H-FER-Catalyzed Conversion of Methanol to Ethanol and Dimethyl Ether: a First-Principles DFT Study

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ABSTRACT

Methanol adsorption and dehydration reactions within zeolites represent important steps in the catalytic conversion process to form long-chain hydrocarbons. Herein, first-principles density functional theory (DFT) is employed in the determination of methanol adsorption and conversion in ferrierite (FER), where we predict the fundamental adsorption geometries and energetics of methanol adsorption. The methanol molecule is shown to physisorb at all explored binding sites, stabilized through hydrogen-bonded interactions with the acid site at O_{meth}—H_{fram} bond distances ranging from 1.33–1.51 Å. We demonstrate that the zeolites' adsorption capability is affected by the silicon/aluminium ratio, with stronger adsorptions predicted in the material with silicon to aluminium fractions of 5 than 8. The adsorption strength is also found to vary depending on the tetrahedral binding site, with the T1O2 site yielding the most stable methanol adsorption structure in the Si/Al ratio = 5 (E_{ads} = –22.5 kcal mol^{-1}), whereas the T1O1 site yields the most stable adsorption geometry (E_{ads} = –19.2 kcal mol^{-1}) in the Si/Al ratio = 8. Upon translational and rotational motion, methanol is protonated resulting in the breaking of its C-O bond to form a methoxy species bound to the framework oxygen (O–CH_3 distance of 1.37 Å), whereas the water molecule is stabilized at the acid site through H-bonding (O_{wat}-H = 2.0 Å). Further reaction between the methoxy species and a second methanol molecule results in the formation of ethanol and protonated dimethyl ether, with adsorption energies of –42 and –25 kcal mol^{-1}, respectively. The results in this study provide atomistic insight into the effect of acidity of the FER zeolite on the adsorption and conversion of methanol.

KEYWORDS

Zeolites, ferrierite, methanol adsorption, acid sites, density functional theory (DFT).

1. Introduction

Methanol is an attractive energy carrier and an abundant resource for the synthesis of important liquid fuels and hydrocarbon products.[1,2] The extensively studied methanol to hydrocarbons process (MTH) is an important step in the promising route to obtaining products that are relevant to the petrochemical industry,[3–5] which is crucial for the 'Methanol Economy' concept. The olefin- and aromatic-cycles are proposed as the central mechanism of methanol conversion, which consists of two catalytic cycles[6] interconverting a range of surface species (hydrocarbon pool). The hydrocarbon pool mechanism can be categorized into two main parts: the olefin cycle which involves the methylation and subsequent cracking of alkenes (both small and large) and the aromatic cycle which is governed by methylation of aromatic compounds with cracking of side chains. The local concentrations of hydrocarbon species within the zeolite dictate the contribution of each cycle.[10]

Earlier reports have shown that the platinum-based catalyst Pt-Re/Al_2O_3 shows great selectivity in the alcohol conversion process with products within the range C_4–C_{12}.[1] Even with a varying yield of 20–50 wt.%, the general implementation in renewable systems is severely limited by the high cost of precious metal catalysts.[7] This has caused interest in the development of more earth-abundant materials as substitutes for precious metal catalysts. Zeolites, also called molecular sieves, are attractive candidates for catalytic applications.[7,8] The three-dimensional (3D) frameworks of zeolites with distinctive molecular-scale features, such as pores, channels and cavities, make them very attractive candidates for methanol conversion catalysis. The channels and cages within zeolites aid distinguishing of molecules of different geometries and sizes.[9] Because of their excellent catalytic activity and high hydrothermal stability under a broad scope of environmental conditions, these aluminosilicate crystals have been utilized in the refining of petrochemical products through ion exchange and adsorption/separation processes.[10–12] The reaction mechanism and product selectivity in zeolites are significantly influenced by the zeolite structure.[13,14] Intermediate formation and hydrocarbon production are shown to be greatly influenced by the acidity of the zeolite.[4,15] For instance, reduced selectivity for light olefin products through coking is promoted by high Brønsted acid concentrations.[16–18] Cleavage of the C-O bond is considered to be the rate-determining step of the overall reaction with some theoretical studies determining its activation barrier to be 72 kcal mol^{-1}.[19]

Methanol conversion to hydrocarbons requires the cleavage of the C-O bond and subsequent formation of C-C bonds, hence the determination of the thermodynamic stabilities of methanol and its dissociated products is of great relevance.[6,20] The activation energy barrier (54 kcal mol^{-1}) for the surface methoxy species formation in FER can be reduced by 10 kcal mol^{-1} when the C-O cleavage occurs near an additional methanol molecule. However, the data are limited to frameworks with a Si/Al ratio of 35 and there is barely any mention of the effect of increased

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acidity.[21] Herein, we investigate the effects of silicon/aluminium ratios (5 and 8) on the methanol adsorption, using first-principles density functional theory (DFT) to elucidate the possible reaction pathways for the methanol C-O bond breaking and C-C bond formation proposed in previous studies. The results obtained give insights, on a molecular level, into the stable adsorption configuration with thermochemical data associated with the dehydrated process when methanol is converted in zeolite H-FER to possible precursors of short-chain hydrocarbons.

2. Computational Details

The optimized structures and energetics were determined from DFT calculations as implemented in the Quantum Espresso package.[22,23] The generalized gradient approximation (GGA) with the Perdew–Burke–Ernzerhof (PBE) exchange-correlation functional was used for geometry optimizations.[24] The kinetic-energy cut-off of the plane–wave was set to 40 Ry and the charge density cut-off to 480 Ry. This ensures that the convergence of the total energy is within 10^{-6} eV and the residual Hellmann–Feynman forces on all relaxed atoms reach 0.01 eV Å^{-1}.[25,26] Due to the very large unit cell of FER (a = 19.0 Å, b = 14.3 Å, c = 7.5 Å),[27] a 1 × 1 × 1 Monkhost-Pack k-point mesh was used for the integration over the Brillouin zone, which was found to be statistically adequate in describing the structural parameters of the zeolite. The lowest-energy adsorption structures and energetics of methanol were determined by adsorbing it at different sites and in different adsorption configurations. The adsorption energy (E_{ads}), which characterized the strength and stability of the adsorbate species in the zeolite framework, was calculated using the relation:

$$E_{ads} = E_{zeo+ads} - (E_{zeo} + E_{ads}) \quad (1)$$

where $E_{zeo+ads}$, E_{zeo}, and E_{ads} are the total adsorption energy of the zeolite with the adsorbate, isolated zeolite framework, and the free adsorbate molecule, respectively. Based on this definition, a negative or positive adsorption energy denotes an exothermic (favourable) or endothermic (unfavourable) process. The visualizations and graphical representation of all structures in this work were obtained using XCRYSDEN[28] and VESTA software[29].

3. Results and Discussion

3.1. Characterization of Ferrierite

All-silica FER was modelled with space group *Immm*, No. 71 with an orthorhombic structure.[30] The initial coordinates (lattice parameters and atomic positions) obtained from the International Zeolite Association (IZA) database were subjected to full geometry optimization to attain the most stable configuration for the structure and lattice parameters such as bond length and angles based on the level of theory. Silicon atoms within the fully optimized FER framework were then substituted for aluminium atoms at the various tetrahedral sites to suit the desired Si/Al ratios of 5 and 8. The distribution of the substituted Al atoms obeyed the Löwenstein's rule,[31] prohibiting Al-O-Al connections and also the Dempsey's rule permitting the maximum allocation of negative charges within the framework.[32] Figure 1 shows the fully optimized all-silica and Al-substituted H-FER. Summarized in Table 1 are the optimized structural parameters including the lattice parameters, interatomic bond distances and angles, which are all in good agreement with known experimental data[33,34] and previous DFT calculations.[35–37]

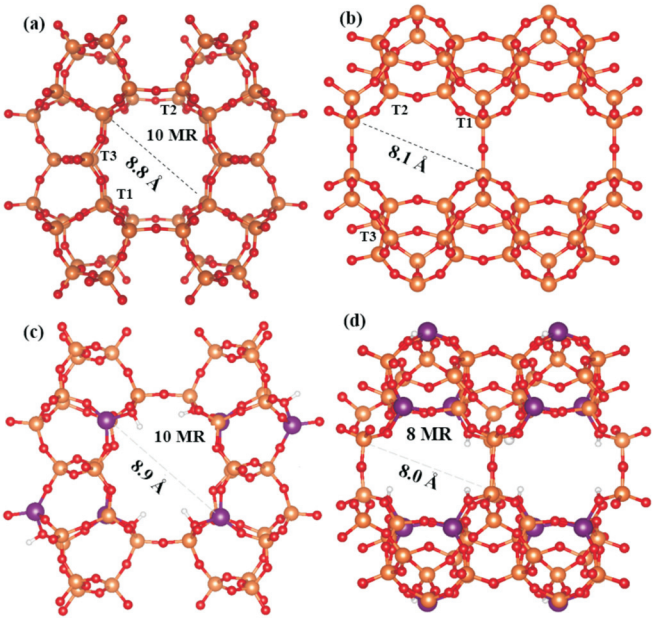

Figure 1 (**a** & **b**) Optimized structures of the purely siliceous ferrierite viewed from the [001] plane and the (**c** & **d**) acidic 10-membered ring channels in the [010] plane and the 8-membered ring channels for the Si/Al = 5 composition. Atomic colour code: Al (purple), H (white), O (red), and Si (orange).

Table 1 The experimentally determined bond distances and angles (in angstrom and degrees) compared to those from the optimization of FER in this work.

Parameters	All-silica	Si/Al = 5	Si/Al = 8	Experiment[30]
Cavity diameter	8.8	8.9	8.6	7.0
Si-O bond lengths	1.61	1.65	1.61	1.61
Al-O bond lengths	–	1.69	1.70	–
Bond angle O-Si-O	108.2	108.4	104.8	109.5
Bond angle Al-O-Si	–	158.6	166.8	–

The charge deficiency created in the Al substituted framework was compensated with H protons at neighbouring oxygen atoms, thereby forming Brønsted acid sites. Two different Si/Al ratios were considered (5 and 8) and the structural parameters in each composition were determined as reported in Table 1. We observed no significant changes in the structural parameters of the Si/Al ratio composition compared to the all-silica FER.

3.2. Methanol Adsorption in Ferrierite

The adsorption and dehydration of a methanol molecule in the zeolite framework is an important starting step in its conversion to safer and more useful renewable fuels. We therefore first determined the lowest-energy adsorption configuration of methanol in the FER framework with Si/Al ratios of 8 and 5, and characterized the extent of C-O bond activation. The preferred methanol adsorption sites within the framework were determined by exploring the T1, T2, and T3 sites in the 10 MR channel of the H-FER zeolite (Fig. 1). The lowest-energy adsorption structures of methanol in the FER framework with ratios of 8 and 5 are shown in Figs. 2 and 3, respectively. The methanol molecule is physisorbed at all explored binding sites where it is stabilized through H-bonding with the acid site at O_{meth}—H_{fram} bond distances ranging from 1.33–1.51 Å. As shown in Table 2, the adsorption energies are found to be generally more stable in the Si/Al ratio of 5 than 8, which can be linked to the high concentra-

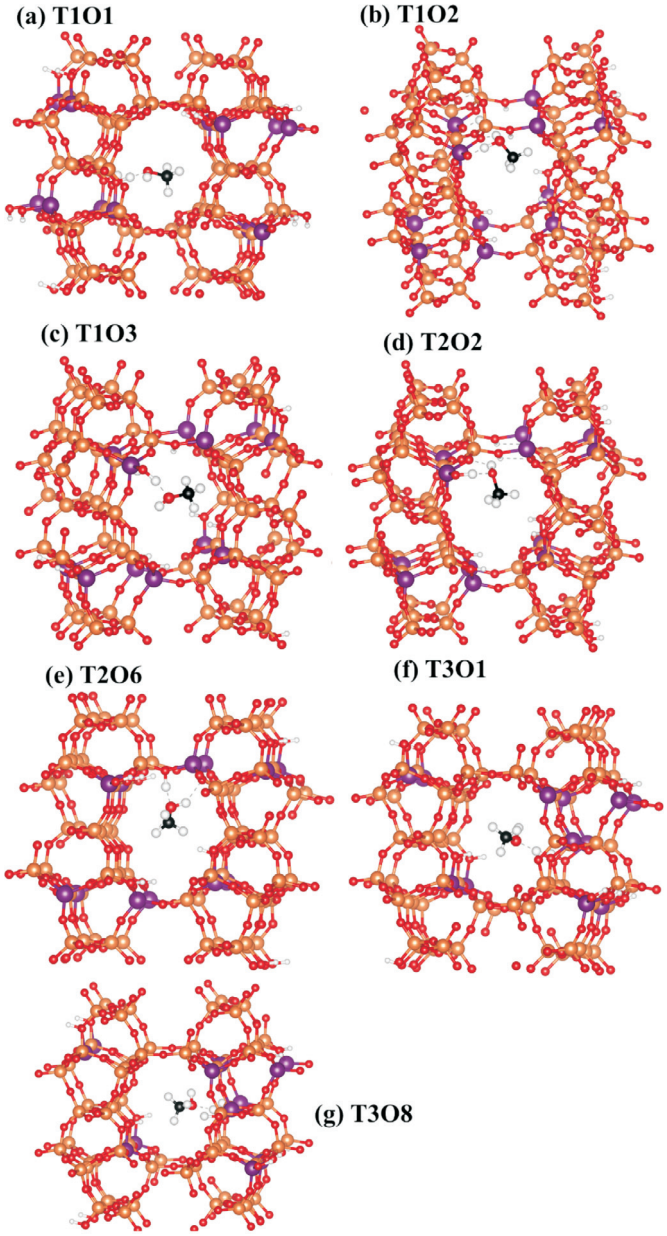

Figure 2 Optimized adsorption structures of methanol in FER with Si/Al of 5. Atomic colour code: Al (purple), C (black), H (white), O (red), Si (orange).

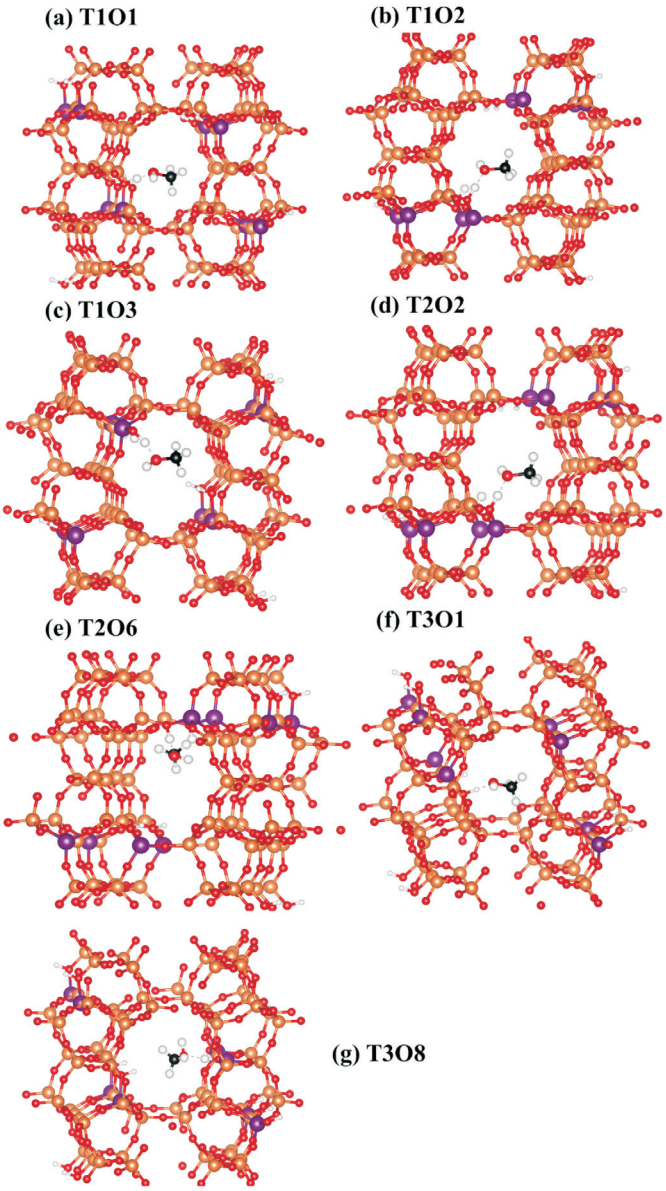

Figure 3 Optimized adsorption structures of methanol in FER with Si/Al of 8. Atomic colour code: Al (purple), C (black), H (white), O (red), Si (orange).

tion of acid sites within the zeolite ratio of 5 that permits the formation of more hydrogen-bonded interactions compared to a ratio of 8. The adsorption strength is found to vary depending on the tetrahedral binding site, with the T1O2 and T1O1 sites yielding the most stable methanol adsorption structure in ratio 5 (E_{ads} = –22.5 kcal mol^{-1}) and 8 (E_{ads} = –19.2 kcal mol^{-1}), respectively. The most stable adsorption structures are characterized by shorter O_{meth}—H_{fram} bond distances as shown in Table 2. The relative energies obtained are in good agreement with previously reported values of 15–27 kcal mol^{-1} in the literature.[38,20]

Table 2 Adsorption energies of methanol at different tetrahedral sites in the FER with Si/Al ratio of 5 and 8.

Tetrahedral sites	Si/Al = 5		Si/Al = 8	
	E_{ads} (kcal mol^{-1})	d(O_{meth}—H_{fram}) Å	E_{ads} (kcal mol^{-1})	d(O_{meth}—H_{fram}) Å
T1O1	–17.1	1.40	–19.2	1.37
T1O2	–22.5	1.33	–10.1	1.47
T1O3	–17.8	1.41	–11.8	1.40
T2O2	–8.8	1.51	–10.3	1.47
T2O6	–16.2	1.41	–12.1	1.35
T3O1	–19.8	1.44	–12.5	1.39
T3O8	–4.7	1.57	3.4	1.55

From the differential charge density isosurface analysis (Fig. 4), we observed electron density accumulation in the O_{meth}—H_{fram} regions, which is consistent with H-bonded interactions.

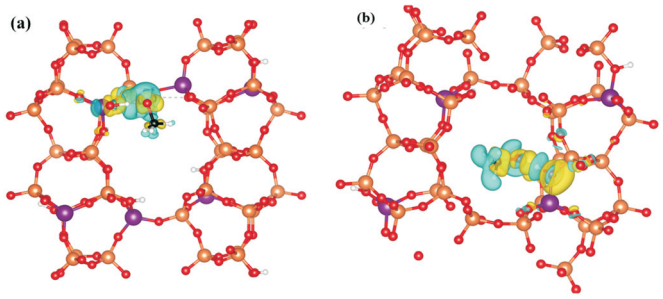

Figure 4 Differential charge density iso-surface contours of the most stable methanol adsorption geometries in FER with Si/Al ratios (**a**) 5 and (**b**) 8. The green and yellow isosurfaces denote accumulation and depletion of electron density by ±0.02 e/Å^3, respectively. Atomic colour code: Al (purple), C (black), H (white), O (red), Si (orange).

3.3. Methanol Dehydration to form Methoxy Species in FER

Protonation of short-chain alcohols in zeolites occurs through geometrical changes owing to a high concentration of charge. The protonation step has been described as a concerted reaction between the O-H bond of the framework and the O-H of methanol, which results in the C-O bond breaking. The protonation process is generally characterized by various translational and rotational motions[39] that leads to the cleavage of the C-O in dehydration. Shown in Fig. 5 is the schematic of the dehydration process of methanol within the FER framework with Si/Al = 5, where the physisorbed methanol attracts a proton at the acid site, reorients such that the –CH_3 end binds at an O-site, followed by the final spontaneous dehydration step. It is worth noting that stable protonated methanol (as observed in Fig. 5b), which was not observed in earlier studies, was obtained after geometry optimization.[40,21] This structure, leading to an adsorption energy of –15 kcal mol^{-1}, is stabilized because of the orientation of the methanol molecule between two close and electro-negatively equivalent framework O2 oxygens (O2 are 2.63 Å apart). The methoxy species is bound at an O–CH_3 distance of 1.37 Å, whereas the water molecule is stabilized at the acid site through H-bonding (O_{wat}-H = 2.0 Å). The co-adsorption of the methoxy species and water molecule releases an energy of 11 kcal mol^{-1}, which compared to the physisorbed methanol molecule, indicates an endothermic reaction. The understanding behind the endothermicity of the methoxy species formation is that breaking a very strong methanol HO-CH_3 bond requires a greater amount of energy compared to forming the weaker framework O-CH_3 and H-bonded H_2O to the framework.

3.4. Post Dehydration Reactions (Ethanol Formation)

The thermodynamic stability of the products formed when a second methanol molecule reacts with the framework methoxy species was also investigated. The incoming methanol molecule can attach to the methoxy species *via* two possible modes: either through its carbon end (forming a C–C bond) or the hydroxyl oxygen (forming an O–C bond). The C–C mode of attachment resulted in the formation of ethanol, which released an energy of 42 kcal mol^{-1}, as clearly illustrated in Fig. 6a. The O–C mode of attachment, on the other hand, resulted in the formation of a stable protonated dimethyl ether species (Fig. 6b), which released an energy of 25 kcal mol^{-1}. The increased stability of the ethanol molecule is a direct result of strong H-bond interaction between the O-H end of the ethanol and the proton of the Brønsted acid sites (O–H = 1.36 Å), which is consistent with the observed electron density accumulation in the interaction regions, as revealed by the differential charge density isosurface contour plot shown in Fig. 7a. A similar observation was made in a previous study, where the product was referred to as an ethoxonium ion.[41] The formation of the ethanol molecule is made possible by hydrogen transfer from the carbon end of the

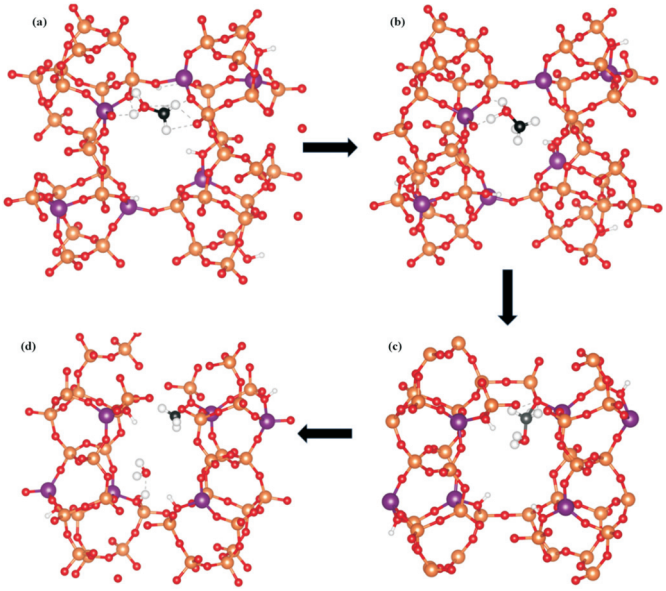

Figure 5 Schematic diagram showing an encounter of the methanol molecule at a Brønsted acid site (conformation before geometry optimization), where (**a**) the methanol molecule attaches to the proton at the acid site, forming (**b**) a methoxonium ion, which appears to be stabilized by two equivalent bridging oxygens. The carbon of the methoxonium ion then forms a C-O bond when brought close to a vacant acid site in (**c**). The H_2O attached to the carbon in the methoxonium system in (**c**) then cleaves off, forming the framework methoxy and 'free' H_2O in (**d**). Atomic colour code: Al (purple), C (black), H (white), O (red), Si (orange).

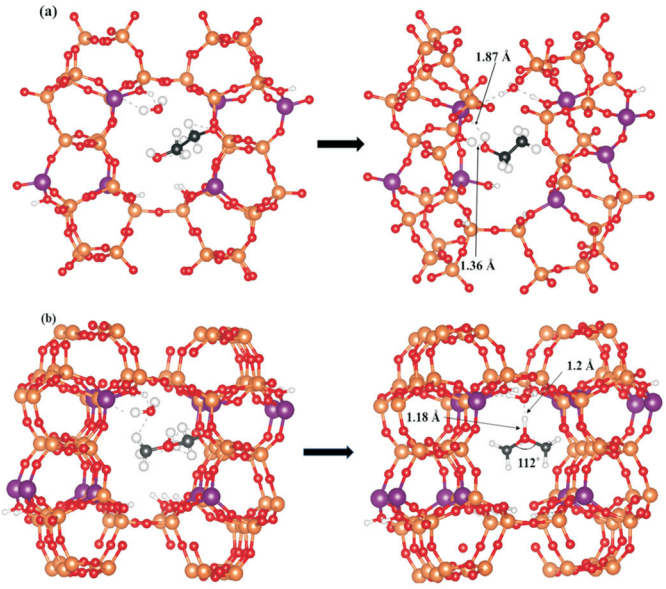

Figure 6 Initial (left) and optimized (right) geometries of ethanol and protonated dimethyl ether species in FER with Si/Al ratio of 5. Atomic colour code: Al (purple), C (black), H (white), O (red), Si (orange).

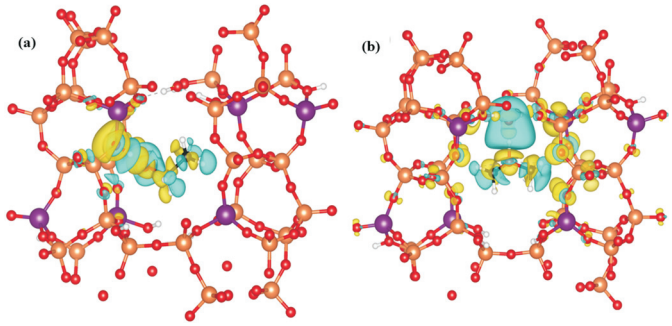

Figure 7 Differential charge density iso-surface contours due to the adsorption of (**a**) ethanol and (**b**) protonated dimethyl ether species in FER with Si/Al ratio of 5. The green and yellow isosurfaces denote accumulation and depletion of electron density by ±0.02 e/Å^3, respectively. Atomic colour code: Al (purple), C (black), H (white), O (red), Si (orange).

incoming methanol molecule to the hydroxyl oxygen end, which finally detaches from the framework O site. Although the protonated dimethyl ether species is lower in thermodynamic stability compared to the formed ethanol, it is known to be the predominant species that is formed in the methanol to gasoline (MTG) process.[42,43] The protonated dimethyl ether is observed in some experiments to form at lower temperatures, but at higher temperatures, it degenerates back to the methoxy species.[33] H-bonding between the proton attached to the dimethyl ether and the water molecule in the channel at 1.2 Å enhances the stabilization of the ion formed (Fig. 7b). An O-H bond distance of 1.18 Å and C-O-C bond angle of 112 ° for dimethyl ether was observed, as can be seen in the optimized structure (Fig. 6b). This result can be attributed to the highly acidic nature of the zeolite and the existence of a water molecule as a product of dehydration in the zeolite. Water molecules are not only speculated to pose as delocalizing agents of protons in the framework, but also facilitate the thermodynamic stability of the products that are formed through H-bonding. It was also observed that the FER pore undergoes a distortion where the T-O-Si bond angle changes by 28° with a corresponding reduction in the pore diameter from 8.9 to 8.3 Å. Since the pore is charge-saturated, the framework oxygens are more likely to cause an elliptical distortion of the channel to better accommodate the ethoxonium, which has been reported previously.[44–46] The adsorbed ethanol molecule could undergo deprotonation and dehydration reactions to produce ethylene, based on the proposed scheme shown in Fig. 8.

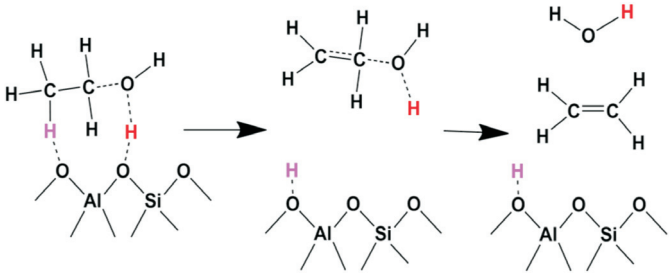

Figure 8 Proposed reaction schematic for the deprotonation and dehydration of ethanol to produce ethylene.

4. Conclusion

The adsorption and conversion reactions of methanol in the FER framework with different Si/Al ratios of 5 and 8, have been studied employing first-principles DFT calculations. Based on predicted adsorption geometries and energetics, it was demonstrated that the methanol molecule is physisorbed at all explored binding sites, where it is stabilized through hydrogen-bonded interactions with the acid site at O_{meth}—H_{fram} bond distances ranging from 1.33–1.51 Å. Stronger adsorption energies were predicted for the FER with Si/Al ratio of 5 than 8, with the most stable adsorption geometries releasing energies of –22.5 and –19.2 kcal mol^{-1}, which suggests that the adsorption strength of methanol is affected by the Si/Al ratio. Protonation of the adsorbed methanol molecule results in translational and rotational motions leading to the breaking of the C-O bond to form methoxy species bound to the framework oxygen (O–CH_3 distance of 1.37 Å), whereas a water molecule is stabilized at the acid site through hydrogen-bonded interactions (O_{wat}-H = 2.0 Å). The formation of stable physisorbed ethanol and protonated dimethyl ether species is demonstrated from further reaction with a second methanol molecule. These results provide atomistic insight into the adsorption geometries and energetics of methanol and its reaction products in the FER zeolite.

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Supplementary Material

The supplementary information contains the optimized atomic coordinates for acidic FER with and without adsorbing species.

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Supplementary material to:

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H-FER-Catalyzed Conversion of Methanol to Ethanol and Dimethyl Ether: a First-Principles DFT Study,

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Supporting Information

H-FER-Catalysed Conversion of Methanol to Ethanol and Dimethyl Ether: A First Principles DFT Study

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Contents

Coordinates for zeolite FER Si/Al =5 Acidic zeolite FER with no methanol				Coordinates for zeolite FER Si/Al =5 Acidic Sites with Methanol adsorbed at various T sites										
					T1O1					T1O2				
O	Si	Al	H	O	Si	Al	H	C	O	Si	Al	H	C	
72	30	6	6	73	30	6	10	1	73	30	6	10	1	
O	6.038347235	1.243893604	2.022031298	O	6.012952763	1.197318219	1.929151818		O	5.805692812	1.257910022	1.941990164		
O	13.070184223	13.173633315	5.798869329	O	13.105723116	13.217485544	5.807890421		O	13.015627564	13.221941822	5.424975587		
O	13.193600083	1.422267511	5.272102671	O	13.108768709	1.481178814	5.174455578		O	13.392913161	1.491902400	5.385129722		
O	12.689418534	13.020600023	1.853759490	O	12.591761151	13.030220560	1.905728536		O	12.700918530	12.958921777	2.149585839		
O	6.255965227	12.978793386	1.883089150	O	6.263581356	12.917709005	1.964930487		O	6.336719467	12.995555625	1.777387398		
O	6.104064790	1.318897538	5.643835833	O	6.060514095	1.357632321	5.622686275		O	6.124696603	1.284015096	5.441048328		
O	6.105835889	13.065715792	5.982422385	O	6.071428387	13.095045883	5.962606780		O	6.409660248	13.021876996	5.781457278		
O	13.021728598	1.287676327	1.908437082	O	12.966850157	1.295452643	1.969330326		O	12.903348524	1.261220029	1.960773475		
O	15.327475530	8.482205416	5.801449547	O	15.422984463	8.398647644	5.684898524		O	15.614004402	8.557693642	5.498896213		
O	3.493400370	5.792432265	1.910992868	O	3.503066225	5.811757453	1.931063732		O	3.284175889	5.966117437	1.922221636		
O	3.699030204	8.375751222	1.795647153	O	3.528830179	8.399132058	1.735287984		O	3.514635663	8.540339505	1.538001133		
O	3.024181287	5.803589101	5.833284868	O	2.959314623	5.811026345	5.793513165		O	2.966353488	5.788732029	5.653849605		
O	15.712695039	5.900491827	5.775947973	O	15.890463275	5.779149028	5.665960023		O	16.007143044	5.986518477	6.172771362		
O	15.770909889	8.538234727	1.695576494	O	15.617050746	8.575776219	1.563305816		O	15.882754395	8.545218914	2.045356247		
O	15.992275881	6.001489993	2.007830416	O	15.715863558	6.029968410	2.121348652		O	15.884548126	5.973145939	1.673353454		
O	3.418188268	8.404922701	5.711911997	O	3.324951596	8.425235506	5.680243231		O	3.519014868	8.364335267	5.501022024		
O	6.774880327	3.579016156	2.908079693	O	6.812126405	3.485888465	2.888270291		O	7.092264611	3.453036979	2.587795387		
O	11.640942141	11.183677740	4.918932096	O	11.765063537	11.261144887	4.751186162		O	11.567684619	11.145858983	4.812397074		
O	11.664876307	3.617197467	4.890732207	O	11.564935672	3.659685821	5.098207510		O	11.853652365	3.628386934	5.154365399		
O	11.380984999	10.701713707	2.310938936	O	11.401960169	10.452643973	2.272692575		O	11.591812095	10.434844847	2.251346502		
O	7.502920434	10.721097714	2.408218128	O	7.491640225	10.626517963	2.372436054		O	7.530313415	10.733196647	2.478392664		
O	7.590005261	3.768006909	5.421347802	O	7.631322514	3.730795611	5.364198580		O	7.473361507	3.771210506	5.228312066		
O	7.614429544	11.010045947	5.278547670	O	7.579093964	11.044641533	5.255356146		O	7.843152160	10.844418877	5.288594214		
O	11.345496439	3.671946100	2.024693926	O	11.549251507	3.517920758	2.210822197		O	11.672562078	3.584426491	2.285268359		
O	16.728397464	10.636317181	6.346343154	O	16.822552202	10.533891081	6.241152959		O	16.624910528	10.859338792	6.349659135		
O	1.839463369	3.784333087	1.329038962	O	1.861659189	3.845697420	1.287971736		O	1.964914605	3.792210841	1.153836932		
O	2.367485637	10.545539281	0.959263934	O	2.322184169	10.669336920	0.985884877		O	2.273332095	10.880089319	1.117373186		
O	2.317737387	3.296914003	6.268028279	O	2.233256508	3.299863629	6.208276367		O	1.875704933	3.412004829	6.032054688		
O	16.697307967	3.523595992	6.416111506	O	16.726318500	3.304800888	6.248690427		O	17.066779696	3.545245154	6.323638738		
O	16.944543029	10.879431119	1.479417304	O	16.905229869	10.857399579	1.389873252		O	17.152562415	10.778703930	1.412010390		
O	17.190163860	3.615837382	1.511698118	O	17.051112293	3.710308914	1.339646797		O	17.214686908	3.688446375	1.443273134		
O	2.122779132	10.995022628	5.894221990	O	2.149564247	11.073420670	5.908422446		O	2.383124266	10.977751550	6.001106110		
O	6.458683374	3.231048815	0.281258769	O	6.530155289	3.217238575	0.262161254		O	6.547708558	3.037661839	0.105745433		
O	12.706917493	11.034836029	-0.186732767	O	12.450142383	11.150957211	-0.227502697		O	12.455379972	11.436012577	-0.236323882		
O	12.107863308	2.764915902	-0.268726376	O	12.267572169	2.641797933	-0.139966460		O	12.627924945	2.861647212	-0.032002978		
O	6.405477367	11.006254935	0.039531044	O	6.372930575	11.036989714	0.029434133		O	6.630198565	11.041739183	0.010961898		
O	16.293229917	9.957399093	3.837231460	O	16.150967655	10.005611011	3.738450062		O	16.230951068	10.480801680	3.792835904		
O	2.688506343	4.126598020	3.805110058	O	2.740699565	4.089353531	3.778239002		O	2.791394230	4.015389255	3.664492662		
O	2.741615447	10.125808836	3.502359498	O	2.696292070	10.166194893	3.507593309		O	2.890177711	10.247900701	3.517015063		
O	15.814909082	3.924173056	3.973784852	O	15.775060324	3.822725184	3.860803045		O	16.180605448	4.439284980	4.001909757		
O	4.347380246	3.266247148	1.900689205	O	4.384038904	3.287947847	1.847130747		O	4.542822154	3.623014445	1.731396341		
O	14.293644178	10.895279235	5.254653640	O	14.317963527	10.860956776	5.446901407		O	14.160373778	10.813774874	5.358671465		
O	14.112241376	3.828756682	5.993830965	O	14.120235186	3.826753703	5.947972518		O	14.451203913	3.860171129	5.934309214		
O	14.336796975	10.742065994	2.153290333	O	14.296731231	10.856094952	1.993613813		O	14.467471784	10.771360549	1.757234087		
O	4.824168884	10.779827326	2.091595710	O	4.807211341	10.714879796	2.085516576		O	4.888807128	10.772980233	1.932139756		
O	4.772802400	3.819462986	5.460059014	O	4.761732035	3.874372767	5.531353380		O	4.525858873	3.633766280	5.665484270		
O	4.980783606	10.732647368	5.282926426	O	4.961292605	10.735560144	5.272943119		O	5.179319399	10.696084034	5.281199980		
O	14.231366174	3.858649466	1.569626989	O	14.143277680	3.670153606	1.520532149		O	14.334458404	3.535648343	1.956079978		
O	2.047876388	1.293265069	0.387923163	O	2.158766780	1.365979975	0.451398435		O	2.508787297	1.434921041	0.146115341		
O	17.193453419	13.009813839	-0.121972015	O	17.029885119	12.962661279	-0.228846014		O	17.234467375	13.103395965	0.104747682		
O	16.936691949	1.280689298	0.313063399	O	16.912942631	1.234245438	0.398897567		O	16.644827796	1.375075504	0.310110911		
O	1.906591481	13.006425316	0.067184099	O	1.814313539	13.107129617	0.047285619		O	1.807654414	13.179216107	-0.146364216		
O	12.110027420	8.766614107	3.971331296	O	12.012441365	8.682949336	4.207621888		O	12.261529395	8.684062949	4.148333406		
O	7.666757842	5.956476476	3.928048806	O	7.556780932	5.932727952	3.847785565		O	7.585733611	5.881789614	3.556822558		
O	7.031022760	8.516655912	4.133597765	O	7.088175272	8.491524264	4.189137449		O	7.072197665	8.419828009	4.096244260		
O	11.336832174	6.202844303	3.623307480	O	11.328646668	6.140722383	3.594930119		O	11.496771977	6.125807542	3.762506074		
O	-0.019114324	2.807105602	-0.270086130	O	-0.027477392	2.717523472	-0.179526768		O	0.035747504	2.349672254	0.040626081		
O	0.024804142	11.131179567	-0.022393302	O	-0.003427519	11.210943325	-0.077482240		O	0.056621830	11.227861395	-0.300446747		
O	9.642268900	9.702560808	4.087930898	O	9.641904212	9.819913992	4.182691954		O	9.738469947	9.466362172	3.909884462		
O	9.329651318	4.004235197	3.400943334	O	9.345812138	4.051368565	3.326125634		O	9.469992806	4.027013141	3.449098242		
O	3.875777333	-0.254676145	1.446515981	O	3.893073069	-0.363330325	1.394953393		O	3.838614130	-0.463040452	1.373539088		
O	15.428720545	0.123877391	6.010690076	O	15.373438511	0.287030696	6.019351423		O	15.494545384	-0.117957195	5.964586319		
O	15.015374890	-0.388325212	1.066178098	O	14.914115799	-0.382207759	1.030928184		O	14.806851735	-0.429149652	0.937948330		
O	3.813105878	0.074862876	6.324199673	O	3.768138911	0.092932595	6.284970620		O	4.013500924	-0.204083476	6.250359422		
O	13.232335126	6.840556452	5.350093763	O	13.488534074	6.678319387	5.013684421		O	13.663249061	6.737929595	5.188013243		
O	5.908071268	6.933623015	2.266212592	O	5.831652022	7.105874386	2.245392615		O	5.684775015	7.118288705	2.235154857		
O	5.302413307	6.668576403	4.857777321	O	5.216170426	6.726505459	4.805550487		O	5.367565661	6.524962362	4.832194244		
O	13.704946556	7.068827013	2.757724785	O	13.383711392	7.318080550	2.409215956		O	13.650421416	7.064430663	2.556884446		
O	4.822412049	-0.251146677	3.889307081	O	4.782526487	-0.202119445	3.862455010		O	4.854676616	-0.414396022	3.797358379		
O	14.396545628	-0.257791462	3.630823826	O	14.394640962	-0.234837837	3.628961052		O	14.583770908	-0.034007790	3.559160272		
O	14.255354236	6.986740195	0.181292018	O	14.321496065	6.844772288	-0.006653173		O	14.405973455	7.540494308	0.068204833		
O	4.846318038	6.917215011	-0.116362270	O	4.757431633	6.959291201	-0.142545547		O	4.694394557	6.868403595	-0.172504526		
Si	5.891926653	2.831534866	1.732959320	O	17.673124471	6.803701660	3.449053696		O	8.977735653	3.203986273	7.453859621		
Si	12.917968350	11.536331182	5.859064527	Si	5.916723474	2.797389320	1.686318696		Si	5.931854863	2.835451628	1.639486210		
Si	6.286343527	11.371356471	1.626029379	Si	12.909470822	11.587722429	5.851717840		Si	12.805956340	11.625182408	5.764564092		

Si	6.161159744	11.461161901	6.054090790	Si	6.270808083	11.319905778	1.632558530	Si	6.382525861	11.367725146	1.588868965
Si	12.820507807	2.922265664	5.733358707	Si	6.133238383	11.487310918	6.042307703	Si	6.399287163	11.418308874	6.002568774
Si	15.614255846	4.282947266	5.504941100	Si	12.765679457	2.923627024	5.881203082	Si	13.084822006	2.992766889	5.965473159
Si	15.783940788	10.076679066	2.291784329	Si	15.626275451	4.146904809	5.410559758	Si	15.930502824	4.436873173	5.572713330
Si	1.546296536	2.802954456	0.054456065	Si	15.694283565	10.102040271	2.177772835	Si	15.878550796	10.182818263	2.235819220
Si	17.450614801	11.412577920	0.031370739	Si	1.548550391	2.816468001	0.053082365	Si	1.587675592	2.758247975	-0.051837860
Si	17.434289311	2.829095938	0.139157571	Si	17.408374321	11.392493616	-0.056032771	Si	17.508146821	11.496199819	0.001869858
Si	1.596451104	11.436971052	-0.201040901	Si	17.394391815	2.772475059	0.091981367	Si	17.489694916	2.771419437	0.156183893
Si	11.164737929	10.086871357	3.788134632	Si	1.565634291	11.523701635	-0.211805966	Si	1.636566526	11.558536931	-0.251907699
Si	7.772997023	4.371470781	3.839990517	Si	11.185613414	10.042560909	3.816768579	Si	11.264336602	9.916562287	3.741092548
Si	5.231476596	-0.138814358	2.322543344	Si	7.768602086	4.362905414	3.792925886	Si	7.818465555	4.310025386	3.759094310
Si	14.030159005	0.025204182	5.191472464	Si	5.224979886	-0.178987509	2.301002163	Si	5.199362871	-0.230541725	2.227693450
Si	13.847419906	-0.043704565	2.121921022	Si	13.988218624	0.118765182	5.179155388	Si	14.116255072	0.077399391	5.124654415
Si	5.196458970	0.014462185	5.454425256	Si	13.796906114	-0.065745320	2.140226403	Si	13.813935786	-0.042649528	2.142866159
Si	14.633636228	7.060087743	6.138897289	Si	5.163657426	0.047155818	5.430613227	Si	5.350542891	-0.108895441	5.324680700
Si	4.492271678	6.984249794	1.457925669	Si	14.769670023	6.943187498	5.970021316	Si	14.922909846	7.209530197	6.090219060
Si	4.130070323	6.994466548	5.949196716	Si	4.418306408	7.052438360	1.435082168	Si	4.308689635	7.111363914	1.377533124
Si	14.849336141	7.215105424	1.654302778	Si	4.054204679	7.019237370	5.915728090	Si	4.128875865	6.922484276	5.828379169
Si	2.922378431	-0.037107353	0.146779182	Si	14.716493087	7.232334437	1.509884075	Si	14.891308672	7.356980533	1.596702109
Si	16.144776591	-0.058349749	-0.074400968	Si	2.921770935	-0.015840212	0.134789157	Si	3.038676445	-0.076355441	0.000838708
Si	12.545319631	7.223614773	3.918094054	Si	16.067610385	-0.046484930	-0.086425281	Si	16.072760228	-0.078611556	-0.057007889
Si	3.458828524	9.952749662	1.962982263	Si	12.519406904	7.206220046	3.804489663	Si	12.717118155	7.152684703	3.917658504
Si	3.090573427	4.249293936	2.247409555	Si	3.388784090	9.984957092	1.957322905	Si	3.435332692	10.100992147	1.908648311
Si	6.453277453	7.085516669	3.804912061	Si	3.125716648	4.255522205	2.219794293	Si	3.125547015	4.356583011	2.127237205
Si	3.225548368	4.254444955	5.340916010	Si	6.403165368	7.128176304	3.782950984	Si	6.419088089	7.031325686	3.698205319
Si	15.640595864	10.000922438	5.325685218	Si	3.206677349	4.253808430	5.334803851	Si	3.075105310	4.203173972	5.261410232
Al	7.986413285	9.888955598	3.817938934	Si	15.647689288	9.958975459	5.279447377	Si	15.641379959	10.173364912	5.268489499
Al	11.164062414	4.508497017	3.507977540	Si	12.773488675	2.842450171	1.397048869	Si	12.924193395	2.874692525	1.560636669
Al	3.399679654	10.043112166	5.256047975	Al	7.992939904	9.891249813	3.833375186	Al	8.075900580	9.756580084	3.777505139
Al	15.744866278	4.148821573	2.286984160	Al	11.201750177	4.438415562	3.621756091	Al	11.312582776	4.424769882	3.746297711
Al	12.814286916	11.182831703	1.499602451	Al	3.370900373	10.071269723	5.244948560	Al	3.586722971	10.036762259	5.230451673
Al	6.043600614	2.936767971	6.165226084	Al	15.639404199	4.181233667	2.198330560	Al	15.854163577	4.214702277	2.353721826
Al	12.812199203	2.947098356	1.461657429	Al	12.707724629	11.187486121	1.450498466	Al	12.848392755	11.217480538	1.401073136
H	8.431730780	11.182918702	5.786430539	Al	6.067139728	2.975104682	6.154884512	Al	6.059015778	2.939360641	5.886015664
H	9.557039414	3.445536261	2.600536528	H	8.412551632	11.221967081	5.738693593	H	8.657846394	10.940250625	5.822150080
H	1.837808435	10.507371759	3.520892523	H	9.476669175	3.410458084	2.585797813	H	9.634252871	3.596633409	2.572766929
H	16.921817382	6.253927060	1.840479212	H	1.818133075	10.601172321	3.530266385	H	2.011675240	10.676239493	3.595415301
H	11.776705361	13.265437988	2.099619857	H	16.577843742	6.395457904	2.667042299	H	16.703060750	6.032614322	1.136922941
H	8.026817321	4.277235046	6.135575930	H	11.684233432	13.379987032	1.987649133	H	12.005676980	12.991127840	2.838244042
H	11.241578349	3.217393190	-0.189208264	H	8.328236086	3.945560499	6.018795785	H	8.917743105	3.614993689	6.553984626
				H	17.534558393	6.442334289	4.351852493	H	7.656658724	3.143254165	7.655222899
				H	19.754875885	6.872744564	3.671655325	H	9.258737159	1.320870186	8.248097344
				H	19.114176916	7.084146674	2.012464871	H	10.493011937	1.799644175	7.056339810
				H	19.133717174	5.443716142	2.752088884	H	8.835426037	1.329823824	6.503201750
				C	19.008100532	6.518692374	2.947604896	C	9.426791625	1.821434754	7.288796797

Coordinates for zeolite FER Si/Al =5
Acidic Sites with Methanol adsorbed at various T sites

	T1O3				**T2O2**				**T2O6**		
O	Si	Al	H	C	O	Si	Al	H	C	O	Si	Al	H	C
73	30	6	10	1	73	30	6	10	1	73	30	6	10	1
O	5.513025804	1.453898386	2.191847094		O	5.804171362	1.202858745	1.965362289		O	5.922808126	1.348720771	1.982388906	
O	12.952751666	13.214139186	5.761268600		O	13.067481045	12.976490970	5.713501933		O	12.981537411	13.375528986	5.690299366	
O	13.148763265	1.471384485	5.205066014		O	13.247374669	1.237704869	5.224408540		O	13.253700772	1.636477121	5.174207529	
O	12.567611236	12.995602806	1.994310093		O	12.731910601	12.982471825	1.868646467		O	12.657862728	13.091545512	1.954144193	
O	6.185282291	13.219002658	1.859120388		O	6.259310169	12.924919389	1.923969064		O	6.353274112	13.078466139	1.902914279	
O	5.990246666	1.330502770	5.612532844		O	6.112223895	1.036492065	5.618822027		O	6.002246620	1.392979672	5.692816486	
O	6.250227850	13.099964053	5.960098021		O	5.649760934	12.828653067	6.085338909		O	6.202169973	13.137109286	5.913405634	
O	13.038780810	1.279242593	2.007653392		O	13.221741488	1.207355702	2.061726909		O	13.089710586	1.368002745	1.958740005	
O	15.325956538	8.466781823	5.679515607		O	15.577282555	8.387526538	5.736141216		O	15.357895157	8.635861293	5.647434984	
O	3.119904286	6.082503077	2.035279418		O	3.346749204	5.876012283	2.024829969		O	3.387775103	5.992191986	1.982430656	
O	3.599958919	8.640065836	1.696486789		O	3.601246372	8.455240961	1.718834515		O	3.636543660	8.563580131	1.678968740	
O	2.875198502	5.839992766	5.609486205		O	3.033849565	5.521495491	5.745051941		O	2.939158264	5.887304685	5.708405678	
O	15.796019916	5.872909909	5.984006178		O	15.602728812	5.795348113	5.890240648		O	15.882492782	6.041346985	5.969902332	
O	15.752441605	8.575716035	1.768331137		O	15.734792715	8.445376709	1.908207548		O	15.875809934	8.693384538	1.733889697	
O	15.875364982	6.001810582	1.890865212		O	15.947303575	5.866981953	1.757709410		O	15.962331511	6.117400252	1.847721975	
O	3.299208614	8.441141546	5.696262062		O	3.087823014	8.114109848	5.615266489		O	3.438560621	8.473224746	5.666849026	
O	6.830011039	3.686685628	2.713028362		O	6.963872915	3.495417284	2.641245769		O	6.955306390	3.643609640	2.849016124	
O	11.626826325	11.151115950	4.847504872		O	12.091216709	10.648006132	4.861749069		O	11.680297489	11.302350593	4.789820141	
O	11.587597624	3.600679604	5.142619750		O	11.463836720	3.184311537	5.108497298		O	11.793319500	3.846443385	5.131380416	
O	11.346623583	10.491520922	2.303221626		O	11.249372266	10.710654422	2.377379675		O	11.396040241	10.614622538	2.258519580	
O	7.456801976	11.013019837	2.609337877		O	7.622802296	10.698673555	2.486922204		O	7.540915914	10.796488587	2.457135486	
O	7.458626296	3.760199384	5.312315674		O	7.640601080	3.499818990	5.252470624		O	7.500122758	3.858040323	5.430744491	
O	7.616665045	10.876931038	5.448847964		O	7.359726354	11.048424315	5.247343751		O	7.676569378	11.019383521	5.325440497	
O	11.576725577	3.477536971	2.259277127		O	11.647868497	3.325503069	2.216753246		O	11.711899007	3.543798719	2.319646912	

O	16.700941489	10.591043967	6.384058081	O	17.165302677	10.432765759	6.287197737	O	16.744976587	10.774406787	6.324273542
O	1.814206839	3.924112624	1.201606556	O	1.899597779	3.835916535	1.143605398	O	1.921833002	3.917164392	1.245429330
O	2.273212445	10.927815026	1.200074940	O	2.593308771	10.846361752	1.093266940	O	2.335380045	10.832913635	1.103561970
O	1.930421642	3.416468483	6.060276349	O	2.277802374	3.042651811	6.103369686	O	1.967680490	3.454096073	6.116010628
O	16.769145504	3.407211972	6.362557384	O	16.552954075	3.362577110	6.385036639	O	16.959769162	3.607655973	6.348560566
O	16.877926739	10.952094795	1.488152715	O	16.675073386	10.835845486	1.363518149	O	16.909312903	11.118941409	1.433784590
O	17.136512891	3.679168977	1.463323355	O	17.161268037	3.507019916	1.456017195	O	17.214330530	3.795434073	1.470797327
O	2.197603343	11.103684868	6.085745841	O	1.916720288	10.749017673	6.055900071	O	2.231130183	11.108399354	6.010462016
O	6.563472583	2.891111983	0.248541885	O	6.633819309	2.985985051	0.143292024	O	6.671876487	3.211531730	0.282587867
O	12.472878769	11.157361688	-0.181933851	O	12.562207459	11.001874914	-0.130716883	O	12.521388585	11.301686987	-0.242920030
O	12.402767085	2.636309379	-0.080300426	O	12.417974118	2.397686698	-0.094685858	O	12.458257665	2.776876905	-0.094197755
O	6.422136592	11.136838698	0.185837818	O	6.339615914	10.883148826	0.164784875	O	6.465836647	11.123355821	0.071044084
O	16.203511374	10.133575364	3.843466671	O	16.295956947	10.105270402	3.840894255	O	16.250896514	10.277880286	3.791702631
O	2.913304078	3.977220447	3.675061022	O	2.844098576	3.839457333	3.656193840	O	2.894790057	4.067618497	3.742444058
O	2.726566617	10.254478615	3.630481378	O	2.701018847	10.109151540	3.591084148	O	2.780086381	10.241831898	3.565226839
O	15.901460603	4.097456595	3.984445958	O	15.820405391	4.002205206	3.931260305	O	15.939820135	4.248735365	3.990803446
O	4.437600620	3.836757902	1.512150219	O	4.480620196	3.512069776	1.574188859	O	4.510261908	3.598392145	1.692048660
O	14.244675023	10.923297084	5.397670835	O	14.618116390	10.886397347	5.740459324	O	14.300126297	11.103130997	5.341608633
O	14.159916707	3.820505509	5.955010202	O	13.970357941	3.750195262	5.801982660	O	14.337173741	3.908408130	6.065878937
O	14.253018666	10.745705763	2.077253549	O	14.173393235	10.591509201	2.256202926	O	14.299598623	10.818215458	1.995774892
O	4.784452910	10.988695776	2.210737823	O	4.945594160	10.684375591	2.385857672	O	4.858652661	10.897028160	2.122332963
O	4.567085127	3.794664262	5.774060692	O	4.799540128	3.557106949	5.432863627	O	4.593756677	3.825274553	5.808034465
O	4.978958206	10.770418280	5.453552232	O	4.790824643	10.344091766	5.595038292	O	5.034231433	10.802615861	5.325445906
O	14.204764290	3.663794912	1.678690691	O	14.252349222	3.584604792	1.521730241	O	14.312133963	3.748340569	1.650984787
O	2.343892767	1.511360917	0.322076939	O	2.020595717	1.285132073	0.507478069	O	2.411269828	1.501173606	0.344445985
O	17.112254760	13.033594395	-0.141828465	O	17.279374802	12.882583716	-0.179956673	O	17.224434774	13.198381742	-0.188094662
O	16.703117325	1.283580705	0.463374362	O	17.015094876	1.152793567	0.268826863	O	16.701618994	1.448692587	0.418490723
O	1.644941718	13.241524893	0.039342781	O	1.750129892	13.033890336	-0.115517957	O	1.773897691	13.218836981	0.067494514
O	12.013077279	8.637372484	4.118744744	O	11.788584248	8.396035319	3.507881583	O	12.142662864	8.791367437	4.078465354
O	7.534047744	6.008827035	3.821247884	O	7.534405550	5.811696922	3.854437828	O	7.665802416	6.023583754	3.819199888
O	6.899095200	8.581048730	3.993295836	O	7.096442159	8.412583662	4.145103336	O	7.036969920	8.559973200	4.125173743
O	11.362700574	6.063521546	3.621284389	O	11.504727275	5.781943589	3.784320061	O	11.439499691	6.226410360	3.538088053
O	-0.057162954	2.502653932	-0.058381940	O	-0.041534336	2.789384281	-0.330781918	O	0.014137379	2.511101278	0.014805640
O	-0.028150306	11.187219699	-0.032172703	O	0.075359554	11.058309258	0.432046173	O	0.022070873	11.263234822	-0.063638373
O	9.575398554	9.663812735	4.122567495	O	9.650408511	9.780425958	4.314922418	O	9.680286790	9.734669708	4.117585044
O	9.300468844	4.076964665	3.373155307	O	9.378803277	3.959966191	3.277244994	O	9.419827264	4.039908997	3.584321904
O	3.657654237	-0.373271311	1.559558617	O	3.820157350	-0.459771728	1.320585071	O	3.925357731	-0.349619723	1.375819511
O	15.327132683	0.147413452	6.058076507	O	15.446402596	-0.037766336	6.038266404	O	15.392251107	0.250830162	6.012358057
O	14.863241939	-0.528304451	1.051163542	O	15.121173116	-0.519164004	1.083921370	O	14.957961096	-0.418835853	1.018270995
O	3.851176817	-0.131107654	6.430910701	O	3.627663574	0.188387250	6.232578422	O	3.792013759	-0.070390799	6.238586445
O	13.341518270	6.694186991	5.273438607	O	13.263670440	7.079001887	5.295213645	O	13.409883682	6.816891263	5.242220700
O	5.621543527	6.990390809	2.302309990	O	5.777391051	6.976039849	2.274517328	O	5.824334088	7.091503390	2.249615317
O	5.252996195	6.728791596	4.936368684	O	5.241084878	6.662148619	4.865181512	O	5.295984580	6.688074650	4.835481814
O	13.629305368	7.111633983	2.700722102	O	13.723551143	6.770794405	2.722622521	O	13.745120437	7.241167160	2.680013391
O	4.703184423	-0.358008331	3.964360351	O	4.694626633	-0.353805939	3.837297074	O	4.835072662	-0.186926709	3.850255929
O	14.401011316	-0.282555878	3.665119662	O	14.533155930	-0.462043291	3.655089285	O	14.470945761	-0.161827800	3.621739514
O	14.197774226	7.153998124	0.140621174	O	14.218192528	7.170482873	0.146149551	O	14.274622356	7.303416051	0.113132070
O	4.526555332	6.887200048	-0.086282403	O	4.638836276	6.841787573	-0.117140273	O	4.734614188	6.941319429	-0.132475994
O	8.256757549	1.073452213	0.135315761	O	8.583880939	13.271481208	4.992819687	O	9.823146955	1.697354749	2.844302778
Si	5.775826097	2.975608791	1.723565902	Si	5.894196785	2.776641017	1.680582408	Si	5.963781293	2.941556704	1.808783334
Si	12.821868589	11.574674530	5.863186293	Si	13.061421193	11.338526267	5.936836410	Si	12.868956052	11.734900614	5.806512894
Si	6.249516021	11.580150487	1.747968885	Si	6.349523063	11.283260119	1.742678143	Si	6.338578700	11.457345071	1.662212919
Si	6.200347406	11.487401788	6.169026704	Si	5.964829613	11.245524201	6.173172876	Si	6.229423885	11.532302587	6.070391530
Si	12.817540284	2.915837041	5.915331406	Si	12.769761222	2.658139711	5.884554224	Si	12.949976767	3.077888538	5.922888203
Si	15.666578177	4.279495734	5.547337674	Si	15.500384373	4.204255108	5.479423611	Si	15.792721065	4.435504160	5.565396891
Si	15.718645743	10.142266414	2.291876490	Si	15.669348148	10.033071775	2.342343483	Si	15.781092881	10.266056257	2.235742504
Si	1.502649164	2.862333421	-0.012250008	Si	1.532228480	2.749831628	-0.030313015	Si	1.576130681	2.863183947	0.036896505
Si	17.395347082	11.440373193	0.032223649	Si	17.525342958	11.295012814	0.076285198	Si	17.457412888	11.591998593	-0.016422246
Si	17.377891349	2.751327963	0.179048613	Si	17.404595967	2.729376526	0.073893660	Si	17.462185057	2.879550479	0.179136204
Si	1.523479020	11.616270795	-0.101068544	Si	1.574303032	11.414450106	-0.068266772	Si	1.593973557	11.609917001	-0.151797027
Si	11.119018596	9.969691104	3.814810555	Si	11.151219984	9.881802722	3.764684283	Si	11.202587138	10.094385563	3.776235729
Si	7.700681631	4.411011572	3.880462827	Si	7.798549650	4.233113697	3.843295271	Si	7.846848758	4.434324045	3.981974891
Si	5.011823609	-0.081999288	2.400054898	Si	5.119872588	-0.267619696	2.269799185	Si	5.239399558	-0.104425224	2.288220909
Si	13.948963164	0.067698730	5.202463100	Si	14.065661133	-0.151980545	5.193724606	Si	14.015678663	0.208911835	5.153966548
Si	13.793356462	-0.115829852	2.180843349	Si	13.985576394	-0.189709035	2.168086851	Si	13.873375196	-0.015712706	2.133884191
Si	5.175774759	-0.038578004	5.491195686	Si	5.018394927	-0.129068855	5.433124962	Si	5.202489409	0.037548422	5.425355035
Si	14.673003226	7.049241801	6.122673133	Si	14.659105661	7.100242204	6.113626877	Si	14.737553566	7.201673782	6.090571191
Si	4.233686758	7.142553492	1.478438963	Si	4.362231000	7.026869645	1.466776178	Si	4.413323221	7.136376128	1.440027794
Si	3.977664884	7.008403827	5.915255968	Si	3.996758330	6.828191545	5.906290617	Si	4.095568326	7.032538232	5.895447337
Si	14.786500043	7.290991203	1.626291536	Si	14.825957533	7.147371626	1.632333579	Si	14.889467728	7.421539907	1.590856372
Si	2.866679258	-0.001109359	0.180910672	Si	2.813047906	-0.063331884	0.087174127	Si	2.971762448	0.011710271	0.100836989
Si	16.017420404	-0.081592154	-0.032801690	Si	16.223106825	-0.196443074	-0.089447726	Si	16.089778900	0.051851900	-0.078130631
Si	12.525772159	7.121630385	3.925438170	Si	12.525562175	7.006786788	3.838055330	Si	12.617509259	7.262555206	3.881649989
Si	3.400254826	10.188335331	2.065040240	Si	3.518597586	10.013611398	2.093554696	Si	3.456356591	10.124764200	2.001204930
Si	3.035509273	4.453993276	2.132014360	Si	3.112693039	4.271094289	2.123946500	Si	3.153538674	4.396834406	2.185196143

Si	6.323217771	7.119743101	3.781359741	Si	6.411927349	7.024651059	3.800437468	Si	6.449353778	7.130798242	3.774597634
Si	3.100037554	4.249584937	5.286713116	Si	3.262511925	3.992007652	5.236163558	Si	3.127279800	4.300169376	5.347269524
Si	15.592775482	10.031911470	5.341468910	Si	15.886742631	9.947536119	5.400256177	Si	15.637507687	10.196293384	5.290506072
Si	12.837017743	2.841094808	1.477711188	Si	12.908815998	2.705523317	1.426673195	Si	12.938823754	2.947115082	1.452002186
Al	7.924416824	9.927910691	3.856088764	Al	7.990661103	9.860334984	3.959544030	Al	8.021906304	9.914570166	3.845038442
Al	11.143280634	4.364418369	3.676536429	Al	11.214658232	4.110358624	3.689006509	Al	11.213792977	4.529405794	3.668533703
Al	3.387509646	10.105559642	5.370450818	Al	3.177140858	9.796460889	5.374307635	Al	3.449282021	10.130163796	5.303026352
Al	15.721499655	4.170184644	2.304798895	Al	15.737268673	4.061590132	2.241414341	Al	15.799553563	4.291399555	2.305849692
Al	12.695533218	11.166741680	1.497673122	Al	12.693995878	11.118191492	1.554458036	Al	12.745517144	11.266126353	1.435297905
Al	6.058064180	3.008476869	6.017149543	Al	6.210947890	2.719803983	5.863158123	Al	6.089460139	3.059320374	6.037369706
H	8.428568317	10.870954700	5.995725649	H	7.901558689	11.936663304	5.166787690	H	8.483015266	11.111919679	5.870134504
H	9.327022014	3.589035756	2.520909599	H	9.430261943	3.442547260	2.445177054	H	9.477726285	3.000537705	3.265885572
H	1.816662569	10.618998084	3.653026664	H	1.817263851	10.528285257	3.542731505	H	1.882164408	10.635429440	3.581969396
H	16.787719795	6.181326479	1.585073386	H	16.836003339	6.026332587	1.383387012	H	16.884138587	6.284039708	1.564520326
H	11.713695656	13.208187478	2.421308452	H	11.838928727	13.362426573	1.972738643	H	11.761968183	13.360395642	2.233712895
H	7.384521150	2.171329535	0.263112960	H	7.399544035	3.599101817	0.160992266	H	7.590578648	3.553648585	0.273579347
H	7.752108641	0.497657932	-0.480963893	H	8.220374659	13.847185070	4.293988915	H	10.744797340	2.008143594	2.613090188
H	10.007984177	0.350353950	-0.769414637	H	10.516910223	12.980931222	4.195643414	H	10.783490815	0.184307678	3.964670481
H	10.219871958	1.695199940	0.389896158	H	10.350647038	12.885579416	5.968342229	H	9.016888273	-0.005528462	3.711931324
H	9.545138016	2.028514750	-1.235634200	H	10.288450362	14.480173466	5.170344101	H	9.663741636	1.208890414	4.880050573
C	9.590547264	1.302273380	-0.415165707	C	10.021656569	13.421005330	5.072467118	C	9.823236122	0.712976042	3.912244543

Coordinates for zeolite FER Si/Al =5 **Acidic Sites with Methanol adsorbed at various T sites**										**Coordinates for FER at Si/Al=8** **Acidic zeolite FER without methanol**			
		T3O1					**T3O8**						
O	Si	Al	H	C	O	Si	Al	H	C	O	Si	Al	H
73	30	6	10	1	73	30	6	10	1	72	32	4	4
O	6.100008782	1.441471702	2.056927732		O	6.305055892	1.393835120	2.072515980		O	6.132056481	1.185759926	1.993253779
O	12.981936699	13.162627612	5.664134871		O	13.091872487	13.213769188	5.741614838		O	12.924106733	13.123499077	5.693179972
O	12.982114619	1.449364508	5.339690309		O	13.107653877	1.497536109	5.267112020		O	12.928463961	1.418459537	5.323782783
O	12.680736800	13.042886867	1.995316979		O	12.705380983	13.014201241	1.936052118		O	12.581758442	13.058374261	1.937273254
O	6.464850219	13.138807990	1.988114904		O	6.453733851	13.097971075	1.786547894		O	6.405345791	12.874361519	1.986526580
O	5.967529342	1.234423611	6.060041355		O	6.068984645	1.254706876	5.742673844		O	6.091368910	1.340111077	5.609113189
O	6.218906556	12.969577165	5.797871792		O	6.110136143	12.986915258	5.809982143		O	6.183990962	13.070571950	5.995629297
O	13.006365585	1.316503192	1.872910576		O	12.976097190	1.290003930	1.922538856		O	12.975996001	1.327459904	1.866452618
O	15.324052472	8.408607311	5.560086345		O	15.376651346	8.461124728	5.619376073		O	15.347821404	8.420534410	5.637826461
O	3.315881575	5.932515246	1.967745576		O	3.394919765	5.720307899	2.236461597		O	3.625463118	5.805653970	1.877468187
O	3.887160388	8.579429081	1.947760208		O	3.870510035	8.541532008	1.984237919		O	3.514652750	8.418099776	1.814275204
O	2.988880385	5.721731645	5.715230134		O	3.088487703	5.697624131	5.246244645		O	3.023148842	5.833433249	5.843682070
O	15.814020735	5.832059651	5.984281229		O	15.856469775	5.863153564	5.933883653		O	15.757052284	5.812328552	5.890394729
O	15.811439856	8.553282850	1.787425227		O	15.787674029	8.542572545	1.756550222		O	15.687578840	8.601053992	1.729201110
O	16.008998045	5.960660091	1.786216870		O	15.946547956	5.952738916	1.838157768		O	15.899989869	6.012002151	1.889591200
O	3.278166249	8.315125018	5.534801899		O	3.303851640	8.310098643	5.450490224		O	3.261965578	8.445545427	5.612189398
O	7.135339556	3.765570832	2.819667164		O	7.060935441	3.852019701	2.723256803		O	6.986236974	3.514984918	2.862392787
O	11.721996081	10.995493863	4.908179690		O	11.955977440	11.067834305	4.780995846		O	11.683053629	10.938272728	4.939374025
O	11.734749770	3.767597653	5.063972299		O	11.644529196	3.680120342	5.049027484		O	11.648135428	3.702306132	5.042953092
O	11.456164161	10.552384994	2.310177224		O	11.539978661	10.483317774	2.233889856		O	11.341806122	10.567554532	2.333876388
O	7.405468368	10.764493441	2.615133046		O	7.475300860	10.777360593	2.455622394		O	7.549238392	10.530325400	2.450064547
O	7.741214557	3.474018506	5.390670291		O	7.748893875	3.533009239	5.283963322		O	7.586659784	3.778769585	5.403588514
O	7.735942950	10.843249550	5.409201653		O	7.683421861	10.955385457	5.300801809		O	7.500589841	10.980025532	5.103449447
O	11.789282942	3.600986289	2.388865819		O	11.840119656	3.622529842	2.361724513		O	11.649880283	3.547136472	2.356131481
O	16.797563970	10.416246066	6.398154258		O	16.974933749	10.430665561	6.336149550		O	16.818346320	10.492590147	6.364140816
O	2.065430244	3.739146242	1.216192601		O	2.033406462	3.667213956	1.273113987		O	1.980490095	3.838077724	1.274055379
O	2.206863239	10.514119718	1.204846852		O	2.281685178	10.484694708	1.085196795		O	2.397379091	10.699567401	0.981268461
O	2.232828560	3.244285478	6.083157925		O	2.234677421	3.369870799	6.131376580		O	2.173329078	3.346485653	6.171381053
O	16.862892544	3.408681761	6.336672085		O	16.734246712	3.378000577	6.378162470		O	16.847590881	3.406865831	6.278758473
O	16.990790212	10.905697741	1.468204837		O	17.025572159	10.864548469	1.428964438		O	16.824181013	10.972502358	1.451943234
O	17.232585944	3.584752149	1.455163282		O	17.244191277	3.611628071	1.470840599		O	17.135279027	3.669257621	1.380060871
O	2.300348511	10.993190076	6.128468269		O	2.218684526	10.938433555	6.027913451		O	2.002602898	11.059524031	5.915863992
O	6.809662434	3.286097925	0.276269174		O	6.868290418	3.179944951	0.196818050		O	6.521985356	3.186101540	0.266727729
O	12.637860759	11.178373676	-0.165903063		O	12.759036732	11.121958852	-0.220835016		O	12.596937027	11.113198862	-0.140178104
O	12.311620972	2.900140336	-0.065605791		O	12.320726648	2.814989202	-0.084621752		O	12.238504777	2.881730271	-0.089679420
O	6.622557303	11.174508770	0.158991767		O	6.494477191	11.054854602	0.048826351		O	6.603594132	11.018462920	0.039627537
O	16.326148564	10.102960505	3.836971539		O	16.410860040	10.047211814	3.803620318		O	16.260043617	10.084977990	3.828127416
O	2.982806735	3.931654514	3.717155684		O	3.147512306	3.509025816	3.700050923		O	2.760148244	4.183808863	3.776241158
O	2.886919995	10.368870478	3.656203641		O	2.808703760	10.347302886	3.574285027		O	2.782556697	10.319127841	3.519162266
O	15.960361581	4.112730969	3.954617387		O	15.904853714	4.058893476	3.963222554		O	15.858435954	4.019574699	3.913935382
O	4.686522824	3.684858527	1.676162369		O	4.654589257	3.444531929	1.531943542		O	4.489912303	3.273431817	1.986370793
O	14.368024448	10.922309818	5.389407602		O	14.559669218	11.027330464	5.392593161		O	14.335048955	10.898985673	5.429010348
O	14.261549464	3.702890832	5.936487176		O	14.161739772	3.858173798	5.931863250		O	14.201905880	3.688306687	5.929589659
O	14.371254856	10.776813307	2.106549202		O	14.434619418	10.810743417	2.127913054		O	14.245326965	10.794729248	2.199419747
O	4.758340162	11.131273484	1.981255171		O	4.779870259	11.076547987	2.006305901		O	4.910886919	10.677075771	2.037983208

O	4.835541574	3.757398532	5.643491634	O	4.850628395	3.795115450	5.755378857	O	4.741235258	3.836965361	5.551781955
O	5.094743538	10.554781009	5.532499990	O	5.053748931	10.561991953	5.365252331	O	4.878318288	10.777619868	5.539750108
O	14.338679214	3.622581335	1.592579645	O	14.368759085	3.539084326	1.546815390	O	14.211939872	3.693375312	1.585250528
O	2.286824152	1.288964637	0.313599641	O	2.138774001	1.256312937	0.185385993	O	2.351411049	1.386719322	0.420909214
O	17.006414923	12.921597382	-0.275252370	O	17.014417022	12.928325765	-0.262853863	O	17.008719334	12.984817364	-0.269105507
O	16.962678454	1.201110756	0.325182587	O	17.018106508	1.203897976	0.366066392	O	16.841537382	1.261855333	0.328989079
O	1.954637576	12.994114676	0.346575532	O	2.151109695	12.971711561	0.242772689	O	1.874315764	13.133555578	0.079833064
O	12.114846244	8.562369065	3.950476106	O	12.003297778	8.534736834	3.994606221	O	11.825852200	8.498427037	3.961744063
O	7.730549295	5.907927398	4.245061927	O	7.847769574	5.946424768	4.138187950	O	7.561469402	5.959632148	3.832598692
O	7.037753685	8.430566875	4.191034131	O	7.199420151	8.491909551	4.096640268	O	7.164633552	8.531203377	4.158844272
O	11.472481077	5.968573413	3.571511457	O	11.463872525	5.934177975	3.618132861	O	11.424205778	5.910940971	3.572385795
O	0.082735722	2.636085785	-0.145856830	O	0.048511200	2.754355489	-0.221655464	O	0.049482733	2.585802195	-0.079063053
O	0.034748455	11.244999196	-0.091308398	O	0.092737698	11.358147643	-0.026100223	O	-0.006077056	11.283877765	0.092112321
O	9.673224650	9.580751286	4.046074185	O	9.731162386	9.865981479	4.086702125	O	9.511812780	9.693285168	4.045943200
O	9.574361025	4.127016787	3.588595573	O	9.569544552	4.079313473	3.437746378	O	9.471502841	4.146228979	3.632710801
O	4.097873116	-0.186734998	1.397252336	O	4.193729868	0.024148191	1.205053739	O	4.050566994	-0.402537075	1.350231772
O	15.259309534	0.247675830	6.103331869	O	15.373152134	0.298746596	6.049284829	O	15.198796441	0.220586088	6.087497697
O	15.003764254	-0.398270427	1.130827179	O	14.988649532	-0.354310947	1.066522899	O	14.944094389	-0.412887404	1.117074692
O	3.782200993	-0.295140883	6.260211185	O	3.762596053	-0.090380583	6.086563415	O	3.833037052	0.004924550	6.237287007
O	13.343510036	6.636234776	5.293952889	O	13.402975511	6.682580732	5.238526146	O	13.311399828	6.712297244	5.241633845
O	6.139925493	6.761183321	2.259412313	O	6.025333955	6.773831532	2.398888857	O	5.869731721	7.216631716	2.234683815
O	5.192779200	6.613131593	4.683720344	O	5.532027464	6.771473074	5.111316445	O	5.253020283	6.827538417	4.811543645
O	13.783219579	6.938792378	2.710046481	O	13.684679219	6.998536204	2.640722983	O	13.614967510	7.068259240	2.644681830
O	4.927413807	-0.030807177	3.903545229	O	4.933804538	-0.153060302	3.735303685	O	4.886777803	-0.289181488	3.853496803
O	14.403327090	-0.062521048	3.680555448	O	14.436562497	-0.125161938	3.648180549	O	14.305054629	-0.129497312	3.667034337
O	14.266415221	7.171985544	0.126238502	O	14.270662994	7.137157647	0.093600119	O	14.216470768	7.089457496	0.096603083
O	4.777923139	6.950043139	-0.253128566	O	4.049200723	6.795268800	-0.107538430	O	4.773018448	7.128183729	-0.152140516
O	1.010474501	7.023221657	2.011064835	O	1.475901773	7.196791612	0.132112251	Si	6.024828754	2.792521071	1.741089062
Si	6.153663998	3.026868811	1.819692007	Si	6.172798615	2.966490321	1.739992409	Si	12.877873150	11.488756146	5.883077533
Si	12.921041768	11.530962239	5.852324511	Si	13.078248376	11.570088571	5.826545101	Si	6.380617117	11.288670849	1.613938779
Si	6.340590806	11.522843221	1.724011777	Si	6.330129571	11.476435387	1.613968540	Si	6.249764667	11.446574629	6.040703645
Si	6.296291362	11.394904946	6.138994096	Si	6.220118930	11.401968954	6.043455161	Si	12.780069675	2.929953385	5.921525424
Si	12.830458926	2.962661748	5.939590397	Si	12.817960163	2.968680802	5.916818920	Si	15.687082134	4.210243467	5.482951915
Si	15.737886997	4.242038148	5.526438145	Si	15.687125842	4.264909779	5.527239016	Si	15.710193138	10.157376954	2.300125645
Si	15.821062917	10.131362839	2.291528130	Si	15.864065579	10.112002127	2.275716661	Si	1.641769834	2.801212581	0.058927286
Si	1.674645166	2.741733432	-0.030606357	Si	1.639645249	2.778060604	-0.033953879	Si	17.410362206	11.431997492	0.011006731
Si	17.452848376	11.381099210	-0.014653383	Si	17.508256132	11.404771307	-0.021725725	Si	17.474622969	2.759046683	0.101322417
Si	17.517538436	2.730230049	0.125703523	Si	17.501669146	2.757575679	0.132690891	Si	1.571221786	11.555800293	-0.165919427
Si	1.639615439	11.444304388	-0.033996839	Si	1.696848193	11.461336040	-0.097499752	Si	11.086377732	9.946843920	3.793310869
Si	11.204216314	9.922546914	3.774726888	Si	11.280853497	9.987572427	3.746867684	Si	7.897393312	4.388054596	3.833296709
Si	8.043807837	4.334446661	4.070173163	Si	8.052859439	4.353525135	3.942009659	Si	5.358385744	-0.211686927	2.303545586
Si	5.386723556	-0.001233863	2.349958164	Si	5.455887781	0.003250875	2.209463521	Si	13.834953721	0.071550930	5.222086695
Si	13.899481384	0.116023920	5.228160796	Si	13.995222336	0.141805185	5.203073271	Si	13.778276665	-0.033402788	2.151986868
Si	13.845747153	-0.015830548	2.173501421	Si	13.852920291	-0.034518024	2.151408694	Si	5.261400566	-0.015834502	5.424390012
Si	5.226330800	-0.066882700	5.510492715	Si	5.219992055	-0.029000611	5.338028110	Si	14.677636170	7.014321656	6.073092088
Si	14.700272274	7.016091157	6.100764658	Si	14.742093988	7.044020053	6.076110259	Si	4.449857940	7.119195356	1.431101976
Si	11.158530055	4.366798440	3.667055047	Si	11.147347434	4.331297245	3.638927679	Si	4.060163135	7.090656120	5.907626240
Si	4.093549040	6.950697048	5.835053451	Si	4.051093945	6.916812918	5.719974496	Si	14.790040140	7.275507444	1.583453546
Si	14.893434598	7.243562299	1.603920489	Si	14.852661292	7.242828414	1.583512414	Si	3.046884967	-0.038807369	0.117767423
Si	3.046360734	-0.121396473	0.164763226	Si	3.085037824	-0.027407362	0.025581169	Si	16.019570700	-0.054487671	-0.076956495
Si	16.074856331	-0.075923601	-0.072147308	Si	16.115136441	-0.045402589	-0.086898175	Si	12.525056072	7.066304760	3.864474561
Si	12.635662651	7.050996817	3.885026472	Si	12.601856796	7.058759714	3.875888989	Si	3.448960399	10.018206061	1.976836639
Si	3.514329008	10.107003854	2.082972538	Si	3.515454973	10.073414379	2.044401967	Si	3.223790095	4.268622299	2.232943464
Si	3.253751135	4.266681307	2.174130591	Si	3.291758063	4.124670460	2.200882129	Si	6.436739872	7.151217085	3.764716368
Si	6.535734250	6.960819208	3.823531774	Si	6.635098167	7.021643605	3.887029203	Si	3.211653089	4.283926169	5.340965247
Si	3.322634088	4.177594738	5.311876717	Si	3.364421565	4.078718821	5.217956964	Si	15.669907493	9.988511978	5.335732899
Si	15.674925149	9.977532840	5.316353133	Si	15.801523386	9.998396692	5.304382789	Si	12.823492370	2.911290106	1.430218768
Si	12.908274454	2.911740501	1.449299990	Si	12.919396945	2.866316162	1.432202553	Si	11.084284715	4.324134276	3.652519515
Al	7.992922283	9.787375732	3.887136548	Al	8.060592712	9.908487985	3.801852375	Si	7.925211545	9.949284975	3.930454156
Al	4.676130964	7.112116035	1.435588570	Al	4.474371198	6.950800705	1.694927459	Al	3.320206675	10.123229294	5.307133244
Al	3.476004589	9.993358027	5.374510083	Al	3.434553924	10.001522799	5.260391663	Al	15.738430993	4.157644133	2.233375489
Al	15.832235894	4.138269044	2.268640029	Al	15.816150014	4.110036022	2.274951741	Al	12.715383762	11.205679692	1.542523963
Al	12.816892991	11.204284689	1.515505044	Al	12.893045999	11.182094044	1.467452170	Al	6.065984472	2.953784904	6.158534242
Al	6.258137399	2.912282487	6.066165979	Al	6.297856203	2.923763195	5.976143539	H	1.933877016	10.809558660	3.509618296
H	8.566836489	11.000097469	5.896941260	H	8.506800534	11.131635801	5.796807492	H	16.826130228	6.218920390	1.647603195
H	2.364314200	6.378892879	1.991147937	H	3.013970065	6.856970441	0.062934078	H	11.661945215	13.375749530	2.037683146
H	2.110167560	10.964873440	3.679368534	H	1.970565243	10.849914525	3.593191528	H	8.307671326	3.869662216	6.058127224
H	16.888692486	6.108200324	1.380913515	H	16.855065117	6.122951775	1.512720432				
H	11.762802043	13.313230571	2.201539594	H	11.782124326	13.281892219	2.112854355				
H	7.665373812	3.760451680	0.246370023	H	7.795564997	3.494285403	0.186710963				
H	1.106391334	7.889537129	1.566397175	H	1.400522233	8.063318502	-0.308396020				
H	1.304732843	7.663898355	4.006558669	H	1.321257368	7.389230618	2.222927011				
H	0.242983555	6.243023713	3.756278832	H	0.275283297	6.164675364	1.447696773				
H	-0.369960897	7.880560932	3.363068710	H	-0.128575968	7.919053012	1.293780594				
C	0.517710488	7.232456778	3.371970870	C	0.685440855	7.180293065	1.350371842				

Coordinates for FER at Si/Al=8
Acidic Sites with Methanol adsorbed at various T sites

T1O1					T1O2					T1O3				
O	Si	Al	H	C	O	Si	Al	H	C	O	Si	Al	H	C
73	32	4	8	1	73	32	4	8	1	73	32	4	8	1
O	6.124608347	1.182913072	1.995970955		O	6.037193338	1.189784310	1.898032573		O	5.745425190	1.390912760	2.264461181	
O	12.998831474	13.132077154	5.681176665		O	12.917691111	13.123674815	5.544990310		O	12.829488743	13.123878693	5.626829721	
O	12.991900660	1.428349544	5.272088662		O	13.200611139	1.405977285	5.303664028		O	12.906581985	1.416199401	5.362707862	
O	12.518070557	13.070037866	1.883228925		O	12.552412706	13.050653882	1.885501393		O	12.514781616	13.072222266	1.949062768	
O	6.351669943	12.869405418	1.975299373		O	6.407850722	12.879691595	1.869043557		O	6.278996361	13.105977068	1.968944590	
O	6.082206594	1.342437326	5.612141698		O	6.120113347	1.275617163	5.533705561		O	6.037168847	1.323464301	5.697313304	
O	6.149773439	13.069616247	5.998068613		O	6.291840290	13.013624068	5.897650623		O	6.287339818	13.093905948	6.012977604	
O	12.891334682	1.344827510	1.862514820		O	12.985613477	1.331655044	1.880412143		O	12.949935601	1.351021221	1.839945179	
O	15.403663087	8.382436497	5.697911223		O	15.406612573	8.464600892	5.673046442		O	15.293203447	8.441874385	5.696097680	
O	3.595790910	5.789135415	1.894879568		O	3.511723354	5.838601775	1.822896021		O	3.255424448	6.000217462	2.038142966	
O	3.475855887	8.395282242	1.822653366		O	3.479696874	8.450884824	1.700447849		O	3.520201517	8.575607946	1.767882320	
O	3.006294610	5.837113210	5.813444336		O	3.032892727	5.811056293	5.806629523		O	2.958536266	5.860417801	5.642331947	
O	15.856405649	5.771424957	5.632714870		O	15.884855531	5.878921600	5.949393599		O	15.718384916	5.840087388	5.888667087	
O	15.515631334	8.601196528	1.574572622		O	15.664261452	8.594903446	1.725708681		O	15.634131932	8.606535652	1.711234762	
O	15.731859410	6.040356263	2.127803364		O	15.923355749	6.035022392	1.825556658		O	15.880588988	6.031819273	1.891650044	
O	3.239812570	8.443932389	5.619677514		O	3.377517533	8.392986959	5.462564995		O	3.260865795	8.472845481	5.690665386	
O	6.944701411	3.523058901	2.877333607		O	7.188223697	3.457947107	2.587826485		O	6.913898519	3.720140066	2.782383868	
O	11.667776620	11.033126456	4.862765121		O	11.640467563	10.938661819	4.871712006		O	11.604966448	10.896316827	4.963234953	
O	11.655943869	3.680092878	4.963574198		O	11.835304992	3.616140553	4.967713015		O	11.573398904	3.655169727	5.028917060	
O	11.373419397	10.473723965	2.292236822		O	11.397242062	10.480751970	2.272321383		O	11.303422078	10.575190925	2.340005486	
O	7.500563980	10.535413746	2.435366241		O	7.569832550	10.555287729	2.447297340		O	7.487249593	10.834884892	2.605062225	
O	7.576850092	3.788374885	5.407920101		O	7.394896926	3.804411374	5.242668772		O	7.476340515	3.812710313	5.375576362	
O	7.486290752	10.995292146	5.094765230		O	7.578878853	10.849901675	5.119815032		O	7.504583017	10.882515107	5.275471175	
O	11.593275758	3.604041138	2.268765359		O	11.660545969	3.569841646	2.282993570		O	11.626151421	3.551862865	2.359596897	
O	16.809028858	10.531571983	6.261901049		O	16.787866510	10.625878572	6.314805292		O	16.751677798	10.522297147	6.367989586	
O	1.948146343	3.824745510	1.289596840		O	2.001860018	3.771884848	1.223924101		O	1.866631459	3.877825778	1.270956441	
O	2.342293028	10.655009810	0.958344003		O	2.435099690	10.815498682	1.000339442		O	2.326177197	10.880737145	1.130555110	
O	2.163103125	3.356336114	6.187034718		O	1.911878240	3.437233470	6.108912979		O	1.970145937	3.462327426	6.129484872	
O	16.826801123	3.346181872	6.203418678		O	17.054245056	3.489884330	6.243553394		O	16.790644570	3.428407422	6.305497759	
O	16.835501537	10.863951557	1.396778612		O	16.880359281	10.910385481	1.427136130		O	16.778963759	10.969817334	1.472307681	
O	17.053492527	3.720938367	1.297398210		O	17.176566579	3.640853952	1.356312759		O	17.141425588	3.667200091	1.396131021	
O	2.006975376	11.070196291	5.892005818		O	2.069459530	10.983798830	5.911486406		O	2.008820484	11.098811484	6.023837171	
O	6.511241168	3.190583442	0.273268969		O	6.318426928	3.207538810	0.149722034		O	6.642273274	2.905242316	0.304105526	
O	12.529341969	11.131420239	-0.188451596		O	12.569499623	11.167437625	-0.212754573		O	12.543182218	11.163141759	-0.141575271	
O	12.197654335	2.849045247	-0.158841314		O	12.481284236	2.886722539	-0.131908482		O	12.264486360	2.942090299	-0.092194443	
O	6.551444437	11.007944581	0.025485025		O	6.623806484	10.968200407	0.011611831		O	6.552955097	11.117664281	0.168924019	
O	16.167367129	9.967856650	3.754826938		O	16.246565147	10.097187158	3.798030205		O	16.191218259	10.060620875	3.836881243	
O	2.743743026	4.154493227	3.782354775		O	2.605267873	4.235710549	3.723235554		O	2.921851558	3.977218742	3.738799556	
O	2.737143134	10.294223741	3.505292814		O	2.814314669	10.310394497	3.495836270		O	2.748319466	10.335711533	3.616186712	
O	15.796677468	3.804717816	3.830811181		O	16.091167031	4.187382890	3.905992804		O	15.912498491	4.058229228	3.914746495	
O	4.464168045	3.251307102	1.972491351		O	4.527701284	3.380244631	2.115131987		O	4.497960861	3.691864544	1.615876510	
O	14.293424992	10.821477072	5.406027002		O	14.293141138	10.877847119	5.356171243		O	14.270546318	10.914551334	5.417009898	
O	14.178274050	3.746916798	5.921915530		O	14.399938124	3.715778998	5.871967106		O	14.156885958	3.726088513	5.835164404	
O	14.254405232	10.894941377	2.120188440		O	14.275830066	10.835472170	2.104085029		O	14.195965998	10.801201378	2.196586600	
O	4.857630632	10.671043354	2.016226203		O	4.947123701	10.651355616	2.030042844		O	4.841240549	10.869942710	2.152338643	
O	4.734485189	3.840612098	5.560539424		O	4.511044921	3.616279823	5.484719438		O	4.605728924	3.778988569	5.825736895	
O	4.870189823	10.768877179	5.488264112		O	4.931603386	10.760879015	5.488471209		O	4.859832950	10.838673977	5.647252151	
O	14.155028087	3.695433601	1.497747372		O	14.271247003	3.696709290	1.718722843		O	14.211935894	3.712205098	1.615013741	
O	2.274358984	1.371384585	0.409505510		O	2.500479689	1.412405970	0.232387350		O	2.375543289	1.491409581	0.344578853	
O	16.963756978	12.965250709	-0.226802369		O	17.155613066	13.031374320	-0.119262285		O	16.990407371	12.998837771	-0.225801157	
O	16.835006164	1.255497305	0.326896005		O	16.673629876	1.321954885	0.197444530		O	16.715695312	1.278113121	0.332906837	
O	1.870041200	13.110117885	0.086988330		O	1.833469095	13.158638567	-0.053241060		O	1.715002008	13.231147342	0.106986574	
O	11.773322651	8.508602549	4.101064123		O	11.886715504	8.471451123	3.993366077		O	11.750825301	8.476665935	3.940627393	
O	7.545795897	5.965284381	3.839899691		O	7.603877487	5.900907343	3.607252954		O	7.576724581	6.044996307	3.835579384	
O	7.164625079	8.541330131	4.145738079		O	7.166519090	8.464188457	4.059215076		O	7.021058237	8.621349253	3.992267611	
O	11.371953008	5.933855489	3.577183903		O	11.449978141	5.874184184	3.623022361		O	11.390897507	5.887102736	3.594649859	
O	0.008647273	2.629083159	-0.088981638		O	0.054910481	2.356528329	0.032873857		O	-0.018174157	2.497604501	-0.066890496	
O	-0.032018436	11.277624963	0.021832874		O	0.033133667	11.211214668	0.034794098		O	-0.061339042	11.260619578	0.096458121	
O	9.496360800	9.750643965	4.012798033		O	9.538913328	9.588666229	3.941185581		O	9.440649553	9.696327181	4.005756145	
O	9.445232446	4.139352661	3.610848646		O	9.521565782	4.076281844	3.718443366		O	9.393638878	4.146381567	3.569331856	
O	4.009836027	-0.360929856	1.368270086		O	4.004914478	-0.462272821	1.289412054		O	3.804477765	-0.339017690	1.550135230	
O	15.278074324	0.225361421	5.988955523		O	15.365578581	-0.079498982	5.907120672		O	15.163526487	0.140316971	6.056718796	
O	14.848512979	-0.351945441	1.010668153		O	14.853540728	-0.434640617	0.935585307		O	14.854123846	-0.445928573	1.084554180	
O	3.815026100	0.029607041	6.250586091		O	3.897227519	-0.141233980	6.154427652		O	3.865126817	-0.140937435	6.422090332	
O	13.428251847	6.692161809	5.053769939		O	13.440109019	6.678780189	5.175805880		O	13.262010609	6.734436450	5.260105585	
O	5.840089776	7.210956787	2.245872189		O	5.787323810	7.185607020	2.201745901		O	5.683774800	7.102882038	2.304454747	
O	5.251648527	6.851096472	4.829089646		O	5.347302108	6.680144241	4.800343981		O	5.295154680	6.863001427	4.936943419	
O	13.357219133	7.224764946	2.418206396		O	13.582102353	7.033266154	2.577355096		O	13.587229548	7.066755312	2.672874829	
O	4.862658353	-0.276497310	3.860218636		O	4.917294866	-0.355800935	3.777169450		O	4.766340013	-0.359540715	3.996018624	
O	14.292022859	-0.147188791	3.590008604		O	14.380586122	-0.201105736	3.536945579		O	14.259712749	-0.102854578	3.647500721	

O	14.313030926	6.808171649	0.001992923	O	14.205404826	7.100667157	0.058108352	O	14.160355353	7.059422022	0.116739336
O	4.738474471	7.105194155	-0.139708167	O	4.761233207	7.089735501	-0.197833034	O	4.573433179	6.973402006	-0.078054120
O	17.695829617	6.812118252	3.420510776	O	8.544625358	4.364486372	7.288241637	O	8.248844341	1.035553977	0.084738363
Si	6.009712156	2.788143123	1.743300945	Si	5.980518098	2.800320797	1.683739458	Si	5.912253198	2.938490764	1.808840916
Si	12.870003189	11.500391939	5.844964669	Si	12.846887467	11.496687728	5.799042897	Si	12.808122116	11.492851500	5.868371873
Si	6.329578922	11.285658585	1.598996039	Si	6.402338362	11.274021424	1.579163189	Si	6.302058093	11.487992932	1.717014932
Si	6.225276392	11.446016663	6.023408936	Si	6.316511353	11.387861546	6.001122622	Si	6.255323478	11.458737302	6.141245834
Si	12.781907013	2.931171443	5.868822101	Si	13.002411243	2.919370417	5.867125351	Si	12.747417564	2.951695475	5.900700424
Si	15.674272894	4.130586759	5.380748338	Si	15.878861324	4.297268598	5.472681724	Si	15.663609653	4.242155399	5.471736798
Si	15.649560182	10.114667127	2.216718464	Si	15.717080071	10.158386887	2.263981937	Si	15.654842006	10.152277074	2.305003417
Si	1.598893291	2.802756754	0.059971288	Si	1.620113451	2.757096136	0.008424332	Si	1.550897946	2.851643353	0.030611264
Si	17.379998829	11.405697035	-0.031221836	Si	17.458744962	11.437335023	0.010249161	Si	17.357274982	11.432978566	0.029232290
Si	17.425492063	2.766398992	0.069326077	Si	17.502489114	2.731261276	0.079317304	Si	17.412979114	2.747433770	0.110495894
Si	1.547511101	11.542864959	-0.190955795	Si	1.598328943	11.552933119	-0.212092015	Si	1.504748291	11.624510766	-0.092476031
Si	11.082792274	9.959377910	3.785081792	Si	11.111606270	9.890317921	3.739814674	Si	11.023679319	9.928385782	3.785350225
Si	7.878568307	4.391879783	3.832042268	Si	7.907357976	4.314095073	3.766508922	Si	7.830967002	4.432583102	3.941000093
Si	5.328944369	-0.202302145	2.308701303	Si	5.328393565	-0.243612029	2.216136989	Si	5.144119374	-0.112985577	2.442952667
Si	13.887488630	0.075090303	5.160160782	Si	13.957461054	-0.017052174	5.106139152	Si	13.786456737	0.060643831	5.205141064
Si	13.715587684	-0.017104566	2.094115360	Si	13.771816606	-0.058814231	2.057795839	Si	13.719544888	-0.022735211	2.136640278
Si	5.239955757	-0.006845938	5.430764208	Si	5.322303491	-0.097383626	5.343912541	Si	5.230197364	-0.052119372	5.532722256
Si	14.746835792	6.930383299	5.976541310	Si	14.752880512	7.039502217	6.063322103	Si	14.625442400	7.024357689	6.094072789
Si	4.421925126	7.102940577	1.444485730	Si	4.389468938	7.118763289	1.372828169	Si	4.276553005	7.146570429	1.496512759
Si	4.046385761	7.091976425	5.911376417	Si	4.116537474	7.025480086	5.835585642	Si	4.010925315	7.076683290	5.926150435
Si	14.698885545	7.210475421	1.518568870	Si	14.775858089	7.270133805	1.546271007	Si	14.744099518	7.272084740	1.593084871
Si	3.013300023	-0.034317715	0.122122512	Si	3.069828969	-0.079783353	0.005056869	Si	2.942642759	-0.007162176	0.205839970
Si	16.003018580	-0.044846989	-0.117092171	Si	16.041581157	-0.104510590	-0.157084186	Si	15.954874795	-0.072152512	-0.080889534
Si	12.482799942	7.103882324	3.792218661	Si	12.564026315	7.029984754	3.854928672	Si	12.474485272	7.050979467	3.875217210
Si	3.402234529	9.999917957	1.961757340	Si	3.465850522	10.040764418	1.945656956	Si	3.409563968	10.148557111	2.054259219
Si	3.204581447	4.243665424	2.236567827	Si	3.175521392	4.294970210	2.216706333	Si	3.118225198	4.382220955	2.185376009
Si	6.428902484	7.161825374	3.770062205	Si	6.458488438	7.065403752	3.683180158	Si	6.389047416	7.151890567	3.780507596
Si	3.204515720	4.276066043	5.345104327	Si	3.058756605	4.257955293	5.289904636	Si	3.154672123	4.262117703	5.340672116
Si	15.647486804	9.943001235	5.291495379	Si	15.667093376	10.029501330	5.308501093	Si	15.604684374	9.998429873	5.347733893
Si	12.765313891	2.919115175	1.369681121	Si	12.902977331	2.920705931	1.443722989	Si	12.815186873	2.949056254	1.438703809
Si	11.060302162	4.340303823	3.604590504	Si	11.130525261	4.277823984	3.653008845	Si	10.994522581	4.308126833	3.650445897
Si	7.908617148	9.970507574	3.913746588	Si	7.952938902	9.873520383	3.883824058	Si	7.859736624	10.002773725	3.961453676
Al	3.309325108	10.118304370	5.285189482	Al	3.386619960	10.082124258	5.259054211	Al	3.311587805	10.153661095	5.401075279
Al	15.661486050	4.190921878	2.175113592	Al	15.832215620	4.195100238	2.238568465	Al	15.747185289	4.181060195	2.239307150
Al	12.691244826	11.211306858	1.493846631	Al	12.722377390	11.199782353	1.469440551	Al	12.668748781	11.220028293	1.540968584
Al	6.064276951	2.955353190	6.162764764	Al	5.984815992	2.921914073	5.974919348	Al	6.112862780	3.015725564	6.078981487
H	1.891141398	10.788999820	3.510458833	H	1.984874121	10.831318893	3.505723601	H	1.876282376	10.783135135	3.623810297
H	16.611289075	6.408712165	2.672854342	H	16.848830027	6.329737731	1.704821836	H	16.806529181	6.288536525	1.703413135
H	11.604147983	13.417591563	1.858215272	H	11.647865641	13.339011291	2.119512034	H	11.611325007	13.342235903	2.205975106
H	8.279783877	3.942270432	6.070539180	H	8.132517208	4.209437387	6.235483710	H	7.454344950	2.172721161	0.286291018
H	17.576659824	6.469201014	4.332959465	H	7.658475252	4.108318444	7.731013421	H	7.712945746	0.564111742	-0.594303010
H	19.780018634	6.894512631	3.625701424	H	9.294623052	2.896868640	8.574680289	H	10.001911352	0.236808329	-0.731469609
H	19.123418045	7.084536777	1.967854653	H	10.456888264	3.586250096	7.394528035	H	10.193289873	1.590491779	0.434685642
H	19.158333382	5.448803456	2.724984891	H	9.216998544	2.417654014	6.835611899	H	9.636185475	1.936759093	-1.231364793
C	19.033449968	6.525952488	2.908469287	C	9.441277067	3.229531132	7.542018464	C	9.605088075	1.209596539	-0.405750097

Coordinates for FER at Si/Al=8
Acidic Sites with Methanol adsorbed at various T sites

T2O2					T2O6					T3O1				
O	Si	Al	H	C	O	Si	Al	H	C	O	Si	Al	H	C
73	32	4	8	1	73	32	4	8	1	73	32	4	8	1
O	5.961947262	1.195736957	1.792883148		O	5.958284543	1.331640505	1.642139284		O	6.170113480	1.156280139	1.999076693	
O	13.075578573	12.924127293	5.855079208		O	13.030032336	13.212581785	5.972891076		O	12.981394633	13.066771817	5.723425296	
O	13.105400323	1.178581210	5.266138986		O	12.979371619	1.464351672	5.331065596		O	12.799225610	1.377509641	5.439853638	
O	12.866753569	12.934964354	1.761638293		O	12.745955770	13.013689269	1.953336510		O	12.577254309	13.151385206	1.880540192	
O	6.274420300	12.923925984	2.091521473		O	6.318747170	13.069331260	2.126828583		O	6.306158065	12.844596963	1.939263469	
O	6.010440941	1.196033727	5.688450807		O	5.936089156	1.447062796	5.804118859		O	6.131219140	1.329750928	5.591097782	
O	5.700814813	12.934870570	5.881944103		O	6.083364677	13.180894485	5.682452883		O	6.140921077	13.057905990	6.005086453	
O	13.272225336	1.194567581	2.122043893		O	13.007464932	1.284703822	2.054035247		O	13.030544164	1.441438618	1.855527730	
O	15.607448196	8.334651282	5.561813031		O	15.401781134	8.454336615	5.520590410		O	15.443293530	8.316820393	5.540649053	
O	3.447344773	5.817206942	2.007415719		O	3.419205021	5.915084008	1.895493161		O	3.659920958	5.757549643	1.885359837	
O	3.573125970	8.402323876	1.857639566		O	3.654583212	8.493752822	1.845698382		O	3.460232694	8.362239546	1.800876322	
O	3.192100709	5.525151391	5.932573405		O	3.155920357	5.750247070	5.930531459		O	3.036810816	5.826816558	5.790052697	
O	15.576849301	5.746551184	5.916157646		O	15.742125675	5.880329899	6.011186720		O	15.847039901	5.723985713	5.384647989	
O	15.631534099	8.445666308	2.062072842		O	15.615625395	8.558098927	1.992199643		O	15.565335383	8.669375020	1.652944813	
O	15.912896268	5.883394448	1.729290140		O	15.894971686	6.002524948	1.777773605		O	15.852919299	5.899667764	2.204068655	
O	3.196640588	8.119403034	5.642650332		O	3.458983661	8.356738704	5.631726466		O	3.294991562	8.426551105	5.575407210	
O	7.008030578	3.536244193	2.422032147		O	6.976900337	3.611675551	2.501170122		O	6.905286367	3.523290123	2.895785010	
O	12.141961805	10.583692975	4.956353427		O	11.852441415	11.064246655	4.982677317		O	11.586338447	10.982168555	4.999114864	
O	11.437416797	3.231620863	5.193953649		O	11.499036010	3.62767633	5.284744507		O	11.534499193	3.677867211	5.061117774	

O	11.438838554	10.783805223	2.420547204	O	11.449302705	10.744435592	2.384196603	O	11.425219272	10.607097349	2.384740125
O	7.577390091	10.615524559	2.436504769	O	7.465426599	10.693491548	2.402148308	O	7.436175969	10.506707173	2.430039687
O	7.458315775	3.344853207	5.098015605	O	7.407570274	3.553050127	5.167120806	O	7.599015666	3.814451862	5.392375226
O	7.397060531	11.095687183	5.190296833	O	7.561991521	11.031322245	5.270459495	O	7.510012209	11.004658149	5.078022856
O	11.714907694	3.331795741	2.296110141	O	11.941033960	3.639296485	2.456205647	O	11.780546871	3.699368677	2.398091228
O	17.144056257	10.394841773	6.248225326	O	16.929731917	10.483624765	6.272783499	O	16.730861725	10.467952716	6.350720391
O	1.893024199	3.796884757	1.240184839	O	1.879467766	3.850218211	1.250828730	O	1.980332930	3.815434664	1.294090983
O	2.493812038	10.754368759	1.147686226	O	2.298078492	10.682101641	1.120379617	O	2.268717015	10.599975471	0.935336618
O	2.452141195	3.033595136	6.236512466	O	2.381093026	3.234719000	6.196620221	O	2.146088749	3.374424140	6.169009235
O	16.602139088	3.336548858	6.314809942	O	16.703478117	3.418970995	6.388006086	O	16.776551721	3.327867977	6.160963169
O	16.630535939	10.775956316	1.328708761	O	16.698510606	10.889817038	1.372095246	O	16.911659155	10.957847337	1.449615858
O	17.178168758	3.525984411	1.389605157	O	17.335744937	3.677438107	1.444561737	O	16.973105648	3.696645423	1.263787415
O	1.932402738	10.713822738	6.091128284	O	2.056185987	10.900083320	6.037466748	O	2.043383490	11.057327640	5.866462595
O	6.289498140	3.114146182	-0.054118274	O	6.162733482	3.422243412	-0.010467690	O	6.596993180	3.154163405	0.270538834
O	12.402757369	11.008416333	-0.000091204	O	12.346098558	11.225411141	0.013223180	O	12.602110572	11.099157249	-0.113068025
O	12.415886071	2.393750113	-0.041437616	O	12.467712741	2.799865110	0.019907687	O	12.365781018	3.072046412	-0.083250863
O	6.375003114	11.113610478	0.120632818	O	6.445504784	11.393373467	0.058157750	O	6.526981503	10.972656922	-0.001453766
O	16.020797309	10.332275231	3.854090110	O	15.962572100	10.409652107	3.834172642	O	16.259264038	10.095833678	3.797777910
O	2.721602101	3.993057984	3.768025873	O	2.627494362	4.244904414	3.771076722	O	2.832184277	4.105812370	3.772219955
O	2.732860267	10.145217348	3.644675034	O	2.778261633	10.250999138	3.605698165	O	2.708077036	10.260663501	3.476577013
O	15.833790849	4.037860373	3.896778718	O	16.049035090	4.209728249	3.967361670	O	15.969323611	3.684070048	3.693708393
O	4.419920262	3.345580551	1.815651444	O	4.385243355	3.424718264	1.960953645	O	4.484068162	3.196177449	1.889755113
O	14.559802405	10.741135410	6.054622694	O	14.359254055	10.897426451	5.895871297	O	14.242179538	10.732295083	5.389225785
O	13.997214107	3.647129135	5.770472250	O	14.136078538	3.810547240	5.779133125	O	14.169878903	3.652246724	5.618265444
O	14.067347073	10.578573108	2.054237403	O	14.090469248	10.716175635	1.965997460	O	14.347034852	11.019045956	2.188305869
O	4.923572561	10.671500718	2.291760783	O	4.821226704	10.883765152	2.064316143	O	4.798795640	10.664336181	1.955137255
O	4.846813798	3.546637638	5.248239800	O	4.777871530	3.756228946	5.232171603	O	4.744787165	3.798451383	5.632913934
O	4.824765126	10.421466226	5.607323938	O	4.924829686	10.777192630	5.436789990	O	4.894258114	10.760721961	5.411190389
O	14.280132259	3.562742580	1.487429720	O	14.494255516	3.490984688	1.600909126	O	14.324049956	3.777336142	1.583409838
O	1.980146783	1.244050777	0.519837939	O	2.210141679	1.347857708	0.443913346	O	2.185177351	1.351614032	0.359953311
O	17.197875658	12.854920818	-0.225901023	O	16.983795640	12.964811887	-0.255884220	O	16.911267210	12.961053329	-0.313365781
O	17.170673196	1.144871491	0.172783462	O	17.074264780	1.236178009	0.353293169	O	16.912843583	1.238174681	0.292666929
O	1.783127666	12.990805847	-0.067591691	O	1.818684079	13.069039839	0.041060688	O	1.916837689	13.081776309	0.070888004
O	11.793889568	8.406292776	3.498575866	O	12.045722844	8.662056220	3.884568704	O	11.778642195	8.526017316	4.077577042
O	7.564432949	5.731794769	3.882020339	O	7.683794341	5.836931579	3.829320253	O	7.597609948	5.966174218	3.781641333
O	7.253892941	8.359773656	4.227596358	O	7.216159586	8.432783755	4.160058626	O	7.160262518	8.538825852	4.175877661
O	11.415095093	5.791737933	3.808849521	O	11.240081705	6.102523757	3.734632726	O	11.231263491	5.975488399	3.714727999
O	0.024620147	2.882614471	-0.377489978	O	0.059810905	2.749736486	-0.327286777	O	-0.008954913	2.776590491	-0.079873152
O	0.025598596	11.062926311	0.401986455	O	-0.043205525	11.236151958	0.149643240	O	-0.047932944	11.333632530	-0.091069038
O	9.694624795	9.907422450	4.210515695	O	9.672993572	9.890674443	4.133429210	O	9.487262485	9.736158261	3.941007179
O	9.369570066	3.841909433	3.300703775	O	9.395376474	3.829560169	3.401167443	O	9.443581148	4.057430408	3.510556855
O	3.900543224	-0.437642362	1.260788600	O	3.956374639	-0.409312593	1.310250168	O	3.989202581	-0.287295033	1.380235596
O	15.347418716	0.034401889	6.145302522	O	15.252078938	0.357009985	6.210261843	O	15.141451216	0.319968227	6.128110029
O	15.286610688	-0.381239994	1.258399526	O	15.108013871	-0.276422537	1.284761116	O	14.978462362	-0.314236810	1.177913690
O	3.578355920	0.176815445	6.200225487	O	3.709198795	0.001419939	6.197690832	O	3.839469928	0.076350181	6.256211402
O	13.282106356	7.045710598	5.235453677	O	13.320156250	6.803214401	5.245129665	O	13.380983318	6.666167575	5.046049586
O	5.820646639	7.018246615	2.384332724	O	5.831970941	7.020003678	2.374012403	O	5.852892815	7.238309179	2.245595712
O	5.366249922	6.650849350	4.979339892	O	5.441318912	6.632999722	4.976279333	O	5.303625907	6.783905331	4.827695602
O	13.609584087	6.708643089	2.620708918	O	13.540037980	6.887741551	2.617152545	O	13.263913738	7.063277467	2.402781133
O	4.665070287	-0.064612186	3.773171336	O	4.759141075	0.194304489	3.763660460	O	4.873169626	-0.280918582	3.859431927
O	14.442567156	-0.539417564	3.738450612	O	14.333552542	-0.238531821	3.805698547	O	14.229138717	-0.037405673	3.704830080
O	14.283459934	7.294392254	0.092470506	O	14.239026849	7.328006211	0.095637688	O	14.480435698	6.658987007	-0.104074912
O	4.756388342	6.970571511	-0.025088041	O	4.852653735	7.060244500	-0.042090452	O	4.760270902	7.099808900	-0.151575710
O	8.587768733	13.279566824	4.734381793	O	9.704733008	1.746008113	2.102244286	O	17.840354335	6.858495908	3.333962833
Si	5.899327883	2.794004647	1.491967914	Si	5.864993229	2.954864997	1.524173847	Si	6.047276612	2.756394431	1.725899651
Si	13.033731985	11.310579935	6.076171254	Si	12.903452747	11.597741053	6.078966633	Si	12.857813887	11.430175488	5.897825366
Si	6.338353049	11.313756218	1.731972814	Si	6.299567422	11.494337824	1.679608076	Si	6.287408836	11.258815517	1.570056934
Si	6.008841277	11.359211931	6.107482747	Si	6.142984908	11.601654534	6.031899274	Si	6.232636260	11.433746314	5.994959398
Si	12.733704037	2.631060583	5.931752323	Si	12.760714689	2.965935652	5.973370457	Si	12.732505062	2.947344756	5.880043219
Si	15.504527162	4.162279330	5.451884827	Si	15.660168364	4.298357932	5.513093966	Si	15.684673613	4.105695988	5.247425087
Si	15.575585080	10.062330228	2.317292651	Si	15.578443239	10.168857243	2.282778681	Si	15.717590198	10.158499213	2.250899063
Si	1.568233115	2.747947586	0.028363511	Si	1.617164051	2.806453083	0.022004753	Si	1.601058559	2.827674807	0.049267786
Si	17.475845434	11.282373939	0.039813301	Si	17.375995499	11.412787004	-0.009401391	Si	17.358143851	11.410201801	-0.032478218
Si	17.464351933	2.744773335	0.014374922	Si	17.510713802	2.796282782	0.108870067	Si	17.412469029	2.755224373	0.005060158
Si	1.550112645	11.379494639	-0.043759168	Si	1.530050941	11.474017101	-0.102321076	Si	1.542927048	11.529810335	-0.230351588
Si	11.227939632	9.902987244	3.788305753	Si	11.230268940	10.064402045	3.853639075	Si	11.085240362	9.971748767	3.819806442
Si	7.755568404	4.149863807	3.718935954	Si	7.821580613	4.233814020	3.740373863	Si	7.896157869	4.384180983	3.799328647
Si	5.182464759	-0.173905272	2.227101839	Si	5.244265179	-0.014557857	2.220636987	Si	5.326433141	-0.204217994	2.303579523
Si	13.999207618	-0.163723683	5.259555546	Si	13.898684024	0.137390656	5.332017944	Si	13.779504038	0.080660491	5.271529723
Si	13.970330405	-0.246006243	2.205187220	Si	13.819331879	-0.098764762	2.265103128	Si	13.769511567	0.036983757	2.169384244
Si	4.969252060	-0.019339794	5.375282321	Si	5.097436280	0.136591019	5.354749715	Si	5.259345609	-0.004590248	5.427103377
Si	14.677202231	7.085187510	6.055770947	Si	14.675042310	7.104201576	6.074305887	Si	14.754655929	6.885518970	5.888103693
Si	4.424540797	7.033348450	1.554888811	Si	4.459756004	7.103003459	1.522436063	Si	4.445993368	7.097006062	1.432365883
Si	4.125195104	6.865930293	6.007115021	Si	4.221742112	6.995978155	5.992288161	Si	4.089109959	7.073150851	5.890196761
Si	14.774506721	7.148413792	1.617919544	Si	14.734273362	7.251931526	1.622576017	Si	15.761380045	4.231700840	2.184262501

Si	2.815600065	-0.075195958	0.088091857	Si	2.926480973	-0.056408654	0.096033990	Si	3.009562089	-0.020795732	0.109155062
Si	16.232306109	-0.146883243	-0.043288192	Si	16.093332519	0.002324627	0.016184608	Si	15.996508202	-0.044099511	-0.077153185
Si	12.482927273	6.975217167	3.807269272	Si	12.477472405	7.100867319	3.874428981	Si	12.446686681	7.090641302	3.773566234
Si	3.490397094	9.981532083	2.124383072	Si	3.445045537	10.066319287	2.046599295	Si	3.355487895	9.968038260	1.926106515
Si	3.112964958	4.242390296	2.211073949	Si	3.078131849	4.361618731	2.216555739	Si	3.262457698	4.214807801	2.218568467
Si	6.508715365	7.000313703	3.880241639	Si	6.550627760	7.024583810	3.850122941	Si	6.461557767	7.152736803	3.761488679
Si	3.285242271	4.040240619	5.293978118	Si	3.222209492	4.259326180	5.283313721	Si	3.238142016	4.260225997	5.348334108
Si	15.817672507	9.939360704	5.417244684	Si	15.641684367	10.052780644	5.382958676	Si	15.641211121	9.913286726	5.279780036
Si	12.937698915	2.668019916	1.479122095	Si	13.015406597	2.867806678	1.554163517	Si	12.886408574	3.020382944	1.444841251
Si	6.131860951	2.801807962	5.899333455	Si	12.674072655	11.433437691	1.584767178	Si	11.035990830	4.379331217	3.672489524
Si	12.700029124	11.330461566	1.562929803	Si	6.059620306	3.061713024	5.942331360	Si	7.904135534	9.963169241	3.898930323
Al	8.015478608	9.864452522	3.933698448	Al	8.003565802	9.900590008	3.825706037	Al	14.708506597	7.199183799	1.498209614
Al	11.192304182	4.095826806	3.739511667	Al	11.116933235	4.380631127	3.764259832	Al	3.331961625	10.102888513	5.241848919
Al	3.229688566	9.807040997	5.413377340	Al	3.373418198	10.029796073	5.352338114	Al	12.776421959	11.244808173	1.560919810
Al	15.753922758	4.054086732	2.202836076	Al	15.908507517	4.164232654	2.278822301	Al	6.116323446	2.934967678	6.164204828
H	7.931376987	11.990822640	5.021556976	H	8.398342132	11.269240376	5.720010436	H	1.863791833	10.759573235	3.496453628
H	9.451955177	3.425464501	2.412497935	H	9.506451005	2.899379608	2.789530740	H	16.732407940	6.299420126	2.698203311
H	1.854329267	10.581296304	3.621076054	H	1.890824134	10.666854548	3.618765813	H	11.643786500	13.441971521	1.935571794
H	16.785335264	6.048541254	1.319437489	H	16.781988366	6.249666741	1.443179155	H	8.271120087	4.025228996	6.070874161
H	8.355125070	13.644578021	3.860587991	H	10.660540774	1.527274043	2.209924848	H	17.767832825	6.759243631	4.305113714
H	10.611397060	13.135017785	4.149871531	H	8.379533789	2.184680826	0.577935693	H	19.888937691	7.288380736	3.219246528
H	10.249669611	12.895885468	5.890334143	H	9.492855123	0.825495700	0.236540636	H	19.138982735	6.556950584	1.768674495
H	10.202129592	14.540616129	5.193696897	H	10.098926207	2.533653140	0.172444129	H	19.483051260	5.527538565	3.205923619
C	10.005410063	13.480137493	4.996559317	C	9.411438222	1.833117425	0.669482055	C	19.177796505	6.528570385	2.865244309

Coordinates for FER at Si/Al=8 Acidic Sites with Methanol adsorbed at various T sites					**Dimethyl ether formation in the framework**					**Ethanol formation in acidic FER framework**				
		T3O8												
O	Si	Al	H	C	O	Si	Al	H	C	O	Si	Al	H	C
73	32	4	8	1	74	30	6	14	2	74	30	6	14	2
O	6.358869351	1.319336265	2.033724085		O	6.572481434	1.543214924	1.904497358		O	6.451911506	1.611026251	1.734103027	
O	13.067577269	13.154456941	5.708697998		O	13.247468490	13.054000266	5.662466375		O	13.394508804	12.994392098	5.800648805	
O	13.134829273	1.444452348	5.257508371		O	13.248614961	1.316536132	4.982981986		O	13.276509555	1.289876709	5.208929113	
O	12.729724961	13.006177827	1.885173380		O	12.928323401	12.780271938	1.594891335		O	12.951543516	12.617934297	1.801147069	
O	6.496593545	13.005599770	1.833258687		O	6.791570787	13.261119643	2.093614818		O	6.731916310	13.340528791	1.923064560	
O	6.041801474	1.170721707	5.713549034		O	6.457332712	1.038257816	5.943777928		O	6.221882949	1.228188158	5.880360119	
O	5.867183536	12.860604241	5.782208360		O	6.241217400	12.797408609	5.357451862		O	6.267805027	12.977038581	5.355531268	
O	13.032841048	1.271352106	1.892943465		O	13.183622819	1.049051884	1.656080624		O	12.917454909	0.928603331	1.863798886	
O	15.432687886	8.476604713	5.698902396		O	16.047328614	8.401959527	5.189627254		O	16.336022456	8.283252761	5.261629172	
O	3.511052274	5.682592012	2.184258755		O	3.696678461	5.940189755	1.690409138		O	3.592871018	6.068147532	1.635445706	
O	3.707537730	8.544759278	2.100030898		O	4.078088975	8.514478723	1.965877140		O	3.964890281	8.605259811	1.988980004	
O	3.245634748	5.777274665	5.246051395		O	3.856421439	5.863787379	5.685862784		O	3.559870209	6.040993852	5.580157359	
O	15.804791415	5.865363784	5.850081998		O	16.003551055	5.795218625	5.599585116		O	15.995436136	5.732079122	5.876709190	
O	15.794340365	8.578865765	1.648803738		O	16.011318861	8.557049034	1.359679403		O	16.157140214	8.350511283	1.847579341	
O	15.848709178	6.014533420	1.932504756		O	15.654133742	5.985768976	1.566834026		O	15.601875404	5.805222000	1.630870464	
O	3.240749561	8.391381228	5.414836992		O	3.564596394	8.443723435	6.030975014		O	3.430048126	8.627735668	5.850810327	
O	7.045841030	3.822242907	2.703284801		O	7.366950232	4.018485737	2.326236024		O	7.494033948	4.011897534	2.202923311	
O	11.850759961	10.982516629	4.856231681		O	12.531257100	10.738179182	4.621743024		O	12.475783846	10.845406783	4.621568183	
O	11.637252538	3.607995592	5.005641790		O	12.194333251	3.719952169	4.805833910		O	12.103699988	3.633651860	5.027125981	
O	11.614090350	10.455035687	2.250149628		O	11.781519127	10.438757481	2.075968799		O	11.733568715	10.314307970	2.127614988	
O	7.440972930	10.602066412	2.452265977		O	7.936586284	10.888438271	2.399016648		O	8.022953472	11.038997590	2.323339832	
O	7.760005095	3.445716475	5.253627918		O	7.663711255	3.111781302	4.842485913		O	7.402140549	3.274946161	4.766104596	
O	7.497816834	10.917918479	5.105819784		O	7.373367867	10.445615932	5.235178593		O	7.272685284	10.582875213	5.108408849	
O	11.769464122	3.526398811	2.316750129		O	11.659848476	3.193572289	2.013508067		O	11.580777743	3.219475317	2.221661591	
O	16.913723569	10.557931541	6.302048991		O	17.774373014	10.757688688	5.775155374		O	17.756426727	10.822719157	5.816457050	
O	2.018466434	3.649213191	1.371994343		O	2.308887244	3.832971604	1.040335789		O	2.330720926	3.974288420	0.880438007	
O	2.210279088	10.592154547	1.332303503		O	2.346545779	10.769743336	1.720292929		O	2.618042876	11.046261518	1.460368415	
O	2.293633270	3.524099205	6.240441854		O	2.246366677	3.444528610	5.940699113		O	1.977098005	3.589432648	5.845595022	
O	16.760541626	3.420527199	6.319898164		O	17.259369536	3.572434854	6.074165597		O	17.204076803	3.430249734	6.158365160	
O	17.081472006	10.879356476	1.412112191		O	16.723658874	10.943473075	0.651745618		O	16.807161869	10.622483157	0.707323875	
O	17.213030318	3.697697777	1.408890956		O	17.229906753	3.647265464	1.254643225		O	17.168659772	3.644885555	1.346869251	
O	2.383679390	10.763759927	6.254534404		O	2.315128793	10.697983634	6.503100085		O	2.162800317	10.884933659	6.336641342	
O	6.876471316	3.120153861	0.183182188		O	6.979913535	3.182256883	-0.136676253		O	6.731442814	3.390314972	-0.218295411	
O	12.834426882	11.058167864	-0.221685851		O	12.942528024	10.922141279	-0.293702758		O	12.688821805	10.941348011	-0.252568122	
O	12.318195929	2.769478317	-0.121476701		O	12.602811192	2.638562687	-0.356099500		O	12.471958921	2.574691437	-0.144865185	
O	6.634248042	11.044523011	0.021197537		O	7.064210382	11.613678529	0.059247868		O	6.919340709	11.566927716	-0.005592519	
O	16.424520786	9.979752498	3.779579960		O	16.733490247	10.339575634	3.231214130		O	16.508741100	10.457724037	3.377104974	
O	3.175396265	3.567160822	3.765801947		O	3.184486649	4.060005021	3.511543249		O	2.919349119	4.191107528	3.430187829	
O	3.038949964	10.483561108	3.782149028		O	3.477507217	10.320663248	4.146665433		O	3.203974128	10.531694469	4.009493991	
O	15.886944752	4.016517436	3.916968782		O	16.242167475	3.994072500	3.655412936		O	16.018112729	3.961926261	3.863986537	
O	4.645641511	3.326740680	1.565802006		O	4.876501460	3.525655119	1.464683432		O	4.869484039	3.698824960	1.672875192	
O	14.488376894	10.960186712	5.262672312		O	15.005904839	11.087182536	5.550788915		O	14.874324991	10.744643729	5.781450390	

O	14.150742370	3.832532811	5.891279203	O	14.670275921	3.443460542	5.788764226	O	14.567759986	3.476759518	6.097619266
O	14.491480364	10.855734113	2.129503755	O	14.433355780	10.659286581	1.938263054	O	14.394009344	10.375379048	1.725647487
O	4.807220134	10.982773907	1.919090692	O	5.265095870	11.072801220	2.055123379	O	5.398685738	11.043293584	2.226331581
O	4.919795783	3.801336946	5.780527992	O	5.061555516	3.234507382	5.547682659	O	4.798546644	3.419546748	5.499133159
O	4.962610462	10.351846249	5.639458224	O	4.940742895	10.717673023	6.385891576	O	4.806006037	10.912278599	6.167168337
O	14.315237795	3.591277521	1.520509417	O	14.287989659	3.463914815	1.608499608	O	14.229530531	3.252648107	1.789313376
O	2.184693773	1.299339192	0.199516648	O	2.505079844	1.324405555	0.067112709	O	2.564124523	1.495516823	-0.119712040
O	17.155803601	12.998601319	-0.207070537	O	17.435356068	13.159546652	-0.580885710	O	17.295264486	13.053540899	-0.282843684
O	16.988393637	1.277510195	0.329394121	O	16.996882007	1.340882144	0.068701656	O	16.972284800	1.294549852	0.282377815
O	2.133222234	12.990773541	0.178863936	O	2.369880290	13.037334161	0.273223561	O	2.132626170	13.254070379	0.071361487
O	11.666134683	8.457379230	4.029210413	O	11.770065751	8.362059968	3.767982433	O	11.850842528	8.377106351	3.959130942
O	7.761636068	5.900305759	4.184183588	O	7.596839370	5.706899519	4.347220252	O	7.496466789	5.832521421	4.171030472
O	7.520888819	8.490328817	4.054317054	O	7.994460587	8.239186928	3.568898045	O	7.839752595	8.371839902	3.455185243
O	11.551510528	5.858004330	3.558603179	O	12.025014569	5.837851721	2.964760792	O	12.097678292	5.808705107	3.322750359
O	0.070092313	2.794769550	-0.216419728	O	0.257358394	2.638036962	-0.077716730	O	0.221022752	2.670682960	0.082216596
O	0.137285389	11.276789299	-0.126239738	O	0.264818966	11.484235204	0.339963186	O	0.247042498	11.484686156	0.450683595
O	9.606071286	10.075479459	3.888311909	O	9.982819695	10.310581366	4.009589790	O	9.942804072	10.233787991	4.075356664
O	9.551797219	4.125553791	3.426898303	O	9.669823166	4.197982869	3.526529496	O	9.610027184	4.284762244	3.700176633
O	4.283889323	-0.047930464	1.062946184	O	4.505837652	0.010618288	1.187635230	O	4.400902243	0.013870733	1.059711465
O	15.379256271	0.202600454	6.048545736	O	15.494324422	0.189760338	5.795696857	O	15.577815261	0.196631376	5.890130327
O	15.052612898	-0.370970734	1.076970862	O	15.283634997	-0.462767179	0.893246465	O	15.097791393	-0.386712354	0.963201501
O	3.656451448	-0.017086467	5.981536627	O	4.049221122	-0.158538434	6.078208672	O	3.946921479	-0.152199209	5.930245224
O	13.381077985	6.811800794	5.197290015	O	13.871327286	6.935303013	4.542669050	O	13.963441880	7.063366438	4.802889145
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O	5.603233815	7.089614448	5.156403627	O	5.835291073	7.567712455	4.984424815	O	5.653911797	7.571128782	4.828508013
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O	4.899152384	-0.160915464	3.661618694	O	5.122664636	0.269012149	3.732402279	O	5.084383230	0.315256678	3.607189485
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O	14.238075220	7.079717576	0.079103446	O	14.482015533	7.344615894	-0.450655858	O	14.744351579	7.585562457	-0.234483799
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Si	1.661344688	2.820187813	0.012598048	Si	6.420025321	11.359032875	6.111949785	Si	6.328613434	11.479637752	6.008499325
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Si	1.733160100	11.435180425	0.034798117	Si	15.948070544	10.111239978	1.817019568	Si	15.952897138	10.002299277	1.942543309
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Si	14.728864452	7.066126773	6.060780522	Si	5.744517752	0.197064388	2.232325343	Si	5.656524015	0.249898491	2.084892423
Si	11.146579071	4.280796447	3.603668239	Si	14.103051680	-0.057082233	4.963716092	Si	14.159828151	-0.062818705	5.102442646
Si	4.106229463	7.050693227	5.742848747	Si	13.985888193	-0.336772806	1.894316074	Si	13.868813207	-0.381721021	2.040993998
Si	14.793697282	7.316333693	1.563836736	Si	5.484958358	-0.084006744	5.281106687	Si	5.395699444	0.020025401	5.180013617
Si	3.082502587	-0.015665629	-0.035277565	Si	15.089392623	7.161251601	5.589793930	Si	15.212801404	7.163810198	5.813902542
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Si	3.435737721	4.139751652	5.272109372	Si	12.796726812	7.185430700	3.326351880	Si	12.862720143	7.178638136	3.573732111
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Al	4.457440291	7.046962931	1.742273915	Si	3.785492086	4.263297489	5.120561950	Si	3.518106912	4.434086645	5.034666160
Al	15.777768162	4.139033831	2.233530894	Al	15.656742097	4.367527725	2.072922881	Al	15.569643402	4.202599282	2.232959079
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H	16.787821886	6.266533454	1.811530532	H	1.113627186	10.511010649	2.781110900	H	1.448682584	10.962098282	4.076859320
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H	7.795600366	3.456258231	0.180089669	H	17.760305889	3.402341744	2.045432038	H	17.874471586	4.265032523	1.627457007
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