	-1.20770000	5.80380000
40	O	3.57090000	-4.20200000	6.24790000
41	O	-0.73790000	-5.99420000	5.72550000
42	H	-1.30770000	8.45280000	5.54490000
43	H	3.53900000	4.98890000	5.43620000
44	H	-5.91550000	5.84190000	-1.27060000

1	H	-6.78570000	6.92250000	2.19890000
2	H	-12.70540000	-0.03450000	-1.12450000
3	H	-13.56750000	1.03610000	2.31350000
4	H	-12.61360000	-4.36250000	-0.43650000
5	H	-12.17550000	-5.02190000	-2.75570000
6	H	-14.47190000	-2.17020000	6.40220000
7	H	-13.77040000	-2.92530000	4.17860000
8	H	6.86450000	-1.88260000	3.83330000
9	H	-2.15040000	-4.10050000	12.78420000
10	H	1.31010000	-8.39770000	-1.01480000
11	H	-12.21020000	-7.97290000	7.89080000
12	H	0.36340000	-1.65380000	11.27870000
13	H	0.62130000	6.05740000	-2.14750000
14	H	0.50140000	4.07440000	-3.47820000
15	H	-2.25700000	7.49990000	7.52180000
16	H	-5.73850000	6.73170000	5.78280000
17	H	-10.96700000	4.40130000	4.09400000
18	H	-11.01960000	5.00810000	1.73210000
19	H	-12.06290000	1.27880000	5.87220000
20	H	-10.59640000	-6.34750000	11.45320000
21	H	-8.66420000	-7.73420000	10.94950000
22	H	2.77450000	1.81970000	10.74640000
23	H	1.80020000	3.79900000	9.78440000
24	H	5.77540000	-0.53010000	8.17660000
25	H	3.24710000	-4.17500000	8.72650000
26	H	0.61160000	-6.65520000	10.31590000
27	H	-1.64370000	-7.57580000	10.07620000
28	H	0.12290000	-9.76940000	3.03170000
29	H	2.36090000	-8.82750000	3.33990000
30	H	-10.15040000	3.92860000	-1.73450000
31	H	-9.16390000	2.16210000	-3.09680000
32	H	3.89500000	1.63920000	-3.49250000
33	H	5.32300000	2.73990000	-1.76330000
34	H	4.42880000	3.88350000	1.88710000
35	H	5.61650000	-1.70970000	-0.58830000
36	H	4.35730000	-5.55350000	4.29820000
37	H	3.22920000	-5.21290000	-0.15130000
38	H	-5.23700000	-6.37850000	11.22840000
39	H	-7.76830000	-9.07120000	6.80850000
40	H	-6.95230000	-10.08460000	3.55430000
41	H	-10.29630000	-10.34930000	0.25900000
42	H	-2.42150000	-9.87450000	0.00040000
43	H	-3.42900000	-8.60990000	3.88980000
44	H	-4.28320000	-7.54880000	7.29620000

1	H	-3.45780000	3.89970000	-3.31080000
2	H	0.59910000	5.23700000	7.81470000
3	H	-9.79240000	-1.54060000	-3.18200000
4	H	-8.38790000	-2.95530000	10.89960000
5	H	-4.87450000	3.78240000	8.02040000
6	H	-2.02270000	2.13730000	10.92000000
7	H	-4.91220000	-7.27130000	-2.96190000
8	H	-8.98790000	-7.09310000	-2.37650000
9	H	1.45740000	-2.18480000	-2.95900000
10	H	-5.88650000	0.35320000	-2.87170000
11	H	-6.57060000	-3.25690000	-2.96870000
12	H	-11.74490000	-3.66940000	8.61800000
13	H	-9.32890000	0.16850000	8.03140000
14	H	-8.19140000	3.21540000	6.31880000
15	H	-5.78340000	-8.84910000	-1.27830000
16	H	-7.97590000	-9.98270000	-0.17660000
17	H	-2.11770000	0.35870000	-2.97420000
18				
19				
20	ZH_CH3OH methylation-TS			
21	Si	-0.03067447	0.03068934	-0.00560284
22	Si	-0.07262076	-0.01232543	5.64667305
23	Si	3.70055727	-0.03254642	2.48284107
24	Si	1.05403147	-3.89298510	2.96185479
25	Al	0.70417282	-0.84860314	2.84754657
26	O	0.29374183	-2.51427730	2.74332538
27	O	2.39059972	-0.66341534	3.12221622
28	O	-0.02331866	0.07012562	1.57479645
29	O	-0.22087324	-0.12431939	4.08905567
30	O	-1.58227919	0.12109565	-0.45726883
31	O	-0.38587675	-1.42134533	6.35596561
32	O	1.35733714	0.51267275	6.19975546
33	O	-1.25763073	1.03447254	5.97983366
34	O	0.81336955	1.28827854	-0.54171889
35	O	3.74753682	1.57256299	2.50125397
36	O	4.98170448	-0.48003700	3.33930047
37	O	2.20069936	-4.00569782	4.11017928
38	O	3.88428723	-0.49617951	0.94578007
39	O	1.79652673	-4.34836889	1.59942173
40	O	0.58967020	-1.28260915	-0.69416868
41	O	-0.14906996	-4.91071980	3.35602959
42	H	-2.07962812	1.27129998	3.74407432
43	C	-3.01973420	-0.82681276	2.61719580
44	H	-3.96144111	-0.50403972	3.02774114

1	H	-2.20177605	-1.05795129	3.28326125
2	H	-2.80438034	-0.69016815	1.57028315
3	O	-2.32521438	1.23155649	2.80691768
4	C	-3.10942862	-3.04566031	2.87669727
5	H	-3.40740062	-3.12300794	3.91699521
6	H	-2.07851853	-3.29397719	2.64760769
7	C	-4.01123763	-2.72815233	1.92103768
8	H	-3.74913462	-2.72506094	0.86985977
9	H	-5.05447335	-2.55708349	2.15882410
10	H	-1.46554801	1.03935295	2.37853229
11	O	0.80120000	-6.00640000	-0.15260000
12	Si	-5.49760000	-0.02110000	-1.47430000
13	Si	-2.51930000	0.76950000	-1.59090000
14	Si	1.67080000	2.63420000	-0.36390000
15	Si	-6.77250000	-2.79180000	-1.55910000
16	Si	-6.65860000	-5.43650000	-0.02630000
17	Si	-0.62800000	-6.20850000	4.15920000
18	Si	-3.21920000	-7.43500000	2.98450000
19	Si	-6.09540000	-6.32220000	2.83000000
20	Si	-7.79180000	-8.89230000	3.21140000
21	Si	-7.85690000	-4.02790000	9.99880000
22	Si	-9.54690000	-6.64300000	10.42590000
23	O	-8.68790000	-5.35140000	10.15840000
24	Si	1.78780000	2.30220000	9.72780000
25	Si	-0.76980000	-1.62740000	10.29930000
26	Si	-1.17800000	1.38380000	9.93890000
27	O	-1.38700000	-0.16320000	10.26480000
28	O	0.35020000	1.77510000	10.12160000
29	O	-1.90930000	-2.64050000	10.65650000
30	Si	-2.31670000	-4.06080000	11.29600000
31	Si	-5.02660000	-5.18350000	10.35000000
32	O	-3.83590000	-4.30830000	10.92640000
33	O	-6.34110000	-4.27000000	10.39930000
34	Si	4.73290000	-0.80100000	7.13550000
35	Si	-7.29070000	2.20560000	5.67640000
36	Si	-4.57940000	3.32750000	6.62400000
37	Si	-1.94070000	7.20800000	6.08700000
38	Si	-4.59330000	6.04430000	5.10460000
39	O	-5.77090000	2.45290000	6.04720000
40	O	-3.26550000	2.41430000	6.57330000
41	O	-0.99450000	5.94280000	5.99240000
42	O	-3.27080000	6.91960000	5.26710000
43	O	-4.35770000	4.58890000	5.69440000
44	O	-7.46660000	2.24720000	4.09540000

1	O	-4.88400000	5.95910000	3.53970000
2	Si	-5.99570000	5.67090000	2.42990000
3	Si	-10.73910000	3.90040000	2.70070000
4	O	-11.73290000	2.70740000	2.34160000
5	Si	-12.07420000	1.15480000	2.31840000
6	O	-11.45520000	0.42330000	3.58130000
7	Si	-11.39460000	-4.15760000	7.24580000
8	Si	-13.29570000	-2.46030000	5.52120000
9	Si	-11.50890000	0.09760000	5.13610000
10	Si	-8.83680000	-0.22830000	6.67330000
11	O	-12.44950000	-3.64190000	6.15630000
12	O	-12.41530000	-1.16550000	5.38290000
13	O	-10.03410000	-0.20050000	5.63860000
14	O	-7.69650000	0.78430000	6.31660000
15	Si	-0.05970000	4.78730000	6.54670000
16	O	-10.24280000	-7.11800000	9.08650000
17	Si	-7.71660000	3.11370000	2.78820000
18	O	-6.95550000	4.50240000	2.92570000
19	O	-9.24950000	3.38730000	2.56950000
20	Si	-4.97250000	-7.60980000	-1.50390000
21	Si	-11.35590000	0.26280000	-0.54610000
22	O	-6.84510000	-7.72030000	2.70470000
23	O	-10.35620000	-0.94150000	-0.80140000
24	Si	-9.16490000	-9.40520000	0.52820000
25	Si	-9.33470000	-6.71560000	-0.96890000
26	Si	-11.54680000	-4.63200000	-1.45310000
27	Si	-9.77590000	-2.05450000	-1.77500000
28	O	-9.58580000	-8.00560000	-0.07990000
29	O	-10.67690000	-5.84320000	-0.91270000
30	O	-10.64710000	-3.36120000	-1.66840000
31	O	-8.28390000	-2.37400000	-1.34130000
32	O	-6.40440000	-3.94670000	-0.53100000
33	O	-8.15250000	-5.87130000	-0.34420000
34	O	-8.84920000	-9.23940000	2.07860000
35	O	-6.41640000	-5.42400000	1.54900000
36	O	-5.61290000	-6.41590000	-0.70840000
37	O	-5.77370000	-1.60340000	-1.35130000
38	Si	-6.81090000	-5.43360000	5.68340000
39	Si	-8.50460000	-8.00720000	6.05360000
40	O	-7.72180000	-6.63160000	6.20070000
41	Si	-10.95800000	-7.17850000	7.67890000
42	Si	-8.42890000	-3.23820000	7.03330000
43	O	-11.40780000	-5.74300000	7.18590000
44	O	-8.21960000	-1.69260000	6.70790000

1	O	-9.95660000	-3.63110000	6.85010000
2	O	-9.98360000	-7.83070000	6.60240000
3	O	-7.53000000	-4.04100000	5.99020000
4	O	-7.92320000	-3.54700000	8.50450000
5	Si	0.12320000	4.64410000	-2.14550000
6	Si	-2.82310000	3.84600000	-1.95510000
7	O	-3.94900000	0.19040000	-1.21850000
8	O	0.75700000	3.77010000	-0.98770000
9	O	-1.45550000	4.66540000	-1.97180000
10	O	-2.55350000	2.34860000	-1.50000000
11	O	-6.33220000	0.83850000	-0.42850000
12	O	-3.77030000	4.57610000	-0.90140000
13	Si	-5.28020000	4.78230000	-0.42350000
14	Si	-7.00390000	2.22870000	-0.05400000
15	Si	-9.63060000	2.52380000	-1.72000000
16	O	-6.07880000	3.41370000	-0.57020000
17	O	-8.42830000	2.36750000	-0.70540000
18	O	-10.83220000	1.58900000	-1.25000000
19	O	-5.20960000	5.26350000	1.09860000
20	O	-7.15700000	2.26930000	1.54270000
21	O	-11.46650000	0.47770000	1.01990000
22	O	-6.60040000	-5.49380000	4.09960000
23	O	-8.61720000	-8.44720000	4.51360000
24	O	-1.68270000	1.69080000	8.46850000
25	Si	-1.74890000	2.17170000	6.97410000
26	O	-0.91870000	3.49570000	6.81430000
27	Si	2.50950000	3.95250000	5.10420000
28	Si	2.56680000	1.37900000	6.82670000
29	Si	3.01120000	-3.35760000	7.49350000
30	Si	-0.01120000	-2.57100000	7.40600000
31	O	2.86460000	2.66320000	5.94590000
32	O	3.90010000	0.51780000	6.89190000
33	O	3.77240000	-1.96900000	7.63100000
34	O	1.47830000	-3.08400000	7.27480000
35	O	2.15450000	1.79120000	8.29130000
36	O	-0.24970000	-2.04670000	8.86410000
37	O	1.05380000	4.47370000	5.45680000
38	O	-1.00420000	-3.76440000	7.04720000
39	Si	0.52350000	-7.58780000	-0.03030000
40	Si	-2.45310000	-8.37930000	0.08690000
41	O	-1.02440000	-7.79970000	-0.28570000
42	O	-3.48040000	-7.82240000	-1.00870000
43	O	-2.05280000	-6.52240000	3.54850000
44	O	-4.53620000	-6.55020000	2.91500000

1	O	-2.87430000	-7.94910000	1.53380000
2	O	0.93450000	-7.98310000	1.44400000
3	O	0.37170000	-7.41290000	3.90390000
4	Si	0.95190000	-8.52590000	2.93030000
5	Si	-1.34640000	-5.31660000	7.02370000
6	Si	-4.32960000	-6.05610000	7.41270000
7	O	-2.92290000	-5.44190000	7.01850000
8	O	-5.41450000	-5.45960000	6.41750000
9	O	-4.71840000	-5.65910000	8.88780000
10	O	-1.36620000	-5.12610000	10.61890000
11	O	-0.72730000	-6.04810000	8.28660000
12	Si	-0.78110000	-6.37380000	9.84140000
13	Si	4.19140000	1.79570000	-2.03280000
14	Si	4.36130000	-0.89370000	-0.53530000
15	Si	1.79920000	-4.81760000	0.05470000
16	Si	1.68560000	-2.17100000	-1.47840000
17	Si	3.22760000	3.05990000	2.24000000
18	Si	5.44840000	-1.68950000	4.28210000
19	Si	3.72400000	-4.24270000	4.65120000
20	O	4.61250000	0.39620000	-1.42440000
21	O	1.43070000	-3.66260000	-0.97320000
22	O	3.17930000	-1.73820000	-1.16020000
23	O	4.64910000	-3.05760000	4.13510000
24	O	2.93740000	2.40540000	-1.28810000
25	O	2.15410000	3.10990000	1.07330000
26	O	2.54300000	3.62280000	3.55350000
27	O	5.51820000	-1.20770000	5.80380000
28	O	3.57090000	-4.20200000	6.24790000
29	O	-0.73790000	-5.99420000	5.72550000
30	H	-1.30770000	8.45280000	5.54490000
31	H	3.53900000	4.98890000	5.43620000
32	H	-5.91550000	5.84190000	-1.27060000
33	H	-6.78570000	6.92250000	2.19890000
34	H	-12.70540000	-0.03450000	-1.12450000
35	H	-13.56750000	1.03610000	2.31350000
36	H	-12.61360000	-4.36250000	-0.43650000
37	H	-12.17550000	-5.02190000	-2.75570000
38	H	-14.47190000	-2.17020000	6.40220000
39	H	-13.77040000	-2.92530000	4.17860000
40	H	6.86450000	-1.88260000	3.83330000
41	H	-2.15040000	-4.10050000	12.78420000
42	H	1.31010000	-8.39770000	-1.01480000
43	H	-12.21020000	-7.97290000	7.89080000
44	H	0.36340000	-1.65380000	11.27870000

1	H	0.62130000	6.05740000	-2.14750000
2	H	0.50140000	4.07440000	-3.47820000
3	H	-2.25700000	7.49990000	7.52180000
4	H	-5.73850000	6.73170000	5.78280000
5	H	-10.96700000	4.40130000	4.09400000
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8	H	-10.59640000	-6.34750000	11.45320000
9	H	-8.66420000	-7.73420000	10.94950000
10	H	2.77450000	1.81970000	10.74640000
11	H	1.80020000	3.79900000	9.78440000
12	H	5.77540000	-0.53010000	8.17660000
13	H	3.24710000	-4.17500000	8.72650000
14	H	0.61160000	-6.65520000	10.31590000
15	H	-1.64370000	-7.57580000	10.07620000
16	H	0.12290000	-9.76940000	3.03170000
17	H	2.36090000	-8.82750000	3.33990000
18	H	-10.15040000	3.92860000	-1.73450000
19	H	-9.16390000	2.16210000	-3.09680000
20	H	3.89500000	1.63920000	-3.49250000
21	H	5.32300000	2.73990000	-1.76330000
22	H	4.42880000	3.88350000	1.88710000
23	H	5.61650000	-1.70970000	-0.58830000
24	H	4.35730000	-5.55350000	4.29820000
25	H	3.22920000	-5.21290000	-0.15130000
26	H	-5.23700000	-6.37850000	11.22840000
27	H	-7.76830000	-9.07120000	6.80850000
28	H	-6.95230000	-10.08460000	3.55430000
29	H	-10.29630000	-10.34930000	0.25900000
30	H	-2.42150000	-9.87450000	0.00040000
31	H	-3.42900000	-8.60990000	3.88980000
32	H	-4.28320000	-7.54880000	7.29620000
33	H	-3.45780000	3.89970000	-3.31080000
34	H	0.59910000	5.23700000	7.81470000
35	H	-9.79240000	-1.54060000	-3.18200000
36	H	-8.38790000	-2.95530000	10.89960000
37	H	-4.87450000	3.78240000	8.02040000
38	H	-2.02270000	2.13730000	10.92000000
39	H	-4.91220000	-7.27130000	-2.96190000
40	H	-8.98790000	-7.09310000	-2.37650000
41	H	1.45740000	-2.18480000	-2.95900000
42	H	-5.88650000	0.35320000	-2.87170000
43	H	-6.57060000	-3.25690000	-2.96870000
44	H	-11.74490000	-3.66940000	8.61800000

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 1  H    -9.32890000    0.16850000     8.03140000
 2  H    -8.19140000    3.21540000     6.31880000
 3  H    -5.78340000   -8.84910000    -1.27830000
 4  H    -7.97590000   -9.98270000    -0.17660000
 5  H    -2.11770000    0.35870000    -2.97420000
 6
 7
 8  ZH_CH3OH(ads)-to-Z-CH3_H2O(ads)-TS
 9  Si -0.04501600   -0.00459468   -0.01667639
10  Si -0.06449751   -0.00154789    5.65236810
11  Si 3.71509749     -0.05003460    2.48688661
12  Si 1.04157309     -3.89709999    2.99305699
13  Al 0.74749410     -0.83382721    2.92009811
14  O   0.22996843     -2.50969345    3.02522472
15  O   2.44998170     -0.78646617    3.11654635
16  O   -0.00673949   -0.23987168    1.52531212
17  O   -0.12891925    0.03108115     4.08655509
18  O   -1.59150643    0.15433761     -0.44160967
19  O   -0.36020123    -1.46513680    6.28567247
20  O   1.36591193     0.48151039     6.24559453
21  O   -1.26618685    0.97252901     6.06630118
22  O   0.81751780     1.28561255     -0.43422830
23  O   3.68736453     1.55330231     2.52968282
24  O   5.01136380     -0.46692803    3.33733692
25  O   2.20271801     -4.06286225    4.10048879
26  O   3.90551348     -0.48355481    0.94512897
27  O   1.71726655     -4.22000720    1.56456058
28  O   0.53650589     -1.24876963    -0.85419256
29  O   -0.15429827    -4.94264783    3.30491953
30  O   0.80133400     -6.00647700    -0.15280300
31  Si -5.49760300    -0.02108800    -1.47429200
32  Si -2.51910400    0.76907700     -1.59036400
33  Si 1.67287300     2.63506400     -0.36445800
34  Si -6.77250000    -2.79180000    -1.55910000
35  Si -6.65860000    -5.43650000    -0.02630000
36  Si -0.62798600    -6.20818700    4.15920500
37  Si -3.21923400    -7.43500800    2.98458400
38  Si -6.09540000    -6.32220000    2.83000000
39  Si -7.79180000    -8.89230000    3.21140000
40  Si -7.85690000    -4.02790000    9.99880000
41  Si -9.54690000    -6.64300000    10.42590000
42  O   -8.68790000    -5.35140000    10.15840000
43  Si 1.78781600     2.30218600     9.72780900
44  Si -0.76980800    -1.62740500    10.29930000
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1	Si	-1.17801000	1.38382800	9.93890900
2	O	-1.38699000	-0.16319600	10.26480100
3	O	0.35018900	1.77512200	10.12159000
4	O	-1.90930600	-2.64049400	10.65649700
5	Si	-2.31670000	-4.06080000	11.29600000
6	Si	-5.02660000	-5.18350000	10.35000000
7	O	-3.83590000	-4.30830000	10.92640000
8	O	-6.34110000	-4.27000000	10.39930000
9	Si	4.73289700	-0.80096600	7.13547100
10	Si	-7.29070000	2.20560000	5.67640000
11	Si	-4.57940700	3.32748900	6.62401900
12	Si	-1.94070000	7.20800000	6.08700000
13	Si	-4.59330000	6.04430000	5.10460000
14	O	-5.77090000	2.45290000	6.04720000
15	O	-3.26560100	2.41457000	6.57334500
16	O	-0.99449900	5.94279900	5.99239600
17	O	-3.27080000	6.91960000	5.26710000
18	O	-4.35770000	4.58890000	5.69440000
19	O	-7.46660000	2.24720000	4.09540000
20	O	-4.88400000	5.95910000	3.53970000
21	Si	-5.99570000	5.67090000	2.42990000
22	Si	-10.73910000	3.90040000	2.70070000
23	O	-11.73290000	2.70740000	2.34160000
24	Si	-12.07420000	1.15480000	2.31840000
25	O	-11.45520000	0.42330000	3.58130000
26	Si	-11.39460000	-4.15760000	7.24580000
27	Si	-13.29570000	-2.46030000	5.52120000
28	Si	-11.50890000	0.09760000	5.13610000
29	Si	-8.83680000	-0.22830000	6.67330000
30	O	-12.44950000	-3.64190000	6.15630000
31	O	-12.41530000	-1.16550000	5.38290000
32	O	-10.03410000	-0.20050000	5.63860000
33	O	-7.69650000	0.78430000	6.31660000
34	Si	-0.05969900	4.78730300	6.54672400
35	O	-10.24280000	-7.11800000	9.08650000
36	Si	-7.71660000	3.11370000	2.78820000
37	O	-6.95550000	4.50240000	2.92570000
38	O	-9.24950000	3.38730000	2.56950000
39	Si	-4.97250000	-7.60980000	-1.50390000
40	Si	-11.35590000	0.26280000	-0.54610000
41	O	-6.84510000	-7.72030000	2.70470000
42	O	-10.35620000	-0.94150000	-0.80140000
43	Si	-9.16490000	-9.40520000	0.52820000
44	Si	-9.33470000	-6.71560000	-0.96890000

1	Si	-11.54680000	-4.63200000	-1.45310000
2	Si	-9.77590000	-2.05450000	-1.77500000
3	O	-9.58580000	-8.00560000	-0.07990000
4	O	-10.67690000	-5.84320000	-0.91270000
5	O	-10.64710000	-3.36120000	-1.66840000
6	O	-8.28390000	-2.37400000	-1.34130000
7	O	-6.40440000	-3.94670000	-0.53100000
8	O	-8.15250000	-5.87130000	-0.34420000
9	O	-8.84920000	-9.23940000	2.07860000
10	O	-6.41640000	-5.42400000	1.54900000
11	O	-5.61290000	-6.41590000	-0.70840000
12	O	-5.77370000	-1.60340000	-1.35130000
13	Si	-6.81090000	-5.43360000	5.68340000
14	Si	-8.50460000	-8.00720000	6.05360000
15	O	-7.72180000	-6.63160000	6.20070000
16	Si	-10.95800000	-7.17850000	7.67890000
17	Si	-8.42890000	-3.23820000	7.03330000
18	O	-11.40780000	-5.74300000	7.18590000
19	O	-8.21960000	-1.69260000	6.70790000
20	O	-9.95660000	-3.63110000	6.85010000
21	O	-9.98360000	-7.83070000	6.60240000
22	O	-7.53000000	-4.04100000	5.99020000
23	O	-7.92320000	-3.54700000	8.50450000
24	Si	0.12366300	4.64446800	-2.14540400
25	Si	-2.82299600	3.84600000	-1.95510200
26	O	-3.94896200	0.19047100	-1.21862900
27	O	0.75594600	3.76941000	-0.98751600
28	O	-1.45550000	4.66540000	-1.97180000
29	O	-2.55362100	2.34860700	-1.50002200
30	O	-6.33220000	0.83850000	-0.42850000
31	O	-3.77030000	4.57610000	-0.90140000
32	Si	-5.28020000	4.78230000	-0.42350000
33	Si	-7.00390000	2.22870000	-0.05400000
34	Si	-9.63060000	2.52380000	-1.72000000
35	O	-6.07880000	3.41370000	-0.57020000
36	O	-8.42830000	2.36750000	-0.70540000
37	O	-10.83220000	1.58900000	-1.25000000
38	O	-5.20960000	5.26350000	1.09860000
39	O	-7.15700000	2.26930000	1.54270000
40	O	-11.46650000	0.47770000	1.01990000
41	O	-6.60040000	-5.49380000	4.09960000
42	O	-8.61720000	-8.44720000	4.51360000
43	O	-1.68267700	1.69080700	8.46850100
44	Si	-1.74883000	2.17137100	6.97378800

1	O	-0.91871000	3.49571700	6.81439200
2	Si	2.50951500	3.95256600	5.10425700
3	Si	2.56655600	1.37886700	6.82672600
4	Si	3.01133200	-3.35747800	7.49346600
5	Si	-0.01128600	-2.57102900	7.40589500
6	O	2.86464300	2.66311100	5.94588500
7	O	3.90010900	0.51781900	6.89195400
8	O	3.77240000	-1.96900000	7.63100000
9	O	1.47827000	-3.08412200	7.27493600
10	O	2.15456400	1.79119200	8.29132000
11	O	-0.24968300	-2.04669800	8.86410200
12	O	1.05379000	4.47370400	5.45678900
13	O	-1.00410100	-3.76441600	7.04698100
14	Si	0.52346500	-7.58778700	-0.03020900
15	Si	-2.45310000	-8.37930000	0.08690000
16	O	-1.02440000	-7.79970000	-0.28570000
17	O	-3.48040000	-7.82240000	-1.00870000
18	O	-2.05273400	-6.52245200	3.54837300
19	O	-4.53620000	-6.55020000	2.91500000
20	O	-2.87430000	-7.94910000	1.53380000
21	O	0.93450000	-7.98310000	1.44400000
22	O	0.37156100	-7.41294100	3.90394100
23	Si	0.95190500	-8.52589500	2.93029800
24	Si	-1.34643500	-5.31655200	7.02384600
25	Si	-4.32960000	-6.05610000	7.41270000
26	O	-2.92290000	-5.44190000	7.01850000
27	O	-5.41450000	-5.45960000	6.41750000
28	O	-4.71840000	-5.65910000	8.88780000
29	O	-1.36620000	-5.12610000	10.61890000
30	O	-0.72730000	-6.04810000	8.28660000
31	Si	-0.78110000	-6.37380000	9.84140000
32	Si	4.19161300	1.79581300	-2.03247800
33	Si	4.36134900	-0.89364500	-0.53540000
34	Si	1.79907000	-4.81750700	0.05494800
35	Si	1.68503400	-2.17067700	-1.47853500
36	Si	3.22795900	3.06040500	2.23972000
37	Si	5.44855100	-1.68947600	4.28209500
38	Si	3.72401800	-4.24258400	4.65111300
39	O	4.61236200	0.39619700	-1.42444400
40	O	1.43075500	-3.66260500	-0.97313200
41	O	3.17929700	-1.73848700	-1.15980900
42	O	4.64904700	-3.05762800	4.13513400
43	O	2.93692900	2.40526700	-1.28875300
44	O	2.15293300	3.10900600	1.07406300

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3	O	3.57067200	-4.20213700	6.24788200
4	O	-0.73796800	-5.99433600	5.72551400
5	H	-1.30770000	8.45280000	5.54490000
6	H	3.53900000	4.98890000	5.43620000
7	H	-5.91550000	5.84190000	-1.27060000
8	H	-6.78570000	6.92250000	2.19890000
9	H	-12.70540000	-0.03450000	-1.12450000
10	H	-13.56750000	1.03610000	2.31350000
11	H	-12.61360000	-4.36250000	-0.43650000
12	H	-12.17550000	-5.02190000	-2.75570000
13	H	-14.47190000	-2.17020000	6.40220000
14	H	-13.77040000	-2.92530000	4.17860000
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18	H	-12.21020000	-7.97290000	7.89080000
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31	H	5.77540000	-0.53010000	8.17660000
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33	H	0.61160000	-6.65520000	10.31590000
34	H	-1.64370000	-7.57580000	10.07620000
35	H	0.12290000	-9.76940000	3.03170000
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38	H	-9.16390000	2.16210000	-3.09680000
39	H	3.89500000	1.63920000	-3.49250000
40	H	5.32300000	2.73990000	-1.76330000
41	H	4.42878700	3.88352300	1.88700900
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44	H	3.22919100	-5.21293700	-0.15129000

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Si 3.71075260 -0.01345539 2.48236305
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6	O	4.98300641	-0.48462047	3.33383096
7	O	2.21160606	-4.04779227	4.10404500
8	O	3.85455621	-0.51615141	0.95231627
9	O	1.76097780	-4.25982184	1.57465162
10	O	0.56935453	-1.27622291	-0.73432394
11	O	-0.13170019	-4.94124860	3.32862935
12	O	0.80129115	-6.00644746	-0.15276631
13	Si	-5.49760388	-0.02108436	-1.47428971
14	Si	-2.51910419	0.76910121	-1.59031438
15	Si	1.67270228	2.63511644	-0.36444392
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17	Si	-6.65860000	-5.43650000	-0.02630000
18	Si	-0.62801094	-6.20806812	4.15924285
19	Si	-3.21922705	-7.43500634	2.98456693
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24	O	-8.68790000	-5.35140000	10.15840000
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27	Si	-1.17801467	1.38384039	9.93891319
28	O	-1.38699037	-0.16319616	10.26480095
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32	Si	-5.02660000	-5.18350000	10.35000000
33	O	-3.83590000	-4.30830000	10.92640000
34	O	-6.34110000	-4.27000000	10.39930000
35	Si	4.73289865	-0.80095376	7.13548346
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37	Si	-4.57940741	3.32748835	6.62402015
38	Si	-1.94070000	7.20800000	6.08700000
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43	O	-3.27080000	6.91960000	5.26710000
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1	O	-7.46660000	2.24720000	4.09540000
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13	O	-12.41530000	-1.16550000	5.38290000
14	O	-10.03410000	-0.20050000	5.63860000
15	O	-7.69650000	0.78430000	6.31660000
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17	O	-10.24280000	-7.11800000	9.08650000
18	Si	-7.71660000	3.11370000	2.78820000
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21	Si	-4.97250000	-7.60980000	-1.50390000
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23	O	-6.84510000	-7.72030000	2.70470000
24	O	-10.35620000	-0.94150000	-0.80140000
25	Si	-9.16490000	-9.40520000	0.52820000
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29	O	-9.58580000	-8.00560000	-0.07990000
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35	O	-8.84920000	-9.23940000	2.07860000
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38	O	-5.77370000	-1.60340000	-1.35130000
39	Si	-6.81090000	-5.43360000	5.68340000
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41	O	-7.72180000	-6.63160000	6.20070000
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1	O	-8.21960000	-1.69260000	6.70790000
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7	Si	-2.82300585	3.84599954	-1.95509769
8	O	-3.94895803	0.19045505	-1.21863858
9	O	0.75596202	3.76943635	-0.98749160
10	O	-1.45550000	4.66540000	-1.97180000
11	O	-2.55361620	2.34860612	-1.50000478
12	O	-6.33220000	0.83850000	-0.42850000
13	O	-3.77030000	4.57610000	-0.90140000
14	Si	-5.28020000	4.78230000	-0.42350000
15	Si	-7.00390000	2.22870000	-0.05400000
16	Si	-9.63060000	2.52380000	-1.72000000
17	O	-6.07880000	3.41370000	-0.57020000
18	O	-8.42830000	2.36750000	-0.70540000
19	O	-10.83220000	1.58900000	-1.25000000
20	O	-5.20960000	5.26350000	1.09860000
21	O	-7.15700000	2.26930000	1.54270000
22	O	-11.46650000	0.47770000	1.01990000
23	O	-6.60040000	-5.49380000	4.09960000
24	O	-8.61720000	-8.44720000	4.51360000
25	O	-1.68266575	1.69077702	8.46849087
26	Si	-1.74880415	2.17126327	6.97368394
27	O	-0.91870177	3.49571089	6.81438411
28	Si	2.50951653	3.95256485	5.10424694
29	Si	2.56656662	1.37880759	6.82671998
30	Si	3.01136733	-3.35744696	7.49345843
31	Si	-0.01127293	-2.57110411	7.40589872
32	O	2.86463359	2.66311660	5.94588998
33	O	3.90011324	0.51782408	6.89193440
34	O	3.77240000	-1.96900000	7.63100000
35	O	1.47826327	-3.08415237	7.27497845
36	O	2.15455350	1.79120031	8.29131471
37	O	-0.24969499	-2.04667692	8.86409246
38	O	1.05378747	4.47370516	5.45678608
39	O	-1.00407609	-3.76442670	7.04694768
40	Si	0.52346965	-7.58778877	-0.03022124
41	Si	-2.45310000	-8.37930000	0.08690000
42	O	-1.02440000	-7.79970000	-0.28570000
43	O	-3.48040000	-7.82240000	-1.00870000
44	O	-2.05274189	-6.52245797	3.54839449

1	O	-4.53620000	-6.55020000	2.91500000
2	O	-2.87430000	-7.94910000	1.53380000
3	O	0.93450000	-7.98310000	1.44400000
4	O	0.37156969	-7.41293544	3.90394876
5	Si	0.95190864	-8.52589162	2.93029631
6	Si	-1.34645722	-5.31655973	7.02387335
7	Si	-4.32960000	-6.05610000	7.41270000
8	O	-2.92290000	-5.44190000	7.01850000
9	O	-5.41450000	-5.45960000	6.41750000
10	O	-4.71840000	-5.65910000	8.88780000
11	O	-1.36620000	-5.12610000	10.61890000
12	O	-0.72730000	-6.04810000	8.28660000
13	Si	-0.78110000	-6.37380000	9.84140000
14	Si	4.19160475	1.79581194	-2.03248380
15	Si	4.36141218	-0.89366105	-0.53545373
16	Si	1.79912304	-4.81749252	0.05506094
17	Si	1.68504206	-2.17066241	-1.47863731
18	Si	3.22797882	3.06040779	2.23969400
19	Si	5.44862124	-1.68947734	4.28206632
20	Si	3.72393295	-4.24258842	4.65129674
21	O	4.61233930	0.39618112	-1.42447344
22	O	1.43078838	-3.66261076	-0.97314971
23	O	3.17928806	-1.73842578	-1.15982521
24	O	4.64902193	-3.05762555	4.13508999
25	O	2.93693579	2.40525709	-1.28874125
26	O	2.15300439	3.10900129	1.07403986
27	O	2.54294349	3.62283243	3.55349929
28	O	5.51813271	-1.20789167	5.80383184
29	O	3.57065810	-4.20217047	6.24788151
30	O	-0.73796008	-5.99432204	5.72551265
31	H	-1.30770000	8.45280000	5.54490000
32	H	3.53900000	4.98890000	5.43620000
33	H	-5.91550000	5.84190000	-1.27060000
34	H	-6.78570000	6.92250000	2.19890000
35	H	-12.70540000	-0.03450000	-1.12450000
36	H	-13.56750000	1.03610000	2.31350000
37	H	-12.61360000	-4.36250000	-0.43650000
38	H	-12.17550000	-5.02190000	-2.75570000
39	H	-14.47190000	-2.17020000	6.40220000
40	H	-13.77040000	-2.92530000	4.17860000
41	H	6.86450122	-1.88259443	3.83330052
42	H	-2.15040000	-4.10050000	12.78420000
43	H	1.31010000	-8.39770000	-1.01480000
44	H	-12.21020000	-7.97290000	7.89080000

1	H	0.36339833	-1.65380566	11.27870165
2	H	0.62130000	6.05740000	-2.14750000
3	H	0.50140000	4.07440000	-3.47820000
4	H	-2.25700000	7.49990000	7.52180000
5	H	-5.73850000	6.73170000	5.78280000
6	H	-10.96700000	4.40130000	4.09400000
7	H	-11.01960000	5.00810000	1.73210000
8	H	-12.06290000	1.27880000	5.87220000
9	H	-10.59640000	-6.34750000	11.45320000
10	H	-8.66420000	-7.73420000	10.94950000
11	H	2.77450362	1.81970528	10.74639888
12	H	1.80018614	3.79900045	9.78439645
13	H	5.77540000	-0.53010000	8.17660000
14	H	3.24710000	-4.17500000	8.72650000
15	H	0.61160000	-6.65520000	10.31590000
16	H	-1.64370000	-7.57580000	10.07620000
17	H	0.12290000	-9.76940000	3.03170000
18	H	2.36090000	-8.82750000	3.33990000
19	H	-10.15040000	3.92860000	-1.73450000
20	H	-9.16390000	2.16210000	-3.09680000
21	H	3.89500000	1.63920000	-3.49250000
22	H	5.32300000	2.73990000	-1.76330000
23	H	4.42878088	3.88353511	1.88701643
24	H	5.61653944	-1.70963641	-0.58833357
25	H	4.35726114	-5.55352127	4.29821060
26	H	3.22918242	-5.21296585	-0.15129419
27	H	-5.23700000	-6.37850000	11.22840000
28	H	-7.76830000	-9.07120000	6.80850000
29	H	-6.95230000	-10.08460000	3.55430000
30	H	-10.29630000	-10.34930000	0.25900000
31	H	-2.42150000	-9.87450000	0.00040000
32	H	-3.42900000	-8.60990000	3.88980000
33	H	-4.28320000	-7.54880000	7.29620000
34	H	-3.45780000	3.89970000	-3.31080000
35	H	0.59911290	5.23699100	7.81469620
36	H	-9.79240000	-1.54060000	-3.18200000
37	H	-8.38790000	-2.95530000	10.89960000
38	H	-4.87450000	3.78240000	8.02040000
39	H	-2.02270000	2.13730000	10.92000000
40	H	-4.91220000	-7.27130000	-2.96190000
41	H	-8.98790000	-7.09310000	-2.37650000
42	H	1.45751762	-2.18477684	-2.95900119
43	H	-5.88650000	0.35320000	-2.87170000
44	H	-6.57060000	-3.25690000	-2.96870000

1	H	-11.74490000	-3.66940000	8.61800000
2	H	-9.32890000	0.16850000	8.03140000
3	H	-8.19140000	3.21540000	6.31880000
4	H	-5.78340000	-8.84910000	-1.27830000
5	H	-7.97590000	-9.98270000	-0.17660000
6	H	-2.11766470	0.35884986	-2.97426343
7	H	-1.16176090	0.40397861	3.64786596
8	C	-3.52279191	0.17888517	3.29963861
9	H	-3.74671509	0.46767327	4.32414865
10	H	-3.44861399	-0.90810687	3.22225331
11	H	-4.30469982	0.54924176	2.63593916
12	O	-2.26576971	0.81087242	2.96203209
13	H	-2.00471756	0.59770520	2.05088749
14				
15				
16	ZH_CH3OH(ads)_C2H4(ads)			
17	Si	-0.03609706	0.01474942	-0.01045367
18	Si	-0.07056979	-0.00641409	5.67411257
19	Si	3.70407924	-0.01451905	2.47869877
20	Si	1.04803121	-3.89910984	2.97561005
21	Al	0.70579057	-0.84732383	2.85807412
22	O	0.31758272	-2.49477033	2.89378990
23	O	2.36795861	-0.56438545	3.14432959
24	O	-0.07701047	0.00265663	1.57429143
25	O	-0.23667272	-0.00192671	4.07797236
26	O	-1.58165654	0.17234294	-0.43541234
27	O	-0.34487757	-1.44659104	6.30342407
28	O	1.36538133	0.51209052	6.18133837
29	O	-1.26634997	0.99832747	6.02391031
30	O	0.83343788	1.27497782	-0.48952209
31	O	3.79386474	1.58750972	2.48036256
32	O	4.97039710	-0.48657406	3.33845315
33	O	2.21084533	-4.03202436	4.10401829
34	O	3.86270089	-0.50913729	0.94845472
35	O	1.77250101	-4.27977270	1.57928353
36	O	0.57803360	-1.28272136	-0.71310993
37	O	-0.12923951	-4.93737073	3.33590367
38	H	-1.28643105	0.56868183	3.58451657
39	C	-3.35230670	0.20386504	3.07981145
40	H	-3.74517805	0.48174181	4.05355417
41	H	-3.16271901	-0.86711657	3.02706440
42	H	-4.03363549	0.51029294	2.29135379
43	O	-2.10285736	0.94843560	2.91136783
44	C	-6.24072962	-1.76529859	3.69672650

1	H	-6.42676939	-1.11678345	4.54539926
2	H	-5.93158978	-2.77789778	3.92513936
3	C	-6.41359172	-1.35897305	2.44354967
4	H	-6.23786822	-2.02853358	1.60879827
5	H	-6.74461716	-0.35391394	2.20569596
6	H	-1.65793694	0.71111403	2.06120387
7	O	0.80120000	-6.00640000	-0.15260000
8	Si	-5.49760000	-0.02110000	-1.47430000
9	Si	-2.51930000	0.76950000	-1.59090000
10	Si	1.67080000	2.63420000	-0.36390000
11	Si	-6.77250000	-2.79180000	-1.55910000
12	Si	-6.65860000	-5.43650000	-0.02630000
13	Si	-0.62800000	-6.20850000	4.15920000
14	Si	-3.21920000	-7.43500000	2.98450000
15	Si	-6.09540000	-6.32220000	2.83000000
16	Si	-7.79180000	-8.89230000	3.21140000
17	Si	-7.85690000	-4.02790000	9.99880000
18	Si	-9.54690000	-6.64300000	10.42590000
19	O	-8.68790000	-5.35140000	10.15840000
20	Si	1.78780000	2.30220000	9.72780000
21	Si	-0.76980000	-1.62740000	10.29930000
22	Si	-1.17800000	1.38380000	9.93890000
23	O	-1.38700000	-0.16320000	10.26480000
24	O	0.35020000	1.77510000	10.12160000
25	O	-1.90930000	-2.64050000	10.65650000
26	Si	-2.31670000	-4.06080000	11.29600000
27	Si	-5.02660000	-5.18350000	10.35000000
28	O	-3.83590000	-4.30830000	10.92640000
29	O	-6.34110000	-4.27000000	10.39930000
30	Si	4.73290000	-0.80100000	7.13550000
31	Si	-7.29070000	2.20560000	5.67640000
32	Si	-4.57940000	3.32750000	6.62400000
33	Si	-1.94070000	7.20800000	6.08700000
34	Si	-4.59330000	6.04430000	5.10460000
35	O	-5.77090000	2.45290000	6.04720000
36	O	-3.26550000	2.41430000	6.57330000
37	O	-0.99450000	5.94280000	5.99240000
38	O	-3.27080000	6.91960000	5.26710000
39	O	-4.35770000	4.58890000	5.69440000
40	O	-7.46660000	2.24720000	4.09540000
41	O	-4.88400000	5.95910000	3.53970000
42	Si	-5.99570000	5.67090000	2.42990000
43	Si	-10.73910000	3.90040000	2.70070000
44	O	-11.73290000	2.70740000	2.34160000

1	Si	-12.07420000	1.15480000	2.31840000
2	O	-11.45520000	0.42330000	3.58130000
3	Si	-11.39460000	-4.15760000	7.24580000
4	Si	-13.29570000	-2.46030000	5.52120000
5	Si	-11.50890000	0.09760000	5.13610000
6	Si	-8.83680000	-0.22830000	6.67330000
7	O	-12.44950000	-3.64190000	6.15630000
8	O	-12.41530000	-1.16550000	5.38290000
9	O	-10.03410000	-0.20050000	5.63860000
10	O	-7.69650000	0.78430000	6.31660000
11	Si	-0.05970000	4.78730000	6.54670000
12	O	-10.24280000	-7.11800000	9.08650000
13	Si	-7.71660000	3.11370000	2.78820000
14	O	-6.95550000	4.50240000	2.92570000
15	O	-9.24950000	3.38730000	2.56950000
16	Si	-4.97250000	-7.60980000	-1.50390000
17	Si	-11.35590000	0.26280000	-0.54610000
18	O	-6.84510000	-7.72030000	2.70470000
19	O	-10.35620000	-0.94150000	-0.80140000
20	Si	-9.16490000	-9.40520000	0.52820000
21	Si	-9.33470000	-6.71560000	-0.96890000
22	Si	-11.54680000	-4.63200000	-1.45310000
23	Si	-9.77590000	-2.05450000	-1.77500000
24	O	-9.58580000	-8.00560000	-0.07990000
25	O	-10.67690000	-5.84320000	-0.91270000
26	O	-10.64710000	-3.36120000	-1.66840000
27	O	-8.28390000	-2.37400000	-1.34130000
28	O	-6.40440000	-3.94670000	-0.53100000
29	O	-8.15250000	-5.87130000	-0.34420000
30	O	-8.84920000	-9.23940000	2.07860000
31	O	-6.41640000	-5.42400000	1.54900000
32	O	-5.61290000	-6.41590000	-0.70840000
33	O	-5.77370000	-1.60340000	-1.35130000
34	Si	-6.81090000	-5.43360000	5.68340000
35	Si	-8.50460000	-8.00720000	6.05360000
36	O	-7.72180000	-6.63160000	6.20070000
37	Si	-10.95800000	-7.17850000	7.67890000
38	Si	-8.42890000	-3.23820000	7.03330000
39	O	-11.40780000	-5.74300000	7.18590000
40	O	-8.21960000	-1.69260000	6.70790000
41	O	-9.95660000	-3.63110000	6.85010000
42	O	-9.98360000	-7.83070000	6.60240000
43	O	-7.53000000	-4.04100000	5.99020000
44	O	-7.92320000	-3.54700000	8.50450000

1	Si	0.12320000	4.64410000	-2.14550000
2	Si	-2.82310000	3.84600000	-1.95510000
3	O	-3.94900000	0.19040000	-1.21850000
4	O	0.75700000	3.77010000	-0.98770000
5	O	-1.45550000	4.66540000	-1.97180000
6	O	-2.55350000	2.34860000	-1.50000000
7	O	-6.33220000	0.83850000	-0.42850000
8	O	-3.77030000	4.57610000	-0.90140000
9	Si	-5.28020000	4.78230000	-0.42350000
10	Si	-7.00390000	2.22870000	-0.05400000
11	Si	-9.63060000	2.52380000	-1.72000000
12	O	-6.07880000	3.41370000	-0.57020000
13	O	-8.42830000	2.36750000	-0.70540000
14	O	-10.83220000	1.58900000	-1.25000000
15	O	-5.20960000	5.26350000	1.09860000
16	O	-7.15700000	2.26930000	1.54270000
17	O	-11.46650000	0.47770000	1.01990000
18	O	-6.60040000	-5.49380000	4.09960000
19	O	-8.61720000	-8.44720000	4.51360000
20	O	-1.68270000	1.69080000	8.46850000
21	Si	-1.74890000	2.17170000	6.97410000
22	O	-0.91870000	3.49570000	6.81430000
23	Si	2.50950000	3.95250000	5.10420000
24	Si	2.56680000	1.37900000	6.82670000
25	Si	3.01120000	-3.35760000	7.49350000
26	Si	-0.01120000	-2.57100000	7.40600000
27	O	2.86460000	2.66320000	5.94590000
28	O	3.90010000	0.51780000	6.89190000
29	O	3.77240000	-1.96900000	7.63100000
30	O	1.47830000	-3.08400000	7.27480000
31	O	2.15450000	1.79120000	8.29130000
32	O	-0.24970000	-2.04670000	8.86410000
33	O	1.05380000	4.47370000	5.45680000
34	O	-1.00420000	-3.76440000	7.04720000
35	Si	0.52350000	-7.58780000	-0.03030000
36	Si	-2.45310000	-8.37930000	0.08690000
37	O	-1.02440000	-7.79970000	-0.28570000
38	O	-3.48040000	-7.82240000	-1.00870000
39	O	-2.05280000	-6.52240000	3.54850000
40	O	-4.53620000	-6.55020000	2.91500000
41	O	-2.87430000	-7.94910000	1.53380000
42	O	0.93450000	-7.98310000	1.44400000
43	O	0.37170000	-7.41290000	3.90390000
44	Si	0.95190000	-8.52590000	2.93030000

1	Si	-1.34640000	-5.31660000	7.02370000
2	Si	-4.32960000	-6.05610000	7.41270000
3	O	-2.92290000	-5.44190000	7.01850000
4	O	-5.41450000	-5.45960000	6.41750000
5	O	-4.71840000	-5.65910000	8.88780000
6	O	-1.36620000	-5.12610000	10.61890000
7	O	-0.72730000	-6.04810000	8.28660000
8	Si	-0.78110000	-6.37380000	9.84140000
9	Si	4.19140000	1.79570000	-2.03280000
10	Si	4.36130000	-0.89370000	-0.53530000
11	Si	1.79920000	-4.81760000	0.05470000
12	Si	1.68560000	-2.17100000	-1.47840000
13	Si	3.22760000	3.05990000	2.24000000
14	Si	5.44840000	-1.68950000	4.28210000
15	Si	3.72400000	-4.24270000	4.65120000
16	O	4.61250000	0.39620000	-1.42440000
17	O	1.43070000	-3.66260000	-0.97320000
18	O	3.17930000	-1.73820000	-1.16020000
19	O	4.64910000	-3.05760000	4.13510000
20	O	2.93740000	2.40540000	-1.28810000
21	O	2.15410000	3.10990000	1.07330000
22	O	2.54300000	3.62280000	3.55350000
23	O	5.51820000	-1.20770000	5.80380000
24	O	3.57090000	-4.20200000	6.24790000
25	O	-0.73790000	-5.99420000	5.72550000
26	H	-1.30770000	8.45280000	5.54490000
27	H	3.53900000	4.98890000	5.43620000
28	H	-5.91550000	5.84190000	-1.27060000
29	H	-6.78570000	6.92250000	2.19890000
30	H	-12.70540000	-0.03450000	-1.12450000
31	H	-13.56750000	1.03610000	2.31350000
32	H	-12.61360000	-4.36250000	-0.43650000
33	H	-12.17550000	-5.02190000	-2.75570000
34	H	-14.47190000	-2.17020000	6.40220000
35	H	-13.77040000	-2.92530000	4.17860000
36	H	6.86450000	-1.88260000	3.83330000
37	H	-2.15040000	-4.10050000	12.78420000
38	H	1.31010000	-8.39770000	-1.01480000
39	H	-12.21020000	-7.97290000	7.89080000
40	H	0.36340000	-1.65380000	11.27870000
41	H	0.62130000	6.05740000	-2.14750000
42	H	0.50140000	4.07440000	-3.47820000
43	H	-2.25700000	7.49990000	7.52180000
44	H	-5.73850000	6.73170000	5.78280000

1	H	-10.96700000	4.40130000	4.09400000
2	H	-11.01960000	5.00810000	1.73210000
3	H	-12.06290000	1.27880000	5.87220000
4	H	-10.59640000	-6.34750000	11.45320000
5	H	-8.66420000	-7.73420000	10.94950000
6	H	2.77450000	1.81970000	10.74640000
7	H	1.80020000	3.79900000	9.78440000
8	H	5.77540000	-0.53010000	8.17660000
9	H	3.24710000	-4.17500000	8.72650000
10	H	0.61160000	-6.65520000	10.31590000
11	H	-1.64370000	-7.57580000	10.07620000
12	H	0.12290000	-9.76940000	3.03170000
13	H	2.36090000	-8.82750000	3.33990000
14	H	-10.15040000	3.92860000	-1.73450000
15	H	-9.16390000	2.16210000	-3.09680000
16	H	3.89500000	1.63920000	-3.49250000
17	H	5.32300000	2.73990000	-1.76330000
18	H	4.42880000	3.88350000	1.88710000
19	H	5.61650000	-1.70970000	-0.58830000
20	H	4.35730000	-5.55350000	4.29820000
21	H	3.22920000	-5.21290000	-0.15130000
22	H	-5.23700000	-6.37850000	11.22840000
23	H	-7.76830000	-9.07120000	6.80850000
24	H	-6.95230000	-10.08460000	3.55430000
25	H	-10.29630000	-10.34930000	0.25900000
26	H	-2.42150000	-9.87450000	0.00040000
27	H	-3.42900000	-8.60990000	3.88980000
28	H	-4.28320000	-7.54880000	7.29620000
29	H	-3.45780000	3.89970000	-3.31080000
30	H	0.59910000	5.23700000	7.81470000
31	H	-9.79240000	-1.54060000	-3.18200000
32	H	-8.38790000	-2.95530000	10.89960000
33	H	-4.87450000	3.78240000	8.02040000
34	H	-2.02270000	2.13730000	10.92000000
35	H	-4.91220000	-7.27130000	-2.96190000
36	H	-8.98790000	-7.09310000	-2.37650000
37	H	1.45740000	-2.18480000	-2.95900000
38	H	-5.88650000	0.35320000	-2.87170000
39	H	-6.57060000	-3.25690000	-2.96870000
40	H	-11.74490000	-3.66940000	8.61800000
41	H	-9.32890000	0.16850000	8.03140000
42	H	-8.19140000	3.21540000	6.31880000
43	H	-5.78340000	-8.84910000	-1.27830000
44	H	-7.97590000	-9.98270000	-0.17660000

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 1  H    -2.11770000    0.35870000     -2.97420000
 2
 3
 4  ZH_CH3OH(ads)_CH3OCH3(ads)-to-Z-(CH3)3O+_H2O(ads)-TS
 5  Si -0.02880249    0.01536290     -0.01165794
 6  Si -0.06574836    -0.00541958    5.65699765
 7  Si 3.70661263     -0.03355079    2.48508253
 8  Si 1.03775272     -3.88356542    2.98219871
 9  Al 0.71310980     -0.83641242    2.88616470
10  O    0.28279740     -2.49097646    2.93253067
11  O    2.40768521     -0.67222581    3.13783757
12  O    -0.00126842    -0.01914260    1.55861018
13  O    -0.15752205    0.05406257     4.08197266
14  O    -1.58506001    0.18474146     -0.42334552
15  O    -0.36753914    -1.45547981    6.29620028
16  O    1.35519886     0.49437975     6.24147811
17  O    -1.28212027    0.97532364     6.04405119
18  O    0.82557975     1.28260981     -0.51463267
19  O    3.74652895     1.57251039     2.50304594
20  O    4.99434056     -0.47652758    3.33575481
21  O    2.20744220     -4.05040499    4.10064935
22  O    3.88544621     -0.49547408    0.94661722
23  O    1.74542187     -4.26872666    1.57637973
24  O    0.55285206     -1.27624216    -0.76441236
25  O    -0.14430614    -4.93209734    3.33743486
26  O    0.80125500     -6.00642900    -0.15268700
27  Si -5.49760300    -0.02108700    -1.47429100
28  Si -2.51934000    0.76934800     -1.59064300
29  Si 1.67272500     2.63501100     -0.36422900
30  Si -6.77250000    -2.79180000    -1.55910000
31  Si -6.65860300    -5.43650800    -0.02630000
32  Si -0.62788700    -6.20816200    4.15925800
33  Si -3.21921500    -7.43500300    2.98453500
34  Si -6.09540700    -6.32220100    2.83000100
35  Si -7.79180000    -8.89230000    3.21140000
36  Si -7.85690000    -4.02790000    9.99880000
37  Si -9.54690000    -6.64300000    10.42590000
38  O    -8.68790000    -5.35140000    10.15840000
39  Si 1.78782000     2.30218800     9.72780900
40  Si -0.76981200    -1.62740600    10.29929900
41  Si -1.17799900    1.38379800     9.93889900
42  O    -1.38697900    -0.16319100    10.26480300
43  O    0.35019100     1.77511800     10.12159200
44  O    -1.90931500    -2.64048600    10.65649100
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1	Si	-2.31670000	-4.06080000	11.29600000
2	Si	-5.02660000	-5.18350000	10.35000000
3	O	-3.83590000	-4.30830000	10.92640000
4	O	-6.34110000	-4.27000000	10.39930000
5	Si	4.73292200	-0.80097300	7.13568700
6	Si	-7.29070000	2.20560000	5.67640000
7	Si	-4.57940800	3.32748800	6.62402000
8	Si	-1.94070000	7.20800000	6.08700000
9	Si	-4.59330000	6.04430000	5.10460000
10	O	-5.77090000	2.45290000	6.04720000
11	O	-3.26559600	2.41455200	6.57331600
12	O	-0.99449900	5.94279800	5.99239400
13	O	-3.27080000	6.91960000	5.26710000
14	O	-4.35770000	4.58890000	5.69440000
15	O	-7.46660000	2.24720000	4.09540000
16	O	-4.88400000	5.95910000	3.53970000
17	Si	-5.99570000	5.67090000	2.42990000
18	Si	-10.73910000	3.90040000	2.70070000
19	O	-11.73290000	2.70740000	2.34160000
20	Si	-12.07420000	1.15480000	2.31840000
21	O	-11.45520000	0.42330000	3.58130000
22	Si	-11.39460000	-4.15760000	7.24580000
23	Si	-13.29570000	-2.46030000	5.52120000
24	Si	-11.50890000	0.09760000	5.13610000
25	Si	-8.83680000	-0.22830000	6.67330000
26	O	-12.44950000	-3.64190000	6.15630000
27	O	-12.41530000	-1.16550000	5.38290000
28	O	-10.03410000	-0.20050000	5.63860000
29	O	-7.69650000	0.78430000	6.31660000
30	Si	-0.05969700	4.78730100	6.54671900
31	O	-10.24280000	-7.11800000	9.08650000
32	Si	-7.71660000	3.11370000	2.78820000
33	O	-6.95550000	4.50240000	2.92570000
34	O	-9.24950000	3.38730000	2.56950000
35	Si	-4.97250000	-7.60980000	-1.50390000
36	Si	-11.35590000	0.26280000	-0.54610000
37	O	-6.84509900	-7.72030100	2.70469900
38	O	-10.35620000	-0.94150000	-0.80140000
39	Si	-9.16490000	-9.40520000	0.52820000
40	Si	-9.33470000	-6.71560000	-0.96890000
41	Si	-11.54680000	-4.63200000	-1.45310000
42	Si	-9.77590000	-2.05450000	-1.77500000
43	O	-9.58580000	-8.00560000	-0.07990000
44	O	-10.67690000	-5.84320000	-0.91270000

1	O	-10.64710000	-3.36120000	-1.66840000
2	O	-8.28390000	-2.37400000	-1.34130000
3	O	-6.40440000	-3.94670000	-0.53100000
4	O	-8.15250100	-5.87129700	-0.34420000
5	O	-8.84920000	-9.23940000	2.07860000
6	O	-6.41638900	-5.42399100	1.54900000
7	O	-5.61289900	-6.41589900	-0.70840000
8	O	-5.77370000	-1.60340000	-1.35130000
9	Si	-6.81090000	-5.43360000	5.68340000
10	Si	-8.50460000	-8.00720000	6.05360000
11	O	-7.72180000	-6.63160000	6.20070000
12	Si	-10.95800000	-7.17850000	7.67890000
13	Si	-8.42890000	-3.23820000	7.03330000
14	O	-11.40780000	-5.74300000	7.18590000
15	O	-8.21960000	-1.69260000	6.70790000
16	O	-9.95660000	-3.63110000	6.85010000
17	O	-9.98360000	-7.83070000	6.60240000
18	O	-7.53000000	-4.04100000	5.99020000
19	O	-7.92320000	-3.54700000	8.50450000
20	Si	0.12357100	4.64438700	-2.14541400
21	Si	-2.82292500	3.84600300	-1.95513300
22	O	-3.94892300	0.19041200	-1.21857400
23	O	0.75613100	3.76954900	-0.98753400
24	O	-1.45550000	4.66540000	-1.97180000
25	O	-2.55373400	2.34859800	-1.49991600
26	O	-6.33220000	0.83850000	-0.42850000
27	O	-3.77030000	4.57610000	-0.90140000
28	Si	-5.28020000	4.78230000	-0.42350000
29	Si	-7.00390000	2.22870000	-0.05400000
30	Si	-9.63060000	2.52380000	-1.72000000
31	O	-6.07880000	3.41370000	-0.57020000
32	O	-8.42830000	2.36750000	-0.70540000
33	O	-10.83220000	1.58900000	-1.25000000
34	O	-5.20960000	5.26350000	1.09860000
35	O	-7.15700000	2.26930000	1.54270000
36	O	-11.46650000	0.47770000	1.01990000
37	O	-6.60039800	-5.49379900	4.09960000
38	O	-8.61720000	-8.44720000	4.51360000
39	O	-1.68270000	1.69084600	8.46851500
40	Si	-1.74880500	2.17141400	6.97381400
41	O	-0.91869800	3.49571100	6.81439900
42	Si	2.50944200	3.95249200	5.10448000
43	Si	2.56639300	1.37898100	6.82716200
44	Si	3.01128100	-3.35752500	7.49347800

1	Si	-0.01120700	-2.57102000	7.40592000
2	O	2.86464800	2.66285700	5.94551500
3	O	3.90008600	0.51775200	6.89155800
4	O	3.77240000	-1.96900000	7.63100000
5	O	1.47827900	-3.08408600	7.27490500
6	O	2.15462600	1.79120100	8.29133500
7	O	-0.24969900	-2.04669800	8.86409900
8	O	1.05379300	4.47370300	5.45679200
9	O	-1.00410300	-3.76441200	7.04697000
10	Si	0.52349000	-7.58779600	-0.03027200
11	Si	-2.45310000	-8.37930000	0.08690000
12	O	-1.02440000	-7.79970000	-0.28570000
13	O	-3.48040000	-7.82240000	-1.00870000
14	O	-2.05276700	-6.52244000	3.54844500
15	O	-4.53620000	-6.55020100	2.91499900
16	O	-2.87430000	-7.94910000	1.53380000
17	O	0.93450000	-7.98310000	1.44400000
18	O	0.37145900	-7.41302300	3.90393500
19	Si	0.95196000	-8.52584400	2.93027300
20	Si	-1.34641400	-5.31653300	7.02384000
21	Si	-4.32960000	-6.05610000	7.41270000
22	O	-2.92290000	-5.44190000	7.01850000
23	O	-5.41450000	-5.45960000	6.41750000
24	O	-4.71840000	-5.65910000	8.88780000
25	O	-1.36620000	-5.12610000	10.61890000
26	O	-0.72730000	-6.04810000	8.28660000
27	Si	-0.78110000	-6.37380000	9.84140000
28	Si	4.19158700	1.79578500	-2.03252600
29	Si	4.36119800	-0.89370300	-0.53511100
30	Si	1.79892900	-4.81750100	0.05498600
31	Si	1.68505600	-2.17138400	-1.47833600
32	Si	3.22781000	3.05995700	2.23972200
33	Si	5.44835900	-1.68932300	4.28202400
34	Si	3.72422300	-4.24271600	4.65118000
35	O	4.61252000	0.39622100	-1.42436200
36	O	1.43105700	-3.66272400	-0.97335700
37	O	3.17925800	-1.73806900	-1.16018600
38	O	4.64902800	-3.05760600	4.13510900
39	O	2.93691400	2.40526500	-1.28877400
40	O	2.15309400	3.10926200	1.07393400
41	O	2.54316000	3.62323600	3.55344100
42	O	5.51821400	-1.20779800	5.80379900
43	O	3.57071800	-4.20206100	6.24788400
44	O	-0.73802000	-5.99434600	5.72551100

1	H	-1.30770000	8.45280000	5.54490000
2	H	3.53900000	4.98890000	5.43620000
3	H	-5.91550000	5.84190000	-1.27060000
4	H	-6.78570000	6.92250000	2.19890000
5	H	-12.70540000	-0.03450000	-1.12450000
6	H	-13.56750000	1.03610000	2.31350000
7	H	-12.61360000	-4.36250000	-0.43650000
8	H	-12.17550000	-5.02190000	-2.75570000
9	H	-14.47190000	-2.17020000	6.40220000
10	H	-13.77040000	-2.92530000	4.17860000
11	H	6.86449600	-1.88264000	3.83330500
12	H	-2.15040000	-4.10050000	12.78420000
13	H	1.31010000	-8.39770000	-1.01480000
14	H	-12.21020000	-7.97290000	7.89080000
15	H	0.36339500	-1.65382200	11.27870600
16	H	0.62130000	6.05740000	-2.14750000
17	H	0.50140000	4.07440000	-3.47820000
18	H	-2.25700000	7.49990000	7.52180000
19	H	-5.73850000	6.73170000	5.78280000
20	H	-10.96700000	4.40130000	4.09400000
21	H	-11.01960000	5.00810000	1.73210000
22	H	-12.06290000	1.27880000	5.87220000
23	H	-10.59640000	-6.34750000	11.45320000
24	H	-8.66420000	-7.73420000	10.94950000
25	H	2.77449300	1.81968900	10.74640200
26	H	1.80020100	3.79900000	9.78440000
27	H	5.77540000	-0.53010000	8.17660000
28	H	3.24710000	-4.17500000	8.72650000
29	H	0.61160000	-6.65520000	10.31590000
30	H	-1.64370000	-7.57580000	10.07620000
31	H	0.12290000	-9.76940000	3.03170000
32	H	2.36090000	-8.82750000	3.33990000
33	H	-10.15040000	3.92860000	-1.73450000
34	H	-9.16390000	2.16210000	-3.09680000
35	H	3.89500000	1.63920000	-3.49250000
36	H	5.32300000	2.73990000	-1.76330000
37	H	4.42878800	3.88353300	1.88703600
38	H	5.61653100	-1.70964900	-0.58834100
39	H	4.35726400	-5.55351700	4.29819900
40	H	3.22919600	-5.21291900	-0.15129400
41	H	-5.23700000	-6.37850000	11.22840000
42	H	-7.76830000	-9.07120000	6.80850000
43	H	-6.95230000	-10.08460000	3.55430000
44	H	-10.29630000	-10.34930000	0.25900000

1	H	-2.42150000	-9.87450000	0.00040000
2	H	-3.42900000	-8.60990000	3.88980000
3	H	-4.28320000	-7.54880000	7.29620000
4	H	-3.45780000	3.89970000	-3.31080000
5	H	0.59910400	5.23699700	7.81469900
6	H	-9.79240000	-1.54060000	-3.18200000
7	H	-8.38790000	-2.95530000	10.89960000
8	H	-4.87450000	3.78240000	8.02040000
9	H	-2.02270000	2.13730000	10.92000000
10	H	-4.91220000	-7.27130000	-2.96190000
11	H	-8.98790000	-7.09310000	-2.37650000
12	H	1.45748500	-2.18462500	-2.95899800
13	H	-5.88650000	0.35320000	-2.87170000
14	H	-6.57060000	-3.25690000	-2.96870000
15	H	-11.74490000	-3.66940000	8.61800000
16	H	-9.32890000	0.16850000	8.03140000
17	H	-8.19140000	3.21540000	6.31880000
18	H	-5.78340000	-8.84910000	-1.27830000
19	H	-7.97590000	-9.98270000	-0.17660000
20	H	-2.11760800	0.35876300	-2.97422100
21	C	-3.48435524	-2.73255462	4.39330053
22	H	-2.92131417	-2.23971910	5.18258514
23	H	-4.12688346	-3.50168736	4.82096076
24	H	-2.79523985	-3.16634017	3.66320891
25	O	-4.31859804	-1.72689258	3.77072340
26	C	-5.13159049	-2.24375247	2.69697076
27	H	-5.77504436	-3.03038252	3.09025662
28	H	-4.50537360	-2.63449772	1.89025100
29	H	-5.74318706	-1.41887065	2.33595177
30	C	-3.28990458	-0.22019550	3.28529703
31	H	-4.08919042	0.22403277	2.71705883
32	H	-2.54440914	-0.82273443	2.79519259
33	H	-3.16995781	0.06337142	4.31663276
34	O	-2.13514514	1.39929146	2.85211318
35	H	-1.34952869	1.11429044	3.38059051
36	H	-1.81813958	1.25031760	1.94863023
37				
38				
39	ZH_CH3OH(ads)_CH3OCH3(ads)			
40	Si	-3.85710031	2.06286966	3.08530430
41	Si	-3.82834869	-0.80358106	-1.82827085
42	Si	-7.33253384	-0.38219373	1.62936710
43	Si	-3.45810808	-2.93086297	2.52549733
44	Al	-4.23539410	-0.30345948	1.13616001

1	O	-3.27846803	-1.51950429	1.82455121
2	O	-5.88663723	-0.75645802	1.08567494
3	O	-3.84179531	1.28973849	1.69773479
4	O	-3.69876318	0.05994685	-0.48901811
5	O	-2.47130897	2.88152474	3.09284292
6	O	-3.04590864	-2.19347852	-1.75358729
7	O	-5.35083992	-1.09943922	-2.26095307
8	O	-3.07806430	0.20768818	-2.82118342
9	O	-5.11953233	3.05309321	3.07991633
10	O	-7.98569626	0.88423475	0.88971098
11	O	-8.35037606	-1.58389402	1.33477425
12	O	-4.49944313	-3.96533147	1.82355908
13	O	-7.30690731	-0.05461372	3.21131337
14	O	-3.99003396	-2.77349054	4.04643988
15	O	-3.95399506	1.16488453	4.40253877
16	O	-1.98778527	-3.58835888	2.47394878
17	O	-2.45890808	-2.98962103	6.17213917
18	Si	1.25748302	4.46325794	3.36327012
19	Si	-1.80497418	4.23306810	3.64024332
20	Si	-6.39090868	3.81884576	2.47581129
21	Si	3.44691500	2.66654000	4.49801200
22	Si	4.29170400	-0.27259400	4.42937300
23	Si	-1.06405719	-4.87258273	2.27535897
24	Si	1.79833604	-4.46676105	3.38985291
25	Si	4.07914900	-2.59647700	2.47630000
26	Si	6.58806600	-4.33423500	3.03682400
27	Si	4.87567900	-3.79606500	-5.11875900
28	Si	7.39476000	-5.59507000	-4.57555300
29	O	6.12805700	-4.68570900	-4.79047700
30	Si	-6.40319600	-1.55205900	-6.07558000
31	Si	-2.60078798	-4.21440658	-5.20185991
32	Si	-3.30637699	-1.47655165	-6.37240328
33	O	-2.55379200	-2.82353200	-5.96949600
34	O	-4.87322500	-1.72786800	-6.43324800
35	O	-1.17328000	-4.85678400	-5.24608900
36	Si	-0.28218600	-6.19726000	-5.20997300
37	Si	2.65261700	-5.78534200	-4.36369400
38	O	1.22482000	-5.73885000	-5.05305100
39	O	3.54852900	-4.66402100	-5.07419000
40	Si	-8.02285810	-3.67102299	-1.84367431
41	Si	2.10800500	3.22800900	-4.19032200
42	Si	-0.82795292	2.81431087	-5.03728010
43	Si	-4.68825600	5.39442100	-5.90308300
44	Si	-1.79199600	5.77370200	-4.99566000

1	O	0.60047800	2.76864200	-4.34819700
2	O	-1.72319807	1.69413212	-4.32606978
3	O	-5.11362200	4.12660100	-5.05651400
4	O	-3.34170900	5.98706600	-5.30295100
5	O	-1.48772400	4.22985400	-4.78231400
6	O	2.26038200	4.11002500	-2.87479000
7	O	-1.48624900	6.58100800	-3.65571500
8	Si	-0.34272100	7.25141600	-2.76493400
9	Si	4.71927000	7.16227500	-3.04087500
10	O	6.07764300	6.68898700	-2.35482800
11	Si	6.95651800	5.55390600	-1.67163000
12	O	6.64022100	4.13703800	-2.30850600
13	Si	8.22843900	-1.41814900	-3.32553100
14	Si	9.39282300	1.40870400	-2.97572200
15	Si	6.80401800	3.11035300	-3.51077700
16	Si	4.42601400	1.24442100	-4.19822100
17	O	9.02871400	-0.12688000	-2.81763700
18	O	8.10468600	2.24912800	-3.29995800
19	O	5.53507700	2.15875700	-3.53578500
20	O	2.99794800	1.88599900	-4.15397100
21	Si	-5.56958000	2.62507100	-4.82453500
22	O	8.21854600	-5.08948200	-3.32269500
23	Si	2.18469900	5.54328600	-2.19485000
24	O	0.97297900	6.35813300	-2.82347900
25	O	3.51571800	6.35070900	-2.41459900
26	Si	3.50763900	-1.80907500	7.03205200
27	Si	6.61583700	6.04871800	1.35427100
28	O	5.28335200	-3.42858200	3.10074300
29	O	6.11899200	4.89407600	2.32115400
30	Si	8.06040100	-2.97394000	5.34547200
31	Si	7.25144300	0.00089300	5.35200600
32	Si	8.56329700	2.61350000	4.39151300
33	Si	5.98208500	4.30418400	3.78972400
34	O	7.94912500	-1.40829200	5.14008400
35	O	8.18800800	1.09420000	4.64967700
36	O	7.26601800	3.46721000	4.14862400
37	O	4.70499000	3.36450500	3.83739500
38	O	3.51804100	1.10392700	4.21611800
39	O	5.84260800	0.00084500	4.63376200
40	O	7.70227800	-3.71670200	3.98497700
41	O	4.05740700	-1.12870100	3.10552500
42	O	3.67182800	-1.04579100	5.66868500
43	O	2.08591700	3.21051800	3.94588200
44	Si	4.41847400	-3.08933200	-0.53789900

1	Si	6.92616500	-4.82513100	0.03444200
2	O	5.69916300	-4.03242400	-0.59227300
3	Si	8.91085100	-4.20916300	-2.20812800
4	Si	5.13140100	-1.49208200	-3.02800800
5	O	8.81327800	-2.66333800	-2.53513600
6	O	4.37888405	-0.14654701	-3.43049707
7	O	6.69833400	-1.24195100	-2.96587300
8	O	8.24031800	-4.49813900	-0.79371900
9	O	4.58553636	-1.89587832	-1.58591005
10	O	4.76759900	-2.63718600	-4.06333700
11	Si	-5.66726243	6.81646758	2.79319740
12	Si	-2.63172919	6.99324599	2.46182411
13	O	-0.26373007	4.02378394	3.32709672
14	O	-5.94418215	5.33243185	2.31663025
15	O	-4.20271300	7.23747000	2.34385000
16	O	-2.34330142	5.47261507	2.81735272
17	O	1.72284900	4.89151100	1.90411800
18	O	-2.01447000	7.34810600	1.03565300
19	Si	-0.68204700	7.74427100	0.24926500
20	Si	1.84639400	6.03429500	0.80736400
21	Si	4.19353700	7.92591300	1.62890500
22	O	0.55715600	6.96191800	0.86946900
23	O	3.12623200	6.91642500	1.04481400
24	O	5.65041200	7.30939000	1.43914700
25	O	-0.92540100	7.34647800	-1.27908900
26	O	1.97061397	5.31300411	-0.62058303
27	O	6.63749400	5.47035800	-0.12078800
28	O	4.24784800	-2.40827300	0.89855600
29	O	7.19385700	-4.37204000	1.55132300
30	O	-2.94291602	-0.33360271	-5.33674342
31	Si	-3.05105101	0.82517039	-4.28077618
32	O	-4.30288197	1.71562802	-4.60976308
33	Si	-7.66044404	1.87626298	-2.71620922
34	Si	-6.78871850	-1.08302541	-2.99276865
35	Si	-5.49524044	-5.37813809	-1.27369222
36	Si	-2.96035214	-3.75927196	-2.11946815
37	O	-7.52819676	0.30285105	-2.77573853
38	O	-7.72169292	-2.22522175	-2.40154040
39	O	-6.70666200	-4.56345300	-1.90213800
40	O	-4.16380520	-4.57089188	-1.49340356
41	O	-6.55720388	-1.35735495	-4.52719899
42	O	-2.93087218	-3.99404290	-3.66934317
43	O	-6.49203400	2.57280900	-3.53128600
44	O	-1.60267909	-4.23324918	-1.43320895

1	Si	-1.62925898	-4.24078402	6.75449193
2	Si	1.43202700	-4.01238800	6.47761800
3	O	-0.10863400	-3.80204300	6.79077700
4	O	2.19170400	-2.69339500	6.97658900
5	O	0.37969393	-4.37630096	2.68939621
6	O	2.70722000	-3.30816400	2.79509000
7	O	1.66590000	-4.26059700	4.94801100
8	O	-1.87349800	-5.42776800	5.73955900
9	O	-1.56037496	-6.02755304	3.24246197
10	Si	-1.69753000	-6.61733400	4.71103900
11	Si	-0.72303399	-5.36766201	-0.75047704
12	Si	2.32497600	-5.23170000	-1.28780400
13	O	0.79239300	-4.97574600	-0.97616700
14	O	3.12382100	-3.91323800	-0.90472800
15	O	2.54055100	-5.53093700	-2.82034400
16	O	-0.78228200	-7.01267100	-3.95228200
17	O	-1.03941300	-6.78455000	-1.38718100
18	Si	-0.87552300	-7.81120400	-2.58947100
19	Si	-8.43273041	3.19561183	4.77249458
20	Si	-7.62362706	0.22077921	4.76560593
21	Si	-3.81904997	-2.44480267	5.61967059
22	Si	-4.66437531	0.49573041	5.68810253
23	Si	-8.00098851	2.37074474	0.31016733
24	Si	-8.36221447	-3.17781275	1.17062118
25	Si	-5.83343695	-4.88731562	1.72884087
26	O	-8.32151793	1.62994403	4.97779602
27	O	-3.89033445	-0.88223648	5.90186083
28	O	-6.21502028	0.22086845	5.48424048
29	O	-7.12244021	-3.95956935	1.79072701
30	O	-7.48457031	3.70435448	3.61447071
31	O	-7.01368386	3.33013129	1.09840070
32	O	-7.56916811	2.37875813	-1.21474003
33	O	-8.60499378	-3.57494516	-0.35774099
34	O	-5.70893287	-5.60835509	0.30080805
35	O	-1.04244998	-5.45208807	0.80067603
36	H	-5.72662400	6.47417600	-5.90006300
37	H	-8.99556600	2.22581200	-3.29884400
38	H	-0.47003900	9.22223000	0.37019800
39	H	-0.05729900	8.62313400	-3.29492200
40	H	7.98308800	6.51897600	1.74614800
41	H	8.39196200	5.92510500	-1.88557100
42	H	9.45831300	2.65246500	3.19084800
43	H	9.29359900	3.14838300	5.58508300
44	H	10.38276100	1.56639900	-4.08879000

1	H	10.00672600	1.85515900	-1.68423400
2	H	-9.61192398	-3.54906706	1.90856701
3	H	-0.42664000	-7.02815200	-6.44800400
4	H	-2.06796100	-4.64477900	8.12865500
5	H	10.36486700	-4.56707200	-2.24956400
6	H	-3.65046000	-5.07993100	-5.82888000
7	H	-6.64155300	7.80293900	2.22577800
8	H	-5.81050200	6.90807500	4.28150200
9	H	-4.50224600	5.00805100	-7.33836100
10	H	-0.97390000	6.34417500	-6.11335400
11	H	4.74749000	6.93789700	-4.52174800
12	H	4.58334600	8.62967800	-2.77232500
13	H	6.89236800	3.86633200	-4.80100300
14	H	8.26423000	-5.54587700	-5.79445300
15	H	6.96425300	-7.01308200	-4.35660100
16	H	-7.15165300	-2.75971500	-6.55017200
17	H	-6.95527900	-0.37644100	-6.82185800
18	H	-9.09540700	-4.29929600	-2.67946800
19	H	-5.42308400	-6.73019300	-1.91476500
20	H	-2.07387200	-8.70973100	-2.61309100
21	H	0.36227100	-8.63072400	-2.38880400
22	H	-0.47568100	-7.41386400	5.05262200
23	H	-2.90355100	-7.50469000	4.75596800
24	H	4.17113500	9.22851700	0.88959000
25	H	3.89232700	8.18005300	3.07420800
26	H	-8.09598400	3.89446700	6.05397700
27	H	-9.82935700	3.47036900	4.30571600
28	H	-9.41743194	2.83882318	0.45033806
29	H	-8.49958298	-0.80145101	5.42305301
30	H	-5.94965801	-5.96480402	2.76278998
31	H	-5.00957096	-3.10525099	6.24499009
32	H	3.27807200	-7.12520300	-4.60339400
33	H	6.62178700	-6.29177200	0.01381300
34	H	6.23479500	-5.72967500	3.45139000
35	H	9.45700900	-3.24870300	5.81221900
36	H	1.94258800	-5.18537000	7.25706900
37	H	2.41589200	-5.80407700	3.11763800
38	H	2.82090800	-6.39220800	-0.48086400
39	H	-2.05569400	7.91465900	3.49282600
40	H	-6.34945600	2.14645900	-6.01059700
41	H	5.81544000	5.43037700	4.76334300
42	H	4.98137900	-3.21756200	-6.49645100
43	H	-0.72039600	2.57206900	-6.51170400
44	H	-2.79313100	-1.09828500	-7.72788200

1	H	3.33282600	-0.82271100	8.14583300
2	H	7.06782700	0.29504300	6.80935800
3	H	-4.44368387	1.29917499	6.93312699
4	H	1.48849800	5.58781000	4.32561400
5	H	3.43005800	2.93607800	5.97148400
6	H	8.37544100	-1.60410700	-4.80464900
7	H	4.73823600	1.03586900	-5.64840100
8	H	2.58172000	4.00057800	-5.38291600
9	H	4.71070900	-2.67015900	7.26758300
10	H	7.16184900	-3.45599800	6.44283000
11	H	-2.02793662	4.47136497	5.10235806
12	C	1.48948989	-0.17865580	-1.01966073
13	H	0.63319233	-0.34297881	-1.67510896
14	H	2.39002057	-0.56757465	-1.50303132
15	H	1.32931183	-0.72061586	-0.07699168
16	O	1.59258614	1.21975618	-0.79947941
17	C	2.68574706	1.55602744	0.04035549
18	H	3.63845168	1.23627692	-0.40073206
19	H	2.58746565	1.08940554	1.02982923
20	H	2.68405768	2.63991957	0.14881140
21	C	-1.10754172	2.08908752	-0.42040492
22	H	-0.69232165	3.03530991	-0.08739340
23	H	-0.76702781	1.27272229	0.20961040
24	H	-0.86281248	1.90703412	-1.46048701
25	O	-2.57321621	2.19689387	-0.34647613
26	H	-3.04052642	1.25629578	-0.59685629
27	H	-2.88846604	2.20153566	0.59845400
28				
29				
30	ZH_CH3OH(ads)_cyclopropane(ads)			
31	Si	-0.03175500	0.02319200	-0.00852700
32	Si	-0.06335700	-0.00787200	5.68430400
33	Si	3.70799600	-0.02463300	2.48745900
34	Si	1.04011200	-3.89566200	2.98563400
35	Al	0.73950300	-0.85900300	2.84096300
36	O	0.30655600	-2.48728500	2.98968700
37	O	2.39842400	-0.60497600	3.18921800
38	O	0.04738800	0.01590900	1.56362900
39	O	-0.20920600	0.05555300	4.05819900
40	O	-1.57784700	0.16858400	-0.43957100
41	O	-0.32957000	-1.46244000	6.27134200
42	O	1.37891800	0.49943000	6.16978000
43	O	-1.24407500	0.98912900	6.04897600
44	O	0.81224400	1.29343300	-0.52547900

1	O	3.76803600	1.57996400	2.49373100
2	O	4.99195700	-0.48025500	3.33245100
3	O	2.21308800	-4.05653200	4.09839100
4	O	3.86048900	-0.50904900	0.95217700
5	O	1.74380300	-4.23820800	1.56799200
6	O	0.57359900	-1.27273000	-0.73640700
7	O	-0.13152800	-4.94437400	3.32539300
8	H	-1.01270100	0.64441800	3.66789600
9	C	-4.66693300	-0.53799400	3.00433300
10	H	-4.62766700	-0.29800100	4.06065200
11	H	-2.81903800	0.78568000	2.92810100
12	H	-5.15769800	0.20885900	2.39053000
13	O	-2.11995400	1.38266900	3.24631500
14	C	-3.52315000	-1.35095500	2.39573700
15	H	-2.70821100	-1.66368300	3.03778600
16	H	-3.23142700	-1.13772700	1.37465300
17	C	-4.86670300	-1.98112500	2.62521600
18	H	-5.47467300	-2.20153300	1.75789600
19	H	-4.95722400	-2.70121800	3.42815500
20	C	-1.97015400	2.52899200	2.38865200
21	H	-1.85957600	2.22820700	1.34777100
22	H	-2.83122400	3.19003600	2.50394400
23	H	-1.07218200	3.05277600	2.71249700
24	O	0.80118600	-6.00638900	-0.15260000
25	Si	-5.49760400	-0.02108300	-1.47429000
26	Si	-2.51944300	0.76946600	-1.59101200
27	Si	1.67073800	2.63422900	-0.36395300
28	Si	-6.77250000	-2.79180000	-1.55910000
29	Si	-6.65860000	-5.43650000	-0.02630000
30	Si	-0.62798400	-6.20843900	4.15918800
31	Si	-3.21920500	-7.43500100	2.98451300
32	Si	-6.09540000	-6.32220000	2.83000000
33	Si	-7.79180000	-8.89230000	3.21140000
34	Si	-7.85690000	-4.02790000	9.99880000
35	Si	-9.54690000	-6.64300000	10.42590000
36	O	-8.68790000	-5.35140000	10.15840000
37	Si	1.78779900	2.30219600	9.72780100
38	Si	-0.76980100	-1.62740100	10.29930000
39	Si	-1.17799700	1.38379200	9.93889700
40	O	-1.38700100	-0.16320100	10.26480000
41	O	0.35019800	1.77510400	10.12159800
42	O	-1.90929700	-2.64050300	10.65650200
43	Si	-2.31670000	-4.06080000	11.29600000
44	Si	-5.02660000	-5.18350000	10.35000000

1	O	-3.83590000	-4.30830000	10.92640000
2	O	-6.34110000	-4.27000000	10.39930000
3	Si	4.73289800	-0.80098700	7.13548400
4	Si	-7.29070000	2.20560000	5.67640000
5	Si	-4.57940000	3.32750100	6.62399900
6	Si	-1.94070000	7.20800000	6.08700000
7	Si	-4.59330000	6.04430000	5.10460000
8	O	-5.77090000	2.45290000	6.04720000
9	O	-3.26549900	2.41429700	6.57329400
10	O	-0.99450200	5.94280300	5.99240900
11	O	-3.27080000	6.91960000	5.26710000
12	O	-4.35770000	4.58890000	5.69440000
13	O	-7.46660000	2.24720000	4.09540000
14	O	-4.88400000	5.95910000	3.53970000
15	Si	-5.99570000	5.67090000	2.42990000
16	Si	-10.73910000	3.90040000	2.70070000
17	O	-11.73290000	2.70740000	2.34160000
18	Si	-12.07420000	1.15480000	2.31840000
19	O	-11.45520000	0.42330000	3.58130000
20	Si	-11.39460000	-4.15760000	7.24580000
21	Si	-13.29570000	-2.46030000	5.52120000
22	Si	-11.50890000	0.09760000	5.13610000
23	Si	-8.83680000	-0.22830000	6.67330000
24	O	-12.44950000	-3.64190000	6.15630000
25	O	-12.41530000	-1.16550000	5.38290000
26	O	-10.03410000	-0.20050000	5.63860000
27	O	-7.69650000	0.78430000	6.31660000
28	Si	-0.05969900	4.78729900	6.54669800
29	O	-10.24280000	-7.11800000	9.08650000
30	Si	-7.71660000	3.11370000	2.78820000
31	O	-6.95550000	4.50240000	2.92570000
32	O	-9.24950000	3.38730000	2.56950000
33	Si	-4.97250000	-7.60980000	-1.50390000
34	Si	-11.35590000	0.26280000	-0.54610000
35	O	-6.84510000	-7.72030000	2.70470000
36	O	-10.35620000	-0.94150000	-0.80140000
37	Si	-9.16490000	-9.40520000	0.52820000
38	Si	-9.33470000	-6.71560000	-0.96890000
39	Si	-11.54680000	-4.63200000	-1.45310000
40	Si	-9.77590000	-2.05450000	-1.77500000
41	O	-9.58580000	-8.00560000	-0.07990000
42	O	-10.67690000	-5.84320000	-0.91270000
43	O	-10.64710000	-3.36120000	-1.66840000
44	O	-8.28390000	-2.37400000	-1.34130000

1	O	-6.40440000	-3.94670000	-0.53100000
2	O	-8.15250000	-5.87130000	-0.34420000
3	O	-8.84920000	-9.23940000	2.07860000
4	O	-6.41640000	-5.42400000	1.54900000
5	O	-5.61290000	-6.41590000	-0.70840000
6	O	-5.77370000	-1.60340000	-1.35130000
7	Si	-6.81090000	-5.43360000	5.68340000
8	Si	-8.50460000	-8.00720000	6.05360000
9	O	-7.72180000	-6.63160000	6.20070000
10	Si	-10.95800000	-7.17850000	7.67890000
11	Si	-8.42890000	-3.23820000	7.03330000
12	O	-11.40780000	-5.74300000	7.18590000
13	O	-8.21960000	-1.69260000	6.70790000
14	O	-9.95660000	-3.63110000	6.85010000
15	O	-9.98360000	-7.83070000	6.60240000
16	O	-7.53000000	-4.04100000	5.99020000
17	O	-7.92320000	-3.54700000	8.50450000
18	Si	0.12316400	4.64406900	-2.14550400
19	Si	-2.82305800	3.84600200	-1.95511800
20	O	-3.94900600	0.19046300	-1.21842400
21	O	0.75709000	3.77017000	-0.98770400
22	O	-1.45550000	4.66540000	-1.97180000
23	O	-2.55345500	2.34860600	-1.50009500
24	O	-6.33220000	0.83850000	-0.42850000
25	O	-3.77030000	4.57610000	-0.90140000
26	Si	-5.28020000	4.78230000	-0.42350000
27	Si	-7.00390000	2.22870000	-0.05400000
28	Si	-9.63060000	2.52380000	-1.72000000
29	O	-6.07880000	3.41370000	-0.57020000
30	O	-8.42830000	2.36750000	-0.70540000
31	O	-10.83220000	1.58900000	-1.25000000
32	O	-5.20960000	5.26350000	1.09860000
33	O	-7.15700000	2.26930000	1.54270000
34	O	-11.46650000	0.47770000	1.01990000
35	O	-6.60040000	-5.49380000	4.09960000
36	O	-8.61720000	-8.44720000	4.51360000
37	O	-1.68271300	1.69079400	8.46849900
38	Si	-1.74889700	2.17161200	6.97406500
39	O	-0.91869600	3.49569700	6.81429700
40	Si	2.50950200	3.95251000	5.10420700
41	Si	2.56679100	1.37897900	6.82672900
42	Si	3.01119600	-3.35762500	7.49352000
43	Si	-0.01123700	-2.57108500	7.40604700
44	O	2.86460400	2.66318900	5.94588500

1	O	3.90009700	0.51779800	6.89193200
2	O	3.77240000	-1.96900000	7.63100000
3	O	1.47831400	-3.08394900	7.27476500
4	O	2.15446900	1.79118500	8.29129500
5	O	-0.24972500	-2.04667900	8.86408800
6	O	1.05379700	4.47370100	5.45679600
7	O	-1.00418000	-3.76440800	7.04717200
8	Si	0.52350100	-7.58780000	-0.03030200
9	Si	-2.45310000	-8.37930000	0.08690000
10	O	-1.02440000	-7.79970000	-0.28570000
11	O	-3.48040000	-7.82240000	-1.00870000
12	O	-2.05279300	-6.52238300	3.54847500
13	O	-4.53620000	-6.55020000	2.91500000
14	O	-2.87430000	-7.94910000	1.53380000
15	O	0.93450000	-7.98310000	1.44400000
16	O	0.37171600	-7.41288500	3.90389100
17	Si	0.95189400	-8.52590600	2.93030300
18	Si	-1.34641000	-5.31659900	7.02371900
19	Si	-4.32960000	-6.05610000	7.41270000
20	O	-2.92290000	-5.44190000	7.01850000
21	O	-5.41450000	-5.45960000	6.41750000
22	O	-4.71840000	-5.65910000	8.88780000
23	O	-1.36620000	-5.12610000	10.61890000
24	O	-0.72730000	-6.04810000	8.28660000
25	Si	-0.78110000	-6.37380000	9.84140000
26	Si	4.19137300	1.79568500	-2.03283300
27	Si	4.36133300	-0.89364000	-0.53536000
28	Si	1.79924600	-4.81758600	0.05467400
29	Si	1.68556600	-2.17089700	-1.47830300
30	Si	3.22764200	3.05983300	2.24005700
31	Si	5.44849500	-1.68948900	4.28208500
32	Si	3.72399600	-4.24268300	4.65119300
33	O	4.61247600	0.39620000	-1.42440700
34	O	1.43066300	-3.66256900	-0.97313900
35	O	3.17929900	-1.73827200	-1.16009500
36	O	4.64913600	-3.05762200	4.13511700
37	O	2.93745700	2.40543500	-1.28803100
38	O	2.15418700	3.10999200	1.07323700
39	O	2.54300400	3.62278800	3.55350700
40	O	5.51820000	-1.20772600	5.80380800
41	O	3.57088900	-4.20199400	6.24789900
42	O	-0.73789800	-5.99418400	5.72549800
43	H	-1.30770000	8.45280000	5.54490000
44	H	3.53900000	4.98890000	5.43620000

1	H	-5.91550000	5.84190000	-1.27060000
2	H	-6.78570000	6.92250000	2.19890000
3	H	-12.70540000	-0.03450000	-1.12450000
4	H	-13.56750000	1.03610000	2.31350000
5	H	-12.61360000	-4.36250000	-0.43650000
6	H	-12.17550000	-5.02190000	-2.75570000
7	H	-14.47190000	-2.17020000	6.40220000
8	H	-13.77040000	-2.92530000	4.17860000
9	H	6.86450200	-1.88261900	3.83331500
10	H	-2.15040000	-4.10050000	12.78420000
11	H	1.31010000	-8.39770000	-1.01480000
12	H	-12.21020000	-7.97290000	7.89080000
13	H	0.36340100	-1.65379500	11.27869900
14	H	0.62130000	6.05740000	-2.14750000
15	H	0.50140000	4.07440000	-3.47820000
16	H	-2.25700000	7.49990000	7.52180000
17	H	-5.73850000	6.73170000	5.78280000
18	H	-10.96700000	4.40130000	4.09400000
19	H	-11.01960000	5.00810000	1.73210000
20	H	-12.06290000	1.27880000	5.87220000
21	H	-10.59640000	-6.34750000	11.45320000
22	H	-8.66420000	-7.73420000	10.94950000
23	H	2.77449800	1.81969700	10.74640000
24	H	1.80020700	3.79900000	9.78440200
25	H	5.77540000	-0.53010000	8.17660000
26	H	3.24710000	-4.17500000	8.72650000
27	H	0.61160000	-6.65520000	10.31590000
28	H	-1.64370000	-7.57580000	10.07620000
29	H	0.12290000	-9.76940000	3.03170000
30	H	2.36090000	-8.82750000	3.33990000
31	H	-10.15040000	3.92860000	-1.73450000
32	H	-9.16390000	2.16210000	-3.09680000
33	H	3.89500000	1.63920000	-3.49250000
34	H	5.32300000	2.73990000	-1.76330000
35	H	4.42878900	3.88351200	1.88708900
36	H	5.61651200	-1.70968100	-0.58831400
37	H	4.35728200	-5.55351000	4.29820200
38	H	3.22919800	-5.21290500	-0.15130800
39	H	-5.23700000	-6.37850000	11.22840000
40	H	-7.76830000	-9.07120000	6.80850000
41	H	-6.95230000	-10.08460000	3.55430000
42	H	-10.29630000	-10.34930000	0.25900000
43	H	-2.42150000	-9.87450000	0.00040000
44	H	-3.42900000	-8.60990000	3.88980000

1	H	-4.28320000	-7.54880000	7.29620000
2	H	-3.45780000	3.89970000	-3.31080000
3	H	0.59910600	5.23699600	7.81469800
4	H	-9.79240000	-1.54060000	-3.18200000
5	H	-8.38790000	-2.95530000	10.89960000
6	H	-4.87450000	3.78240000	8.02040000
7	H	-2.02270000	2.13730000	10.92000000
8	H	-4.91220000	-7.27130000	-2.96190000
9	H	-8.98790000	-7.09310000	-2.37650000
10	H	1.45736900	-2.18480400	-2.95899500
11	H	-5.88650000	0.35320000	-2.87170000
12	H	-6.57060000	-3.25690000	-2.96870000
13	H	-11.74490000	-3.66940000	8.61800000
14	H	-9.32890000	0.16850000	8.03140000
15	H	-8.19140000	3.21540000	6.31880000
16	H	-5.78340000	-8.84910000	-1.27830000
17	H	-7.97590000	-9.98270000	-0.17660000
18	H	-2.11778000	0.35849800	-2.97416300
19				
20				
21	ZH_cyclopropane(ads)-to-Z-CH2CH2CH3-TS			
22	Si	-0.02755874	0.02313073	-0.02050090
23	Si	-0.07502111	-0.00765977	5.63905451
24	Si	3.72361872	-0.03404327	2.48952349
25	Si	1.04762206	-3.89428180	2.97784386
26	Al	0.75843211	-0.83119222	2.89468707
27	O	0.29919863	-2.49848213	2.85412835
28	O	2.44612313	-0.68393421	3.17854935
29	O	0.07182029	-0.05742460	1.53651180
30	O	-0.21455171	-0.06737928	4.07483322
31	O	-1.60107508	0.13868604	-0.42577762
32	O	-0.36041129	-1.44244820	6.32258555
33	O	1.36148058	0.50995206	6.19778470
34	O	-1.26041694	0.99505459	6.04163713
35	O	0.79914684	1.29912675	-0.54272912
36	O	3.74798832	1.57130066	2.49667151
37	O	5.02406937	-0.47397465	3.32194057
38	O	2.20248244	-4.04313406	4.10768040
39	O	3.87792720	-0.50268749	0.94830393
40	O	1.76514240	-4.30303062	1.58588023
41	O	0.53903293	-1.26795044	-0.80084094
42	O	-0.15365846	-4.92332583	3.33667820
43	C	-2.36937726	-1.78566877	2.64229181
44	H	-1.93291346	-0.87783949	3.05466080

1	H	-1.79751283	-2.30535975	1.88672123
2	C	-3.57958268	-2.30549121	3.12947337
3	H	-3.97041418	-1.92040812	4.06329833
4	H	-3.83893656	-3.33259601	2.90429489
5	C	-4.02151147	-1.31892895	1.88165319
6	H	-3.23066892	-0.81395140	1.28421928
7	H	-4.53197806	-1.96280192	1.17143191
8	H	-4.61430823	-0.52130497	2.31710302
9	O	0.80120000	-6.00640000	-0.15260000
10	Si	-5.49760000	-0.02110000	-1.47430000
11	Si	-2.51950000	0.76950000	-1.59080000
12	Si	1.67330000	2.63520000	-0.36440000
13	Si	-6.77250000	-2.79180000	-1.55910000
14	Si	-6.65860000	-5.43650000	-0.02630000
15	Si	-0.62810000	-6.20860000	4.15920000
16	Si	-3.21920000	-7.43500000	2.98450000
17	Si	-6.09540000	-6.32220000	2.83000000
18	Si	-7.79180000	-8.89230000	3.21140000
19	Si	-7.85690000	-4.02790000	9.99880000
20	Si	-9.54690000	-6.64300000	10.42590000
21	O	-8.68790000	-5.35140000	10.15840000
22	Si	1.78780000	2.30220000	9.72780000
23	Si	-0.76980000	-1.62740000	10.29930000
24	Si	-1.17800000	1.38380000	9.93890000
25	O	-1.38700000	-0.16320000	10.26480000
26	O	0.35020000	1.77510000	10.12160000
27	O	-1.90930000	-2.64050000	10.65650000
28	Si	-2.31670000	-4.06080000	11.29600000
29	Si	-5.02660000	-5.18350000	10.35000000
30	O	-3.83590000	-4.30830000	10.92640000
31	O	-6.34110000	-4.27000000	10.39930000
32	Si	4.73290000	-0.80100000	7.13550000
33	Si	-7.29070000	2.20560000	5.67640000
34	Si	-4.57940000	3.32750000	6.62400000
35	Si	-1.94070000	7.20800000	6.08700000
36	Si	-4.59330000	6.04430000	5.10460000
37	O	-5.77090000	2.45290000	6.04720000
38	O	-3.26550000	2.41430000	6.57330000
39	O	-0.99450000	5.94280000	5.99240000
40	O	-3.27080000	6.91960000	5.26710000
41	O	-4.35770000	4.58890000	5.69440000
42	O	-7.46660000	2.24720000	4.09540000
43	O	-4.88400000	5.95910000	3.53970000
44	Si	-5.99570000	5.67090000	2.42990000

1	Si	-10.73910000	3.90040000	2.70070000
2	O	-11.73290000	2.70740000	2.34160000
3	Si	-12.07420000	1.15480000	2.31840000
4	O	-11.45520000	0.42330000	3.58130000
5	Si	-11.39460000	-4.15760000	7.24580000
6	Si	-13.29570000	-2.46030000	5.52120000
7	Si	-11.50890000	0.09760000	5.13610000
8	Si	-8.83680000	-0.22830000	6.67330000
9	O	-12.44950000	-3.64190000	6.15630000
10	O	-12.41530000	-1.16550000	5.38290000
11	O	-10.03410000	-0.20050000	5.63860000
12	O	-7.69650000	0.78430000	6.31660000
13	Si	-0.05970000	4.78730000	6.54670000
14	O	-10.24280000	-7.11800000	9.08650000
15	Si	-7.71660000	3.11370000	2.78820000
16	O	-6.95550000	4.50240000	2.92570000
17	O	-9.24950000	3.38730000	2.56950000
18	Si	-4.97250000	-7.60980000	-1.50390000
19	Si	-11.35590000	0.26280000	-0.54610000
20	O	-6.84510000	-7.72030000	2.70470000
21	O	-10.35620000	-0.94150000	-0.80140000
22	Si	-9.16490000	-9.40520000	0.52820000
23	Si	-9.33470000	-6.71560000	-0.96890000
24	Si	-11.54680000	-4.63200000	-1.45310000
25	Si	-9.77590000	-2.05450000	-1.77500000
26	O	-9.58580000	-8.00560000	-0.07990000
27	O	-10.67690000	-5.84320000	-0.91270000
28	O	-10.64710000	-3.36120000	-1.66840000
29	O	-8.28390000	-2.37400000	-1.34130000
30	O	-6.40440000	-3.94670000	-0.53100000
31	O	-8.15250000	-5.87130000	-0.34420000
32	O	-8.84920000	-9.23940000	2.07860000
33	O	-6.41640000	-5.42400000	1.54900000
34	O	-5.61290000	-6.41590000	-0.70840000
35	O	-5.77370000	-1.60340000	-1.35130000
36	Si	-6.81090000	-5.43360000	5.68340000
37	Si	-8.50460000	-8.00720000	6.05360000
38	O	-7.72180000	-6.63160000	6.20070000
39	Si	-10.95800000	-7.17850000	7.67890000
40	Si	-8.42890000	-3.23820000	7.03330000
41	O	-11.40780000	-5.74300000	7.18590000
42	O	-8.21960000	-1.69260000	6.70790000
43	O	-9.95660000	-3.63110000	6.85010000
44	O	-9.98360000	-7.83070000	6.60240000

1	O	-7.53000000	-4.04100000	5.99020000
2	O	-7.92320000	-3.54700000	8.50450000
3	Si	0.12370000	4.64450000	-2.14540000
4	Si	-2.82300000	3.84600000	-1.95510000
5	O	-3.94900000	0.19040000	-1.21860000
6	O	0.75580000	3.76930000	-0.98750000
7	O	-1.45550000	4.66540000	-1.97180000
8	O	-2.55360000	2.34860000	-1.49990000
9	O	-6.33220000	0.83850000	-0.42850000
10	O	-3.77030000	4.57610000	-0.90140000
11	Si	-5.28020000	4.78230000	-0.42350000
12	Si	-7.00390000	2.22870000	-0.05400000
13	Si	-9.63060000	2.52380000	-1.72000000
14	O	-6.07880000	3.41370000	-0.57020000
15	O	-8.42830000	2.36750000	-0.70540000
16	O	-10.83220000	1.58900000	-1.25000000
17	O	-5.20960000	5.26350000	1.09860000
18	O	-7.15700000	2.26930000	1.54270000
19	O	-11.46650000	0.47770000	1.01990000
20	O	-6.60040000	-5.49380000	4.09960000
21	O	-8.61720000	-8.44720000	4.51360000
22	O	-1.68270000	1.69080000	8.46850000
23	Si	-1.74890000	2.17180000	6.97420000
24	O	-0.91870000	3.49570000	6.81430000
25	Si	2.50950000	3.95250000	5.10420000
26	Si	2.56680000	1.37890000	6.82680000
27	Si	3.01120000	-3.35760000	7.49350000
28	Si	-0.01130000	-2.57100000	7.40600000
29	O	2.86460000	2.66320000	5.94590000
30	O	3.90010000	0.51780000	6.89190000
31	O	3.77240000	-1.96900000	7.63100000
32	O	1.47830000	-3.08400000	7.27480000
33	O	2.15450000	1.79120000	8.29130000
34	O	-0.24970000	-2.04670000	8.86410000
35	O	1.05380000	4.47370000	5.45680000
36	O	-1.00420000	-3.76440000	7.04720000
37	Si	0.52350000	-7.58780000	-0.03030000
38	Si	-2.45310000	-8.37930000	0.08690000
39	O	-1.02440000	-7.79970000	-0.28570000
40	O	-3.48040000	-7.82240000	-1.00870000
41	O	-2.05280000	-6.52240000	3.54850000
42	O	-4.53620000	-6.55020000	2.91500000
43	O	-2.87430000	-7.94910000	1.53380000
44	O	0.93450000	-7.98310000	1.44400000

1	O	0.37170000	-7.41290000	3.90390000
2	Si	0.95190000	-8.52590000	2.93030000
3	Si	-1.34640000	-5.31660000	7.02370000
4	Si	-4.32960000	-6.05610000	7.41270000
5	O	-2.92290000	-5.44190000	7.01850000
6	O	-5.41450000	-5.45960000	6.41750000
7	O	-4.71840000	-5.65910000	8.88780000
8	O	-1.36620000	-5.12610000	10.61890000
9	O	-0.72730000	-6.04810000	8.28660000
10	Si	-0.78110000	-6.37380000	9.84140000
11	Si	4.19160000	1.79580000	-2.03250000
12	Si	4.36130000	-0.89370000	-0.53530000
13	Si	1.79910000	-4.81760000	0.05480000
14	Si	1.68500000	-2.17150000	-1.47840000
15	Si	3.22790000	3.06050000	2.23970000
16	Si	5.44850000	-1.68950000	4.28210000
17	Si	3.72400000	-4.24270000	4.65120000
18	O	4.61250000	0.39620000	-1.42440000
19	O	1.43100000	-3.66270000	-0.97330000
20	O	3.17920000	-1.73800000	-1.16010000
21	O	4.64900000	-3.05760000	4.13510000
22	O	2.93690000	2.40530000	-1.28880000
23	O	2.15280000	3.10900000	1.07410000
24	O	2.54300000	3.62290000	3.55350000
25	O	5.51820000	-1.20780000	5.80380000
26	O	3.57090000	-4.20200000	6.24790000
27	O	-0.73790000	-5.99420000	5.72550000
28	H	-1.30770000	8.45280000	5.54490000
29	H	3.53900000	4.98890000	5.43620000
30	H	-5.91550000	5.84190000	-1.27060000
31	H	-6.78570000	6.92250000	2.19890000
32	H	-12.70540000	-0.03450000	-1.12450000
33	H	-13.56750000	1.03610000	2.31350000
34	H	-12.61360000	-4.36250000	-0.43650000
35	H	-12.17550000	-5.02190000	-2.75570000
36	H	-14.47190000	-2.17020000	6.40220000
37	H	-13.77040000	-2.92530000	4.17860000
38	H	6.86450000	-1.88260000	3.83330000
39	H	-2.15040000	-4.10050000	12.78420000
40	H	1.31010000	-8.39770000	-1.01480000
41	H	-12.21020000	-7.97290000	7.89080000
42	H	0.36340000	-1.65380000	11.27870000
43	H	0.62130000	6.05740000	-2.14750000
44	H	0.50140000	4.07440000	-3.47820000

1	H	-2.25700000	7.49990000	7.52180000
2	H	-5.73850000	6.73170000	5.78280000
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4	H	-11.01960000	5.00810000	1.73210000
5	H	-12.06290000	1.27880000	5.87220000
6	H	-10.59640000	-6.34750000	11.45320000
7	H	-8.66420000	-7.73420000	10.94950000
8	H	2.77450000	1.81970000	10.74640000
9	H	1.80020000	3.79900000	9.78440000
10	H	5.77540000	-0.53010000	8.17660000
11	H	3.24710000	-4.17500000	8.72650000
12	H	0.61160000	-6.65520000	10.31590000
13	H	-1.64370000	-7.57580000	10.07620000
14	H	0.12290000	-9.76940000	3.03170000
15	H	2.36090000	-8.82750000	3.33990000
16	H	-10.15040000	3.92860000	-1.73450000
17	H	-9.16390000	2.16210000	-3.09680000
18	H	3.89500000	1.63920000	-3.49250000
19	H	5.32300000	2.73990000	-1.76330000
20	H	4.42880000	3.88350000	1.88700000
21	H	5.61650000	-1.70970000	-0.58830000
22	H	4.35730000	-5.55350000	4.29820000
23	H	3.22920000	-5.21290000	-0.15130000
24	H	-5.23700000	-6.37850000	11.22840000
25	H	-7.76830000	-9.07120000	6.80850000
26	H	-6.95230000	-10.08460000	3.55430000
27	H	-10.29630000	-10.34930000	0.25900000
28	H	-2.42150000	-9.87450000	0.00040000
29	H	-3.42900000	-8.60990000	3.88980000
30	H	-4.28320000	-7.54880000	7.29620000
31	H	-3.45780000	3.89970000	-3.31080000
32	H	0.59910000	5.23700000	7.81470000
33	H	-9.79240000	-1.54060000	-3.18200000
34	H	-8.38790000	-2.95530000	10.89960000
35	H	-4.87450000	3.78240000	8.02040000
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38	H	-8.98790000	-7.09310000	-2.37650000
39	H	1.45750000	-2.18460000	-2.95900000
40	H	-5.88650000	0.35320000	-2.87170000
41	H	-6.57060000	-3.25690000	-2.96870000
42	H	-11.74490000	-3.66940000	8.61800000
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H    -5.78340000    -8.84910000    -1.27830000
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ZH_cyclopropane(ads)
Si -0.03581151    0.02837502     -0.00514870
Si -0.06876134    -0.00401076    5.69880341
Si 3.71735126     -0.01239532    2.48507579
Si 1.04708573     -3.90415942    2.98177362
Al 0.76680199     -0.86729852    2.79744598
O    0.32600576     -2.48958417    2.94845291
O    2.39797854     -0.56443000    3.20037127
O    0.01401437     0.02880620     1.57426666
O    -0.22860802    -0.01253233    4.05698756
O    -1.57136105    0.15215577     -0.45560327
O    -0.34679485    -1.44716853    6.29374258
O    1.37552266     0.50853320     6.14774797
O    -1.25328356    1.00956982     6.00569266
O    0.82940494     1.28363091     -0.51778132
O    3.79427289     1.58837917     2.48591392
O    4.99198474     -0.48113895    3.33367813
O    2.21096043     -4.04362749    4.10617700
O    3.85439985     -0.51801253    0.95600070
O    1.76149415     -4.26077771    1.57607037
O    0.59317784     -1.27927799    -0.69801962
O    -0.13288632    -4.93725581    3.33347387
C    -4.25511300    0.17609755     2.66233592
H    -5.14360601    0.38501953     3.24339395
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C    -2.99216889    0.91487503     3.02377187
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C    -3.14446794    -0.58339297    3.31887555
H    -1.12537540    0.22621331     3.71771694
H    -3.27997992    -0.88242742    4.35141642
H    -2.58899833    -1.28717380    2.71107922
O    0.80124623     -6.00642317    -0.15269612
Si -5.49758205    -0.02118381    -1.47434488
Si -2.51956998    0.76944607     -1.59082939
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Si -6.77250000    -2.79180000    -1.55910000
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2	Si	-6.09539800	-6.32220400	2.82995300
3	Si	-7.79180000	-8.89230000	3.21140000
4	Si	-7.85690000	-4.02790000	9.99880000
5	Si	-9.54690000	-6.64300000	10.42590000
6	O	-8.68790000	-5.35140000	10.15840000
7	Si	1.78779900	2.30221100	9.72779700
8	Si	-0.76979722	-1.62740335	10.29930173
9	Si	-1.17781899	1.38331097	9.93873499
10	O	-1.38699700	-0.16319900	10.26480100
11	O	0.35020400	1.77509200	10.12160400
12	O	-1.90930400	-2.64049600	10.65649800
13	Si	-2.31670000	-4.06080000	11.29600000
14	Si	-5.02660000	-5.18350000	10.35000000
15	O	-3.83590000	-4.30830000	10.92640000
16	O	-6.34110000	-4.27000000	10.39930000
17	Si	4.73290894	-0.80094887	7.13557244
18	Si	-7.29070000	2.20560000	5.67640000
19	Si	-4.57937608	3.32753688	6.62397422
20	Si	-1.94070000	7.20800000	6.08700000
21	Si	-4.59330000	6.04430000	5.10460000
22	O	-5.77090400	2.45289300	6.04722000
23	O	-3.26562277	2.41443875	6.57334460
24	O	-0.99449700	5.94279600	5.99238700
25	O	-3.27080000	6.91960000	5.26710000
26	O	-4.35770700	4.58889100	5.69438500
27	O	-7.46660400	2.24719800	4.09540000
28	O	-4.88400000	5.95910000	3.53970000
29	Si	-5.99570000	5.67090000	2.42990000
30	Si	-10.73910000	3.90040000	2.70070000
31	O	-11.73290000	2.70740000	2.34160000
32	Si	-12.07420000	1.15480000	2.31840000
33	O	-11.45520000	0.42330000	3.58130000
34	Si	-11.39460000	-4.15760000	7.24580000
35	Si	-13.29570000	-2.46030000	5.52120000
36	Si	-11.50890000	0.09760000	5.13610000
37	Si	-8.83680000	-0.22830000	6.67330000
38	O	-12.44950000	-3.64190000	6.15630000
39	O	-12.41530000	-1.16550000	5.38290000
40	O	-10.03410000	-0.20050000	5.63860000
41	O	-7.69650000	0.78430000	6.31660000
42	Si	-0.05970700	4.78730400	6.54670000
43	O	-10.24280000	-7.11800000	9.08650000
44	Si	-7.71658800	3.11368700	2.78821400

1	O	-6.95550500	4.50240300	2.92569500
2	O	-9.24949900	3.38730300	2.56949800
3	Si	-4.97250000	-7.60980000	-1.50390000
4	Si	-11.35590000	0.26280000	-0.54610000
5	O	-6.84510100	-7.72030100	2.70471300
6	O	-10.35620000	-0.94150000	-0.80140000
7	Si	-9.16490000	-9.40520000	0.52820000
8	Si	-9.33470000	-6.71560000	-0.96890000
9	Si	-11.54680000	-4.63200000	-1.45310000
10	Si	-9.77590000	-2.05450000	-1.77500000
11	O	-9.58580000	-8.00560000	-0.07990000
12	O	-10.67690000	-5.84320000	-0.91270000
13	O	-10.64710000	-3.36120000	-1.66840000
14	O	-8.28390000	-2.37400000	-1.34130000
15	O	-6.40440000	-3.94670000	-0.53100000
16	O	-8.15250000	-5.87130000	-0.34420000
17	O	-8.84920000	-9.23940000	2.07860000
18	O	-6.41639900	-5.42399100	1.54900600
19	O	-5.61290000	-6.41590000	-0.70840000
20	O	-5.77369900	-1.60340100	-1.35130800
21	Si	-6.81090000	-5.43360000	5.68340000
22	Si	-8.50460000	-8.00720000	6.05360000
23	O	-7.72180000	-6.63160000	6.20070000
24	Si	-10.95800000	-7.17850000	7.67890000
25	Si	-8.42890000	-3.23820000	7.03330000
26	O	-11.40780000	-5.74300000	7.18590000
27	O	-8.21960000	-1.69260000	6.70790000
28	O	-9.95660000	-3.63110000	6.85010000
29	O	-9.98360000	-7.83070000	6.60240000
30	O	-7.53000000	-4.04100000	5.99020000
31	O	-7.92320000	-3.54700000	8.50450000
32	Si	0.12382596	4.64460997	-2.14538500
33	Si	-2.82302197	3.84599900	-1.95509001
34	O	-3.94895894	0.19055563	-1.21839635
35	O	0.75553200	3.76907500	-0.98751400
36	O	-1.45550000	4.66540000	-1.97180000
37	O	-2.55354404	2.34860100	-1.49991005
38	O	-6.33219400	0.83850000	-0.42849800
39	O	-3.77030000	4.57610000	-0.90140000
40	Si	-5.28020000	4.78230000	-0.42350000
41	Si	-7.00390800	2.22869100	-0.05400100
42	Si	-9.63060000	2.52380000	-1.72000000
43	O	-6.07880100	3.41370100	-0.57020000
44	O	-8.42830000	2.36750200	-0.70540000

1	O	-10.83220000	1.58900000	-1.25000000
2	O	-5.20960000	5.26350000	1.09860000
3	O	-7.15699800	2.26931200	1.54268600
4	O	-11.46650000	0.47770000	1.01990000
5	O	-6.60040100	-5.49380600	4.09960400
6	O	-8.61720000	-8.44720000	4.51360000
7	O	-1.68298449	1.69185121	8.46884904
8	Si	-1.74885787	2.17101509	6.97394002
9	O	-0.91872260	3.49571375	6.81429902
10	Si	2.50953984	3.95246592	5.10393566
11	Si	2.56686130	1.37860419	6.82659179
12	Si	3.01134213	-3.35731935	7.49333138
13	Si	-0.01124296	-2.57086916	7.40581753
14	O	2.86460340	2.66354806	5.94640976
15	O	3.90009356	0.51777641	6.89173319
16	O	3.77240000	-1.96900000	7.63100000
17	O	1.47817612	-3.08444946	7.27517021
18	O	2.15450892	1.79122625	8.29129519
19	O	-0.24969930	-2.04667530	8.86409142
20	O	1.05380700	4.47369700	5.45680800
21	O	-1.00418633	-3.76439462	7.04717465
22	Si	0.52348296	-7.58779398	-0.03025388
23	Si	-2.45310000	-8.37930000	0.08690000
24	O	-1.02440000	-7.79970000	-0.28570000
25	O	-3.48040000	-7.82240000	-1.00870000
26	O	-2.05303516	-6.52251123	3.54920450
27	O	-4.53620000	-6.55018600	2.91508700
28	O	-2.87429900	-7.94911100	1.53380500
29	O	0.93450000	-7.98310000	1.44400000
30	O	0.37158733	-7.41299674	3.90391306
31	Si	0.95194584	-8.52585615	2.93027808
32	Si	-1.34639839	-5.31658925	7.02371730
33	Si	-4.32960000	-6.05610000	7.41270000
34	O	-2.92290100	-5.44189600	7.01849400
35	O	-5.41450000	-5.45960000	6.41750000
36	O	-4.71840000	-5.65910000	8.88780000
37	O	-1.36620000	-5.12610000	10.61890000
38	O	-0.72730000	-6.04810000	8.28660000
39	Si	-0.78110000	-6.37380000	9.84140000
40	Si	4.19139089	1.79568588	-2.03275520
41	Si	4.36125848	-0.89338247	-0.53563582
42	Si	1.79903688	-4.81759430	0.05485548
43	Si	1.68494409	-2.17117347	-1.47873107
44	Si	3.22825605	3.06095224	2.23946362

1	Si	5.44838326	-1.68943860	4.28205473
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3	O	4.61248122	0.39620629	-1.42439651
4	O	1.43104151	-3.66271245	-0.97332770
5	O	3.17923286	-1.73854524	-1.15942822
6	O	4.64917604	-3.05770535	4.13519061
7	O	2.93731901	2.40549405	-1.28827399
8	O	2.15237908	3.10847541	1.07443183
9	O	2.54286455	3.62263224	3.55354276
10	O	5.51820137	-1.20786140	5.80381915
11	O	3.57074674	-4.20209830	6.24788598
12	O	-0.73792722	-5.99421968	5.72550201
13	H	-1.30770000	8.45280000	5.54490000
14	H	3.53900000	4.98890000	5.43620000
15	H	-5.91550000	5.84190000	-1.27060000
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24	H	-2.15040000	-4.10050000	12.78420000
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26	H	-12.21020000	-7.97290000	7.89080000
27	H	0.36339800	-1.65380900	11.27870200
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21	H	-2.02270000	2.13730000	10.92000000
22	H	-4.91220000	-7.27130000	-2.96190000
23	H	-8.98790000	-7.09310000	-2.37650000
24	H	1.45750113	-2.18460625	-2.95900102
25	H	-5.88650100	0.35320300	-2.87169900
26	H	-6.57060000	-3.25690000	-2.96870000
27	H	-11.74490000	-3.66940000	8.61800000
28	H	-9.32890000	0.16850000	8.03140000
29	H	-8.19140000	3.21540000	6.31880000
30	H	-5.78340000	-8.84910000	-1.27830000
31	H	-7.97590000	-9.98270000	-0.17660000
32	H	-2.11757394	0.35871304	-2.97419599
33				

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