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 ($E_{ads} = -19.2 \text{ kcal mol}^{-1}$) 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–CH₃ 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 cycles⁶ 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/Al₂O₃ shows great selectivity in the alcohol conversion process with products within the range C4-C12.1 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 threedimensional (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 firstprinciples 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) exchangecorrelation 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 $10^{-6}\,\mathrm{eV}$ 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 $1 \times 1 \times 1$ 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:

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

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 XCRYSDEN²⁸ and VESTA software²⁹.

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 Alsubstituted 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 data33,34 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).

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 yield-ing the most stable methanol adsorption structure in ratio

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).

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.

	Si/A	l = 5	Si/Al = 8						
Tetrahedral sites	E _{ads} (kcal mol ⁻¹)	$d(O_{meth} - H_{fram}) \mathring{A}$	E _{ads} (kcal mol ⁻¹)	$d(O_{meth} - H_{fram}) \dot{A}$					
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					

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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 $\pm 0.02 \text{ e/Å}^3$, 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 motions³⁹ 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



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).

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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 $\pm 0.02 \text{ e/Å}^3$, 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-CH₃ 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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Supporting Information

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

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	Coordinates f	or zeolite FER	R Si/Al =5	/Al =5 Coordinates for zeolite FER Si/Al =5							
	Acidic zeolite	FER with no 1	methanol			Acidic Site	s with Methano	l adsorl	oed at various 🛾	l'sites	
	0 Si	Δ1	н	0	c:	T101	ц	0	c:	T102	и с
	72 30) 6	6	73	S1 30	AI	н (73	51 30	AI 6	H C
0	6.038347235	1.243893604	2.022031298	0	6.012952763	1.197318219	1.929151818	0	5.805692812	1.257910022	1.941990164
ŏ	13.070184223	13.173633315	5 5.798869329	õ	13.105723116	13.217485544	5.807890421	õ	13.015627564	13.221941822	5.424975587
0	13.193600083	1.422267511	5.272102671	0	13.108768709	1.481178814	5.174455578	0	13.392913161	1.491902400	5.385129722
0	12.689418534	13.020600023	3 1.853759490	0	12.591761151	13.030220560	1.905728536	0	12.700918530	12.958921777	2.149585839
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0	6.104064790	1.318897538	5.643835833	0	6.060514095	1.357632321	5.622686275	0	6.124696603	1.284015096	5.441048328
0	6.105835889	13.065/15/92	5.982422385	0	6.0/142838/	13.095045883	5.962606780	0	6.409660248	13.0218/6996	5./8145/2/8
0	15.021/28598	8 482205416	5 801449547	0	12.900830137	8 398647644	5 684898524	0	12.905348524	8 557693642	5 498896213
ŏ	3 493400370	5 792432265	1 910992868	ő	3 503066225	5 811757453	1 931063732	0	3 284175889	5 966117437	1 922221636
ŏ	3.699030204	8.375751222	1.795647153	Õ	3.528830179	8.399132058	1.735287984	õ	3.514635663	8.540339505	1.538001133
0	3.024181287	5.803589101	5.833284868	0	2.959314623	5.811026345	5.793513165	0	2.966353488	5.788732029	5.653849605
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0	5.418188208 6.774880327	8.404922701 3.579016156	2 908079693	0	6 812126405	8.423233300 3.485888465	2 888270291	0	7.092264611	8.304333207 3.453036979	2 587795387
ŏ	11 640942141	11 183677740	4 918932096	ő	11 765063537	11 261144887	4 751186162	ŏ	11 567684619	11 145858983	4 812397074
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ŏ	2.367485637	10.545539281	0.959263934	ŏ	2.322184169	10 669336920	0.985884877	ŏ	2.273332095	10.880089319	1.117373186
ŏ	2.317737387	3.296914003	6.268028279	Õ	2.233256508	3.299863629	6.208276367	õ	1.875704933	3.412004829	6.032054688
0	16.697307967	3.523595992	6.416111506	0	16.726318500	3.304800888	6.248690427	0	17.066779696	3.545245154	6.323638738
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ŏ	14.112241376	3.828756682	5.993830965	ő	14.120235186	3 826753703	5.947972518	ő	14 451203913	3.860171129	5.934309214
ŏ	14.336796975	10.742065994	2.153290333	ŏ	14.296731231	10.856094952	1.993613813	ŏ	14.467471784	10.771360549	1.757234087
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ŏ	1.906591481	13.006425316	0.067184099	ŏ	1.814313539	13.107129617	0.047285619	ŏ	1.807654414	13.179216107	-0.146364216
0	12.110027420	8.766614107	3.971331296	0	12.012441365	8.682949336	4.207621888	0	12.261529395	8.684062949	4.148333406
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ŏ	9.329651318	4.004235197	3.400943334	ŏ	9.345812138	4.051368565	3.326125634	ŏ	9.469992806	4.027013141	3.449098242
õ	3.875777333	-0.254676145	1.446515981	õ	3.893073069	-0.363330325	1.394953393	õ	3.838614130	-0.463040452	1.373539088
0	15.428720545	0.123877391	6.010690076	0	15.373438511	0.287030696	6.019351423	0	15.494545384	-0.117957195	5.964586319
0	15.015374890	-0.388325212	1.066178098	0	14.914115799	-0.382207759	1.030928184	0	14.806851735	-0.429149652	0.937948330
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0	5 302413307	6 668576403	4 857777321	0	5.216170426	6 726505459	4 805550487	0	5 367565661	6 524962362	4 832194204
ŏ	13,704946556	7.068827013	2.757724785	ŏ	13.383711392	7.318080550	2.409215956	ŏ	13.650421416	7.064430663	2.556884446
ŏ	4.822412049	-0.251146677	3.889307081	ŏ	4.782526487	-0.202119445	3.862455010	õ	4.854676616	-0.414396022	3.797358379
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0	14.255354236	6.986740195	0.181292018	0	14.321496065	6.844772288	-0.006653173	0	14.405973455	7.540494308	0.068204833
0	4.846318038	6.917215011	-0.116362270	0	4.757431633	6.959291201	-0.142545547	0	4.694394557	6.868403595	-0.172504526
S1 C:	5.891926653	2.831534866	1./32959320		17.673124471	0.803701660	5.449053696 1.686318606		8.977735653	5.203986273	/.453859621
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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
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Si	7.772997023 4.371470781 3.839990517	Si	11.185613414 10.042560909 3.816768579	Si	11.264336602 9.916562287 3.741092548
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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
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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
Н	8.431730780 11.182918702 5.786430539	Al	6.067139728 2.975104682 6.154884512	Al	6.059015778 2.939360641 5.886015664
Н	9.557039414 3.445536261 2.600536528	Н	8.412551632 11.221967081 5.738693593	Н	8.657846394 10.940250625 5.822150080
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Н	16.921817382 6.253927060 1.840479212	Н	1.818133075 10.601172321 3.530266385	Н	2.011675240 10.676239493 3.595415301
Н	11.776705361 13.265437988 2.099619857	Н	16.577843742 6.395457904 2.667042299	Н	16.703060750 6.032614322 1.136922941
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Н	11.241578349 3.217393190 -0.189208264	Н	8.328236086 3.945560499 6.018795785	Н	8.917743105 3.614993689 6.553984626
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		Н	19.754875885 6.872744564 3.671655325	Н	9.258737159 1.320870186 8.248097344
		Н	19.114176916 7.084146674 2.012464871	Н	10.493011937 1.799644175 7.056339810
		Н	19.133717174 5.443716142 2.752088884	Н	8.835426037 1.329823824 6.503201750
		С	19.008100532 6.518692374 2.947604896	С	9.426791625 1.821434754 7.288796797

	Coordinates for zeolite FER Si/Al =5												
		T1O2		P	ciule	Sites with Meth	T2O2	at various 1 s	ne	•		T206	
0	Si		н	c	0	Si	1202 ΔI	н	c	0	Si		н с
73	30	6	10	1	73	30	6	10	1	73	30	6	10 1
0	5.513025804	1.453898386	2.191847094	-	0	5.804171362	1.202858745	1.965362289	-	0	5.922808126	1.348720771	1.982388906
0	12 952751666	13 214139186	5 761268600)	0	13 067481045	12 976490970	5 713501933		0	12 981537411	13 375528986	5 690299366
0	13.148763265	1.471384485	5.205066014		0	13.247374669	1.237704869	5.224408540		0	13.253700772	1.636477121	5.174207529
ō	12.567611236	12.995602806	1.994310093		ō	12.731910601	12.982471825	1.868646467		ō	12.657862728	13.091545512	1.954144193
0	6.185282291	13.219002658	1.859120388		0	6.259310169	12.924919389	1.923969064		0	6.353274112	13.078466139	1.902914279
0	5.990246666	1.330502770	5.612532844		0	6.112223895	1.036492065	5.618822027		0	6.002246620	1.392979672	5.692816486
0	6.250227850	13.099964053	5.960098021		0	5.649760934	12.828653067	6.085338909		0	6.202169973	13.137109286	5.913405634
0	13.038780810	1.279242593	2.007653392		0	13.221741488	1.207355702	2.061726909		0	13.089710586	1.368002745	1.958740005
0	15.325956538	8.466781823	5.679515607		0	15.577282555	8.387526538	5.736141216		0	15.357895157	8.635861293	5.647434984
0	3.119904286	6.082503077	2.035279418		0	3.346749204	5.876012283	2.024829969		0	3.387775103	5.992191986	1.982430656
0	3.599958919	8.640065836	1.696486789		0	3.601246372	8.455240961	1.718834515		0	3.636543660	8.563580131	1.678968740
0	2.875198502	5.839992766	5.609486205		0	3.033849565	5.521495491	5.745051941		0	2.939158264	5.887304685	5.708405678
0	15.796019916	5.872909909	5.984006178		0	15.602728812	5.795348113	5.890240648		0	15.882492782	6.041346985	5.969902332
0	15.752441605	8.575716035	1.768331137		0	15.734792715	8.445376709	1.908207548		0	15.875809934	8.693384538	1.733889697
0	15.875364982	6.001810582	1.890865212		0	15.947303575	5.866981953	1.757709410		0	15.962331511	6.117400252	1.847721975
0	3.299208614	8.441141546	5.696262062		0	3.087823014	8.114109848	5.615266489		0	3.438560621	8.473224746	5.666849026
0	6.830011039	3.686685628	2.713028362		0	6.963872915	3.495417284	2.641245769		0	6.955306390	3.643609640	2.849016124
0	11.626826325	11.151115950	4.847504872	2	0	12.091216709	10.648006132	4.861749069		0	11.680297489	11.302350593	4.789820141
0	11.587597624	3.600679604	5.142619750		0	11.463836720	3.184311537	5.108497298		0	11.793319500	3.846443385	5.131380416
0	11.346623583	10.491520922	2.303221626	;	0	11.249372266	10.710654422	2.377379675		0	11.396040241	10.614622538	2.258519580
0	7.456801976	11.013019837	2.609337877		0	7.622802296	10.698673555	2.486922204		0	7.540915914	10.796488587	2.457135486
0	7.458626296	3.760199384	5.312315674		0	7.640601080	3.499818990	5.252470624		0	7.500122758	3.858040323	5.430744491
0	7.616665045	10.876931038	5.448847964		0	7.359726354	11.048424315	5.247343751		0	7.676569378	11.019383521	5.325440497
0	11.576725577	3.477536971	2.259277127		0	11.647868497	3.325503069	2.216753246		0	11.711899007	3.543798719	2.319646912

	0 16.700941489 10.591043967 6.384058081	0	17.165302677 10.432765759 6.287197737	0	16.744976587 10.774406787 6.324273542
	0 1.814206839 3.924112624 1.201606556	0	1 899597779 3 835916535 1 143605398	0	1 921833002 3 917164392 1 245429330
	0 2 273212445 10 927815026 1 200074940	õ	2 593308771 10 846361752 1 093266940	0	2 3353800/5 10 832913635 1 103561970
	0 1 020421642 2 416469492 6 060276240	0	2.333300771 10.840301732 1.033200340	0	1 067680400 2 464006072 6 116010628
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	0 16.769145504 3.407211972 6.362557384	0	16.552954075 3.362577110 6.385036639	0	16.959769162 3.607655973 6.348560566
	0 16.877926739 10.952094795 1.488152715	0	16.675073386 10.835845486 1.363518149	0	16.909312903 11.118941409 1.433784590
	0 17.136512891 3.679168977 1.463323355	0	17.161268037 3.507019916 1.456017195	0	17.214330530 3.795434073 1.470797327
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	0 6.563472583 2.891111983 0.248541885	0	6.633819309 2.985985051 0.143292024	0	6.671876487 3.211531730 0.282587867
	0 12 472878769 11 157361688 -0 181933851	0	12 562207459 11 001874914 -0 130716883	0	12 521388585 11 301686987 -0 242920030
	0 12.47267085 2.626209279 0.080200426	0	12,11707/118 2,207686608 0.00/685858	0	12.521500505 11.501000507 0.242520050
		0		0	
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	0 14 244675023 10 923297084 5 397670835	0	14 618116390 10 886397347 5 740459324	0	14 300126297 11 103130997 5 341608633
	0 1/ 159916707 3 820505509 5 955010202	õ	13 9703579/1 3 750195262 5 801982660	0	1/ 3371737/1 3 908/08130 6 065878937
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	0 9 575398554 9 663812735 4 122567495	õ	9 650408511 9 780425958 4 314922418	0	9 680286790 9 734669708 4 117585044
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	0 14.401011316 -0.282555878 3.665119662	0	14.533155930 -0.462043291 3.655089285	0	14.470945761 -0.161827800 3.621739514
	0 14.197774226 7.153998124 0.140621174	0	14.218192528 7.170482873 0.146149551	0	14.274622356 7.303416051 0.113132070
	0 4.526555332 6.887200048 -0.086282403	0	4.638836276 6.841787573 -0.117140273	0	4.734614188 6.941319429 -0.132475994
	0 8.256757549 1.073452213 0.135315761	0	8.583880939 13.271481208 4.992819687	0	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
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	Si 12 817540284 2 915837041 5 915331406	Si	12 769761222 2 658139711 5 884554224	si	12 949976767 3 077888538 5 077888202
	C: 15 CCCE70177 A 370405734 5 547337674	с:	100000000000000000000000000000000000000		1E 7027210EE & A2EE041C0 E ECE20C204
	JI 10000/01// 4.2/9495/34 5.54/33/6/4	21	15.500384373 4.204255108 5.479423611	51	13./32/21005 4.435504160 5.565396891
	51 15./18645/43 10.142266414 2.291876490	51	15.009348148 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 700691621 / /11011572 2 990/62927	Si	7 708540650 / 222112607 2 842205271	Ci	7 846848758 4 424224045 2 081074801
	Ci 5 011822600 0 001000200 2 400054000	с:	5 110070500200110007 - 3.040200105	- Ci	5 220200559 0 104425234 2 200220000
	51 5.011823609 -0.081999288 2.400054898	21	5.1198/2588 -0.20/019090 2.209/99185	21	5.239399558 -0.104425224 2.288220909
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	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 0.190010672	Si	2 813047906 -0 063331884 0 097174127	Si.	2 971762448 0 011710271 0 100226090
	2: 15 012430404 0 001203124 0 033004000	וכ יי	2.01304/300 -0.003331004 0.00/1/412/	ונ יי	2.371702440 0.011710271 0.100030383
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L	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
н	8.428568317 10.870954700 5.995725649	н	7.901558689 11.936663304 5.166787690	н	8.483015266 11.111919679 5.870134504
н	9.327022014 3.589035756 2.520909599	н	9.430261943 3.442547260 2.445177054	н	9.477726285 3.000537705 3.265885572
н	1.816662569 10.618998084 3.653026664	н	1.817263851 10.528285257 3.542731505	н	1.882164408 10.635429440 3.581969396
н	16.787719795 6.181326479 1.585073386	н	16.836003339 6.026332587 1.383387012	н	16.884138587 6.284039708 1.564520326
н	11.713695656 13.208187478 2.421308452	н	11.838928727 13.362426573 1.972738643	н	11.761968183 13.360395642 2.233712895
н	7.384521150 2.171329535 0.263112960	н	7.399544035 3.599101817 0.160992266	н	7.590578648 3.553648585 0.273579347
н	7.752108641 0.497657932 -0.480963893	н	8.220374659 13.847185070 4.293988915	н	10.744797340 2.008143594 2.613090188
н	10.007984177 0.350353950 -0.769414637	н	10.516910223 12.980931222 4.195643414	н	10.783490815 0.184307678 3.964670481
н	10.219871958 1.695199940 0.389896158	н	10.350647038 12.885579416 5.968342229	н	9.016888273 -0.005528462 3.711931324
н	9.545138016 2.028514750 -1.235634200	н	10.288450362 14.480173466 5.170344101	н	9.663741636 1.208890414 4.880050573
С	9.590547264 1.302273380 -0.415165707	С	10.021656569 13.421005330 5.072467118	С	9.823236122 0.712976042 3.912244543

Coordinates for zeolite FER Si/Al =5										Coc	ordinates	for FER at S	i/Al=8	
		Acidic Site	es with Metha	nol	adsor	bed at various	T sites				Acidic	zeolite F	FER without	methanol
0	c;	1301	ц	c	0	с;	1308	ц	c		•	C:		
72	30	AI 6	10	1	72	30	AI	10	1		0	22	AI	H
73	C 100008782	1 441471702	2 05 (027722	1	73	C 205055802	1 202825120	2 072515080	T	~	72	32	4	4
0	0.100008782	1.4414/1/02	2.050927732		0	0.305055892	1.393835120	2.072515980	2	0	12 024	100722 1	1.185/59926	1.993253779
0	12.981930099	1 440264509	E 220600200	L	0	13.0918/248/	1 407526100	5.74101483	5	0	12.924	100/33 1	1 419450527	5.0931/99/2
0	12.962114019	1.449504506	3.339090309	•	0	13.10/0556//	12 01 4201241	1 02605211	5	0	12.920	403901 . 750113 1	1.410439337	1 027272254
0	6 464850210	12 128807000	1.999310975	,	0	6 452722851	12 007071075	1 7865/780/	5	0	6 4052	7 JO442 1	2 87/261510	1.096526590
0	5 967529242	1 22//22611	6.060041255		0	6.068084645	1 25/706876	5 742672844		0	6 0012	062010 1	2/0111077	5 600112190
0	6 218906556	12 969577165	5 797871792		0	6 1101361/3	12 986915258	5 8099821/3		0	6 1830	12000510 1	3 070571950	5 995629297
0	13 006365585	1 316503102	1 872910576		0	12 976097190	1 200003030	1 922538856		0	12 975	90902 I.	1 3 2 7 4 5 9 9 0 4	1 866452618
0	15 32/052/72	8 /08607311	5 560086345		0	15 3766513/6	8 461124728	5 619376073		0	15 3/7	821/0/	8 4 2 0 5 3 4 4 1 0	5 637826461
0	3 315881575	5 932515246	1 967745576		0	3 394919765	5 720307899	2 236461597		0	3 6254	163118 5	805653970	1 877468187
0	3 887160388	8 579429081	1 947760208		0	3 870510035	8 541532008	1 984237919		õ	3 5146	52750 8	418099776	1 814275204
0	2.988880385	5.721731645	5.715230134		õ	3.088487703	5.697624131	5.246244645		õ	3.0231	48842 5	.833433249	5.843682070
0	15.814020735	5.832059651	5.984281229		õ	15.856469775	5.863153564	5.933883653		0	15 757	052284	5 812328552	5 890394729
0	15.811439856	8.553282850	1.787425227		0	15.787674029	8.542572545	1.756550222		õ	15.687	578840	8.601053992	1.729201110
0	16.008998045	5.960660091	1.786216870		0	15.946547956	5.952738916	1.838157768		ō	15.899	989869	6.012002151	1.889591200
0	3.278166249	8.315125018	5.534801899		0	3.303851640	8.310098643	5.450490224		ō	3.2619	65578 8	3.445545427	5.612189398
0	7.135339556	3.765570832	2.819667164		0	7.060935441	3.852019701	2.723256803		0	6.9862	36974 3	3.514984918	2.862392787
0	11.721996081	10.995493863	4.908179690)	0	11.955977440	11.067834305	4.78099584	5	0	11.683	053629 1	0.938272728	4,939374025
0	11.734749770	3.767597653	5.063972299		0	11.644529196	3.680120342	5.049027484		0	11.648	135428	3.702306132	5.042953092
0	11.456164161	10.552384994	2.310177224	1	0	11.539978661	10.483317774	2.23388985	5	0	11.341	806122 1	10.567554532	2.333876388
0	7.405468368	10.764493441	2.615133046		0	7.475300860	10.777360593	2.455622394		0	7.5492	238392 10	0.530325400	2.450064547
0	7.741214557	3.474018506	5.390670291		0	7.748893875	3.533009239	5.283963322		0	7.5866	59784 3	8.778769585	5.403588514
0	7.735942950	10.843249550	5.409201653		0	7.683421861	10.955385457	5.300801809		0	7.5005	89841 10	0.980025532	5.103449447
0	11.789282942	3.600986289	2.388865819		0	11.840119656	3.622529842	2.361724513		0	11.649	880283	3.547136472	2.356131481
0	16.797563970	10.416246066	6.398154258	3	0	16.974933749	10.430665561	6.33614955)	0	16.818	346320 1	10.492590147	6.364140816
0	2.065430244	3.739146242	1.216192601		0	2.033406462	3.667213956	1.273113987		0	1.9804	90095 3	3.838077724	1.274055379
0	2.206863239	10.514119718	1.204846852		0	2.281685178	10.484694708	1.085196795		0	2.3973	379091 10	0.699567401	0.981268461
0	2.232828560	3.244285478	6.083157925		0	2.234677421	3.369870799	6.131376580		0	2.1733	329078 3	3.346485653	6.171381053
0	16.862892544	3.408681761	6.336672085		0	16.734246712	3.378000577	6.378162470		0	16.847	590881	3.406865831	6.278758473
0	16.990790212	10.905697741	1.468204837	7	0	17.025572159	10.864548469	1.42896443	3	0	16.824	181013 1	10.972502358	1.451943234
0	17.232585944	3.584752149	1.455163282		0	17.244191277	3.611628071	1.470840599		0	17.135	279027	3.669257621	1.380060871
0	2.300348511	10.993190076	6.128468269		0	2.218684526	10.938433555	6.027913451		0	2.0026	502898 1	1.059524031	5.915863992
0	6.809662434	3.286097925	0.276269174		0	6.868290418	3.179944951	0.196818050		0	6.5219	85356 3	8.186101540	0.266727729
0	12.637860759	11.178373676	-0.165903063	3	0	12.759036732	11.121958852	2 -0.22083501	6	0	12.596	937027 1	1.113198862	-0.140178104
0	12.311620972	2.900140336	-0.065605791		0	12.320726648	2.814989202	-0.084621752		0	12.238	504777	2.881730271	-0.089679420
0	6.622557303	11.174508770	0.158991767		0	6.494477191	11.054854602	0.048826351		0	6.6035	594132 1	1.018462920	0.039627537
0	16.326148564	10.102960505	3.836971539	9	0	16.410860040	10.047211814	3.80362031	3	0	16.260	043617 1	10.084977990	3.828127416
0	2.982806735	3.931654514	3.717155684		0	3.147512306	3.509025816	3.700050923		0	2.7601	48244 4	1.183808863	3.776241158
0	2.886919995	10.368870478	3.656203641		0	2.808703760	10.347302886	3.574285027		0	2.7825	556697 10	0.319127841	3.519162266
0	15.960361581	4.112730969	3.954617387		0	15.904853714	4.058893476	3.963222554		0	15.858	435954	4.019574699	3.913935382
0	4.686522824	3.684858527	1.676162369		0	4.654589257	3.444531929	1.531943542		0	4.4899	12303 3	3.273431817	1.986370793
0	14.368024448	10.922309818	5.389407602	2	0	14.559669218	11.027330464	5.39259316	1	0	14.335	048955 1	10.898985673	5.429010348
0	14.261549464	3.702890832	5.936487176		0	14.161739772	3.858173798	5.931863250		0	14.201	905880	3.688306687	5.929589659
0	14.371254856	10.776813307	2.106549202	<u>′</u>	0	14.434619418	10.810743417	2.12791305	4	0	14.245	326965 1	10.794729248	2.199419747
0	4.758340162	11.131273484	1.981255171		0	4.779870259	11.076547987	2.006305901		0	4.9108	386919 10	0.677075771	2.037983208

		-			
0	4.835541574 3.757398532 5.643491634	0	4.850628395 3.795115450 5.755378857	0	4.741235258 3.836965361 5.551781955
0	5 004742528 10 554781000 5 522400000	0	5 052748021 10 561001052 5 265252221	0	A 979219299 10 777610969 5 520750109
0	5.054745550 10.554761005 5.552455550		5:055740551 10:501551555 5:505252551	0	4.070310200 10.777013000 5.535750100
0	14.338679214 3.622581335 1.592579645	0	14.368759085 3.539084326 1.546815390	0	14.211939872 3.693375312 1.585250528
0	2 286824152 1 288964637 0 313599641	0	2 138774001 1 256312937 0 185385993	0	2 351411049 1 386719322 0 420909214
U	2.200024132 1.200304037 0.313333041	0	2.130774001 1.230312337 0.103303333	0	2.551411045 1.500715522 0.420505214
0	17.006414923 12.921597382 -0.275252370	0	17.014417022 12.928325765 -0.262853863	0	17.008719334 12.984817364 -0.269105507
0	16 962678454 1 201110756 0 325182587	0	17 018106508 1 203897976 0 366066392	0	16 8/1537382 1 261855333 0 328989079
0	10.502070454 1.201110750 0.525102507	0	17.010100000 1.200007770 0.000000052	U	10.041337362 1.201033333 0.320303075
0	1.954637576 12.994114676 0.346575532	0	2.151109695 12.971711561 0.242772689	0	1.874315764 13.133555578 0.079833064
0	12 11/8/62// 8 562369065 3 950/76106	0	12 003297778 8 534736834 3 994606221	0	11 825852200 8 498427037 3 961744063
U	12.114040244 0.302303003 3.330470100	0	12.005257770 0.554750054 5.554000221	0	11.023032200 0.430427037 3.301744003
0	7.730549295 5.907927398 4.245061927	0	7.847769574 5.946424768 4.138187950	0	7.561469402 5.959632148 3.832598692
0	7 037753685 8 430566875 4 191034131	0	7 199420151 8 491909551 4 096640268	0	7 164633552 8 531203377 4 158844272
0	7:057755005 0:450500075 4:151054151	0	7:155420151 0:451505551 4:050040200	U	7.104035352 0.351205377 4.150044272
0	11.472481077 5.968573413 3.571511457	0	11.463872525 5.934177975 3.618132861	0	11.424205778 5.910940971 3.572385795
0	0 082735722 2 636085785 -0 145856830	0	0 048511200 2 754355489 -0 221655464	0	0 0/9/82733 2 585802195 -0 079063053
Ŭ	0.002/33/22 2.030003/05 0.143030030	Ŭ	0.040311200 2.734333405 0.221033404	U	0.049402793 2.909002199 0.079003095
0	0.034748455 11.244999196 -0.091308398	0	0.092737698 11.358147643 -0.026100223	0	-0.006077056 11.283877765 0.092112321
0	9 673224650 9 580751286 4 046074185	0	9 731162386 9 865981479 4 086702125	0	9 511812780 9 693285168 4 045943200
0	5.075224050 5.500751200 4.040074105	0	5.751102500 5.805581475 4.888702125	U	5.511012700 5.055205100 4.045545200
0	9.574361025 4.127016787 3.588595573	0	9.569544552 4.079313473 3.437746378	0	9.471502841 4.146228979 3.632710801
0	4 097873116 -0 186734998 1 397252336	0	4 193729868 0 024148191 1 205053739	0	
Ŭ	4.057075110 0.100754550 1.557252550	Ŭ	4.155725000 0.024140151 1.205055755	U	4.050500554 0.402557075 1.550251772
0	15.259309534 0.247675830 6.103331869	0	15.373152134 0.298746596 6.049284829	0	15.198796441 0.220586088 6.087497697
0	15 003764254 -0 398270427 1 130827179	0	14 988649532 -0 354310947 1 066522899	0	1/ 9//09/389 -0/12887/0/ 111707/692
0	15.005704254 0.550270427 1.150027175	0	14:500045552 0:554510547 1:000522055	U	14.544654565 0.412667464 1.117674652
0	3.782200993 -0.295140883 6.260211185	0	3.762596053 -0.090380583 6.086563415	0	3.833037052 0.004924550 6.237287007
0	13 343510036 6 636234776 5 293952889	0	13 402975511 6 682580732 5 238526146	0	13 311399828 6 712297244 5 241633845
	15.5+5510050 0.05025+770 5.255552005		13:402575511 0:002500752 5:250520140		13.511355620 0.712257244 5.241055045
0	6.139925493 6.761183321 2.259412313	0	6.025333955 6.773831532 2.3988888857	0	5.869731721 7.216631716 2.234683815
0	5 192779200 6 613131593 / 6837203//	0	5 532027464 6 771473074 5 111316445	0	5 253020283 6 827538417 4 811543645
0	5.152775200 0.015151555 4.005720544		5:552027404 0:771475074 5:111510445	0	5.255020205 0.027550417 4.011545045
0	13.783219579 6.938792378 2.710046481	0	13.684679219 6.998536204 2.640722983	0	13.614967510 7.068259240 2.644681830
0	4 927413807 -0 030807177 3 903545229	0	4 933804538 -0 153060302 3 735303685	0	4 886777803 -0 289181488 3 853496803
	4.527415667 0.050607177 5.505545225		4.555004550 0.155000502 5.755505005		4.000777003 0.203101400 3.033490003
0	14.403327090 -0.062521048 3.680555448	0	14.436562497 -0.125161938 3.648180549	0	14.305054629 -0.129497312 3.667034337
0	14 266415221 7 171985544 0 126238502	0	14 270662994 7 137157647 0 093600119	0	14 216470768 7 089457496 0 096603083
U	14.200415221 7.171505544 0.120250502	0	14.270002554 7.157157047 0.055000115	0	14.210470708 7.005457450 0.050005005
0	4.777923139 6.950043139 -0.253128566	0	4.049200723 6.795268800 -0.107538430	0	4.773018448 7.128183729 -0.152140516
0	1 010/7/501 7 023221657 2 01106/835	0	1 / 75901773 7 196791612 0 132112251	Si	6 02/82875/ 2 792521071 1 7/1089062
0	1.010474501 7.025221057 2.011004055	U	1.475501775 7.150751012 0.152112251	51	0.024020/34 2./323210/1 1./41003002
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
51	12:521041700 11:550502255 5:052524511	51	15.070240570 11.570000571 5.020545101	51	0.50001/11/ 11.2000/0045 1.015550///5
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
0.					
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
51	13:7378888337 4:242838148 3:328438143	51	13.00/123042 4.204303/75 5.327233010	51	15.710155150 10.157570554 2.500125045
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
51	1.074045100 2.741755452 0.050000557	51	1.055045245 2.770000004 0.055555075	51	17.410502200 11.451557452 0.011000751
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
51	17.517550450 2.750250045 0.125705525	51	17.501005140 2.757575075 0.152050051	51	1.571221700 11.555000255 0.105515427
Si	1.639615439 11.444304388 -0.033996839	Si	1.696848193 11.461336040 -0.097499752	Si	11.086377732 9.946843920 3.793310869
Si	11 20/21631/ 9 9225/691/ 3 77/726888	Si	11 280853/97 9 987572/27 3 7/686768/	Si	7 897393312 / 38805/596 3 833296709
51	11.204210314 5.522540514 5.774720000	51	11.200055457 5.507572427 5.740007004	51	7.857555512 4.588054556 5.855250705
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
51	5.500725550 0.001255005 2.545550104	51	5.455667761 0.005256675 2.205405521	51	15.054555721 0.071550550 5.222000055
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
0.					
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
51	14.700272274 7.010051157 0.100704050		14.742055500 7.044020055 0.070110255		4.449057940 7.1191955500 1.491101970
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
		<i>.</i>		<u> </u>	
SI	14.893434598 /.243562299 1.603920489	51	14.852661292 /.242828414 1.583512414	51	3.040884967 -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
<u> </u>	16.074956221 0.07502201 0.0724 47202	<u>.</u>	16 116126441 0.045402500 0.000000475		
51	10.074820331 -0.072923601 -0.072147308	51	10.113130441 -0.043402589 -0.0868981/5	51	12.3230300/2 /.000304/60 3.8644/4561
Si	12.635662651 7.050996817 3.885026472	Si	12.601856796 7.058759714 3.875888989	Si	3.448960399 10.018206061 1.976836639
ci	3 514329008 10 107003854 2 082072529	C;	3 515454973 10 073/1/279 2 0///01067	Ci	3 223790095 4 268622299 2 222942464
5	3.31+323000 10.107003034 2.002372330	5	3.515454575 10.075414575 2.044401907	5	5.225750055 4.200022255 2.252545404
Si	3.253/51135 4.266681307 2.174130591	Si	3.291/58063 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
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SI	12.9082/4454 2.911/40501 1.449299990	51	12.919390945 2.800310102 1.432202553	51	11.084284/15 4.3241342/6 3.652519515
Al	7.992922283 9.787375732 3.887136548	AI	8.060592712 9.908487985 3.801852375	Si	7.925211545 9.949284975 3.930454156
	A 676120064 7 112116025 1 425500570		4 474271109 6 05000705 1 004027450	A1	2 220206675 10 122220204 5 207122244
AI	4.0/0130904 /.112110035 1.4355885/0	AI	4.4/43/1198 0.930800/05 1.69492/459	AI	5.5202000/5 10.123229294 5.30/133244
AI	3.476004589 9.993358027 5 374510083	AI	3,434553924 10.001522799 5 260391663	AI	15,738430993 4.157644133 2 233375489
AI	15.832235894 4.138269044 2.268640029	AI	15.816150014 4.110036022 2.274951741	AI	12.715383762 11.205679692 1.542523963
Al	12.816892991 11.204284689 1.515505044	AI	12.893045999 11.182094044 1.467452170	Al	6.065984472 2.953784904 6.158534242
	6 259127200 2 012202407 C 000405020	A 1	6 207856202 2 022762105 5 076142520	ц.	1 022077016 10 000550560 2 500540205
AI	0.23013/399 2.91228248/ 0.0001059/9	AI	0.231830203 2.323103195 5.970143539	п	1.322011010 10.903220000 3.203018530
н	8.566836489 11.000097469 5.896941260	н	8.506800534 11.131635801 5.796807492	н	16.826130228 6.218920390 1.647603195
	2 264214200 6 270002070 1 001147027		2 012070065 6 856070444 0 062024070		11 66104E31E 12 27E740E30 2 027C0244C
н	2.304314200 0.378892879 1.991147937	н	3.013370005 0.850970441 0.062934078	н	11.001945215 13.375749530 2.037683146
н	2.110167560 10.964873440 3.679368534	н	1.970565243 10.849914525 3.593191528	н	8.307671326 3.869662216 6.058127224
	16 000603406 6 100300334 1 300043545		16 9EE06E117 6 1220E177E 1 512720422	1	
н	10.000092400 0.108200324 1.380913515	н	10.00000111/ 0.122951775 1.512720432	l	
н	11.762802043 13.313230571 2.201539594	н	11.782124326 13.281892219 2.112854355	I	
	7 665272912 2 760451690 0 246270022		7 705564007 2 404285402 0 486740062	1	
н	/.0033/3812 3./00451680 0.2463/0023	н	7.735564997 3.494285403 0.186710963	1	
н	1.106391334 7.889537129 1.566397175	н	1.400522233 8.063318502 -0.308396020	1	
	1 204722942 7 002000255 4 000050000		1 221257260 7 200220640 2 222022064	l	
н	1.304/32843 /.003898355 4.006558669	н	1.32125/308 /.389230618 2.22292/011	l I	
н	0.242983555 6.243023713 3.756278832	н	0.275283297 6.164675364 1.447696773	1	
			0 139575069 7 010053013 1 303780504	1	
н	-0.303500871 1.880560932 3.363068/10	н	-0.1283/308 /.919053012 1.293/80594	l	
	0.517710488 7.232456778 3.371970870	С	0.685440855 7.180293065 1.350371842	l	
C			· · · · · · · · · · · · · · · · · · ·		

				Acidic	Coordinate Sites with Meth	es for FER at S	Si/Al=8 Lat various T sit	06			
		T101		Actuic	Sites with Meth	T102	at various 1 si			T103	
0	Si	Al	н	со	Si	Al	н с	0	Si	Al	н с
73	32	4	8 1	1 73	32	4	8 1	L 73	32	4	8 1
0	12.998831474	13.132077154	5.681176665	0	12.917691111	13.123674815	5.544990310	0	5.745425190 12 829488743	1.390912760	5 626829721
0	12.991900660	1.428349544	5.272088662	0	13.200611139	1.405977285	5.303664028	o	12.906581985	1.416199401	5.362707862
0	12.518070557	13.070037866	1.883228925	0	12.552412706	13.050653882	1.885501393	0	12.514781616	13.072222266	1.949062768
0	6.351669943	12.869405418	1.975299373	0	6.407850722	12.879691595	1.869043557	0	6.278996361	13.105977068	1.968944590
0	6.082206594	1.342437326	5.612141698	0	6.120113347	1.275617163	5.533705561	0	6.037168847	1.323464301	5.697313304
0	6.149//3439 12 20122/622	13.069616247	5.998068613	0	6.291840290	1 221655044	5.897650623	0	0.28/339818	1251021221	6.012977604 1 820045170
0	15.403663087	8.382436497	5.697911223	0	15.406612573	8.464600892	5.673046442	0	15.293203447	8.441874385	5.696097680
0	3.595790910	5.789135415	1.894879568	0	3.511723354	5.838601775	1.822896021	0	3.255424448	6.000217462	2.038142966
0	3.475855887	8.395282242	1.822653366	0	3.479696874	8.450884824	1.700447849	0	3.520201517	8.575607946	1.767882320
0	3.006294610	5.837113210	5.813444336	0	3.032892727	5.811056293	5.806629523	0	2.958536266	5.860417801	5.642331947
0	15.856405649	5.771424957	5.632714870	0	15.884855531	5.878921600	5.949393599	0	15.718384916	5.840087388	5.888667087
0	15.731859410	6.040356263	2.127803364	0	15.923355749	6.035022392	1.825556658	0	15.880588988	6.031819273	1.891650044
0	3.239812570	8.443932389	5.619677514	0	3.377517533	8.392986959	5.462564995	0	3.260865795	8.472845481	5.690665386
0	6.944701411	3.523058901	2.877333607	0	7.188223697	3.457947107	2.587826485	0	6.913898519	3.720140066	2.782383868
0	11.667776620	11.033126456	4.862765121	0	11.640467563	10.938661819	4.871712006	0	11.604966448	10.896316827	4.963234953
0	11.655943869	3.680092878	4.963574198	0	11.835304992	3.616140553	4.967713015	0	11.573398904	3.655169727	5.028917060
0	7 500563980	10.4/3/23965	2.292236822	0	7 569832550	10.480/519/0	2.2/2321383	0	7 /872/0503	10.575190925	2.340005486
0	7.576850092	3.788374885	5.407920101	o	7.394896926	3.804411374	5.242668772	0	7.476340515	3.812710313	5.375576362
0	7.486290752	10.995292146	5.094765230	0	7.578878853	10.849901675	5.119815032	0	7.504583017	10.882515107	5.275471175
0	11.593275758	3.604041138	2.268765359	0	11.660545969	3.569841646	2.282993570	0	11.626151421	3.551862865	2.359596897
0	16.809028858	10.531571983	6.261901049	0	16.787866510	10.625878572	6.314805292	0	16.751677798	10.522297147	6.367989586
0	1.948146343	3.824745510	1.289596840	0	2.001860018	3.771884848	1.223924101	0	1.866631459	3.877825778	1.270956441
0	2.163103125	3.356336114	6.187034718	0	1.911878240	3.437233470	6.108912979	0	1.970145937	3.462327426	6.129484872
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0	16.835501537	10.863951557	1.396778612	0	16.880359281	10.910385481	1.427136130	0	16.778963759	10.969817334	1.472307681
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0	2.006975376	11.070196291	5.892005818	0	2.069459530	10.983798830	5.911486406	0	2.008820484	11.098811484	6.023837171
0	6.511241168 12 529341969	3.190583442	-0 188451596	0	6.318426928	3.207538810	0.149722034	0	6.6422/32/4 12 5/3182218	2.905242316	-0 1/157525
0	12.197654335	2.849045247	-0.158841314	o	12.481284236	2.886722539	-0.131908482	0	12.264486360	2.942090299	-0.092194443
0	6.551444437	11.007944581	0.025485025	0	6.623806484	10.968200407	0.011611831	0	6.552955097	11.117664281	0.168924019
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0	2.743743026	4.154493227	3.782354775	0	2.605267873	4.235710549	3.723235554	0	2.921851558	3.977218742	3.738799556
0	2.737143134	10.294223741	3.505292814	0	2.814314669	10.310394497	3.495836270	0	2.748319466	10.335711533	3.616186712
0	4 464168045	3.804717816	1 972491351	0	4 527701284	4.18/382890	3.905992804 2 115131987	0	4 497960861	4.058229228	3.914746495
0	14.293424992	10.821477072	5.406027002	0	14.293141138	10.877847119	5.356171243	o	14.270546318	10.914551334	5.417009898
0	14.178274050	3.746916798	5.921915530	0	14.399938124	3.715778998	5.871967106	0	14.156885958	3.726088513	5.835164404
0	14.254405232	10.894941377	2.120188440	0	14.275830066	10.835472170	2.104085029	0	14.195965998	10.801201378	2.196586600
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0	16.963756978	12.965250709	-0.226802369	0	17.155613066	13.031374320	-0.119262285	0	16.990407371	12.998837771	-0.225801157
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0	1.8/0041200	13.110117885	0.086988330	0	1.833469095	13.158638567	-0.053241060	0	1./15002008	13.23114/342	0.106986574
0	7.545795897	5.965284381	3.839899691	0	7.603877487	5.900907343	3.607252954	0	7.576724581	6.044996307	3.835579384
0	7.164625079	8.541330131	4.145738079	0	7.166519090	8.464188457	4.059215076	0	7.021058237	8.621349253	3.992267611
0	11.371953008	5.933855489	3.577183903	0	11.449978141	5.874184184	3.623022361	0	11.390897507	5.887102736	3.594649859
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0	-0.032018436	11.277624963	0.021832874	0	0.033133667	11.211214668	0.034794098	0	-0.061339042	11.260619578	0.096458121
0	9.445232446	9.730043905 4.139352661	4.012/98033 3.610848646	0	9.521565782	9.30000229 4.076281844	3.718443366	0	9.393638878	2.02032/181 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
0	15.278074324	0.225361421	5.988955523	0	15.365578581	-0.079498982	5.907120672	0	15.163526487	0.140316971	6.056718796
0	14.848512979	-0.351945441	1.010668153	0	14.853540728	-0.434640617	0.935585307	0	14.854123846	-0.445928573	1.084554180
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0	13.428251847	0.692161809	5.053/69939 2.245872190	0	13.440109019	0.0/8/80189 7 185607020	5.1/5805880	0	13.262010609	b./34436450	5.260105585
0	5.251648527	6.851096472	4.829089646	0	5.347302108	6.680144241	4.800343981	0	5.295154680	6.863001427	4.936943419
0	13.357219133	7.224764946	2.418206396	o	13.582102353	7.033266154	2.577355096	0	13.587229548	7.066755312	2.672874829
0	4.862658353	-0.276497310	3.860218636	0	4.917294866	-0.355800935	3.777169450	0	4.766340013	-0.359540715	3.996018624
0	14.292022859	-0.147188791	3.590008604	0	14.380586122	-0.201105736	3.536945579	0	14.259712749	-0.102854578	3.647500721

0	14 313030926 6 808171649 0 001992923	0	14 205404826 7 100667157 0 058108352	0	14 160355353 7 059422022 0 116739336
0	A 738474471 7 105194155 -0 139708167	0	A 761233207 7 089735501 -0 197833034	0	A 573A33179 6 973A02006 -0 07805A120
0	17 695829617 6 812118252 3 420510776	0	8 544625358 4 364486372 7 288241637	0	8 248844341 1 035553977 0 084738363
Si	6 009712156 2 7881/3123 1 7/33009/5	Si	5 980518098 2 800320797 1 683739458	Si	5 912253198 2 938/9076/ 1 8088/0916
5	12 970002190 11 500201020 5 944054650	с;	12 946997467 11 406697729 E 700042907	C:	12 20212235136 2.336430764 1.606840310
51		51		21	
21		21	6.402338362 11.274021424 1.579163189	21	6.302058093 11.487992932 1.717014932
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SI	15.6/42/2894 4.130586/59 5.380/48338	SI	15.8/8861324 4.29/268598 5.4/2681/24	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
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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
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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 0/1581157 -0 10/510590 -0 15708/186	Si	
Si	12 482700042 7 102882224 2 702218661	Si Si	12 564026215 7 020084754 2 854028672	Ci	12 474485272 7 050070467 2 875217210
51	2 402224520 0 000017057 1 061757240	51	2 465950522 10 040764419 1 045656056	51	2 400562069 10 149567111 2 054250210
51	3.402234329 9.99991/937 1.901/3/340	51	3.403830322 10.040704418 1.943030930	21	2 119225109 4 292220055 2 19527600
21	3.204581447 4.243005424 2.230507827	21	3.175521392 4.294970210 2.210700333	21	3.118225198 4.382220955 2.185376009
21	0.428902484 /.101825374 3.770062205	21		21	
51	3.204515720 4.276066043 5.345104327	51	3.058756605 4.257955293 5.289904636	SI	3.1546/2123 4.26211//03 5.3406/2116
SI	15.64/486804 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
н	1.891141398 10.788999820 3.510458833	н	1.984874121 10.831318893 3.505723601	н	1.876282376 10.783135135 3.623810297
н	16.611289075 6.408712165 2.672854342	н	16.848830027 6.329737731 1.704821836	н	16.806529181 6.288536525 1.703413135
н	11.604147983 13.417591563 1.858215272	н	11.647865641 13.339011291 2.119512034	н	11.611325007 13.342235903 2.205975106
н	8.279783877 3.942270432 6.070539180	н	8.132517208 4.209437387 6.235483710	н	7.454344950 2.172721161 0.286291018
н	17.576659824 6.469201014 4.332959465	н	7.658475252 4.108318444 7.731013421	н	7.712945746 0.564111742 -0.594303010
н	19.780018634 6.894512631 3.625701424	н	9.294623052 2.896868640 8.574680289	Н	10.001911352 0.236808329 -0.731469609
н	19.123418045 7.084536777 1.967854653	н	10.456888264 3.586250096 7.394528035	н	10.193289873 1.590491779 0.434685642
н	19 158333382 5 448803456 2 724984891	н	9 216998544 2 417654014 6 835611899	н	9 636185475 1 936759093 -1 231364793
Ċ	19 033449968 6 525952488 2 908469287	Ċ	9 441277067 3 229531132 7 542018/64	l c	9 605088075 1 209596539 -0 405750097
Č	13.033443300 0.323332400 2.300403287	Ľ	5.7712//00/ 5.225551132 /.342010404		5.005000075 1.205550355 -0.405750097

	Coordinates for FER at Si/Al=8													
				Α	cidic	Sites with Meth	nanol adsorbed	at various T s	ites	;				
		T2O2					T2O6					T3O1		1
0	Si	Al	н	С	0	Si	Al	н	С	0	Si	Al	н	С
73	32	4	8	1	73	32	4	8	1	73	32	4	8	1
0	5.961947262	1.195736957	1.792883148	-1	0	5.958284543	1.331640505	1.642139284		0	6.170113480	1.156280139	1.999076693	
0	13.075578573	12.924127293	5.855079208		0	13.030032336	13.212581785	5.972891076		0	12.981394633	13.066771817	5.723425296	;
0	13.105400323	1.178581210	5.266138986		0	12.979371619	1.464351672	5.331065596		0	12.799225610	1.377509641	5.439853638	- 1
0	12.866753569	12.934964354	1.761638293		0	12.745955770	13.013689269	1.953336510		0	12.577254309	13.151385206	1.880540192	2
0	6.274420300	12.923925984	2.091521473		0	6.318747170	13.069331260	2.126828583		0	6.306158065	12.844596963	1.939263469	
0	6.010440941	1.196033727	5.688450807		0	5.936089156	1.447062796	5.804118859		0	6.131219140	1.329750928	5.591097782	
0	5.700814813	12.934870570	5.881944103		0	6.083364677	13.180894485	5.682452883		0	6.140921077	13.057905990	6.005086453	
0	13.272225336	1.194567581	2.122043893		0	13.007464932	1.284703822	2.054035247		0	13.030544164	1.441438618	1.855527730	
0	15.607448196	8.334651282	5.561813031		0	15.401781134	8.454336615	5.520590410		0	15.443293530	8.316820393	5.540649053	
0	3.447344773	5.817206942	2.007415719		0	3.419205021	5.915084008	1.895493161		0	3.659920958	5.757549643	1.885359837	
0	3.573125970	8.402323876	1.857639566		0	3.654583212	8.493752822	1.845698382		0	3.460232694	8.362239546	1.800876322	
0	3.192100709	5.525151391	5.932573405	1	0	3.155920357	5.750247070	5.930531459		0	3.036810816	5.826816558	5.790052697	
0	15.576849301	5.746551184	5.916157646		0	15.742125675	5.880329899	6.011186720		0	15.847039901	5.723985713	5.384647989	
0	15.631534099	8.445666308	2.062072842		0	15.615625395	8.558098927	1.992199643		0	15.565335383	8.669375020	1.652944813	
0	15.912896268	5.883394448	1.729290140		0	15.894971686	6.002524948	1.777773605		0	15.852919299	5.899667764	2.204068655	1
0	3.196640588	8.119403034	5.642650332		0	3.458983661	8.356738704	5.631726466		0	3.294991562	8.426551105	5.575407210	1
0	7.008030578	3.536244193	2.422032147		0	6.976900337	3.611675551	2.501170122		0	6.905286367	3.523290123	2.895785010	1
0	12.141961805	10.583692975	4.956353427		0	11.852441415	11.064246655	4.982677317		0	11.586338447	10.982168555	4.999114864	ŧ.
0	11.437416797	3.231620863	5.193953649		0	11.499036010	3.62767633	5.284744507		0	11.534499193	3.677867211	5.061117774	

 7.45523999 1.9773920091 1.9773920091 1.9773920091 1.9773920071 1.9773920071 1.9773920071 1.97732072 1.97732072 1.97732072071 1.97732072071 1.97732072071 1.97732072071 1.97732072071 1.9774207471 1.977420741 1.9777772074074741 1.9777777474741<th>0</th><th>11 420020554 10 702005222 2 420547204</th><th>0</th><th>11 440202705 10 744425502 2 284106602</th><th>0</th><th>11 425210272 10 607007240 2 284740125</th>	0	11 420020554 10 702005222 2 420547204	0	11 440202705 10 744425502 2 284106602	0	11 425210272 10 607007240 2 284740125
0 7.48531271 1.5382328 7.48531271 1.5382328 7.58502586 1.51728576 2.58572587 0 7.48531277 1.53823428 2.58523687 7.58502586 1.78545185 5.58722856 0 1.14403589 1.58524458 2.52857357 1.586234278 2.728501278 1.586234278 1.57285478 1.57285478 1.57285478 1.57285478 1.57285478 1.57285478 1.57285478 1.57285478 1.57285478 1.57285478 1.57285478 1.57285478 1.57285478 1.57285478 1.572854778 1.57285478 1.572854778 1.57285778 1.58632883 1.5518588 1.572857171 3.57287843 1.5518588 1.551857883 1.5518588 1.5518588 1.5518588 1.5518588 1.55185883 1.5518588 1.55185883 1.55185883 1.55185883 1.55185883 1.55185883 1.55185883 1.55185883 1.55185883 1.55185883 1.55185883 1.55185883 1.55185883 1.55185883 1.55185883 1.55185883 1.55185883 1.55185883 1.55185883 1.5518583278333 1.55185883	0		0	7 465 4265 00 10 602401548 2 402148208	0	
0 7.40831377 3.5483207 5.0881280 7.4073707 3.53303127 5.16712000 6 7.20901386 3.4484245 5.9327232 0 1.716405627 5.30844173 3.2482235 6 3.24827136 6 3.3078941 6 3.3078941 6 3.3078941 6 3.3078941 6 3.3078941 6 3.3078941 6 3.3078941 6 3.3078941 6 3.3078941 6 3.3078941 6 3.3078941 6 3.3078941 6 3.3078941 6 3.3078941 6 3.3078941 6 3.3078941 6 3.3078941 3.307841 1.3078047111 1.307804711 1.	0	7.577390091 10.615524559 2.436504769	0	7.465426599 10.693491548 2.402148308	0	7.436175969 10.506707173 2.430039687
0 7.450000511 1.937040051 7.45001251 1.93704005 0.93704005 0 7.45001200 1.93704070 1.93704070 0.9370407 0.9370407 0 7.44001200 1.93704070 0.93704070 0.93704070 0.93704070 0.93704070 0 2.938070401 0.93704070 0.93704070 0.93704070 0.93704070 0.93704070 0.93704070 0.93704070 0.93704070 0.93704070 0.93704070 0.93704070 0.93704070 0.93704070 0.93704070 0.93704070 0.93704070 0.93704070 0.937047070 0.937047070 0.93704707070 0.93704707070707070707070707070707070707070	0	7.458315775 3.344853207 5.098015605	0	7.407570274 3.553050127 5.167120806	0	7.599015666 3.814451862 5.392375226
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c) 1:4:00227 0:4:00227 0:4:00227 0:4:00228 0:7:00127 0:4:002087 0:4:000083 c) 1:8:0021018 3:3:0844701 2:4:000083 0:4:000083 0:4:000083 c) 2:8:07:0818 3:3:0844661 3:0:000083 0:4:0:000287 0:4:0000281 c) 2:8:07:0818 3:3:0:00007 3:0:0:0:0:0:0:0:0:0:0:0:0:0:0:0:0:0:0:0	0	11 714907694 3 331795741 2 296110141	0	11 941033960 3 639296485 2 456205647	0	11 780546871 3 699368677 2 398091228
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0 16.00213908 3.3584888 6.34600902 0 16.07855170 3.27785170 6.1005155 5.105785737 4.4465188 0 17.37816878 5.35984411 3.184605150 0 17.33748483 3.077438107 14.6451374 0 16.07327404 5.66462950 0 5.66462950 0 5.66462950 0 5.66462950 0 5.666697100 10.07327404 5.66462950 0 5.66697100 10.07327404 5.66462950 0 5.66697100 10.07327404 5.66462950 0 5.66697100 10.07327404 5.0692209718 5.0672071014521748 0 5.666971001 10.07237404 5.77777110 0 5.56277101 0 5.56277101 0 5.56277101 0 5.56277101 0 5.78671013 5.77777120 0 1.552677101 0 1.562877101 0 1.6649851061 1.6649851061 1.6649851061 1.6649851061 1.6649851061 1.5697710261 1.78517551 1.56677101 1.77217551751 1.56677101 1.77217577771 1.56877110 1.77217577771	0	2.452141195 3.033595136 6.236512466	0	2.381093026 3.234719000 6.196620221	0	2.146088749 3.374424140 6.169009235
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Si7.7555684044.1498638073.718935954Si7.8215806134.2338140203.740373863Si7.8261578694.384180983.799328647Si5.182464759-0.1739052722.227101839Si5.244265179-0.0145578572.220636987Si5.326433141-0.2042179942.303579523Si13.999207618-0.1637236835.25955546Si13.8986840240.1373906565.332017944Si13.7795040380.0806604915.271529723Si13.970330405-0.2460062432.205187220Si13.819331879-0.0987647622.265103128Si13.7695115670.0369837572.169384244Si4.969252060-0.0193397945.375282321Si5.0974362800.1365910195.354749715Si5.259345609-0.0045902485.427103377Si14.677022317.0851875106.055770947Si14.6750423107.1042015766.074305887Si14.7546559296.8855189705.888103693Si4.4245407977.0333484501.554888811Si4.4257560047.1030034591.522436063Si4.485933687.0970060621.432365883Si4.1251951046.8659302936.007115021Si4.2217421126.9959781555.992288161Si4.0891099597.0731508515.890196761Si14.7745067217.1484137921.617919544Si14.7342733627.2519315261.622576017Si15.7613800454.2317008402.184262501	Si	11.227939632 9.902987244 3.788305753	Si	11.230268940 10.064402045 3.853639075	Si	11.085240362 9.971748767 3.819806442
Si1.125050404Si1.221701839Si1.2242651791.27390405Si1.350176094.3641603693.364260369Si13.999207618-0.1637236835.25955546Si5.244265179-0.0145578722.200636987Si5.32646712.303579223Si13.970330405-0.2460062432.205187220Si13.8986840240.1373906565.332017944Si13.7795040380.0806604915.271529723Si13.970330405-0.2460062432.205187220Si13.819331879-0.0987647622.265103128Si13.7695115670.0369837572.169384244Si4.969252060-0.0193397945.375282321Si5.0974362800.1365910195.354749715Si5.259345609-0.0045902485.427103377Si14.677022317.0851875106.055770947Si14.6750423107.1042015766.074305887Si14.7546559296.8855189705.88103693Si4.42540777.033344501.554888811Si4.425407421126.9959781555.992288161Si4.0891099597.0731508515.890196761Si14.7745067217.1484137921.617919544Si14.7342733627.2519315261.622576017Si15.7613800454.2317008402.184262501	Si.	7 755568404 4 149863807 3 718935954	si	7 821580613 4 233814020 3 740373962	Si	7 896157869 4 384180983 3 799328647
Si5.1.02404/7350.1/15002/22.22/101839Si5.2442051/90.01453/85/22.20050887SiSi5.320431410.20421/9942.3035/95/23Si13.9992076180.1637236835.259555546Si13.898640240.1373906565.32017944Si13.7795040380.0806604915.271529723Si13.9703304050.2460062432.205187220Si13.819331879-0.0987647622.265103128Si13.7695115670.0369837572.169384244Si4.969252060-0.0193397945.375282321Si5.0974362800.1365910195.354749715Si5.259345609-0.0045902485.427103377Si14.6772022317.0851875106.055770947Si14.6750423107.1042015766.074305887Si14.7546559296.8855189705.888103693Si4.425407977.0333484501.554888811Si4.4597560047.1030034591.522436063Si4.4459933687.0970060621.432365883Si4.1251951046.8659302936.007115021Si4.2217421126.9959781555.992288161Si4.0891099597.0731508515.890196761Si14.7745067217.1484137921.617919544Si14.7342733627.2519315261.622576017Si15.7613800454.2317008402.184262501	- C:	E 1004647E0 0 172005007 3.710303934	- C:	- 24426E170 0.014EE78E7 2.230C2C007		E 236422141 0 204247004 2 202570522
Si13.99920/018 -0.163/236835.25955546Si13.8986840240.1373906565.332017944Si13.7795040380.0806604915.271529723Si13.970330405 -0.2460062432.205187220Si13.819331879-0.0987647622.265103128Si13.7695115670.0369837572.169384244Si4.969252060-0.0193397945.375282321Si5.0974362800.1365910195.354749715Si5.259345609-0.0045902485.427103377Si14.6772022317.0851875106.055770947Si14.6750423107.1042015766.074305887Si14.7546559296.8855189705.888103693Si4.4245407977.0333484501.554888811Si4.4597560047.1030034591.522436063Si4.445933687.0970060621.432365883Si4.1251951046.8659302936.007115021Si4.2217421126.9959781555.992288161Si4.0891099597.0731508515.890196761Si14.7745067217.1484137921.617919544Si14.7342733627.2519315261.622576017Si15.7613800454.2317008402.184262501	51	5.162404/59 -0.1/39052/2 2.22/101839	21	3.2442031/9 -0.01433/85/ 2.22003098/	21	5.520433141 -U.2U421/994 2.3U35/9523
Si13.970330405 -0.2460062432.205187220Si13.819331879-0.0987647622.265103128Si13.7695115670.0369837572.169384244Si4.969252060-0.0193397945.375282321Si5.0974362800.1365910195.354749715Si5.259345609-0.0045902485.427103377Si14.677022317.0851875106.055770947Si14.6750423107.1042015766.074305887Si14.7546559296.8855189705.888103693Si4.4245407977.0333484501.554888811Si4.4597560047.1030034591.522436063Si4.459930887.0970060621.432365883Si4.1251951046.8659302936.007115021Si4.2217421126.9959781555.992288161Si4.0891099597.0731508515.890196761Si14.7745067217.1484137921.617919544Si14.734273627.2519315261.622576017Si15.7613800454.2317008402.184262501	Si	13.999207618 -0.163723683 5.259555546	Si	13.898684024 0.137390656 5.332017944	Si	13.779504038 0.080660491 5.271529723
Si4.969252060-0.0193397945.375282321Si5.0974362800.1365910195.354749715Si5.259345609-0.0045902485.427103377Si14.6772022317.0851875106.055770947Si14.6750423107.1042015766.074305887Si14.7546559296.8855189705.888103693Si4.4245407977.0333484501.55488811Si4.4597560047.1030034591.522436063Si4.4459933687.0970060621.432365883Si4.1251951046.8659302936.007115021Si4.2217421126.9959781555.992288161Si4.0891099597.0731508515.890196761Si14.7745067217.1484137921.617919544Si14.734273627.2519315261.622576017Si15.7613800454.2317008402.184262501	Si	13.970330405 -0.246006243 2.205187220	Si	13.819331879 -0.098764762 2.265103128	Si	13.769511567 0.036983757 2.169384244
Si14.6772022317.0851875106.055770947Si14.6750423107.1042015766.074305887Si14.7546559296.8855189705.888103693Si4.4245407977.0333484501.554888811Si4.4597560047.1030034591.522436063Si4.4459933687.0970060621.432365883Si4.1251951046.8659302936.007115021Si4.2217421126.9959781555.992288161Si4.0891099597.0731508515.890196761Si14.7745067217.1484137921.617919544Si14.7342733627.2519315261.622576017Si15.7613800454.2317008402.184262501	Si	4.969252060 -0.019339794 5.375282321	Si	5.097436280 0.136591019 5.354749715	Si	5.259345609 -0.004590248 5.427103377
Si 4.424540797 7.033348450 1.554888811 Si 4.459756004 7.103003459 1.522436063 Si 4.45993068 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	14.677202231 7.085187510 6.055770947	Si	14.675042310 7.104201576 6.074305887	Si	14.754655929 6.885518970 5 888103693
Si 4.425750004 7.103003459 1.32430005 Si 4.44355300 7.03700002 1.43250583 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	Ci	A A2A5A0797 7 0333A9A50 1 55A999911	¢;	A 459756004 7 103002450 1 522426062	s:	A AA5993368 7 097006062 1 A22265992
Si 4.125135104 0.855330235 0.00/115021 Si 4.221742112 0.9959/8155 5.992288161 Si 4.089109959 7.0/3150851 5.890196/61 Si 14.774506721 7.148413792 1.617919544 Si 14.734273362 7.251931526 1.622576017 Si 15.761380045 4.231700840 2.184262501	51		51		5	
Si 14.774506721 7.148413792 1.617919544 Si 14.734273362 7.251931526 1.622576017 Si 15.761380045 4.231700840 2.184262501	51	4.125195104 0.855930293 0.00/115021	51	4.221/42112 0.9959/8155 5.992288161	51	4.003103323 /.0/3120821 2.890196/61
	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
н	7.931376987 11.990822640 5.021556976	н	8.398342132 11.269240376 5.720010436	н	1.863791833 10.759573235 3.496453628
н	9.451955177 3.425464501 2.412497935	н	9.506451005 2.899379608 2.789530740	н	16.732407940 6.299420126 2.698203311
н	1.854329267 10.581296304 3.621076054	н	1.890824134 10.666854548 3.618765813	н	11.643786500 13.441971521 1.935571794
н	16.785335264 6.048541254 1.319437489	н	16.781988366 6.249666741 1.443179155	н	8.271120087 4.025228996 6.070874161
н	8.355125070 13.644578021 3.860587991	н	10.660540774 1.527274043 2.209924848	н	17.767832825 6.759243631 4.305113714
н	10.611397060 13.135017785 4.149871531	н	8.379533789 2.184680826 0.577935693	н	19.888937691 7.288380736 3.219246528
н	10.249669611 12.895885468 5.890334143	н	9.492855123 0.825495700 0.236540636	н	19.138982735 6.556950584 1.768674495
н	10.202129592 14.540616129 5.193696897	н	10.098926207 2.533653140 0.172444129	н	19.483051260 5.527538565 3.205923619
С	10.005410063 13.480137493 4.996559317	С	9.411438222 1.833117425 0.669482055	С	19.177796505 6.528570385 2.865244309

Coordinates for FER at Si/Al=8					Dimethyl ether formation in the framework					Ethanol formation in acidic FER framework				
Acidic Sites with Methanol adsorbed at various														
		T sites												
		T3O8			~	~ .			~					
0	Si	Al	н	С	0	Si	Al	Н	С	0	Si	Al	н	С
73	32	4	8	1	/4	30	6	14	- 2	74	30	6	14	2
0	6.358869351	1.319336265	2.033724085		0	6.572481434	1.543214	924 1.9	04497358	0	6.451911506	1.61102	5251 1.7341	03027
0	13.067577269	13.154456941	5.708697998	8	0	13.247468490	13.05400	0266 5	5.662466375	0	13.39450880	4 12.9943	92098 5.80	0648805
0	13.134829273	1.444452348	5.257508371		0	13.248614961	1.31653	6132 4	.982981986	0	13.27650955	5 1.2898	76709 5.208	3929113
0	12.729724961	13.006177827	1.88517338	D	0	12.928323401	12.78027	1938 1	L.594891335	0	12.95154351	6 12.6179	34297 1.80	1147069
0	6.496593545	13.005599770	1.833258687		0	6.791570787	13.26111	9643 2	.093614818	0	6.731916310	13.34052	8791 1.923	064560
0	6.041801474	1.170721707	5.713549034		0	6.457332712	1.038257	816 5.	943777928	0	6.221882949	1.22818	8158 5.8803	860119
0	5.867183536	12.860604241	5.782208360		0	6.241217400	12.79740	8609 5	.357451862	0	6.267805027	12.97703	8581 5.355	531268
0	13.032841048	1.271352106	1.892943465		0	13.183622819	1.04905	1884 1	.656080624	0	12.91745490	9 0.9286	03331 1.863	3798886
0	15.432687886	8.476604713	5.698902396		0	16.047328614	8.40195	9527 5	.189627254	0	16.33602245	6 8.2832	52761 5.261	629172
0	3.511052274	5.682592012	2.184258755		0	3.696678461	5.940189	755 1.	690409138	0	3.592871018	6.06814	7532 1.6354	45706
0	3.707537730	8.544759278	2.100030898		0	4.078088975	8.514478	723 1.	965877140	0	3.964890281	8.60525	9811 1.9889	80004
0	3.245634748	5.777274665	5.246051395		0	3.856421439	5.863787	379 5.	685862784	0	3.559870209	6.04099	3852 5.5801	57359
0	15.804791415	5.865363784	5.850081998		0	16.003551055	5.79521	8625 5	.599585116	0	15.99543613	6 5.7320	79122 5.876	5709190
0	15.794340365	8.578865765	1.648803738		0	16.011318861	8.55704	9034 1	.359679403	0	16.15714021	4 8.3505	11283 1.847	579341
0	15.848709178	6.014533420	1.932504756		0	15.654133742	2 5.98576	8976 1	.566834026	0	15.60187540	4 5.8052	22000 1.630	0870464
0	3.240749561	8.391381228	5.414836992		0	3.564596394	8.443723	435 6.	030975014	0	3.430048126	8.62773	5668 5.8508	310327
0	7.045841030	3.822242907	2.703284801		0	7.366950232	4.018485	737 2.	326236024	0	7.494033948	4.01189	7534 2.2029	23311
0	11.850759961	10.982516629	4.85623168	1	0	12.531257100	0 10.73817	9182 4	1.621743024	0	12.47578384	6 10.8454	06783 4.62	1568183
0	11.637252538	3.607995592	5.005641790)	0	12.194333251	3.71995	2169 4	.805833910	0	12.10369998	8 3.6336	51860 5.027	125981
0	11.614090350	10.455035687	2.250149628	8	0	11.781519127	7 10.43875	7481 2	2.075968799	0	11.73356871	5 10.3143	07970 2.12	7614988
0	7.440972930	10.602066412	2.452265977		0	7.936586284	10.88843	8271 2	.399016648	0	8.022953472	11.03899	7590 2.323	339832
0	7.760005095	3.445716475	5.253627918		0	7.663711255	3.111781	302 4.	842485913	0	7.402140549	3.27494	5161 4.7661	04596
0	7.497816834	10.917918479	5.105819784		0	7.373367867	10.44561	5932 5	.235178593	0	7.272685284	10.58287	5213 5.108	408849
0	11.769464122	3.526398811	2.316750129		0	11.659848476	5 3.19357	2289 2	.013508067	0	11.58077774	3 3.2194	75317 2.221	661591
0	16.913723569	10.557931541	6.302048993	1	0	17.774373014	10.75768	8688 5	5.775155374	0	17.75642672	7 10.8227	19157 5.81	6457050
0	2.018466434	3.649213191	1.371994343		0	2.308887244	3.832971	.604 1.	040335789	0	2.330720926	3.97428	8420 0.8804	38007
0	2.210279088	10.592154547	1.332303503		0	2.346545779	10.76974	3336 1	.720292929	0	2.618042876	11.04626	1518 1.460	368415
0	2.293633270	3.524099205	6.240441854		0	2.246366677	3.444528	610 5.	940699113	0	1.977098005	3.58943	2648 5.8455	95022
0	16.760541626	3.420527199	6.319898164		0	17.259369536	5 3.57243	4854 6	.074165597	0	17.20407680	3 3.4302	49734 6.158	365160
0	17.081472006	10.879356476	5 1.41211219	1	0	16.723658874	10.94347	3075 (0.651745618	0	16.80716186	9 10.6224	83157 0.70	7323875
0	17.213030318	3.697697777	1.408890956	i	0	17.229906753	3.64726	5464 1	.254643225	0	17.16865977	2 3.6448	85555 1.346	869251
0	2.383679390	10.763759927	6.254534404		0	2.315128793	10.69798	3634 6	.503100085	0	2.162800317	10.88493	3659 6.336	641342
0	6.876471316	3.120153861	0.183182188		0	6.979913535	3.182256	883 -0.	136676253	0	6.731442814	3.39031	4972 -0.2182	295411
0	12.834426882	11.058167864	-0.22168585	1	0	12.942528024	10.92214	1279 -(0.293702758	0	12.68882180	5 10.9413	48011 -0.25	2568122
0	12.318195929	2.769478317	-0.121476701	_	0	12.602811192	2.63856	2687 -0	.356099500	0	12.47195892	1 2.5746	91437 -0.144	1865185
0	6.634248042	11.044523011	0.021197537		0	7.064210382	11.61367	8529 0	.059247868	0	6.919340709	11.56692	7716 -0.005	592519
0	16.424520786	9.979752498	3.779579960)	0	16.733490247	10.33957	5634 3	3.231214130	0	16.50874110	0 10.4577	24037 3.37	7104974
0	3.175396265	3.567160822	3.765801947		0	3.184486649	4.060005	021 3.	511543249	0	2.919349119	4.19110	7528 3.4301	87829
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0	15.886944752	4.016517436	3.916968782		0	16.242167475	3.99407	2500 3	.655412936	0	16.01811272	9 3.9619	26261 3.863	986537
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0	14.488376894	10.960186712	5.262672312	2	0	15.005904839	11.08718	82536 5	5.550788915	0	14.87432499	1 10.7446	43729 5.78	1450390

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0	14.491480364 10.855734113 2.129503755	0	14.433355780 10.659286581 1.938263054	0	14.394009344 10.375379048 1.725647487
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