Supporting Information

Methanol to Olefins Reaction over Cavity-type Zeolite: Cavity Controls the Critical Intermediates and Product Selectivity

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1. Catalyst Characterizations

1.1 Powder X-ray Diffraction (XRD)

Powder X-ray diffraction (XRD) pattern of H-RUB-50 was recorded on a PANalytical X'Pert PRO X-ray diffractometer equipped with Cu Kα radiation (λ = 0.15418 nm) from 5 and 50° with a scan speed of 2θ =5.0°/min at 40 kV and 40 mA. The reflection peaks are in good agreement with the standard sample and no other impurity phases were observed as presented in **Figure S1**.

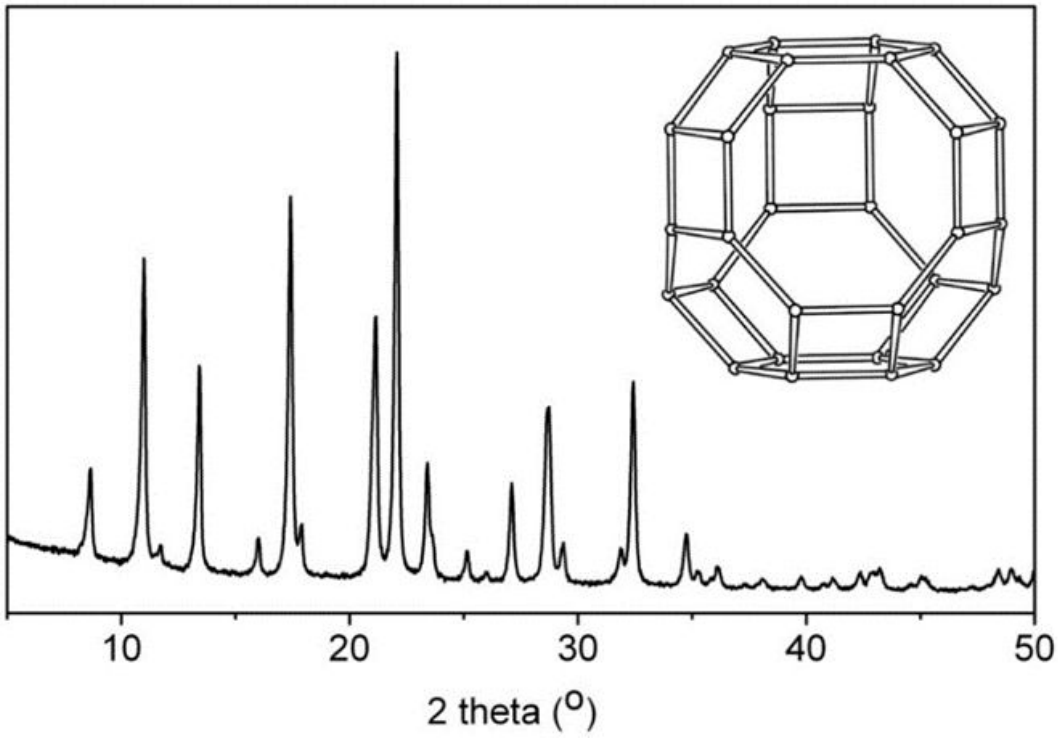


Figure S1. XRD pattern of H-RUB-50.

1.2 Scanning Electron Microscopy (SEM)

To investigate the crystal size and morphology of H-RUB-50 catalyst, a HITACHI SU8020 Scanning Electron Microscope was employed.

Figure S2. The scanning electron microscope (SEM) images of as-synthesized H-RUB-50.

1.3 N_2 Adsorption

Textural properties of the calcined H-RUB-50 were determined by N_2 adsorption at 77 K on a Micromeritics ASAP 2020 system. The total surface area was calculated based on the BET equation. The microspore volume and microspore surface area were evaluated using the t-plot method.

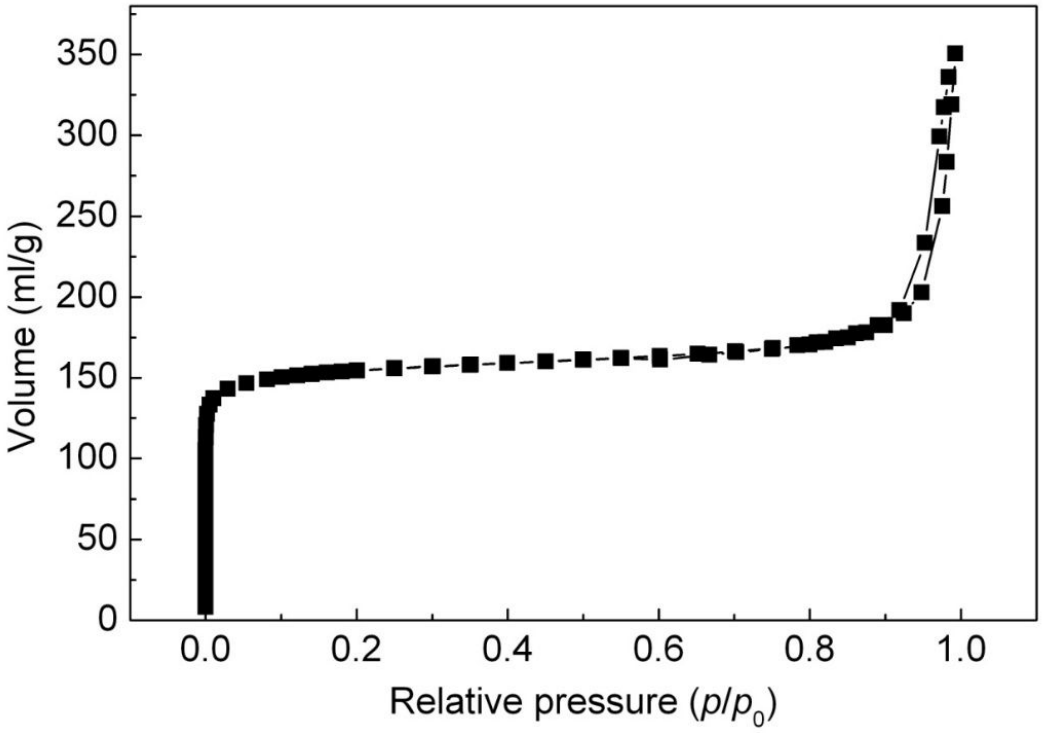


Figure S3. N_2 adsorption-desorption isotherms of as-synthesized H-RUB-50 sample.

Table S1. Textural properties of calcined H-RUB-50 catalyst.

Sample	Surface area (m^2/g)			Pore volume (cm^3/g)	
	Micropore	External	Total	Micropore	Total
H-RUB-50	406.6	93.1	499.7	0.20	0.40

1.4 NH_3-TPD Experiment

The NH_3-TPD experiments were measured on a chemical adsorption analyzer (Autochem 2920, Micromeritics) with a TCD detector. About 0.1 g of calcined pellet sample (40-60 mesh) was loaded in a U-tube reactor. The catalyst was initially heated at 300 ^oC in He flow for activation. After the pre-treatment, the sample was cooled to 100 ^oC and saturated with ammonia. Physically adsorbed ammonia

was removed by purging a He flow of 40 ml min^{-1} for 30 min. Finally, the catalyst was heated to 700 ^{o}C with a heating rate of 10 ^{o}C/min in a He flow.

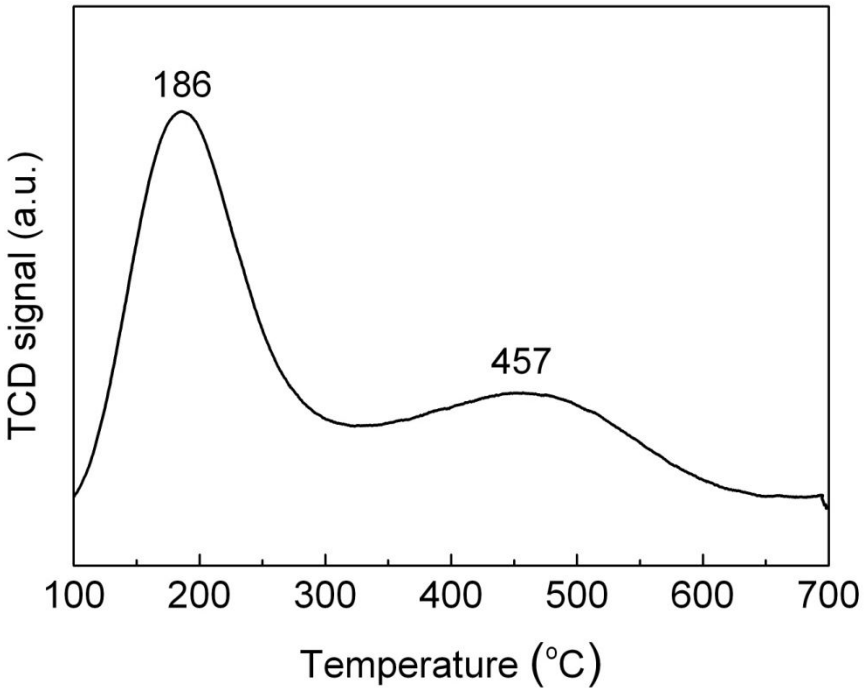


Figure S4. NH_3-TPD curves of H-RUB-50.

2. Theoretical Calculation Model

For theoretical calculations, a 52T cluster model ($Si_{51}AlO_{82}H_{45}$) represents the structure of H-RUB-50 zeolite as shown in Figure S5, which was extracted from the crystallographic of the LEV structure (**Figure S5**).

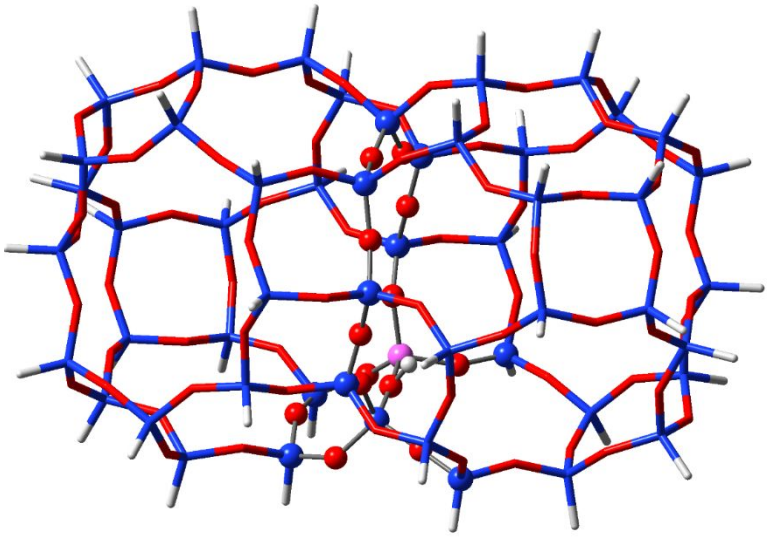


Figure S5. Representations of H-RUB-50 framework structures by 52T cluster models. The eight-MR window and $(SiO)_3$-Si-OH-Al-$(SiO)_3$ active center in the extended cluster model represented as ball and stick view is treated as the high-layer atoms during the ONIOM calculations.

3. Methanol to Olefins Conversion and Product Distribution over H-RUB-50 Zeolite

The catalytic performances of methanol conversion over H-RUB-50 at the temperature range of 275 ~ 400 °C are shown in **Figure S6**. At low temperature of 275 and 300 °C, an obvious induction period and low conversion are observed, while at temperature of 350 °C and 400 °C, complete methanol conversion is realized. With the increase of reaction temperature, methanol conversion is enhanced, while H-RUB-50 catalyst suffers from rapid deactivation as the performance over other catalysts with cavity structure and narrow eight-MR pore opening[1-3]. The product distribution of MTO conversion over H-RUB-50 as shown in **Figure S7** indicates that ethene and propene appear as the main products, especially ethene, consistent with the characteristic of product selectivity on other LEV-type catalysts, which is quite different from the reaction over other cavity-type catalysts, such as H-SSZ-13[1], H-SAPO-34[2] and DNL-6[3, 4], where propene or butene are formed as the main products. All these studies confirmed that light olefins can be selectively generated and the difference in the olefin product selectivity implies the

chemical environment of cavity-type catalyst plays a central role in determining the products distribution.

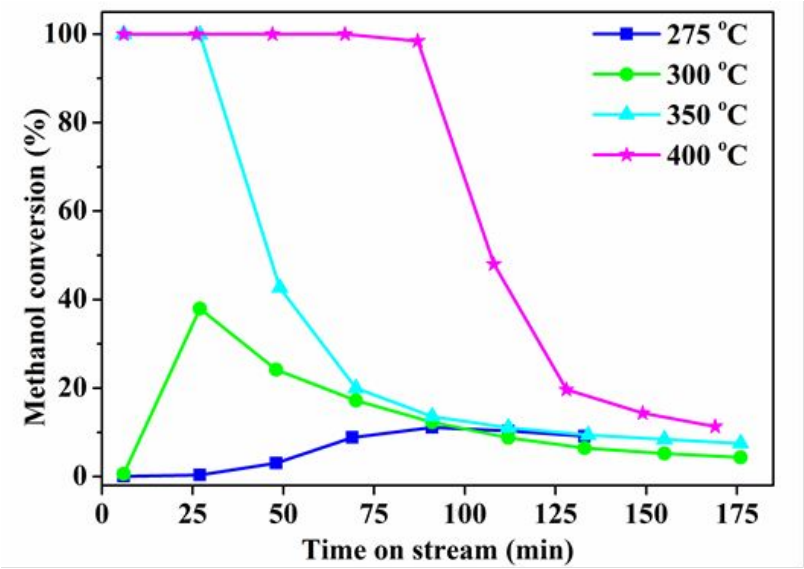


Figure S6. Methanol conversion over H-RUB-50 catalyst with time on stream at various temperatures.

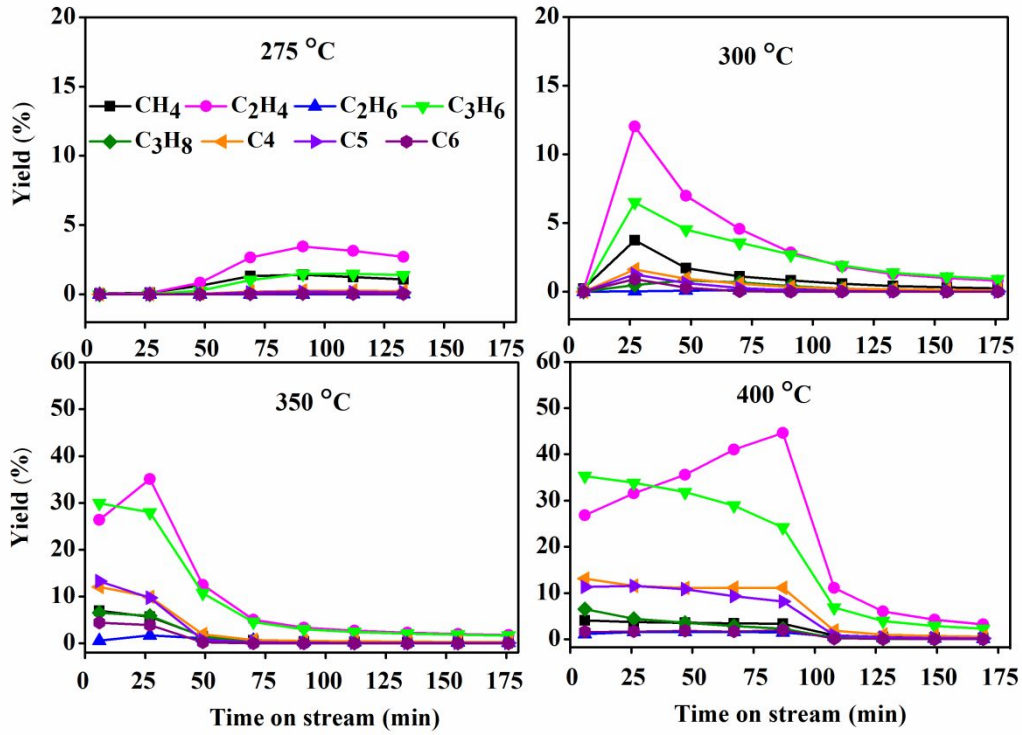


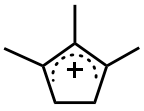
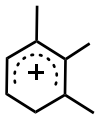
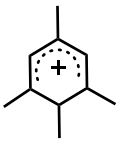
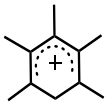
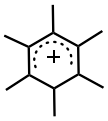
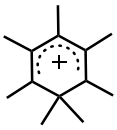
Figure S7. The yields of hydrocarbon products of methanol conversion over H-RUB-50 with time on stream at various reaction temperatures.

4. Carbenium Ions Capture and Identification by ^{13}C MAS NMR and GC-MS in Combination with Theoretical Calculation

4.1 The Stabilities of the Carbenium Ions

The stabilities of the active intermediates, methylcyclopentenyl and methylbenzenium cations, is explored in term of the calculated adsorption energy as detailed in **Table S2**. Obviously, from trimethylbenzenium to heptamethylbenzenium, the adsorption energy increases from -114.3 kcal/mol to -29.6 kcal/mol due to the steric confinement effect, indicating trimethylcyclopenyl, trimethylbenzenium and tetramethylbenzenium cations are more stabilized in the LEV cavity of H-RUB-50.

Table S2 The adsorption energy (ΔE_{ads}**)** of different adsorbed species within H-RUB-50 zeolite

Carbenium ions	$TriMCP^+$	$TriMB^+$	$TetraMB^+$	$PentaMB^+$	$HexaMB^+$	$HeptaMB^+$
E_{ads} (kcal/mol)						
	-111.4	-114.3	-109.0	-40.5	-33.4	-29.6

4.2 The Identification of the Captured Carbenium Ions with Theoretical Calculation

The theoretical calculation predicts 1, 2, 5-trimethylcyclopentenyl cation with ^{13}C chemical shift at 45, 158 and 240 ppm, 1, 2, 3-trimethylbenzenium cation with ^{13}C chemical shift at 51, 136, 145, 187 and 201 ppm, and 1, 3, 4, 5-tetramethylbenzenium cation with ^{13}C chemical shift at 56, 132, 182 and 206 ppm, respectively. **Figure S8** presents the optimized structures of $triMCP^+$, $triMB^+$ and $tetraMB^+$ cations inside the H-RUB-50 zeolite.

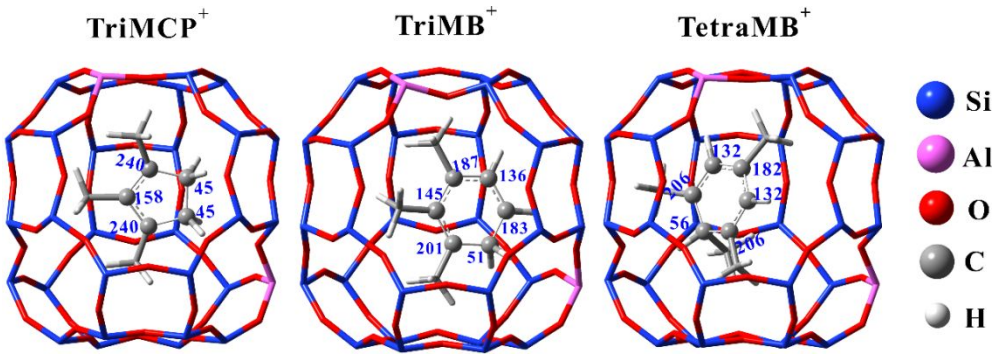


Figure S8. Optimized structures of triMCP$^+$, triMB$^+$ and tetraMB$^+$ cations inside the H-RUB-50 zeolite. The calculated ^{13}C chemical shifts of ring atoms are indicated with the unit of ppm.

4.3 Identification of the Confined Carbenium Ions Using GC-MS

The identification of the carbenium ions formed in H-RUB-50 has been also consolidated by the GC-MS analysis of the confined organic species in the zeolite catalyst after a parallel $^{12}CH_3OH$ reaction as shown in **Figure S9.**

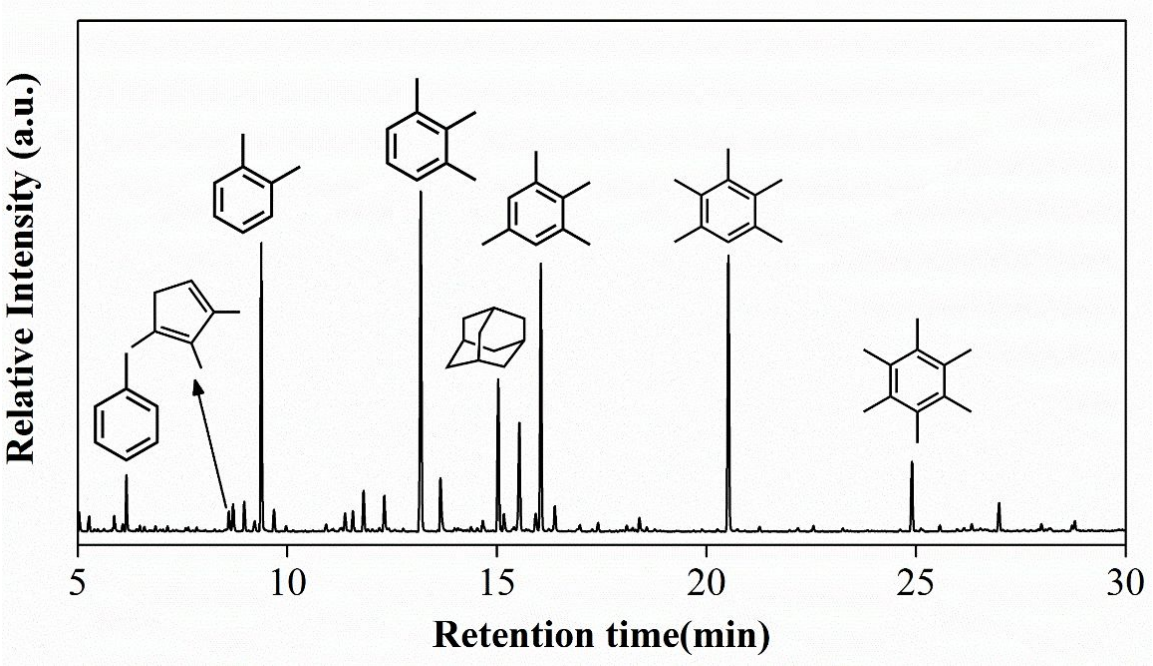


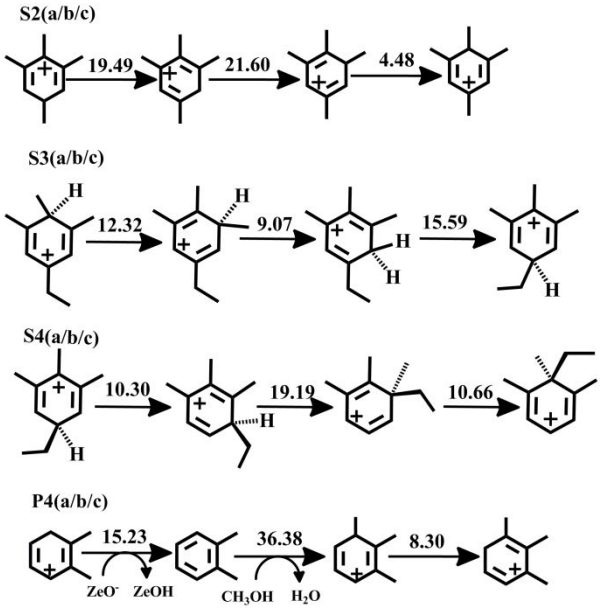
Figure S9. GC-MS chromatograms of the organic species retained in H-RUB-50 catalyst after CH_3OH conversion at 300 ^oC. WHSV of CH_3OH = 2.0 h^{-1}.

5. Theoretical Study of Ethene Formation via the Catalytic Cycles of Side-chain Methylation and Paring

Scheme S1 provides the reactions of H, CH_2CH_3 group transfer (**S2, S3, S4**) in side-chain cycle and deprotonation (**P4(a))**, methylation (**P4(b))** and hydride transfer (**P4(c)**) paring cycle as given in Scheme 1. The migration reactions (**S2, S3, S4**) are easily accomplished by the free energy barriers of 4.48-21.60 kcal/mol in side-chain methylation cycle, and in paring cycle, the migration reactions need to overcome relatively high free energy barriers of 8.30-36.38 kcal/mol.

Table S3 lists the free energy barriers at 300 °C of ethene formation via side-chain methylation and paring routes without water.

Table S4 provides the comparison of the calculated free energy barriers ($\Delta G^{\ddagger}$) of the elementary reactions for ethene formation via side-chain cycle at 300 °C based on different calculation levels on a 52T cluster model of H-RUB-50.



Scheme S1 The details of migration reactions involved in the catalytic cycle of side-chain methylation and paring routes.

Table S3. Calculated free energy barriers ($\Delta G^{\ddagger}$) at 300 °C of ethene formation via the side-chain methylation and paring routes without water assistance in methanol conversion over H-RUB-50 Zeolite.

Side-Chain Route		**Paring Route**	
Reactions	$\Delta G^{\ddagger}$ (kcal/mol)	Reactions	$\Delta G^{\ddagger}$ (kcal/mol)
M1	36.31	M1	36.31
S2(a/b/c)	19.73/20.74/15.17	P1	30.77
D1	14.24	PE	44.87
M2	16.78	P2	27.17
S3(a/b/c)	15.83/6.75/15.85	P3	23.93
S4(a/b/c)	10.10/14.15/10.09	P4(a/b/c)	8.26/28.86/2.38
E1	38.15	P5	21.25

Table S4. Comparison of the calculated free energy barriers ($\Delta G^{\ddagger}$) of the elementary reactions for ethene formation via side-chain cycle at 300 °C based on different calculation levels on a 52T cluster model of H-RUB-50.

Calculated Methods	ωB97XD/6-31G (d, p)	ωB97XD/6-311G (2df, 2p)
Reaction	$\Delta G^{\ddagger}$ (kcal/mol)	$\Delta G^{\ddagger}$ (kcal/mol)
M1	37.01	35.89
S2(a/b/c)	19.49/21.60/4.48	18.68/20.94/3.95
D1	11.27	12.75
M2	23.15	22.65
S3(a/b/c)	12.32/9.07/15.59	10.87/8.39/14.97
S4(a/b/c)	10.30/19.19/10.66	9.29/19.15/9.99
E1	15.52	15.88

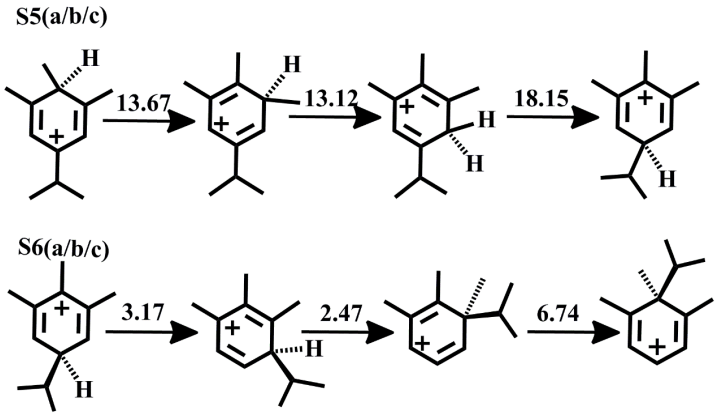
6. Cavity-controlled Product Selectivity Derived from the Host-guest Interaction

Scheme S2 provides the hydride(**S5**) and propyl side-chain group transfer (**S6**) for the formation of propene in side-chain methylation cycle, which exhibits the low reaction barriers of 2.47-18.15 kcal/mol.

Table S5 provides the comparison of the calculated free energy barriers of the elementary reactions for ethene and propene formation via side-chain cycle at 300 ^{o}C without water.

Table S6 provides the adsorption energy of the 3, 4, 5-trimethyl-1-ethylbenzenium ($TMEB^{+}$) and 3, 4, 5-trimethyl-1-propylbenzenium ($TMPB^{+}$) adsorbed within RUB-50 zeolite. It is found that the stabilization energy of ethene precursor, $TMEB^{+}$ was -106.63 kcal/mol and that of propene precursor $TMPB^{+}$ is -86.86 kcal/mol. This indicates that the ethene precursor can be more easily formed and stabilized than propene precursor in H-RUB-50 with small cavity. The spatial confinement effect of LEV cavity is of great significance for the critical intermediates and olefins precursors generation in the catalyst.

Figure S10 provides the energy barrier of ethene and propene precursors formed in MTO reaction catalyzed over CHA and LEV.



Scheme S2 The details of hydride and propyl side-chain group transfer for the formation of ethene and propene in side-chain cycle.

Table S5. Comparison of the calculated free energy barriers ($\Delta G^{\ddagger}$) at 300 °C of the elementary reactions for ethene and propene formation via side-chain cycle without water assistance in methanol conversion over H-RUB-50 Zeolite.

The cycle of ethene		**The cycle of propene**	
Reactions	$\Delta G^{\ddagger}$ (kcal/mol)	Reactions	$\Delta G^{\ddagger}$ (kcal/mol)
M1	36.31	M1	36.31
S2(a/b/c)	19.73/20.74/15.17	S2(a/b/c)	19.73/20.74/15.17
D1	14.24	D1	14.24
M2	16.78	M2	16.78
S3(a/b/c)	15.83/6.75/15.85	D2	15.70
S4(a/b/c)	10.10/14.15/10.09	M3	22.39
E1	38.15	S5(a/b/c)	15.77/11.07/17.45
		S6(a/b/c)	1.54/12.43/4.49
		E2	9.53

Table S6 The adsorption energy (ΔE_{ads}) of the $TMEB^{+}$ and $TMPB^{+}$ adsorbed within RUB-50 zeolite.

	$TMEB^{+}$	$TMPB^{+}$
		
E_{ads} (kcal/mol)	-106.63	-86.86

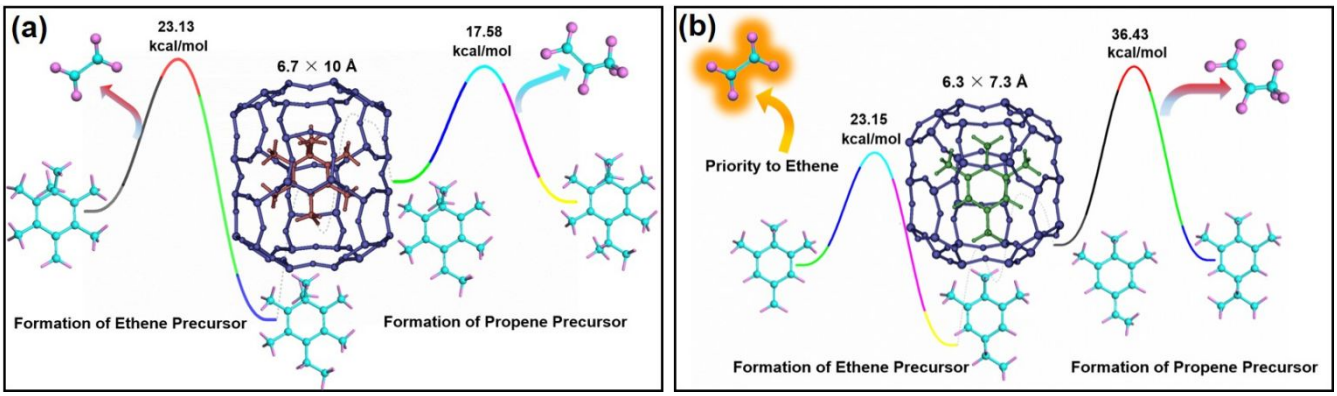


Figure S10. The energy barrier of ethene and propene precursors formed in MTO reaction catalyzed over (a) CHA and (b) LEV

REFERENCE

(1) Xu, S.; Zheng, A.; Wei, Y.; Chen, J.; Li, J.; Chu, Y.; Zhang, M.; Wang, Q.; Zhou, Y.; Wang, J.; Deng, F.; Liu, Z. Direct Observation of Cyclic Carbenium Ions and Their Role in the Catalytic Cycle of the Methanol-to-Olefin Reaction over Chabazite Zeolites. *Angew. Chem., Int. Ed.* **2013,** *52***,** 11564-11568.

(2) Chen, J.; Li, J.; Wei, Y.; Yuan, C.; Li, B.; Xu, S.; Zhou, Y.; Wang, J.; Zhang, M.; Liu, Z. Spatial Confinement Effects of Cage-type SAPO Molecular Sieves on Product Distribution and Coke Formation in Methanol-to-Olefin Reaction. *Catal. Commun.* **2014,** *46*, 36-40.

(3) Li, J.; Wei, Y.; Xu, S.; Tian, P.; Chen, J.; Liu, Z. Heptamethylbenzenium Cation Formation and the Correlated Reaction Pathway during Methanol-to-Olefins Conversion over DNL-6. *Catal. Today* **2014,** *226,* 47-51.

(4) Li, J.; Wei, Y.; Chen, J.; Xu, S.; Tian, P.; Yang, X.; Li, B.; Wang, J.; Liu, Z. Cavity Controls the Selectivity: Insights of Confinement Effects on MTO Reaction. *ACS. Catal.* **2015,** *5*, 661-665.

7. The calculated Energies and the Coordinates of Structures

The energies in Figure 4, 5 and 7 are listed as Table S6, S7 and S8.

Table S6. Relative Gibbs free barriers for methanol conversion to ethene over H-RUB-50 following the side-chain methylation route at 300 °C.

Side-chain route	**G (kcal/mol)**
ZeOH + CH_3OH(g) + TriMB(g) +H_2O(g)	0
ZeOH+CH_3OH(Ads)+TriMB(Ads) +H_2O(Ads)	-3.36884
TS-M1	33.63703
ZeO^- + 1, 2, 4, 6-tetraMB^+(Ads) +2H_2O(Ads)	17.549
ZeO^- + 1, 2, 4, 6-tetraMB^+(Ads) + H_2O(Ads) +H_2O(g)	0.47493
TS-S2a	19.96908
ZeO^- + 1, 2, 3, 5-tetraMB^++H_2O(Ads)	5.59478
TS-S2b	27.19247
ZeO^-+ 2, 3, 4, 6-tetraMB^++H_2O(Ads)	21.63443
TS-S2c	26.11271
ZeO^- + 1, 3, 4, 5-tetraMB^++H_2O(Ads)	-11.3631
TS-D1	-0.0897
ZeOH+TMMC+H_2O(Ads)	0.09642
ZeOH+TMMC+MeOH(Ads) +H_2O(Ads)	7.11616
TS-M2	30.26442
ZeO^- + TMEB^++2H_2O(Ads)	-8.5087
ZeO^- + 3, 4, 5-TriM-1-EB^++H_2O(Ads)+H_2O(g)	10.73139
TS-S3a	23.04664
ZeO^- + 4, 5, 6-TriM-2-EB^++H_2O(Ads)	16.70685
TS-S3b	25.78133
ZeO^- + 1, 5, 6-TriM-3-EB^++H_2O(Ads)	2.32659
TS-S3c	17.91255
ZeO^-+1, 2, 6-TriM-4-EB^++H_2O(Ads)	-6.04533
TS-S4a	4.25744
ZeO^-+ 1, 2, 3-TriM-4-EB^++H_2O(Ads)	-7.17691
TS-S4b	12.01333
ZeO^-+ 2, 3, 4-TriM-4-EB^++H_2O(Ads)	-5.76414
TS-S4c	4.89091
ZeO^-+ 3, 4, 5-TriM-4-EB^++H_2O(Ads)	-7.07639
TS-E1	8.44644
ZeOH+1,2,3-triMB(Ads) +C_2H_4(Ads) +H_2O(Ads)	-12.35537

Table S7. Relative Gibbs free barriers for methanol conversion to ethene over H-RUB-50 following the paring route at 300 ^{o}C.

Paring route	**G (kcal/mol)**
ZeOH+CH_3OH(g)+TriMB(g) +H_2O(g)	0
ZeOH+CH_3OH(Ads)+TriMB(Ads) +H_2O(Ads)	-3.368841226
TS-M1	33.63702551
ZeO^- + 1, 2, 4, 6-tetraMB$^+$(Ads) +2H_2O(Ads)	17.5489997
ZeO^- + 1, 2, 4, 6-tetraMB$^+$(Ads) + H_2O(Ads) +H_2O(g)	14.98006366
TS-P1	46.89224753
ZeO^- +1, 2, 3, 5-tetramethylbicyclo-[3.1.0] hexenyl cation +H_2O	28.04349368
TS-PE	73.83989
ZeO^- + 1, 2, 5-triMCP$^+$+C_2H_4(Ads) +H_2O(Ads)	31.59268741
ZeO^- + 1, 2, 5-triMCP$^+$+C_2H_4(g) +H_2O(Ads)	25.53667836
TS-P2	59.0852151
ZeO^- +1, 2-dimethylbicyclo-[3.1.0]hexenyl cation+H_2O (Ads)	20.13017835
TS-P3	41.92245377
ZeO^- + diMB$^+$+H_2O(Ads)	0.564620392
TS-P4a	15.7939622
ZeOH+diMB+H_2O(Ads)	0.340662251
ZeOH+diMB+ CH_3OH(Ads) +H_2O(Ads)	-9.695537749
TS-P4b	26.68846708
ZeO^-+2,3,4-triMB$^+$+H_2O(Ads)	12.29948599
TS-P4c	20.60357021
ZeO^-+1, 2, 3- triMB$^+$+H_2O(Ads)	5.438673622
TS-P5	7.329422495
ZeOH+1, 2, 3- triMB +H_2O(Ads)	-9.491659912

Table S8. Relative Gibbs free barriers for methanol conversion to propene over H-RUB-50 following the side-chain methylation route at 300 °C.

Side-chain route	**G（kcal/mol）**
ZeOH + CH_3OH(g)+TriMB(g) +H_2O(g)	0
ZeOH + CH_3OH(Ads)+TriMB(Ads) +H_2O(Ads)	-3.368841226
TS-M1	33.63702551
$ZeOH^-$ +1, 2, 4, 6-tetraMB$^+$(Ads) +2H_2O(Ads)	17.5489997
ZeO^- +1, 2, 4, 6-tetraMB$^+$(Ads) + H_2O(Ads) +H_2O(g)	0.474930565
TS-S2a	19.96907794
ZeO^- +1, 2, 3, 5-tetraMB$^+$+H_2O(Ads)	5.594780574
TS-S2b	27.1924653
ZeO^-+2, 3, 4, 6-tetraMB$^+$+H_2O(Ads)	21.6344254
TS-S2c	26.1127097
ZeO^-+1, 3, 4, 5-tetraMB$^+$+H_2O(Ads)	-11.3630989
TS-D1	-0.089702486
ZeOH+TMMC+H_2O(Ads)	0.096416838
ZeOH+TMMC+MeOH(Ads) +H_2O(Ads)	7.116158536
TS-M2	30.26441923
ZeO^-+TMEB$^+$+2H_2O(Ads)	-8.508702511
ZeO^-+3, 4, 5-TriM-EB$^+$+H_2O(Ads)+H_2O(g)	3.318119638
TS-D2	21.13041605
ZeOH+TMEC+H_2O(Ads)	19.65595698
ZeOH+TMEC+CH_3OH(Ads)+H_2O(Ads)	10.9826901
TS-M3	47.41664468
ZeO^-+TMEB$^+$+2H_2O(Ads)	8.025175073
ZeO^-+3, 4, 5-TriM-1-PB$^+$+H_2O(Ads)+H_2O(g)	19.88023515
TS-S5a	33.5468273
ZeO^-+4, 5, 6-TriM-2-EB$^+$+H_2O(Ads)	20.30179603
TS-S5b	33.42151365
ZeO^-+1, 5, 6-TriM-3-EB$^+$+H_2O(Ads)	12.40258095
TS-S5c	30.554611
ZeO^-+1, 2, 6-TriM-4-EB$^+$+H_2O(Ads)	-3.896539062
TS-S6a	-0.724164786
ZeO^-+1, 2, 3-TriM-4-EB$^+$+H_2O(Ads)	-15.75188779
TS-S6b	-13.28219866
ZeO^-+2, 3, 4-TriM-4-EB$^+$+H_2O(Ads)	-16.34419401
TS-S6c	-9.602922206
ZeO^-+3, 4, 5-TriM-4-EB$^+$+H_2O(Ads)	-25.35585794
TS-E2	-11.8337875
ZeOH+1, 2, 3-triMB(Ads) +C_3H_6(Ads) +H_2O(Ads)	-30.33029518

The DFT coordinates for the models in the manuscript.

The rate-determining transition state (**M2**) for ethene formation via side-chain methylation.

O	-3.35570300	4.94406800	-0.09346500
O	3.85600500	5.05721000	-2.32642300
O	-6.36567500	3.93404300	1.76963700
O	-7.04995300	1.39759800	4.42409700
O	-6.36592800	3.85440900	-1.91069300
O	-7.05061200	1.20550900	-4.45287800
O	3.85627000	5.15365200	2.13144100
O	-8.08057500	3.09391600	-0.05311600
O	-3.90879400	4.60404700	2.46538300
O	-3.90911400	4.49369700	-2.63515000
O	-8.64218600	-0.78963900	0.03094000
O	-8.09984100	-4.83338000	0.11839800
O	-4.53400300	-5.94367400	0.14213500
O	-1.90776400	1.47018100	-4.13748400
O	-1.90717500	1.64834300	4.09678800
O	-0.20315000	-1.97490300	4.88559500
O	8.44573200	4.96784200	-0.09486300
O	4.87994200	6.07823500	-0.11866000
O	8.98805100	0.92421000	-0.00741300
O	0.54909500	2.10935200	-4.86197000
O	1.23371500	4.75838900	-2.31981300
O	0.54974800	2.31828600	4.79256600
O	1.23400100	4.85480800	2.13810900
O	2.25367200	-1.33556800	4.16106900
O	8.42660100	-2.95939200	0.07668000
O	4.25503700	-4.35912600	2.65865200
O	4.25469000	-4.46954700	-2.44180200
O	-3.51060100	-5.01891400	-2.10810400
O	6.71187400	-3.71991100	1.93430800
O	7.39655700	-1.07101300	4.47649400
O	6.71162200	-3.79955500	-1.74601600
O	7.39589800	-1.26310400	-4.40048100
O	-3.50997500	-4.92259600	2.34983900
Si	6.09379000	-2.03869500	-5.01535700
Si	-4.81217900	-5.69840500	1.73531300
Si	8.70758300	-0.94245100	3.50703800
Si	-4.81222700	-5.76755200	-1.45965900
Si	6.09450300	-1.81929900	5.12446900
Si	8.70707000	-1.09273000	-3.43777100
Si	-5.74855700	1.95379400	-5.10085700

Si	5.15832600	5.90194200	1.48346000
Si	2.54480500	4.88681300	-3.28919700
Si	-8.36117100	1.22720700	3.46129800
Si	5.15807300	5.83279500	-1.71164100
Si	-5.74788600	2.17318100	5.03888100
Si	-8.36163600	1.07694700	-3.48342400
Si	2.54524600	5.02509300	3.10089200
O	3.05513000	0.96651900	-4.91532500
O	-7.85072000	-2.69307300	1.83507600
O	-2.71002300	-1.04426400	-4.87140600
O	8.19687900	2.90392000	1.71290100
O	8.19666900	2.82767100	-1.81160000
O	-2.70930500	-0.83195000	4.93892300
O	-7.85096500	-2.76933200	-1.68928800
O	3.05591900	1.17881500	4.89502200
Si	-7.99224300	3.67725200	1.48385300
O	-8.61114900	2.55229600	2.51482000
Si	-5.46229700	4.45924800	-3.17994100
O	-5.54150800	3.47190200	-4.49540700
Si	-2.92842800	5.44334500	1.44325600
O	-1.36167100	5.06606200	1.78147500
Si	-7.99246300	3.61022200	-1.61382800
O	-8.61149700	2.44173200	-2.59515700
Si	-5.46186700	4.59321400	3.01139000
O	-5.54080200	3.66372100	4.36826000
Si	-2.92862800	5.37641300	-1.65039300
O	-1.36195100	4.98481300	-1.97226700
Si	9.07646400	1.50757300	1.52950500
O	8.45760500	0.38263700	2.56056000
O	4.80022500	-1.05173300	-4.75711100
Si	-7.67242700	-4.33404200	1.65513800
O	-6.10572700	-4.71136100	1.99324300
Si	2.17562800	2.35356800	-5.15886800
O	2.79461500	3.52212700	-4.17748500
Si	-8.73026100	-1.30604200	1.59165300
O	-8.11126400	-0.13745600	2.57298200
Si	-2.88809200	0.58737800	-5.12224100
O	-4.45494300	0.97901600	-4.80034800
Si	8.01866400	4.53551300	1.46207000
O	6.45193300	4.92715800	1.78393600
Si	-8.73048700	-1.37307100	-1.50602900
O	-8.11169500	-0.24805000	-2.53694600
Si	2.17631600	2.57503800	5.07834800
O	2.79518900	3.70009800	4.04737100

Si	8.01846000	4.46857800	-1.63158200
O	6.45165400	4.84593000	-1.96980200
Si	-2.88748800	0.80896900	5.11895600
O	-4.45422000	1.18634500	4.78067000
Si	9.07624200	1.44054400	-1.56817400
O	8.45725600	0.27207400	-2.54941900
Si	-1.82972200	-2.21908600	5.18241300
O	-2.44871000	-3.38745200	4.20105100
Si	-7.67268500	-4.40100800	-1.43859200
O	-6.10601800	-4.79256700	-1.76032200
Si	3.23412200	-0.45288700	5.14576600
O	4.80086200	-0.84442100	4.82399100
Si	8.33841000	-3.47572600	1.63744200
O	8.95739600	-2.30725600	2.61868600
Si	5.80777200	-4.45871900	-2.98784200
O	5.88682700	-3.52920600	-4.34470300
Si	8.33818600	-3.54275600	-1.46023900
O	8.95709400	-2.41780300	-2.49120600
Si	5.80821900	-4.32478700	3.20361700
O	5.88740300	-3.33743400	4.51894300
H	-5.99785500	2.39376900	6.47057700
H	-9.53948200	1.11174900	4.33259300
H	-10.16084900	-1.52082400	1.85278400
H	-8.77092600	4.91346800	1.64609300
H	-10.16112300	-1.59894300	-1.75733000
H	-9.54004400	0.92391800	-4.34878100
H	-8.77116300	4.83826300	-1.82933500
H	-8.54783800	-5.08343900	2.56782800
H	-1.90837500	-2.68010700	6.57595900
H	-2.51169200	1.24808500	6.47054600
H	2.85849300	-0.83314200	6.51516100
H	6.34463500	-1.97768200	6.56434600
H	2.25523100	3.09601900	6.45066000
H	6.27509500	-5.65744400	3.61207200
H	9.88603900	-0.78932400	4.37230700
H	9.11711000	-4.70376800	1.85294900
H	9.11682800	-4.77898900	-1.62255500
H	9.88541700	-0.97716700	-4.30900400
H	6.27456500	-5.80785700	-3.33839500
H	6.34372400	-2.25921300	-6.44706800
H	2.85762600	-1.11359200	-6.44694100
H	2.25432400	2.81466000	-6.55240200
H	-2.51265000	0.96762100	-6.49164900
H	-5.99874500	2.11223600	-6.54071800

H	-1.97636700	-6.10847200	-3.86986900
H	3.43222300	-6.76166300	-1.57901300
H	3.43247400	-6.68653900	1.89598100
H	-1.97582100	-5.93470500	4.15738500
H	-4.99718000	-7.12199600	-2.00016500
H	-4.99683600	-7.02823100	2.33361000
H	-8.54823200	-5.18920500	-2.31783300
H	-5.92861900	5.94233100	3.36199600
H	-5.92914400	5.79193500	-3.58847600
H	-3.08622700	6.89612700	1.60262000
H	-3.08643300	6.82093800	-1.87245800
H	2.32229700	6.24287800	3.89348000
H	2.32173900	6.06916500	-4.13374100
H	5.34307300	7.25653000	2.02369600
H	5.34277800	7.16275000	-2.30997600
H	8.89411100	5.32377100	2.34135500
H	8.89379900	5.21806500	-2.54424200
H	10.50709700	1.73343200	1.78086300
H	10.50684800	1.65532800	-1.82919800
H	-1.99524600	-2.92363800	-6.43321300
Si	3.16300100	-0.74014400	-5.08010800
Si	-1.88118900	-2.53118800	-5.07334400
O	2.32662200	-1.54879500	-4.01137400
O	-0.34164200	-2.36094900	-4.69687400
O	-2.61035300	-3.67900300	-4.17796400
Al	0.44656600	-3.91420900	1.68947600
Si	0.46314500	-3.97640800	-1.56892500
Si	3.13912600	-5.33533800	-1.43907200
Si	-2.15847900	-4.93667000	-3.10576500
Si	0.67631900	-1.60566700	-3.49436600
Si	3.13388200	-5.27341200	1.72623500
Si	0.68669600	-1.39466300	3.51657000
Si	-2.12121800	-4.80885400	3.30219900
O	0.55440500	-2.22495800	2.17342400
O	1.71026900	-4.91821300	2.29239900
O	-0.95950700	-4.63892800	2.28454100
O	0.40381100	-3.85611800	-0.01767200
O	3.32650500	-4.89244600	0.11466400
O	1.69070100	-4.94342000	-2.05704500
O	0.56798200	-2.44913700	-2.16366800
O	-0.85855500	-4.61413200	-2.24935300
O	0.16104700	0.13178800	3.21710600
O	0.16862600	-0.06738000	-3.27537000
O	-0.15327100	2.45004400	-2.29144500

O	-0.19563500	2.56921600	2.19280000
O	0.09927000	3.74964000	-0.07452700
Si	-0.33011200	1.63824500	3.49039600
Si	-0.32617800	1.46711600	-3.54353000
Si	-0.05910000	3.93346100	-1.64825600
Si	-0.05942800	4.00912700	1.49285800
C	-4.16930300	-1.05183100	1.27268000
C	-4.13334000	-1.92202300	0.04247400
C	-4.19522700	-1.15261600	-1.25245500
C	-3.68687300	0.08814800	-1.29066600
C	-3.22442300	0.72891200	-0.07476600
C	-3.66399800	0.18950000	1.19676000
C	-2.35122700	1.77601900	-0.12690300
H	-2.16857000	2.25716000	-1.07832400
H	-2.14081300	2.33049800	0.77764900
C	-2.79260800	-2.70445700	0.06556500
H	-2.71526400	-3.37800100	-0.78703600
H	-1.95321600	-2.00816900	0.02650800
H	-2.69167700	-3.30591300	0.96879300
H	-4.95277400	-2.64702900	0.08093300
C	-0.58240800	0.38781400	-0.03506200
H	-0.05130600	1.32000700	-0.08590800
H	-0.84865500	-0.13887200	-0.93799700
H	-0.91143500	0.00715100	0.91899800
O	1.10304900	-0.52258200	0.20696900
H	0.92565800	-1.23216400	0.86475200
H	1.63738200	-0.95196500	-0.49049900
C	-4.75687700	-1.83017600	-2.45750800
H	-5.84348000	-1.94034700	-2.34287900
H	-4.56949600	-1.25435800	-3.36926200
H	-4.34854700	-2.83861700	-2.58490200
C	-4.68962100	-1.64327700	2.53934300
H	-4.51808900	-0.98069800	3.39366500
H	-5.77014300	-1.81572000	2.44893800
H	-4.22837900	-2.61552900	2.74698300
H	-3.58065800	0.82069300	2.07963200
H	-3.62229000	0.64264600	-2.22636700
O	3.17557900	-1.94800700	-0.93613800
H	3.44039800	-2.20389200	-1.82536700
H	3.47159300	-2.66556100	-0.36208600

The rate-determining intermediate (1, 3, 4, 5- tetraMB$^+$ cation) for ethene formation via side-chain methylation.

O	-3.31191400	4.93233200	-0.07515700
O	3.89920100	5.04461600	-2.30865800

O	-6.32388100	3.91786900	1.78291900
O	-7.01242600	1.36814200	4.42351300
O	-6.32491400	3.85840800	-1.89776900
O	-7.01486000	1.22488300	-4.45432600
O	3.90036100	5.11656300	2.14966900
O	-8.04062400	3.09094600	-0.04413100
O	-3.86558000	4.57940500	2.48191400
O	-3.86697700	4.49715500	-2.61914500
O	-8.60941000	-0.79196500	0.01867200
O	-8.07453300	-4.83711000	0.08380600
O	-4.51074000	-5.95412100	0.10081100
O	-1.87148900	1.47834500	-4.13846500
O	-1.86924100	1.61125900	4.09683500
O	-0.17180600	-2.01948200	4.86528900
O	8.48911300	4.93449700	-0.07840800
O	4.92538300	6.05159800	-0.09548900
O	9.02396000	0.88944900	-0.01327700
O	0.58647500	2.11686000	-4.85977300
O	1.27598700	4.75062000	-2.30355400
O	0.58903500	2.27275700	4.79574500
O	1.27756300	4.82231900	2.15507000
O	2.28609100	-1.38063500	4.14371300
O	8.45533700	-2.99351200	0.04956600
O	4.28158800	-4.39970400	2.62451900
O	4.28019400	-4.48209000	-2.47648900
O	-3.48612200	-5.01871100	-2.14450100
O	6.73950300	-3.76105100	1.90327900
O	7.42950000	-1.12744100	4.45986800
O	6.73851300	-3.82047300	-1.77742400
O	7.42705500	-1.27073600	-4.41802800
O	-3.48429900	-4.94682700	2.31383800
Si	6.12341500	-2.04052500	-5.03693300
Si	-4.78807100	-5.71727200	1.69524000
Si	8.74060500	-0.99597900	3.49090900
Si	-4.78896900	-5.76861100	-1.49994800
Si	6.12616700	-1.87686900	5.10394400
Si	8.73869600	-1.10808100	-3.45462000
Si	-5.71159500	1.97415500	-5.09859900
Si	5.20369700	5.86598800	1.50559000
Si	2.58771200	4.88185800	-3.27190000
Si	-8.32411200	1.20547200	3.46001900
Si	5.20280100	5.81440500	-1.68984300
Si	-5.70882600	2.13792600	5.04232900
Si	-8.32597200	1.09338500	-3.48542600

Si	2.58923400	4.98516700	3.11864400
O	3.09034000	0.96970900	-4.91987000
O	-7.82118200	-2.70674700	1.81218400
O	-2.67835800	-1.03072700	-4.88597700
O	8.23673200	2.86113400	1.71802700
O	8.23581400	2.80425900	-1.80683900
O	-2.67583600	-0.87223200	4.92535000
O	-7.82213000	-2.76363000	-1.71253300
O	3.09311200	1.12807600	4.89149600
Si	-7.95096700	3.66566200	1.49600400
O	-8.57178800	2.53620300	2.52088100
Si	-5.42033100	4.46859900	-3.16385400
O	-5.50155100	3.48866800	-4.48477700
Si	-2.88409500	5.42278800	1.46420300
O	-1.31778500	5.04049800	1.80025800
Si	-7.95181100	3.61566100	-1.60199600
O	-8.57316300	2.45372900	-2.58962900
Si	-5.41865500	4.56853100	3.02812200
O	-5.49909000	3.63174200	4.37987400
Si	-2.88469900	5.37271400	-1.62962200
O	-1.31884800	4.98014800	-1.95405300
Si	9.11370000	1.46419100	1.52681000
O	8.49292600	0.33475000	2.55177300
O	4.83172100	-1.05261700	-4.77305600
Si	-7.64595800	-4.34704600	1.62320800
O	-6.07990800	-4.72905600	1.95908300
Si	2.21336500	2.35970600	-5.15563800
O	2.83465700	3.52171100	-4.16796600
Si	-8.69819100	-1.31677500	1.57654000
O	-8.07687300	-0.15474800	2.56417100
Si	-2.85358700	0.60276300	-5.12792900
O	-4.41949800	0.99547900	-4.80301900
Si	8.06149800	4.49440900	1.47619900
O	6.49554500	4.88717500	1.80048300
Si	-8.69903800	-1.36677300	-1.52146300
O	-8.07833100	-0.23725100	-2.54628800
Si	2.21611700	2.52488300	5.08263600
O	2.83690200	3.65446100	4.05776600
Si	8.06067200	4.44447700	-1.61777300
O	6.49451300	4.82658400	-1.95364800
Si	-2.85095600	0.76794600	5.11435700
O	-4.41703100	1.15012500	4.77847000
Si	9.11285700	1.41419000	-1.57119000
O	8.49155100	0.25227800	-2.55873700

Si	-1.79876100	-2.26237200	5.16114000
O	-2.42011500	-3.42406600	4.17329900
Si	-7.64683600	-4.39693600	-1.47092000
O	-6.08107800	-4.78981200	-1.79499700
Si	3.26829200	-0.50539200	5.13334600
O	4.83428400	-0.89797100	4.80905900
Si	8.36644300	-3.51825200	1.60748400
O	8.98774800	-2.35633900	2.59502700
Si	5.83325300	-4.47110900	-3.02267600
O	5.91380200	-3.53431400	-4.37444700
Si	8.36559600	-3.56825500	-1.49052200
O	8.98641800	-2.43879800	-2.51539500
Si	5.83493200	-4.37123200	3.16940900
O	5.91616000	-3.39127000	4.49012100
H	-5.95815700	2.35110200	6.47525700
H	-9.50249500	1.08740500	4.33086700
H	-10.12913200	-1.53034300	1.83673300
H	-8.72733400	4.90240600	1.66517100
H	-10.13013200	-1.58861600	-1.77375800
H	-9.50480000	0.94729800	-4.35140800
H	-8.72827100	4.84630700	-1.81061700
H	-8.52260400	-5.09982700	2.53189400
H	-1.87804700	-2.73082800	6.55205400
H	-2.47413500	1.19900400	6.46833200
H	2.89219300	-0.89237000	6.50059100
H	6.37623500	-2.04362500	6.54288700
H	2.29621400	3.03818100	6.45778700
H	6.29941500	-5.70697100	3.57043600
H	9.91948000	-0.84979100	4.35680500
H	9.14290200	-4.74889800	1.81610200
H	9.14192100	-4.80501300	-1.65976200
H	9.91711200	-0.98991300	-4.32540500
H	6.29748000	-5.81917400	-3.38075400
H	6.37271100	-2.25363200	-6.46987900
H	2.88873600	-1.10158200	-6.46285800
H	2.29269200	2.82830300	-6.54662200
H	-2.47773500	0.98972400	-6.49523700
H	-5.96169300	2.14105200	-6.53738700
H	-1.95394100	-6.10157600	-3.91243300
H	3.45364600	-6.77735700	-1.62614100
H	3.45460900	-6.72137900	1.84920600
H	-1.95201400	-5.97196900	4.11567500
H	-4.97645300	-7.11979000	-2.04784400
H	-4.97531900	-7.04981700	2.28645600

H	-8.52398000	-5.17873900	-2.35424200
H	-5.88285200	5.91656300	3.38621500
H	-5.88477400	5.80437300	-3.56497800
H	-3.03900600	6.87475100	1.63163200
H	-3.03996800	6.81865100	-1.84388400
H	2.36868400	6.19891000	3.91794300
H	2.36652600	6.06933700	-4.11011400
H	5.39103600	7.21724200	2.05323100
H	5.38987100	7.14728500	-2.28089100
H	8.93854300	5.27620000	2.35965400
H	8.93724900	5.19735000	-2.52644900
H	10.54478900	1.68601800	1.77916100
H	10.54381700	1.62775800	-1.83127400
H	-1.96748800	-2.90273200	-6.45823700
Si	3.19500400	-0.73624900	-5.09408700
Si	-1.85268400	-2.51789500	-5.09644800
O	2.35731200	-1.54913200	-4.02952600
O	-0.31256200	-2.35256300	-4.71909200
O	-2.58352000	-3.66944200	-4.20706600
Al	0.48651100	-3.91076500	1.65369800
Si	0.50543000	-3.99059500	-1.60065500
Si	3.17160700	-5.34487800	-1.47437700
Si	-2.12619700	-4.93236400	-3.14295200
Si	0.72060300	-1.61185000	-3.50449900
Si	3.14780500	-5.30349300	1.69360300
Si	0.72211400	-1.43593000	3.48474200
Si	-2.08228700	-4.83843900	3.26136800
O	0.55469600	-2.22441600	2.12972800
O	1.72942400	-4.93078400	2.27591100
O	-0.94222600	-4.63471200	2.23047100
O	0.38650400	-3.90171400	-0.05401800
O	3.31097200	-4.95599000	0.08719400
O	1.71576800	-4.95788600	-2.10155800
O	0.64286500	-2.43556000	-2.14903500
O	-0.82859300	-4.57499200	-2.31045300
O	0.20765300	0.10095600	3.22782600
O	0.19880000	-0.07815900	-3.29486200
O	-0.14812900	2.42924700	-2.26612700
O	-0.17262900	2.53517900	2.18674200
O	0.13839300	3.76081100	-0.06519300
Si	-0.28792600	1.60017100	3.48174000
Si	-0.28729000	1.46022100	-3.53324700
Si	-0.01778000	3.91408800	-1.63780000
Si	-0.01551700	3.97771400	1.50330800

C	-4.24316500	-1.05596900	-1.17536200
C	-3.70671600	0.19719800	-1.18507400
C	-3.32157100	0.81783000	0.02217600
C	-3.62585000	0.25079200	1.27501200
C	-4.19268000	-0.98892800	1.34690700
C	-4.29072100	-1.79931800	0.10973800
C	-4.65202000	-1.75533200	-2.42193000
H	-5.60877900	-2.27358400	-2.29112100
H	-4.72710000	-1.06246200	-3.26478600
H	-3.91769400	-2.52583100	-2.68771400
H	-5.15232200	-2.46944500	0.15395600
C	-2.98940400	-2.70515600	0.08947200
H	-2.84186600	-3.19043800	1.05296500
H	-3.15580800	-3.47924000	-0.65879600
H	-2.11434000	-2.09581200	-0.14271800

The rate-determining transition state (**P(E)**) for ethene formation via paring mechanism.

O	-3.31705000	4.92015000	-0.06708600
O	3.88339800	5.04580400	-2.33535100
O	-6.31635500	3.90439800	1.81002400
O	-6.98378600	1.36508400	4.46603000
O	-6.33455200	3.82731600	-1.87031600
O	-7.02771900	1.17915100	-4.41096400
O	3.90539600	5.13915800	2.12252400
O	-8.03891500	3.06295200	-0.00488100
O	-3.85709600	4.57761500	2.49417800
O	-3.88228300	4.47080800	-2.60637200
O	-8.59426700	-0.82150100	0.07920600
O	-8.04541800	-4.86446800	0.16116300
O	-4.47791200	-5.96950900	0.16663100
O	-1.88385900	1.45115600	-4.12038900
O	-1.84312700	1.62378700	4.11360500
O	-0.12971300	-1.99757600	4.89148300
O	8.48415200	4.96180700	-0.12639900
O	4.91662200	6.06684200	-0.13192000
O	9.03297000	0.91893800	-0.04444700
O	0.56851100	2.09472100	-4.85669400
O	1.26162300	4.74301900	-2.31606300
O	0.61627000	2.29697300	4.79788100
O	1.28364000	4.83636000	2.14186000
O	2.32254500	-1.35385000	4.15545000
O	8.47778100	-2.96556500	0.03967700
O	4.32105100	-4.37337200	2.64110600
O	4.29583000	-4.48024000	-2.45934300
O	-3.46689000	-5.04155500	-2.08794000

O	6.77333500	-3.72995300	1.90516400
O	7.46650300	-1.08179200	4.44581500
O	6.75514300	-3.80704500	-1.77517000
O	7.42256900	-1.26772500	-4.43118300
O	-3.44439500	-4.94837100	2.37003700
Si	6.11862700	-2.04485100	-5.04020500
Si	-4.74852300	-5.72554500	1.76124800
Si	8.77255900	-0.95058100	3.47003100
Si	-4.76419900	-5.79259400	-1.43366100
Si	6.16877100	-1.83248700	5.09964800
Si	8.73819300	-1.09604400	-3.47479700
Si	-5.72998600	1.92984700	-5.06480100
Si	5.20313000	5.88985900	1.46869100
Si	2.56773600	4.87411300	-3.29181000
Si	-8.29945500	1.19338600	3.50955800
Si	5.18730100	5.82292700	-1.72642000
Si	-5.67988600	2.14220300	5.07496400
Si	-8.33377500	1.04794300	-3.43518200
Si	2.59934300	5.00794800	3.09830400
O	3.07597700	0.95571300	-4.92315600
O	-7.79105900	-2.72496900	1.87794000
O	-2.68582000	-1.06382600	-4.85227600
O	8.24727700	2.89626100	1.68111500
O	8.22988200	2.82245600	-1.84339400
O	-2.63743500	-0.85868900	4.95831500
O	-7.80852100	-2.79880500	-1.64627000
O	3.12459200	1.16120300	4.88721500
Si	-7.94392000	3.64535300	1.53204400
O	-8.55606600	2.51875300	2.56524800
Si	-5.43807100	4.43439800	-3.14355700
O	-5.52225300	3.44784500	-4.45931000
Si	-2.88303100	5.41915600	1.46782400
O	-1.31406000	5.04395700	1.79810000
Si	-7.95924300	3.58047300	-1.56564300
O	-8.58132500	2.41173300	-2.54474500
Si	-5.40745900	4.56406800	3.04779000
O	-5.47833400	3.63351500	4.40437900
Si	-2.89832600	5.35432500	-1.62582600
O	-1.33264400	4.96531600	-1.95564100
Si	9.12804900	1.50136600	1.49242900
O	8.51594800	0.37478400	2.52572000
O	4.82486400	-1.06001800	-4.77492400
Si	-7.61134300	-4.36576700	1.69648100
O	-6.04220100	-4.74042300	2.02570700

Si	2.19320500	2.34160900	-5.16142400
O	2.81524800	3.51040900	-4.18225500
Si	-8.67390700	-1.33912000	1.63997100
O	-8.05185800	-0.17028200	2.61906900
Si	-2.86766200	0.56774800	-5.10111200
O	-4.43345100	0.95685100	-4.77137900
Si	8.06538000	4.52775500	1.43230700
O	6.49965800	4.91681500	1.76213300
Si	-8.68923200	-1.40400000	-1.45771800
O	-8.07720100	-0.27733300	-2.49087200
Si	2.24380300	2.55597000	5.07583300
O	2.85591800	3.68267700	4.04261900
Si	8.05009400	4.46296700	-1.66135200
O	6.48108100	4.83819300	-1.99161600
Si	-2.81709500	0.78227300	5.13986400
O	-4.38602000	1.15751100	4.80973800
Si	9.11272600	1.43648700	-1.60525800
O	8.49069000	0.26776600	-2.58427300
Si	-1.75431100	-2.24406400	5.19618800
O	-2.37652400	-3.41254100	4.21687700
Si	-7.62656300	-4.43038500	-1.39759500
O	-6.06090700	-4.81936100	-1.72728600
Si	3.30647800	-0.47040700	5.13593800
O	4.87220700	-0.85935200	4.80620400
Si	8.39802600	-3.48311400	1.60049300
O	9.02006300	-2.31439200	2.57950600
Si	5.84619800	-4.46671400	-3.01301600
O	5.91719900	-3.53613800	-4.36959000
Si	8.38270200	-3.54799300	-1.49719700
O	8.99485100	-2.42139300	-2.53039900
Si	5.87683200	-4.33707000	3.17846500
O	5.96098300	-3.35051500	4.49408200
H	-5.92315700	2.36142000	6.50802200
H	-9.47330200	1.07554600	4.38654100
H	-10.10287100	-1.55623900	1.90796900
H	-8.72365400	4.88028200	1.69897000
H	-10.12074500	-1.63185200	-1.70215600
H	-9.51618400	0.89373700	-4.29485300
H	-8.74083500	4.80748800	-1.77646600
H	-8.48101300	-5.11685600	2.61264100
H	-1.82553600	-2.70628500	6.58980800
H	-2.43532900	1.22098200	6.49009100
H	2.93814800	-0.85217700	6.50689000
H	6.42620300	-1.99149200	6.53816900

H	2.32866700	3.07611900	6.44810400
H	6.34771000	-5.66930600	3.58369000
H	9.95501600	-0.79627900	4.32961200
H	9.17961900	-4.71012900	1.81131300
H	9.16239500	-4.78293800	-1.66419800
H	9.91207300	-0.97810100	-4.35172000
H	6.31329700	-5.81489800	-3.36679400
H	6.36186300	-2.26399900	-6.47328000
H	2.87409100	-1.12363700	-6.45524300
H	2.26437200	2.80377400	-6.55499200
H	-2.49947100	0.94951800	-6.47214400
H	-5.98747800	2.08890900	-6.50330500
H	-1.93968300	-6.12757000	-3.85798100
H	3.48105100	-6.77419600	-1.59416000
H	3.49824800	-6.70149100	1.88084400
H	-1.90010300	-5.95949900	4.16938100
H	-4.94975500	-7.14695000	-1.97419500
H	-4.92825900	-7.05615600	2.35966900
H	-8.50522700	-5.21929100	-2.27308200
H	-5.87451100	5.91223900	3.40162700
H	-5.90891900	5.76666200	-3.54886200
H	-3.04223200	6.87153400	1.62900400
H	-3.05937600	6.79875500	-1.84609500
H	2.37845200	6.22484800	3.89283400
H	2.33876500	6.05670400	-4.13440600
H	5.38848800	7.24434700	2.00896300
H	5.36706700	7.15357300	-2.32472100
H	8.94394500	5.31672200	2.30783800
H	8.91981600	5.21440400	-2.57777100
H	10.55955600	1.72920600	1.73692200
H	10.54171100	1.65360700	-1.87314700
H	-1.97594900	-2.94101300	-6.41897100
Si	3.18560200	-0.75066700	-5.08966300
Si	-1.85577600	-2.54928700	-5.05947600
O	2.35568300	-1.56132200	-4.01739700
O	-0.31466800	-2.37702500	-4.69039100
O	-2.57881000	-3.69885600	-4.16126400
Al	0.55919700	-3.92501200	1.68367900
Si	0.55933300	-4.04483500	-1.57602900
Si	3.19132100	-5.34899000	-1.45512500
Si	-2.11736100	-4.95193700	-3.09169000
Si	0.72355100	-1.65283300	-3.46192100
Si	3.18175500	-5.29120600	1.72233200
Si	0.76047400	-1.43827300	3.49179400

Si	-2.04433100	-4.82432400	3.30709800
O	0.62458600	-2.25416400	2.15983700
O	1.77517100	-4.94917200	2.35756400
O	-0.92654300	-4.59795200	2.23760100
O	0.55901600	-4.08351800	-0.02197800
O	3.33012100	-4.95566600	0.10892100
O	1.75229000	-5.00100600	-2.14644800
O	0.67613300	-2.50083200	-2.12789300
O	-0.82702400	-4.61965200	-2.22003900
O	0.24752700	0.10916600	3.23433000
O	0.20129400	-0.10660300	-3.26971200
O	-0.17663500	2.40312300	-2.26042300
O	-0.18426100	2.53141100	2.18842200
O	0.07536100	3.73783000	-0.06774600
Si	-0.26088100	1.59589200	3.49949300
Si	-0.29251100	1.41720700	-3.53051200
Si	-0.02541800	3.89085900	-1.64907500
Si	-0.00789500	3.97140600	1.50783500
C	-4.16781600	-0.75447900	-1.46048500
C	-3.32185000	0.29876500	-1.53284300
C	-3.33779100	1.74093100	0.49559400
C	-2.69918700	0.53072100	-0.17850200
C	-3.24872700	-0.60310400	0.63769000
C	-4.17168700	-1.26705200	-0.09295300
C	-4.99411900	-2.40819900	0.37381800
H	-5.41554100	-2.21594100	1.36718100
H	-5.81184100	-2.62108000	-0.32214300
H	-4.34933300	-3.29090000	0.44393700
C	-4.37499500	2.43085000	-0.17483000
H	-4.37851100	2.48817400	-1.26020100
H	-5.10389700	3.04404000	0.36121800
H	-2.83015000	2.76207100	0.22371500
H	-3.35568500	1.75489600	1.58617900
C	-4.93550900	-1.39301100	-2.56681400
H	-4.64686600	-2.44769500	-2.64727700
H	-6.01606800	-1.36871700	-2.37618200
H	-4.73437100	-0.91266000	-3.52818900
C	-2.73490500	-0.97275600	1.97304200
H	-3.37023100	-1.71974000	2.45746700
H	-1.73796000	-1.40685200	1.84916700
H	-2.64682800	-0.11364400	2.64921100
H	-3.12734400	0.89797600	-2.41467500
H	-1.60909800	0.58785800	-0.18319600
O	-2.21355500	-3.32682300	0.06959600

H	-1.96241500	-3.97450200	-0.59412400
H	-1.93890700	-3.76592100	0.89061100

The rate-determining intermediate (methanol and 1, 2, 3-triMB adsorbed on zeolite) for ethene formation via paring mechanism.

O	-3.40113900	4.92232200	-0.09253400
O	3.80702500	5.05605200	-2.33576600
O	-6.40505700	3.90536300	1.77655700
O	-7.07699900	1.37131700	4.43645500
O	-6.41016200	3.81919900	-1.90362300
O	-7.08935300	1.16347800	-4.44015400
O	3.81316500	5.16040400	2.12191500
O	-8.11962000	3.05616900	-0.04230900
O	-3.94951000	4.58496000	2.46768300
O	-3.95655000	4.46556000	-2.63264300
O	-8.66788100	-0.82911900	0.04940400
O	-8.11163800	-4.87081500	0.14325600
O	-4.54200900	-5.96889100	0.16397600
O	-1.94703000	1.44619300	-4.13237300
O	-1.93556200	1.63898900	4.10150600
O	-0.21810800	-1.97702800	4.89435100
O	8.40013200	4.98626900	-0.11046700
O	4.83055200	6.08447200	-0.13124500
O	8.95634400	0.94466700	-0.01661800
O	0.50665400	2.09246300	-4.86146200
O	1.18578200	4.74831300	-2.32496000
O	0.52002800	2.31852800	4.79267000
O	1.19194200	4.85264600	2.13277800
O	2.23550300	-1.33060900	4.16524200
O	8.40824500	-2.94066800	0.07513200
O	4.24507300	-4.35000700	2.66539600
O	4.23800500	-4.46948400	-2.43484200
O	-3.52489900	-5.04468700	-2.08932100
O	6.69870500	-3.70372200	1.93649600
O	7.37789800	-1.04800200	4.47303200
O	6.69360500	-3.78989800	-1.74367600
O	7.36554100	-1.25584600	-4.40358000
O	-3.51837600	-4.94055400	2.36857100
Si	6.06522800	-2.03695400	-5.01526200
Si	-4.81881100	-5.72170100	1.75697600
Si	8.68712700	-0.91669800	3.50151900
Si	-4.82305800	-5.79661100	-1.43773200
Si	6.07930300	-1.79956600	5.12414900
Si	8.67746400	-1.07930100	-3.44300500
Si	-5.79076200	1.91503400	-5.09127900

Si	5.11176200	5.91197100	1.47079600
Si	2.49507600	4.87948500	-3.29640400
Si	-8.38896600	1.19475700	3.47579400
Si	5.10729800	5.83715500	-1.72417700
Si	-5.77672700	2.15241900	5.04804500
Si	-8.39858200	1.03217200	-3.46864500
Si	2.50393700	5.02910300	3.09342500
O	3.01648900	0.95807000	-4.91630300
O	-7.86742800	-2.72664200	1.85579700
O	-2.74169200	-1.07225900	-4.86096200
O	8.16082600	2.92472200	1.70129300
O	8.15597200	2.84222000	-1.82306400
O	-2.72805600	-0.84252000	4.94915300
O	-7.87231500	-2.80915500	-1.66842100
O	3.03020700	1.18777500	4.89364400
Si	-8.03113800	3.64252900	1.49350100
O	-8.64477300	2.51730500	2.52732200
Si	-5.51036300	4.42485600	-3.17520100
O	-5.58803900	3.43491600	-4.48881000
Si	-2.97343100	5.42577700	1.44270300
O	-1.40492900	5.05442700	1.77939900
Si	-8.03544100	3.57000200	-1.60405400
O	-8.65185500	2.39767400	-2.58244800
Si	-5.50177500	4.56981000	3.01587800
O	-5.57565400	3.64246200	4.37449900
Si	-2.97770800	5.35335300	-1.65082300
O	-1.41015200	4.96651300	-1.97418900
Si	9.04490800	1.53105500	1.51914000
O	8.43131900	0.40584800	2.55304800
O	4.76867100	-1.05394400	-4.75695500
Si	-7.68379900	-4.36732800	1.67852500
O	-6.11536700	-4.73868200	2.01528300
Si	2.13193100	2.34168400	-5.16106900
O	2.74829800	3.51408200	-4.18262300
Si	-8.75202500	-1.34304900	1.61115100
O	-8.13564600	-0.17062200	2.58954400
Si	-2.92569200	0.55834800	-5.11419700
O	-4.49340900	0.94519800	-4.79084900
Si	7.97670700	4.55525200	1.44782400
O	6.40909900	4.94213000	1.77118700
Si	-8.75633100	-1.41557400	-1.48640300
O	-8.14281100	-0.29028500	-2.52017400
Si	2.14610900	2.58131600	5.07572800
O	2.75971000	3.70664900	4.04189700

Si	7.97242600	4.48282600	-1.64570000
O	6.40387300	4.85424200	-1.98239900
Si	-2.91159300	0.79809600	5.12653200
O	-4.48006700	1.16953100	4.78976900
Si	9.04060400	1.45852800	-1.57841300
O	8.42423800	0.28621800	-2.55672300
Si	-1.84340800	-2.22620900	5.19384800
O	-2.45983200	-3.39842900	4.21548100
Si	-7.68812900	-4.43976800	-1.41508700
O	-6.12058600	-4.82656200	-1.73831200
Si	3.21431500	-0.44287300	5.14703400
O	4.78193200	-0.82963400	4.82375800
Si	8.32398600	-3.45453000	1.63692700
O	8.94035300	-2.28221900	2.61523500
Si	5.79027800	-4.45433700	-2.98306900
O	5.86427800	-3.52696900	-4.34168200
Si	8.31968000	-3.52705600	-1.46062800
O	8.93331800	-2.40183300	-2.49444800
Si	5.79888300	-4.30942300	3.20813800
O	5.87653500	-3.31946900	4.52160100
H	-6.02545400	2.37469600	6.47969700
H	-9.56566500	1.07683200	4.34893600
H	-10.18150800	-1.56223600	1.87466200
H	-8.81380100	4.87637200	1.65464200
H	-10.18654000	-1.64676100	-1.73530600
H	-9.57766500	0.87359700	-4.33208200
H	-8.81861900	4.79500200	-1.82064300
H	-8.55537700	-5.11808000	2.59374000
H	-1.91857200	-2.68503400	6.58834300
H	-2.53541600	1.24089200	6.47682100
H	2.84189000	-0.82196500	6.51761500
H	6.33197700	-1.95454100	6.56395400
H	2.22515900	3.10500100	6.44700300
H	6.27086600	-5.63975100	3.61829500
H	9.86625900	-0.75802600	4.36486800
H	9.10716400	-4.67952900	1.85351700
H	9.10230200	-4.76091600	-1.62184400
H	9.85419500	-0.96127400	-4.31608800
H	6.26117600	-5.80249800	-3.33188700
H	6.31392000	-2.25916000	-6.44692800
H	2.82394200	-1.12541600	-6.44395600
H	2.20711600	2.80056700	-6.55552500
H	-2.55344200	0.93742900	-6.48483800
H	-6.04349300	2.07006800	-6.53106500

H	-1.98942000	-6.13214100	-3.85129600
H	3.42455200	-6.76285300	-1.56685100
H	3.42937900	-6.68155800	1.90800300
H	-1.97830400	-5.94413500	4.17560300
H	-5.00415400	-7.15262400	-1.97558500
H	-4.99808600	-7.05119300	2.35796800
H	-8.56220700	-5.23250000	-2.29170600
H	-5.97263200	5.91795000	3.36474600
H	-5.98231600	5.75521900	-3.58544100
H	-3.13595600	6.87829500	1.59971500
H	-3.14074200	6.79693800	-1.87522100
H	2.27794300	6.24752500	3.88416800
H	2.26680900	6.05956800	-4.14272600
H	5.29264500	7.26813600	2.00837300
H	5.28663900	7.16666700	-2.32512300
H	8.85068500	5.34804400	2.32448900
H	8.84393500	5.23366800	-2.56090800
H	10.47511100	1.76222700	1.76809700
H	10.47010700	1.67771800	-1.84181500
H	-2.02270100	-2.95193700	-6.42024700
Si	3.12994500	-0.74850700	-5.07821800
Si	-1.90808200	-2.55669200	-5.06121000
O	2.29782000	-1.55810000	-4.00688900
O	-0.36862300	-2.38056200	-4.68719100
O	-2.63210500	-3.70538800	-4.16280600
Al	0.43112200	-3.91508700	1.69350000
Si	0.45049400	-3.97737600	-1.56075300
Si	3.12906500	-5.34932300	-1.43371600
Si	-2.18168200	-4.95231700	-3.08468500
Si	0.64688500	-1.61278200	-3.49990400
Si	3.13716800	-5.27013100	1.72583600
Si	0.66575100	-1.38167700	3.53929200
Si	-2.14091000	-4.81619800	3.31785700
O	0.61948800	-2.20807700	2.16663400
O	1.70476900	-4.92082200	2.26611100
O	-0.95934100	-4.60697600	2.32587100
O	0.42603100	-3.79574100	-0.01095000
O	3.35391800	-4.87087000	0.11133600
O	1.66707600	-4.97737100	-2.02017700
O	0.66217500	-2.45989100	-2.15947100
O	-0.87422600	-4.58430100	-2.24154100
O	0.15644200	0.13475300	3.21244500
O	0.14519400	-0.08126800	-3.28892100
O	-0.20195500	2.40971200	-2.26055400

O	-0.22704300	2.54471600	2.17328800
O	0.04840900	3.74263700	-0.07730600
Si	-0.36621100	1.63832300	3.48652200
Si	-0.37450500	1.45317500	-3.53408600
Si	-0.11039200	3.91007800	-1.65056300
Si	-0.10561100	3.99687600	1.48761700
C	-4.10856000	-1.26434900	-0.05999300
C	-3.98467400	-0.68816400	-1.32753200
C	-3.40582600	0.57704000	-1.43875900
C	-2.97088200	1.26210000	-0.30979400
C	-3.17498300	0.71639900	0.95115500
C	-3.76783200	-0.53885000	1.08495100
C	-4.69255300	-2.63403000	0.09298700
H	-4.52097000	-3.24105000	-0.80031500
H	-4.25785300	-3.16736400	0.94489300
H	-5.77830800	-2.58683600	0.26080500
C	0.74623500	0.06556100	-0.16798100
H	0.39460400	0.74249900	0.60631600
H	-0.07782600	-0.51225000	-0.58317300
H	1.25816000	0.62486600	-0.94612400
O	1.71607400	-0.81732800	0.44006600
H	2.34384500	-1.33892800	-0.19822600
H	1.25587600	-1.44948200	1.12519200
H	-2.54104600	2.25339500	-0.40736900
H	-3.34854600	1.05199400	-2.41597000
H	-2.93297500	1.29673200	1.83804400
C	-4.56324000	-1.40256800	-2.51970800
H	-4.04578300	-2.34371000	-2.73846200
H	-5.61701100	-1.65130200	-2.34992600
H	-4.51572900	-0.78247200	-3.41795900
C	-4.13955800	-1.10016600	2.42535600
H	-5.16077200	-1.49401300	2.41909800
H	-3.48553100	-1.92141200	2.74318800
H	-4.10287300	-0.32041200	3.18710700
O	3.40328400	-2.06277300	-0.89902200
H	3.68822000	-2.87848000	-0.45412400
H	3.27112700	-2.28291300	-1.82992600

The rate-determining transition state for propene formation (**M3**) via side-chain methylation.

O	-3.31939600	4.95269000	-0.13426600
O	3.88738800	5.02666200	-2.38469300
O	-6.32694200	3.96984900	1.74720200
O	-7.00977800	1.46554600	4.43237400
O	-6.33574400	3.84765200	-1.93195000
O	-7.03105800	1.17079600	-4.44176000

O	3.89800900	5.17465900	2.07174500
O	-8.04752800	3.11186700	-0.06182400
O	-3.86726100	4.64331200	2.42958900
O	-3.87942900	4.47397400	-2.66931200
O	-8.61602300	-0.76941100	0.06843200
O	-8.08085100	-4.81286500	0.20144600
O	-4.51699700	-5.92940200	0.22996200
O	-1.88702900	1.42958900	-4.14108500
O	-1.86731300	1.70297900	4.09055200
O	-0.16809800	-1.91404500	4.91737300
O	8.48202900	4.95462600	-0.16263700
O	4.91822300	6.07126000	-0.19121400
O	9.01717500	0.91128000	-0.02963200
O	0.56933000	2.05579300	-4.87847400
O	1.26458000	4.73278700	-2.36869400
O	0.59241000	2.37638200	4.77297200
O	1.27522100	4.88076100	2.08780200
O	2.28822500	-1.28767600	4.17994200
O	8.44884100	-2.97004500	0.10066100
O	4.28064000	-4.33210500	2.70808700
O	4.26844400	-4.50151300	-2.39073500
O	-3.49705300	-5.03262500	-2.03313600
O	6.73697700	-3.70585500	1.97083900
O	7.43229000	-1.02900000	4.48064900
O	6.72817600	-3.82806100	-1.70830700
O	7.41101100	-1.32375300	-4.39348400
O	-3.48607200	-4.88475100	2.42338100
Si	6.10609000	-2.10399500	-4.99639800
Si	-4.79108700	-5.66520700	1.82082100
Si	8.74133100	-0.91408400	3.50680700
Si	-4.79855700	-5.77130400	-1.37312900
Si	6.13035800	-1.76733300	5.14018300
Si	8.72468600	-1.14467900	-3.43577900
Si	-5.72912400	1.90912700	-5.10129700
Si	5.19994300	5.91299600	1.41220500
Si	2.57368500	4.84756600	-3.34246200
Si	-8.32350000	1.28645500	3.47458000
Si	5.19226800	5.80689800	-1.78187300
Si	-5.70489900	2.24577900	5.03519600
Si	-8.34009700	1.05588000	-3.46792000
Si	2.58897000	5.05974600	3.04558200
O	3.07314900	0.90778800	-4.92427100
O	-7.82391000	-2.65331000	1.89267700
O	-2.69554400	-1.09168900	-4.84404700

O	8.23354300	2.91221500	1.66944500
O	8.22514600	2.79520600	-1.85392800
O	-2.67203700	-0.76592000	4.96314200
O	-7.83234200	-2.77032800	-1.63055900
O	3.09672700	1.23354000	4.88293600
Si	-7.95462300	3.71277800	1.46808900
O	-8.57322300	2.60096800	2.51340100
Si	-5.43391300	4.43609800	-3.21015200
O	-5.51792700	3.43375100	-4.51392400
Si	-2.88770400	5.46891700	1.39560400
O	-1.32086900	5.09267500	1.73462100
Si	-7.96203900	3.60992300	-1.62860100
O	-8.58544100	2.43130700	-2.59494100
Si	-5.41910100	4.64166700	2.97919700
O	-5.49663100	3.72807800	4.34690600
Si	-2.89509000	5.36620700	-1.69705500
O	-1.32986900	4.96801400	-2.01792000
Si	9.11016000	1.51221600	1.50022900
O	8.49160800	0.40042800	2.54562800
O	4.81492000	-1.11172200	-4.74666300
Si	-7.64901900	-4.29657700	1.73133500
O	-6.08224200	-4.67285600	2.07023800
Si	2.19562300	2.29355100	-5.18185700
O	2.81897800	3.47223700	-4.21546300
Si	-8.70147500	-1.26756300	1.63521100
O	-8.07811000	-0.08885100	2.60155000
Si	-2.87121100	0.53726900	-5.11334100
O	-4.43660600	0.93550000	-4.79245700
Si	8.05773000	4.54112500	1.40015600
O	6.49245400	4.93936200	1.72101200
Si	-8.70889700	-1.37041700	-1.46147900
O	-8.09041100	-0.25854100	-2.50674200
Si	2.22009100	2.63341400	5.05208400
O	2.83865800	3.74532800	4.00676100
Si	8.05033900	4.43841200	-1.69250600
O	6.48345600	4.81472300	-2.03152400
Si	-2.84681700	0.87729900	5.12457900
O	-4.41362700	1.25363300	4.78549500
Si	9.10274300	1.40936300	-1.59645900
O	8.47938900	0.23076800	-2.56271500
Si	-1.79443000	-2.15177000	5.22067600
O	-2.41778600	-3.33026300	4.25430100
Si	-7.65646400	-4.39932200	-1.36140500
O	-6.09125200	-4.79747200	-1.68212600

Si	3.27252800	-0.39547900	5.15213900
O	4.83781300	-0.79360500	4.83137300
Si	8.36327300	-3.46812800	1.66748800
O	8.98662700	-2.28953300	2.63374400
Si	5.82029300	-4.49987300	-2.94037500
O	5.89794300	-3.58626400	-4.30807600
Si	8.35585400	-3.57098200	-1.42920100
O	8.97445500	-2.45917500	-2.47451300
Si	5.83512200	-4.29433700	3.24910300
O	5.91910900	-3.29198400	4.55273400
H	-5.95119600	2.48337400	6.46480500
H	-9.50002700	1.18326100	4.34981600
H	-10.13185200	-1.47666500	1.90204600
H	-8.73067900	4.95222500	1.61777500
H	-10.14051200	-1.59653500	-1.70691300
H	-9.52075500	0.89503100	-4.32878000
H	-8.73899000	4.83682700	-1.85654000
H	-8.52370800	-5.03374700	2.65461300
H	-1.87074100	-2.59649600	6.61963700
H	-2.46713600	1.33132300	6.47014400
H	2.89933400	-0.75917400	6.52668900
H	6.38348800	-1.90951300	6.58122700
H	2.30308900	3.17008600	6.41809400
H	6.30050000	-5.62304100	3.67189300
H	9.92203700	-0.75313800	4.36757800
H	9.14022400	-4.69503200	1.89542800
H	9.13186800	-4.81044700	-1.57896300
H	9.90124900	-1.04138000	-4.31095400
H	6.28382400	-5.85383600	-3.27635000
H	6.35235200	-2.34152000	-6.42602300
H	2.86835700	-1.18953000	-6.43126500
H	2.27197700	2.73834800	-6.58080700
H	-2.49820500	0.90095200	-6.48790300
H	-5.98231000	2.05136600	-6.54232600
H	-1.96883400	-6.14532200	-3.78564200
H	3.44377300	-6.78197100	-1.49962300
H	3.45209600	-6.66665900	1.97425900
H	-1.94964100	-5.87872000	4.23904200
H	-4.98721200	-7.13156500	-1.89750700
H	-4.97680100	-6.98768100	2.43488100
H	-8.53545200	-5.19601600	-2.22948400
H	-5.88259100	5.99560900	3.31522400
H	-5.89926200	5.76483200	-3.63302300
H	-3.04249000	6.92373500	1.53850400

H	-3.05076900	6.80835600	-1.93546200
H	2.37005100	6.28702800	3.82452800
H	2.35084600	6.02048000	-4.20012400
H	5.38839200	7.27339800	1.93631200
H	5.37803000	7.12949900	-2.39597300
H	8.93661800	5.33788000	2.26827900
H	8.92495700	5.17567200	-2.61575500
H	10.54177300	1.73832200	1.74571900
H	10.53313800	1.61846800	-1.86318600
H	-1.98776200	-2.99032100	-6.38561600
Si	3.17753300	-0.80086300	-5.06953900
Si	-1.86988500	-2.58238000	-5.03064100
O	2.34212400	-1.59555100	-3.98963100
O	-0.32917400	-2.41064400	-4.65965000
O	-2.59909300	-3.71841100	-4.12039300
Al	0.47298800	-3.88836700	1.73775000
Si	0.48395000	-3.99258200	-1.52094100
Si	3.15644400	-5.35135200	-1.37514900
Si	-2.14449400	-4.96661200	-3.03757700
Si	0.69310600	-1.64323100	-3.47015100
Si	3.15446900	-5.25537300	1.79105500
Si	0.72018300	-1.35481000	3.53978300
Si	-2.09361100	-4.76323600	3.37127800
O	0.57848500	-2.19177000	2.20021300
O	1.73463400	-4.88499700	2.35727000
O	-0.93071600	-4.60315500	2.35337000
O	0.41623500	-3.86616400	0.02988700
O	3.33933600	-4.89446100	0.17514400
O	1.71200800	-4.95887500	-2.00153100
O	0.56502200	-2.46598900	-2.12665900
O	-0.83007200	-4.65130200	-2.20100100
O	0.19030000	0.16488400	3.22855800
O	0.19255200	-0.09954400	-3.26759500
O	-0.15031600	2.42193600	-2.29718400
O	-0.10908100	2.58705000	2.17352200
O	0.13586400	3.75480100	-0.10703600
Si	-0.28587400	1.67892900	3.48030300
Si	-0.30495000	1.43243400	-3.54798600
Si	-0.02922300	3.91608100	-1.68138100
Si	-0.01568800	4.02385700	1.46194200
C	-4.37442700	-1.38219400	1.00016800
C	-4.15065700	-2.31518100	-0.16672500
C	-4.27026600	-1.62515100	-1.51186700
C	-3.82894700	-0.36371900	-1.61137600

C	-3.52468900	0.38613300	-0.41944500
C	-4.05152100	-0.09398900	0.84172500
C	-2.76663000	1.51811600	-0.44789600
H	-2.50971900	1.93742300	-1.41813700
C	-2.70642800	-2.85887300	0.00030800
H	-1.98946100	-2.04095500	-0.05382700
H	-2.57768100	-3.36319900	0.95768400
H	-2.45089900	-3.57551800	-0.77254200
H	-4.83663800	-3.16835400	-0.11952900
C	-0.88232600	0.29537500	-0.14223400
H	-0.43146200	1.27192500	-0.16217400
H	-1.03252300	-0.25782600	-1.05479200
H	-1.26322000	-0.09592500	0.78959900
O	0.84915500	-0.47628500	0.18909800
H	0.74558600	-1.14999900	0.90161100
H	1.35310400	-0.94205400	-0.50386400
C	-4.87031700	-2.30517000	-2.69547300
H	-5.95943500	-2.34218600	-2.56742200
H	-4.66194400	-1.75230100	-3.61501800
H	-4.53630800	-3.33558200	-2.81993700
C	-4.76016600	-1.91165900	2.33927400
H	-4.81376300	-1.10913500	3.07923100
H	-5.72737000	-2.42336700	2.31100600
H	-4.03353400	-2.65017700	2.69217500
H	-4.13687000	0.58742200	1.67939700
H	-3.78831900	0.14554400	-2.57435400
O	3.07474300	-1.95192900	-0.79917000
H	3.47514300	-2.13327700	-1.65521300
H	3.36736500	-2.67128500	-0.22580900
C	-2.77381100	2.41875900	0.73722100
H	-2.05268600	3.20711400	0.58246300
H	-3.76036800	2.88881400	0.86311700
H	-2.52219600	1.91455800	1.67073900

The rate-determining intermediates (1, 3, 4, 5- tetraMB$^+$ cation) for propene formation via side-chain methylation.

O	-3.31191400	4.93233200	-0.07515700
O	3.89920100	5.04461600	-2.30865800
O	-6.32388100	3.91786900	1.78291900
O	-7.01242600	1.36814200	4.42351300
O	-6.32491400	3.85840800	-1.89776900
O	-7.01486000	1.22488300	-4.45432600
O	3.90036100	5.11656300	2.14966900
O	-8.04062400	3.09094600	-0.04413100
O	-3.86558000	4.57940500	2.48191400

O	-3.86697700	4.49715500	-2.61914500
O	-8.60941000	-0.79196500	0.01867200
O	-8.07453300	-4.83711000	0.08380600
O	-4.51074000	-5.95412100	0.10081100
O	-1.87148900	1.47834500	-4.13846500
O	-1.86924100	1.61125900	4.09683500
O	-0.17180600	-2.01948200	4.86528900
O	8.48911300	4.93449700	-0.07840800
O	4.92538300	6.05159800	-0.09548900
O	9.02396000	0.88944900	-0.01327700
O	0.58647500	2.11686000	-4.85977300
O	1.27598700	4.75062000	-2.30355400
O	0.58903500	2.27275700	4.79574500
O	1.27756300	4.82231900	2.15507000
O	2.28609100	-1.38063500	4.14371300
O	8.45533700	-2.99351200	0.04956600
O	4.28158800	-4.39970400	2.62451900
O	4.28019400	-4.48209000	-2.47648900
O	-3.48612200	-5.01871100	-2.14450100
O	6.73950300	-3.76105100	1.90327900
O	7.42950000	-1.12744100	4.45986800
O	6.73851300	-3.82047300	-1.77742400
O	7.42705500	-1.27073600	-4.41802800
O	-3.48429900	-4.94682700	2.31383800
Si	6.12341500	-2.04052500	-5.03693300
Si	-4.78807100	-5.71727200	1.69524000
Si	8.74060500	-0.99597900	3.49090900
Si	-4.78896900	-5.76861100	-1.49994800
Si	6.12616700	-1.87686900	5.10394400
Si	8.73869600	-1.10808100	-3.45462000
Si	-5.71159500	1.97415500	-5.09859900
Si	5.20369700	5.86598800	1.50559000
Si	2.58771200	4.88185800	-3.27190000
Si	-8.32411200	1.20547200	3.46001900
Si	5.20280100	5.81440500	-1.68984300
Si	-5.70882600	2.13792600	5.04232900
Si	-8.32597200	1.09338500	-3.48542600
Si	2.58923400	4.98516700	3.11864400
O	3.09034000	0.96970900	-4.91987000
O	-7.82118200	-2.70674700	1.81218400
O	-2.67835800	-1.03072700	-4.88597700
O	8.23673200	2.86113400	1.71802700
O	8.23581400	2.80425900	-1.80683900
O	-2.67583600	-0.87223200	4.92535000

O	-7.82213000	-2.76363000	-1.71253300
O	3.09311200	1.12807600	4.89149600
Si	-7.95096700	3.66566200	1.49600400
O	-8.57178800	2.53620300	2.52088100
Si	-5.42033100	4.46859900	-3.16385400
O	-5.50155100	3.48866800	-4.48477700
Si	-2.88409500	5.42278800	1.46420300
O	-1.31778500	5.04049800	1.80025800
Si	-7.95181100	3.61566100	-1.60199600
O	-8.57316300	2.45372900	-2.58962900
Si	-5.41865500	4.56853100	3.02812200
O	-5.49909000	3.63174200	4.37987400
Si	-2.88469900	5.37271400	-1.62962200
O	-1.31884800	4.98014800	-1.95405300
Si	9.11370000	1.46419100	1.52681000
O	8.49292600	0.33475000	2.55177300
O	4.83172100	-1.05261700	-4.77305600
Si	-7.64595800	-4.34704600	1.62320800
O	-6.07990800	-4.72905600	1.95908300
Si	2.21336500	2.35970600	-5.15563800
O	2.83465700	3.52171100	-4.16796600
Si	-8.69819100	-1.31677500	1.57654000
O	-8.07687300	-0.15474800	2.56417100
Si	-2.85358700	0.60276300	-5.12792900
O	-4.41949800	0.99547900	-4.80301900
Si	8.06149800	4.49440900	1.47619900
O	6.49554500	4.88717500	1.80048300
Si	-8.69903800	-1.36677300	-1.52146300
O	-8.07833100	-0.23725100	-2.54628800
Si	2.21611700	2.52488300	5.08263600
O	2.83690200	3.65446100	4.05776600
Si	8.06067200	4.44447700	-1.61777300
O	6.49451300	4.82658400	-1.95364800
Si	-2.85095600	0.76794600	5.11435700
O	-4.41703100	1.15012500	4.77847000
Si	9.11285700	1.41419000	-1.57119000
O	8.49155100	0.25227800	-2.55873700
Si	-1.79876100	-2.26237200	5.16114000
O	-2.42011500	-3.42406600	4.17329900
Si	-7.64683600	-4.39693600	-1.47092000
O	-6.08107800	-4.78981200	-1.79499700
Si	3.26829200	-0.50539200	5.13334600
O	4.83428400	-0.89797100	4.80905900
Si	8.36644300	-3.51825200	1.60748400

O	8.98774800	-2.35633900	2.59502700
Si	5.83325300	-4.47110900	-3.02267600
O	5.91380200	-3.53431400	-4.37444700
Si	8.36559600	-3.56825500	-1.49052200
O	8.98641800	-2.43879800	-2.51539500
Si	5.83493200	-4.37123200	3.16940900
O	5.91616000	-3.39127000	4.49012100
H	-5.95815700	2.35110200	6.47525700
H	-9.50249500	1.08740500	4.33086700
H	-10.12913200	-1.53034300	1.83673300
H	-8.72733400	4.90240600	1.66517100
H	-10.13013200	-1.58861600	-1.77375800
H	-9.50480000	0.94729800	-4.35140800
H	-8.72827100	4.84630700	-1.81061700
H	-8.52260400	-5.09982700	2.53189400
H	-1.87804700	-2.73082800	6.55205400
H	-2.47413500	1.19900400	6.46833200
H	2.89219300	-0.89237000	6.50059100
H	6.37623500	-2.04362500	6.54288700
H	2.29621400	3.03818100	6.45778700
H	6.29941500	-5.70697100	3.57043600
H	9.91948000	-0.84979100	4.35680500
H	9.14290200	-4.74889800	1.81610200
H	9.14192100	-4.80501300	-1.65976200
H	9.91711200	-0.98991300	-4.32540500
H	6.29748000	-5.81917400	-3.38075400
H	6.37271100	-2.25363200	-6.46987900
H	2.88873600	-1.10158200	-6.46285800
H	2.29269200	2.82830300	-6.54662200
H	-2.47773500	0.98972400	-6.49523700
H	-5.96169300	2.14105200	-6.53738700
H	-1.95394100	-6.10157600	-3.91243300
H	3.45364600	-6.77735700	-1.62614100
H	3.45460900	-6.72137900	1.84920600
H	-1.95201400	-5.97196900	4.11567500
H	-4.97645300	-7.11979000	-2.04784400
H	-4.97531900	-7.04981700	2.28645600
H	-8.52398000	-5.17873900	-2.35424200
H	-5.88285200	5.91656300	3.38621500
H	-5.88477400	5.80437300	-3.56497800
H	-3.03900600	6.87475100	1.63163200
H	-3.03996800	6.81865100	-1.84388400
H	2.36868400	6.19891000	3.91794300
H	2.36652600	6.06933700	-4.11011400

H	5.39103600	7.21724200	2.05323100
H	5.38987100	7.14728500	-2.28089100
H	8.93854300	5.27620000	2.35965400
H	8.93724900	5.19735000	-2.52644900
H	10.54478900	1.68601800	1.77916100
H	10.54381700	1.62775800	-1.83127400
H	-1.96748800	-2.90273200	-6.45823700
Si	3.19500400	-0.73624900	-5.09408700
Si	-1.85268400	-2.51789500	-5.09644800
O	2.35731200	-1.54913200	-4.02952600
O	-0.31256200	-2.35256300	-4.71909200
O	-2.58352000	-3.66944200	-4.20706600
Al	0.48651100	-3.91076500	1.65369800
Si	0.50543000	-3.99059500	-1.60065500
Si	3.17160700	-5.34487800	-1.47437700
Si	-2.12619700	-4.93236400	-3.14295200
Si	0.72060300	-1.61185000	-3.50449900
Si	3.14780500	-5.30349300	1.69360300
Si	0.72211400	-1.43593000	3.48474200
Si	-2.08228700	-4.83843900	3.26136800
O	0.55469600	-2.22441600	2.12972800
O	1.72942400	-4.93078400	2.27591100
O	-0.94222600	-4.63471200	2.23047100
O	0.38650400	-3.90171400	-0.05401800
O	3.31097200	-4.95599000	0.08719400
O	1.71576800	-4.95788600	-2.10155800
O	0.64286500	-2.43556000	-2.14903500
O	-0.82859300	-4.57499200	-2.31045300
O	0.20765300	0.10095600	3.22782600
O	0.19880000	-0.07815900	-3.29486200
O	-0.14812900	2.42924700	-2.26612700
O	-0.17262900	2.53517900	2.18674200
O	0.13839300	3.76081100	-0.06519300
Si	-0.28792600	1.60017100	3.48174000
Si	-0.28729000	1.46022100	-3.53324700
Si	-0.01778000	3.91408800	-1.63780000
Si	-0.01551700	3.97771400	1.50330800
C	-4.24316500	-1.05596900	-1.17536200
C	-3.70671600	0.19719800	-1.18507400
C	-3.32157100	0.81783000	0.02217600
C	-3.62585000	0.25079200	1.27501200
C	-4.19268000	-0.98892800	1.34690700
C	-4.29072100	-1.79931800	0.10973800
C	-4.65202000	-1.75533200	-2.42193000

H	-5.60877900	-2.27358400	-2.29112100
H	-4.72710000	-1.06246200	-3.26478600
H	-3.91769400	-2.52583100	-2.68771400
H	-5.15232200	-2.46944500	0.15395600
C	-2.98940400	-2.70515600	0.08947200
H	-2.84186600	-3.19043800	1.05296500
H	-3.15580800	-3.47924000	-0.65879600
H	-2.11434000	-2.09581200	-0.14271800

The transition state forming ethyl precursor (**M2**) via side-chain methylation.

O	-3.35570300	4.94406800	-0.09346500
O	3.85600500	5.05721000	-2.32642300
O	-6.36567500	3.93404300	1.76963700
O	-7.04995300	1.39759800	4.42409700
O	-6.36592800	3.85440900	-1.91069300
O	-7.05061200	1.20550900	-4.45287800
O	3.85627000	5.15365200	2.13144100
O	-8.08057500	3.09391600	-0.05311600
O	-3.90879400	4.60404700	2.46538300
O	-3.90911400	4.49369700	-2.63515000
O	-8.64218600	-0.78963900	0.03094000
O	-8.09984100	-4.83338000	0.11839800
O	-4.53400300	-5.94367400	0.14213500
O	-1.90776400	1.47018100	-4.13748400
O	-1.90717500	1.64834300	4.09678800
O	-0.20315000	-1.97490300	4.88559500
O	8.44573200	4.96784200	-0.09486300
O	4.87994200	6.07823500	-0.11866000
O	8.98805100	0.92421000	-0.00741300
O	0.54909500	2.10935200	-4.86197000
O	1.23371500	4.75838900	-2.31981300
O	0.54974800	2.31828600	4.79256600
O	1.23400100	4.85480800	2.13810900
O	2.25367200	-1.33556800	4.16106900
O	8.42660100	-2.95939200	0.07668000
O	4.25503700	-4.35912600	2.65865200
O	4.25469000	-4.46954700	-2.44180200
O	-3.51060100	-5.01891400	-2.10810400
O	6.71187400	-3.71991100	1.93430800
O	7.39655700	-1.07101300	4.47649400
O	6.71162200	-3.79955500	-1.74601600
O	7.39589800	-1.26310400	-4.40048100
O	-3.50997500	-4.92259600	2.34983900
Si	6.09379000	-2.03869500	-5.01535700
Si	-4.81217900	-5.69840500	1.73531300

Si	8.70758300	-0.94245100	3.50703800
Si	-4.81222700	-5.76755200	-1.45965900
Si	6.09450300	-1.81929900	5.12446900
Si	8.70707000	-1.09273000	-3.43777100
Si	-5.74855700	1.95379400	-5.10085700
Si	5.15832600	5.90194200	1.48346000
Si	2.54480500	4.88681300	-3.28919700
Si	-8.36117100	1.22720700	3.46129800
Si	5.15807300	5.83279500	-1.71164100
Si	-5.74788600	2.17318100	5.03888100
Si	-8.36163600	1.07694700	-3.48342400
Si	2.54524600	5.02509300	3.10089200
O	3.05513000	0.96651900	-4.91532500
O	-7.85072000	-2.69307300	1.83507600
O	-2.71002300	-1.04426400	-4.87140600
O	8.19687900	2.90392000	1.71290100
O	8.19666900	2.82767100	-1.81160000
O	-2.70930500	-0.83195000	4.93892300
O	-7.85096500	-2.76933200	-1.68928800
O	3.05591900	1.17881500	4.89502200
Si	-7.99224300	3.67725200	1.48385300
O	-8.61114900	2.55229600	2.51482000
Si	-5.46229700	4.45924800	-3.17994100
O	-5.54150800	3.47190200	-4.49540700
Si	-2.92842800	5.44334500	1.44325600
O	-1.36167100	5.06606200	1.78147500
Si	-7.99246300	3.61022200	-1.61382800
O	-8.61149700	2.44173200	-2.59515700
Si	-5.46186700	4.59321400	3.01139000
O	-5.54080200	3.66372100	4.36826000
Si	-2.92862800	5.37641300	-1.65039300
O	-1.36195100	4.98481300	-1.97226700
Si	9.07646400	1.50757300	1.52950500
O	8.45760500	0.38263700	2.56056000
O	4.80022500	-1.05173300	-4.75711100
Si	-7.67242700	-4.33404200	1.65513800
O	-6.10572700	-4.71136100	1.99324300
Si	2.17562800	2.35356800	-5.15886800
O	2.79461500	3.52212700	-4.17748500
Si	-8.73026100	-1.30604200	1.59165300
O	-8.11126400	-0.13745600	2.57298200
Si	-2.88809200	0.58737800	-5.12224100
O	-4.45494300	0.97901600	-4.80034800
Si	8.01866400	4.53551300	1.46207000

O	6.45193300	4.92715800	1.78393600
Si	-8.73048700	-1.37307100	-1.50602900
O	-8.11169500	-0.24805000	-2.53694600
Si	2.17631600	2.57503800	5.07834800
O	2.79518900	3.70009800	4.04737100
Si	8.01846000	4.46857800	-1.63158200
O	6.45165400	4.84593000	-1.96980200
Si	-2.88748800	0.80896900	5.11895600
O	-4.45422000	1.18634500	4.78067000
Si	9.07624200	1.44054400	-1.56817400
O	8.45725600	0.27207400	-2.54941900
Si	-1.82972200	-2.21908600	5.18241300
O	-2.44871000	-3.38745200	4.20105100
Si	-7.67268500	-4.40100800	-1.43859200
O	-6.10601800	-4.79256700	-1.76032200
Si	3.23412200	-0.45288700	5.14576600
O	4.80086200	-0.84442100	4.82399100
Si	8.33841000	-3.47572600	1.63744200
O	8.95739600	-2.30725600	2.61868600
Si	5.80777200	-4.45871900	-2.98784200
O	5.88682700	-3.52920600	-4.34470300
Si	8.33818600	-3.54275600	-1.46023900
O	8.95709400	-2.41780300	-2.49120600
Si	5.80821900	-4.32478700	3.20361700
O	5.88740300	-3.33743400	4.51894300
H	-5.99785500	2.39376900	6.47057700
H	-9.53948200	1.11174900	4.33259300
H	-10.16084900	-1.52082400	1.85278400
H	-8.77092600	4.91346800	1.64609300
H	-10.16112300	-1.59894300	-1.75733000
H	-9.54004400	0.92391800	-4.34878100
H	-8.77116300	4.83826300	-1.82933500
H	-8.54783800	-5.08343900	2.56782800
H	-1.90837500	-2.68010700	6.57595900
H	-2.51169200	1.24808500	6.47054600
H	2.85849300	-0.83314200	6.51516100
H	6.34463500	-1.97768200	6.56434600
H	2.25523100	3.09601900	6.45066000
H	6.27509500	-5.65744400	3.61207200
H	9.88603900	-0.78932400	4.37230700
H	9.11711000	-4.70376800	1.85294900
H	9.11682800	-4.77898900	-1.62255500
H	9.88541700	-0.97716700	-4.30900400
H	6.27456500	-5.80785700	-3.33839500

H	6.34372400	-2.25921300	-6.44706800
H	2.85762600	-1.11359200	-6.44694100
H	2.25432400	2.81466000	-6.55240200
H	-2.51265000	0.96762100	-6.49164900
H	-5.99874500	2.11223600	-6.54071800
H	-1.97636700	-6.10847200	-3.86986900
H	3.43222300	-6.76166300	-1.57901300
H	3.43247400	-6.68653900	1.89598100
H	-1.97582100	-5.93470500	4.15738500
H	-4.99718000	-7.12199600	-2.00016500
H	-4.99683600	-7.02823100	2.33361000
H	-8.54823200	-5.18920500	-2.31783300
H	-5.92861900	5.94233100	3.36199600
H	-5.92914400	5.79193500	-3.58847600
H	-3.08622700	6.89612700	1.60262000
H	-3.08643300	6.82093800	-1.87245800
H	2.32229700	6.24287800	3.89348000
H	2.32173900	6.06916500	-4.13374100
H	5.34307300	7.25653000	2.02369600
H	5.34277800	7.16275000	-2.30997600
H	8.89411100	5.32377100	2.34135500
H	8.89379900	5.21806500	-2.54424200
H	10.50709700	1.73343200	1.78086300
H	10.50684800	1.65532800	-1.82919800
H	-1.99524600	-2.92363800	-6.43321300
Si	3.16300100	-0.74014400	-5.08010800
Si	-1.88118900	-2.53118800	-5.07334400
O	2.32662200	-1.54879500	-4.01137400
O	-0.34164200	-2.36094900	-4.69687400
O	-2.61035300	-3.67900300	-4.17796400
Al	0.44656600	-3.91420900	1.68947600
Si	0.46314500	-3.97640800	-1.56892500
Si	3.13912600	-5.33533800	-1.43907200
Si	-2.15847900	-4.93667000	-3.10576500
Si	0.67631900	-1.60566700	-3.49436600
Si	3.13388200	-5.27341200	1.72623500
Si	0.68669600	-1.39466300	3.51657000
Si	-2.12121800	-4.80885400	3.30219900
O	0.55440500	-2.22495800	2.17342400
O	1.71026900	-4.91821300	2.29239900
O	-0.95950700	-4.63892800	2.28454100
O	0.40381100	-3.85611800	-0.01767200
O	3.32650500	-4.89244600	0.11466400
O	1.69070100	-4.94342000	-2.05704500

O	0.56798200	-2.44913700	-2.16366800
O	-0.85855500	-4.61413200	-2.24935300
O	0.16104700	0.13178800	3.21710600
O	0.16862600	-0.06738000	-3.27537000
O	-0.15327100	2.45004400	-2.29144500
O	-0.19563500	2.56921600	2.19280000
O	0.09927000	3.74964000	-0.07452700
Si	-0.33011200	1.63824500	3.49039600
Si	-0.32617800	1.46711600	-3.54353000
Si	-0.05910000	3.93346100	-1.64825600
Si	-0.05942800	4.00912700	1.49285800
C	-4.16930300	-1.05183100	1.27268000
C	-4.13334000	-1.92202300	0.04247400
C	-4.19522700	-1.15261600	-1.25245500
C	-3.68687300	0.08814800	-1.29066600
C	-3.22442300	0.72891200	-0.07476600
C	-3.66399800	0.18950000	1.19676000
C	-2.35122700	1.77601900	-0.12690300
H	-2.16857000	2.25716000	-1.07832400
H	-2.14081300	2.33049800	0.77764900
C	-2.79260800	-2.70445700	0.06556500
H	-2.71526400	-3.37800100	-0.78703600
H	-1.95321600	-2.00816900	0.02650800
H	-2.69167700	-3.30591300	0.96879300
H	-4.95277400	-2.64702900	0.08093300
C	-0.58240800	0.38781400	-0.03506200
H	-0.05130600	1.32000700	-0.08590800
H	-0.84865500	-0.13887200	-0.93799700
H	-0.91143500	0.00715100	0.91899800
O	1.10304900	-0.52258200	0.20696900
H	0.92565800	-1.23216400	0.86475200
H	1.63738200	-0.95196500	-0.49049900
C	-4.75687700	-1.83017600	-2.45750800
H	-5.84348000	-1.94034700	-2.34287900
H	-4.56949600	-1.25435800	-3.36926200
H	-4.34854700	-2.83861700	-2.58490200
C	-4.68962100	-1.64327700	2.53934300
H	-4.51808900	-0.98069800	3.39366500
H	-5.77014300	-1.81572000	2.44893800
H	-4.22837900	-2.61552900	2.74698300
H	-3.58065800	0.82069300	2.07963200
H	-3.62229000	0.64264600	-2.22636700
O	3.17557900	-1.94800700	-0.93613800
H	3.44039800	-2.20389200	-1.82536700

H	3.47159300	-2.66556100	-0.36208600

The transition state forming propyl precursor (**M3**) via side-chain methylation.

O	-3.31939600	4.95269000	-0.13426600
O	3.88738800	5.02666200	-2.38469300
O	-6.32694200	3.96984900	1.74720200
O	-7.00977800	1.46554600	4.43237400
O	-6.33574400	3.84765200	-1.93195000
O	-7.03105800	1.17079600	-4.44176000
O	3.89800900	5.17465900	2.07174500
O	-8.04752800	3.11186700	-0.06182400
O	-3.86726100	4.64331200	2.42958900
O	-3.87942900	4.47397400	-2.66931200
O	-8.61602300	-0.76941100	0.06843200
O	-8.08085100	-4.81286500	0.20144600
O	-4.51699700	-5.92940200	0.22996200
O	-1.88702900	1.42958900	-4.14108500
O	-1.86731300	1.70297900	4.09055200
O	-0.16809800	-1.91404500	4.91737300
O	8.48202900	4.95462600	-0.16263700
O	4.91822300	6.07126000	-0.19121400
O	9.01717500	0.91128000	-0.02963200
O	0.56933000	2.05579300	-4.87847400
O	1.26458000	4.73278700	-2.36869400
O	0.59241000	2.37638200	4.77297200
O	1.27522100	4.88076100	2.08780200
O	2.28822500	-1.28767600	4.17994200
O	8.44884100	-2.97004500	0.10066100
O	4.28064000	-4.33210500	2.70808700
O	4.26844400	-4.50151300	-2.39073500
O	-3.49705300	-5.03262500	-2.03313600
O	6.73697700	-3.70585500	1.97083900
O	7.43229000	-1.02900000	4.48064900
O	6.72817600	-3.82806100	-1.70830700
O	7.41101100	-1.32375300	-4.39348400
O	-3.48607200	-4.88475100	2.42338100
Si	6.10609000	-2.10399500	-4.99639800
Si	-4.79108700	-5.66520700	1.82082100
Si	8.74133100	-0.91408400	3.50680700
Si	-4.79855700	-5.77130400	-1.37312900
Si	6.13035800	-1.76733300	5.14018300
Si	8.72468600	-1.14467900	-3.43577900
Si	-5.72912400	1.90912700	-5.10129700
Si	5.19994300	5.91299600	1.41220500
Si	2.57368500	4.84756600	-3.34246200

Si	-8.32350000	1.28645500	3.47458000
Si	5.19226800	5.80689800	-1.78187300
Si	-5.70489900	2.24577900	5.03519600
Si	-8.34009700	1.05588000	-3.46792000
Si	2.58897000	5.05974600	3.04558200
O	3.07314900	0.90778800	-4.92427100
O	-7.82391000	-2.65331000	1.89267700
O	-2.69554400	-1.09168900	-4.84404700
O	8.23354300	2.91221500	1.66944500
O	8.22514600	2.79520600	-1.85392800
O	-2.67203700	-0.76592000	4.96314200
O	-7.83234200	-2.77032800	-1.63055900
O	3.09672700	1.23354000	4.88293600
Si	-7.95462300	3.71277800	1.46808900
O	-8.57322300	2.60096800	2.51340100
Si	-5.43391300	4.43609800	-3.21015200
O	-5.51792700	3.43375100	-4.51392400
Si	-2.88770400	5.46891700	1.39560400
O	-1.32086900	5.09267500	1.73462100
Si	-7.96203900	3.60992300	-1.62860100
O	-8.58544100	2.43130700	-2.59494100
Si	-5.41910100	4.64166700	2.97919700
O	-5.49663100	3.72807800	4.34690600
Si	-2.89509000	5.36620700	-1.69705500
O	-1.32986900	4.96801400	-2.01792000
Si	9.11016000	1.51221600	1.50022900
O	8.49160800	0.40042800	2.54562800
O	4.81492000	-1.11172200	-4.74666300
Si	-7.64901900	-4.29657700	1.73133500
O	-6.08224200	-4.67285600	2.07023800
Si	2.19562300	2.29355100	-5.18185700
O	2.81897800	3.47223700	-4.21546300
Si	-8.70147500	-1.26756300	1.63521100
O	-8.07811000	-0.08885100	2.60155000
Si	-2.87121100	0.53726900	-5.11334100
O	-4.43660600	0.93550000	-4.79245700
Si	8.05773000	4.54112500	1.40015600
O	6.49245400	4.93936200	1.72101200
Si	-8.70889700	-1.37041700	-1.46147900
O	-8.09041100	-0.25854100	-2.50674200
Si	2.22009100	2.63341400	5.05208400
O	2.83865800	3.74532800	4.00676100
Si	8.05033900	4.43841200	-1.69250600
O	6.48345600	4.81472300	-2.03152400

Si	-2.84681700	0.87729900	5.12457900
O	-4.41362700	1.25363300	4.78549500
Si	9.10274300	1.40936300	-1.59645900
O	8.47938900	0.23076800	-2.56271500
Si	-1.79443000	-2.15177000	5.22067600
O	-2.41778600	-3.33026300	4.25430100
Si	-7.65646400	-4.39932200	-1.36140500
O	-6.09125200	-4.79747200	-1.68212600
Si	3.27252800	-0.39547900	5.15213900
O	4.83781300	-0.79360500	4.83137300
Si	8.36327300	-3.46812800	1.66748800
O	8.98662700	-2.28953300	2.63374400
Si	5.82029300	-4.49987300	-2.94037500
O	5.89794300	-3.58626400	-4.30807600
Si	8.35585400	-3.57098200	-1.42920100
O	8.97445500	-2.45917500	-2.47451300
Si	5.83512200	-4.29433700	3.24910300
O	5.91910900	-3.29198400	4.55273400
H	-5.95119600	2.48337400	6.46480500
H	-9.50002700	1.18326100	4.34981600
H	-10.13185200	-1.47666500	1.90204600
H	-8.73067900	4.95222500	1.61777500
H	-10.14051200	-1.59653500	-1.70691300
H	-9.52075500	0.89503100	-4.32878000
H	-8.73899000	4.83682700	-1.85654000
H	-8.52370800	-5.03374700	2.65461300
H	-1.87074100	-2.59649600	6.61963700
H	-2.46713600	1.33132300	6.47014400
H	2.89933400	-0.75917400	6.52668900
H	6.38348800	-1.90951300	6.58122700
H	2.30308900	3.17008600	6.41809400
H	6.30050000	-5.62304100	3.67189300
H	9.92203700	-0.75313800	4.36757800
H	9.14022400	-4.69503200	1.89542800
H	9.13186800	-4.81044700	-1.57896300
H	9.90124900	-1.04138000	-4.31095400
H	6.28382400	-5.85383600	-3.27635000
H	6.35235200	-2.34152000	-6.42602300
H	2.86835700	-1.18953000	-6.43126500
H	2.27197700	2.73834800	-6.58080700
H	-2.49820500	0.90095200	-6.48790300
H	-5.98231000	2.05136600	-6.54232600
H	-1.96883400	-6.14532200	-3.78564200
H	3.44377300	-6.78197100	-1.49962300

H	3.45209600	-6.66665900	1.97425900
H	-1.94964100	-5.87872000	4.23904200
H	-4.98721200	-7.13156500	-1.89750700
H	-4.97680100	-6.98768100	2.43488100
H	-8.53545200	-5.19601600	-2.22948400
H	-5.88259100	5.99560900	3.31522400
H	-5.89926200	5.76483200	-3.63302300
H	-3.04249000	6.92373500	1.53850400
H	-3.05076900	6.80835600	-1.93546200
H	2.37005100	6.28702800	3.82452800
H	2.35084600	6.02048000	-4.20012400
H	5.38839200	7.27339800	1.93631200
H	5.37803000	7.12949900	-2.39597300
H	8.93661800	5.33788000	2.26827900
H	8.92495700	5.17567200	-2.61575500
H	10.54177300	1.73832200	1.74571900
H	10.53313800	1.61846800	-1.86318600
H	-1.98776200	-2.99032100	-6.38561600
Si	3.17753300	-0.80086300	-5.06953900
Si	-1.86988500	-2.58238000	-5.03064100
O	2.34212400	-1.59555100	-3.98963100
O	-0.32917400	-2.41064400	-4.65965000
O	-2.59909300	-3.71841100	-4.12039300
Al	0.47298800	-3.88836700	1.73775000
Si	0.48395000	-3.99258200	-1.52094100
Si	3.15644400	-5.35135200	-1.37514900
Si	-2.14449400	-4.96661200	-3.03757700
Si	0.69310600	-1.64323100	-3.47015100
Si	3.15446900	-5.25537300	1.79105500
Si	0.72018300	-1.35481000	3.53978300
Si	-2.09361100	-4.76323600	3.37127800
O	0.57848500	-2.19177000	2.20021300
O	1.73463400	-4.88499700	2.35727000
O	-0.93071600	-4.60315500	2.35337000
O	0.41623500	-3.86616400	0.02988700
O	3.33933600	-4.89446100	0.17514400
O	1.71200800	-4.95887500	-2.00153100
O	0.56502200	-2.46598900	-2.12665900
O	-0.83007200	-4.65130200	-2.20100100
O	0.19030000	0.16488400	3.22855800
O	0.19255200	-0.09954400	-3.26759500
O	-0.15031600	2.42193600	-2.29718400
O	-0.10908100	2.58705000	2.17352200
O	0.13586400	3.75480100	-0.10703600

Si	-0.28587400	1.67892900	3.48030300
Si	-0.30495000	1.43243400	-3.54798600
Si	-0.02922300	3.91608100	-1.68138100
Si	-0.01568800	4.02385700	1.46194200
C	-4.37442700	-1.38219400	1.00016800
C	-4.15065700	-2.31518100	-0.16672500
C	-4.27026600	-1.62515100	-1.51186700
C	-3.82894700	-0.36371900	-1.61137600
C	-3.52468900	0.38613300	-0.41944500
C	-4.05152100	-0.09398900	0.84172500
C	-2.76663000	1.51811600	-0.44789600
H	-2.50971900	1.93742300	-1.41813700
C	-2.70642800	-2.85887300	0.00030800
H	-1.98946100	-2.04095500	-0.05382700
H	-2.57768100	-3.36319900	0.95768400
H	-2.45089900	-3.57551800	-0.77254200
H	-4.83663800	-3.16835400	-0.11952900
C	-0.88232600	0.29537500	-0.14223400
H	-0.43146200	1.27192500	-0.16217400
H	-1.03252300	-0.25782600	-1.05479200
H	-1.26322000	-0.09592500	0.78959900
O	0.84915500	-0.47628500	0.18909800
H	0.74558600	-1.14999900	0.90161100
H	1.35310400	-0.94205400	-0.50386400
C	-4.87031700	-2.30517000	-2.69547300
H	-5.95943500	-2.34218600	-2.56742200
H	-4.66194400	-1.75230100	-3.61501800
H	-4.53630800	-3.33558200	-2.81993700
C	-4.76016600	-1.91165900	2.33927400
H	-4.81376300	-1.10913500	3.07923100
H	-5.72737000	-2.42336700	2.31100600
H	-4.03353400	-2.65017700	2.69217500
H	-4.13687000	0.58742200	1.67939700
H	-3.78831900	0.14554400	-2.57435400
O	3.07474300	-1.95192900	-0.79917000
H	3.47514300	-2.13327700	-1.65521300
H	3.36736500	-2.67128500	-0.22580900
C	-2.77381100	2.41875900	0.73722100
H	-2.05268600	3.20711400	0.58246300
H	-3.76036800	2.88881400	0.86311700
H	-2.52219600	1.91455800	1.67073900