Supporting Information

Cooperative Catalytically Active Sites for Methanol Activation by Single Metal Ion-doped H-ZSM-5

Wei-Che Lin[a†], Simson Wu[a†], Guangchao Li[a], Ping-Luen Ho[a], Yichen Ye[a], Pu Zhao[a], , Sarah Day[b], Chiu Tang[b], Wei Chen[c], Anmin Zheng[c], Benedict T.W. Lo[d*], Shik Chi Edman Tsang[a*]

[a] Wolfson Catalysis Centre, Department of Chemistry, University of Oxford, Oxford OX1 3QR, UK

[b] Diamond Light Source Ltd, Harwell Science and Innovation Campus, Didcot, Oxfordshire, OX11 0DE, UK

[c] Wuhan Institute of Physics and Mathematics, CAS, Wuhan 430071, China

[d] Department of Applied Biology and Chemical Technology, Hong Kong Polytechnic University, Hong Kong, China

[†]These authors contributed equally.
[*]Email: edman.tsang@chem.ox.ac.uk

Catalyst preparation:

H-ZSM-5 was provided by Sinopec, China. According to inductively coupled plasma-atomic emission spectroscopy (P-4010/ICP-AES), the Si/Al ratio in this material was 19.25. Before using the sample, it was calcined in air at 480 °C for 2 hours with a ramp rate of 1 °C min^{-1}. In terms of the preparation of ion-exchanged for example Zn-ZSM-5, 2 g of unmodified ZSM-5 was soaked in a 30 mL zinc nitrate solution composed of 10.32 g of zinc nitrate hexahydrate (Sigma-Aldrich, 98%) and 30 mL deionized water. An extra precaution was taken to adjust the pH to avoid any precipitation during the ion exchange. After agitation at room temperature in a round bottom flask for 24 hours, the sample was washed with deionized water and subsequently dried at 100 °C overnight. Finally, the powder was calcined in air at 550 °C for 12 hours with a ramp rate of 5 °C min^{-1}. The procedure for preparation of Cu-ZSM-5 was similar to Zn-ZSM-5, 10.9 g copper(II) acetate monohydrate (Sigma-Aldrich, 98%) was dissolved in 30 mL deionized water in order to have the comparable concentration with Zn-ZSM-5. The rest processes were the same as Zn-ZSM-5. In terms of Fe-ZSM-5, 22 g iron(III) nitrate nonahydrate (Sigma-Aldrich, 98%) was used to keep the same concentration with previous catalysts. In addition, higher temperature (80 °C) has been employed to increase the efficiency of iron(III) exchanged onto the H-ZSM-5 framework. Other procedures remained the same. Finally, 9.27 g silver nitrate (Sigma-Aldrich, 99%) was dissolved in 30 mL deionized water for the Ag-ZSM-5 ion-exchange process. In addition, in order to avoid the aggregation of silver atoms forming cluster under light illumination, all the procedures were done under covering by alumina foil.

Catalytic evaluation:

1. *Reactor*

The catalytic reaction took place in a HEL fix bed reactor. Figure S1 showed the configuration of the reactor. A 2 hours pre-treatment under 400 °C with a ramp rate of 10 °C min^{-1} was performed for all catalysts. During the reaction, liquid methanol with a flow rate of 0.016 mL min^{-1} was pumped into a fixed bed stainless steel reactor that hosted the catalysts sandwiched by quartz wool plugs. The carrier gas was N_2 with a feed rate of 3 mL min^{-1} at reaction conditions of 397 °C and 10 bar. The liquid reaction products were collected in a container that was immersed in a dry ice bath. After condensation, the products were separated into an organic layer and an aqueous layer. Each layer was injected into a gas chromatography instrument for analysis. The gas-phase product, however, was collected in an inverted bottle *via* water drain. The collected gas was analyzed by gas chromatography.

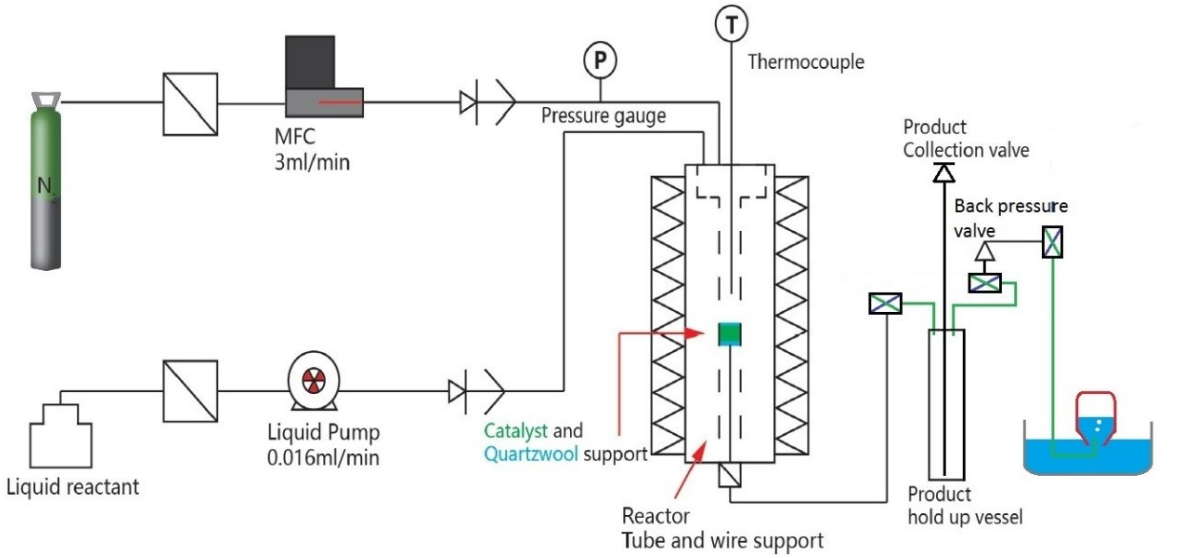


Figure S1. The configuration of the fix bed reactor.

2. *Gas chromatography (GC)*

Liquid product:
Both organic layer and aqueous layer products were added 1% 2-isopropylphenol as an internal standard before injection into an Agilent 7890B GC for analysis. In addition, a relative respond factor to the internal standard was added as a parameter to make the calculation more accurate.

The relative response factor can be obtained by injecting the same weight of each known compound and 2-isopropylphenol. The reciprocal of peak area ratio is equal to their relative respond factors to the internal standard.

The weight percentage of each product can be inferred from the formula below:

$$\frac{Product\ weight\ percentage}{1\%} = \left(\frac{Product\ peak\ area}{Internal\ product\ peak\ area}\right) \times \left(\frac{Internal\ standard\ respond\ factor}{Product\ respond\ factor}\right)$$

The product produced in weight equal to its weight percentage times the total weight of the liquid collected.
Gas product:
The total volume of the gas product was recorded under normal pressure. Subsequently, the gas was taken out from the bottle by a syringe and injected into the GC for analysis. The total amount of the gas compound produced equal to its concertation multiple the total volume of the gas collected.
A 5% methane in argon mixture gas was used as an external standard to calibrate the concentration of hydrocarbon in the gas collected. The concentration of hydrocarbon produced is equal to the integration of the total peak area on the FID result multiplied by 5% divided by the peak area of the external standard methane. In this case, the calculated concentration assumed that the entire light hydrocarbon was methane. The relative response factor for most of the light hydrocarbon is similar to that of methane. It was assumed that their response factors to FID detector are the same.

Table S1(a). The products produced from each catalyst at steady state.

Products (% mol of carbon)	**H-ZSM-5**	**Fe-ZSM-5**	**Cu-ZSM-5**	**Zn-ZSM-5**	**Ag-ZSM-5**
Methanol (reactant) conv/%	89.3	90.1	88.2	93.5	99.3
BTX	15.2	11.1	11.3	14.8	16.8
Other aromatics	32.4	26.8	34.2	43.1	45.5
DME	trace	0.1	0.2	Trace	Trace
Alkanes/alkenes	41.5	52.9	42.5	35.6	37.0

Table S1(b). The products in mol% produced at steady state.

Products (mol of carbon)	**H-ZSM-5**	**Fe-ZSM-5**	**Cu-ZSM-5**	**Zn-ZSM-5**	**Ag-ZSM-5**
Methanol (reactant)	0.0546	0.0481	0.0629	0.0346	0.004
BTX	0.0775	0.0586	0.06	0.0792	0.0884
Other aromatics	0.165	0.142	0.182	0.23	0.24
DME	0.0005	0.0003	0.0012	9×10^{-6}	1×10^{-5}
Alkane/alkene	0.211	0.28	0.226	0.19	0.195

Table S2. The composition of alkanes/alkenes.

Compounds	**Carbon contribution percentage (%)**

C_2-C_3 (gas phase)	67.6
2-methylbutane	4.9
2-methylpentane	9.7
3-methylpentane	3.3
2-methylhextane	4.5
3-methylbutane	10

Table S3. The composition of other aromatics.

Compounds	Carbon contribution percentage (%)
1-ethyl-4-methyl benzene	10.9
Mesitylene	25.3
1-ethyl-2,4-dimethyl benzene	3.3
1,2,4,5-tetramethyl benzene	24
Benzene derivatives with >C10	33.4
Naphthalene	3.1

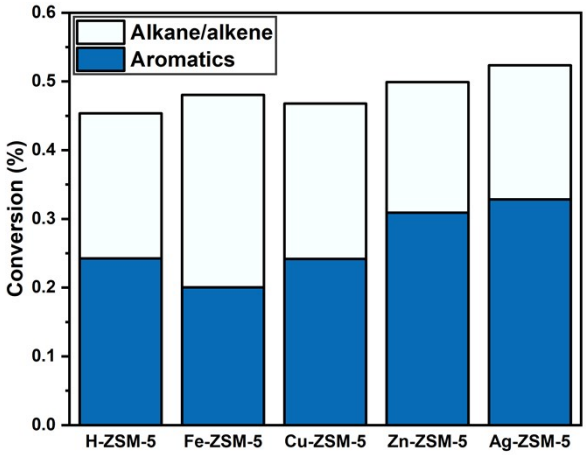


Figure S2. The product selectivity over different ZSM-5 catalysts.

We have also further compared the product selectivity with different framework-Al and doped-metal contents to investigate the structure-activity relationship of the FLPs. Briefly, H-ZSM-5 of Al_2O_3-to-SiO_2 ratios of 25 and 38 were used (denoted as 'H-ZSM-5(25) and H-ZSM-5(38)'). Different contents of doped-metal were achieved by performing an additional ion-exchange procedure with the corresponding metal nitrate precursor, where these samples are denoted as '2Fe/Zn-ZSM-5(25/38)'. The product distribution is presented in Figure S2. Upon increasing Fe content, it can be seen that the selectivity toward aliphatic products increases. The selectivity toward aromatic products, in contrast, increases with the Zn content. This clearly suggests that the role of the metal sites does not merely contribute toward the formation of M-OCH_3, but gives an additional impact towards either aliphatic or aromatic products. This clearly suggests that the role of the metal sites does not merely contribute toward the formation of M-OCH_3, but gives an additional impact towards either aliphatic or aromatic products. In particular, it is believed that the Fe(III) sites can readily activate dihydrogen in the form of Fe(III)-H_2. Note that there is an abundant source of dihydrogen which is formed in-situ during the methanol conversion reactions that involves numerous dehydrogenation and dehydration steps. The Fe(III)-H_2 can readily react with the reactive species at the 'hydrocarbon pool' to increase their

molecular hydrogen content. This leads to the fall of aromatic products (with a lower C:H ratio) but a rise in aliphatic products (with a higher C:H ratio).

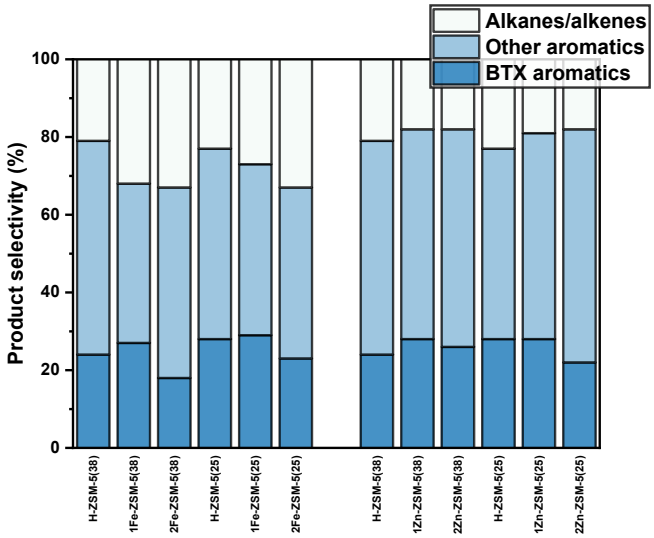


Figure S3. Product selectivity within the oil phase products over the number of ZSM-5 based catalysts. Increasing Fe content appears to increase alkanes/alkenes whereas the increase in Zn content gives lower alkanes/alkenes ratios.

Characterization:

1. *Extended X-Ray absorption fine structure (EXAFS)*

The chemical states of Fe, Zn and Ag local structures in the metal-doped catalysts were probed by using the extended X-ray absorption fine structure (EXAFS) technique. The Fe, Zn and Ag K-edge EXAFS measurements were all performed at beamline BL07A of the Taiwan light source at National Synchrotron Radiation Research Centre in Taiwan. A Si (111) Double Crystal Monochromator (DCM) was used to scan the photon energy. The EXAFS spectra were measured in the fluorescence mode using a Lytle fluorescence detector for all metal-doped ZSM-5 samples. The IFEFFIT software package was used to analyze the EXAFS data to obtain the local structural parameters of Fe, Zn and Ag respectively. Several constraints were applied to the fitting parameters to exclude unphysical results.

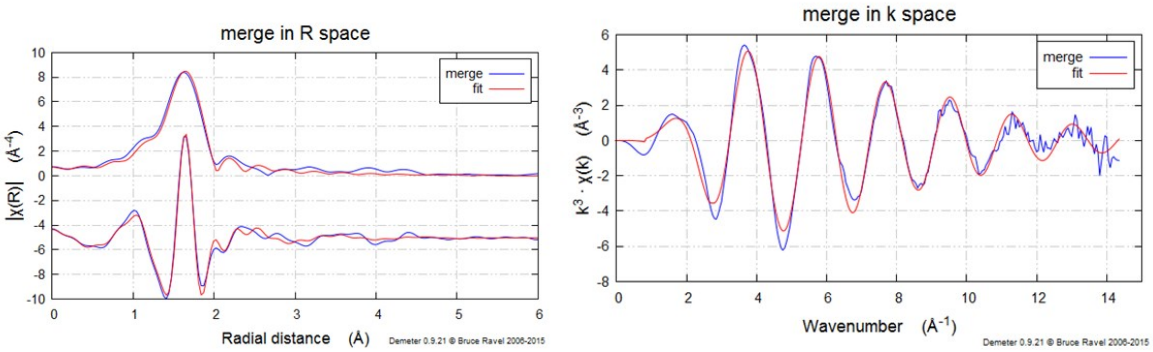


Figure S4. The best-fitted EXAFS data of Zn-ZSM-5.
R-factor: 0.1%
k-range: 3-12
R-range: 1.35-2.5

Table S4. The energy difference between the theoretical path and calculated path: 1.2 eV

Scattering path	Bond length (Å)	Coordination number	Debye-Waller factor
Zn-O1	2.03 (1)	5.7 (3)	0.009

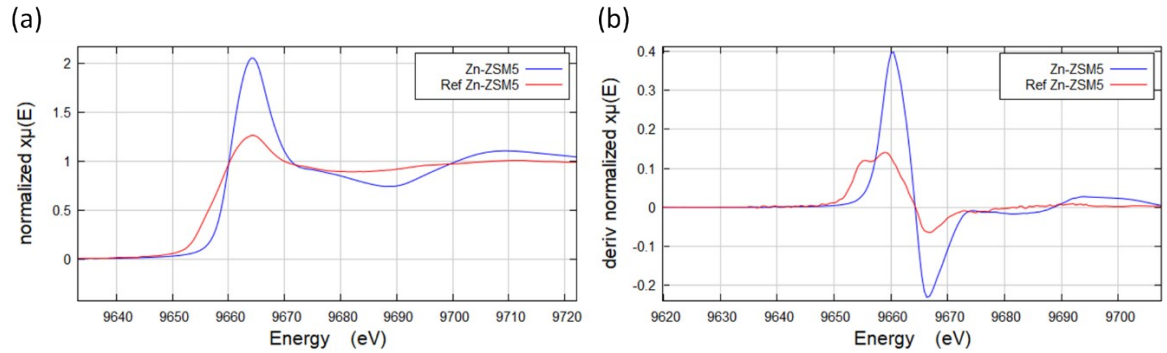


Figure S5. (a) XANES spectra, (b) first derivative of XANES spectra for Zn-ZSM-5 and reference Zn foil.

Zn^{II} XANES is characterized by a well-defined peak at 9664 eV, which corresponds to the 1s → 4p electronic transition.[1]

Zn-ZSM5 absorption edge shift to higher energy implies an oxidation state of II.

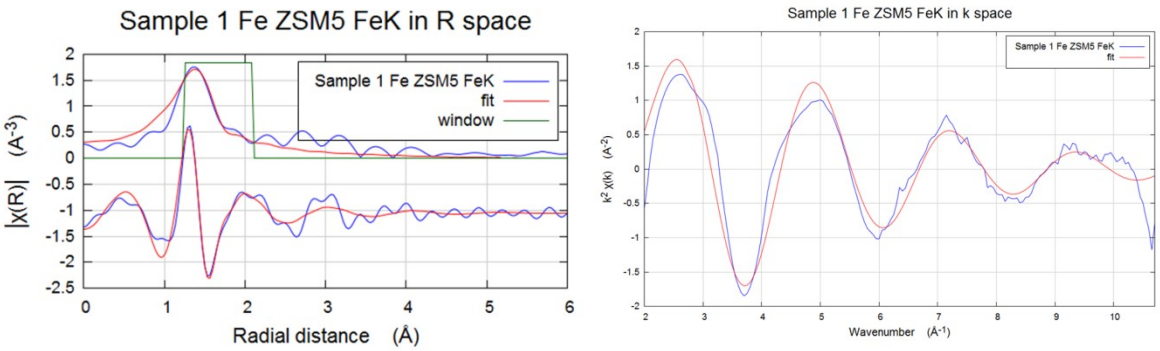


Figure S6. The best-fitted EXAFS data of Fe-ZSM-5.
R-factor: 1.0%
k-range: 3-12.3
R-range: 1.25-2.1

Table S5. The energy difference between the theoretical path and calculated path: 3.1 eV

Scattering path	**Bond length (Å)**	**Coordination number**	**Debye-Waller factor**
Fe-O1	1.81 (3)	5.3 (3)	0.008

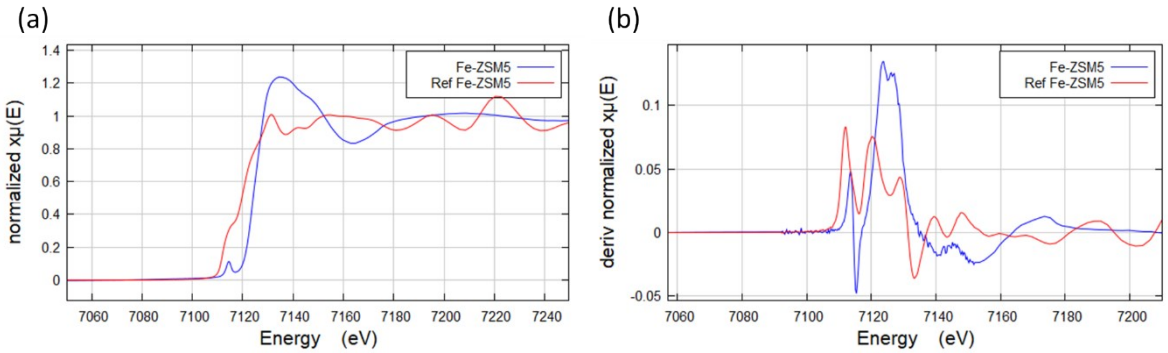


Figure S7. (a) XANES spectra, (b) first derivative of XANES spectra for Fe-ZSM5 and reference Fe foil. Fe(III) is characterized by the pre-edge peak at 7114 eV that corresponds to 1s → 3d electronic transition and peak at 7135 eV.[2]

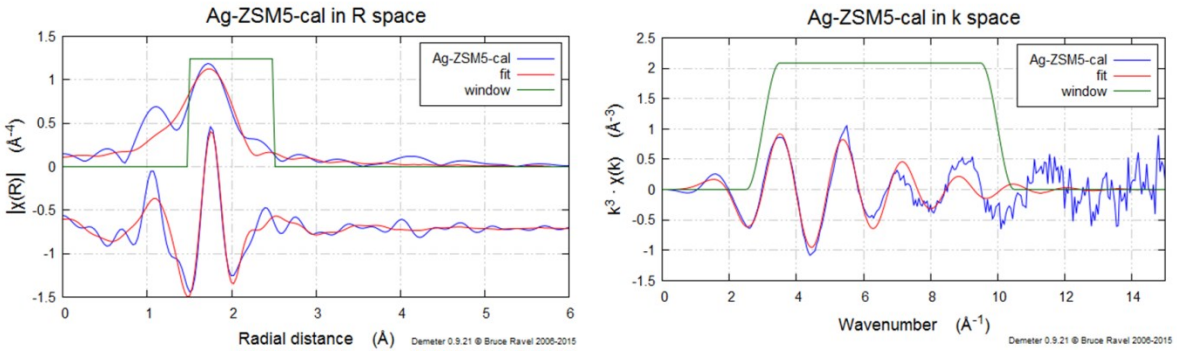


Figure S8. The best-fitted EXAFS data of Ag-ZSM-5.
R-factor: 1.3%
k-range: 3-8
R-range: 1.25-3

Table S6. The energy difference between the theoretical path and calculated path: 3.0 eV

Scattering path	**Bond length (Å)**	**Coordination number**	**Debye-Waller factor**
Ag-O1	2.22 (3)	3.0 (6)	0.015
Ag-O2	2.43 (4)	0.8 (3)	0.003

Given the low metal loading of the samples, the EXAFS signal is relatively weak as evidenced by the signal-to-noise ratio in the k-space beyond 10.5 $Å^{-1}$. As a result, it is not as accurate and precise as we hope in considering the peak fitting at and beyond 2.0 Å. On the other hand, the intensity of the shoulder peak/noise at around 2 Å is small compared with the main peak at 1.4Å and is also similar in intensity to that of the noise levels from beyond 2.0 Å. Therefore, we attribute this shoulder peak to the backscattering ripples rather than a meaningful peak contributed by the scattering paths. Similarly, the peak at around 1.2 Å was found in the three Ag containing samples, which appears to be even shorter than any typical Ag-X interaction hence making no sense for chemical interaction with Ag. Again, we attribute this peak as an artefact. In fact, the signal-to-noise ratio of the k-space spectrum is low such that it gives rise to high uncertainty in the extra peaks and in turn introduced unwanted artefacts to the spectra. We further adjusted the spline range and chose a smaller k-range for fitting.

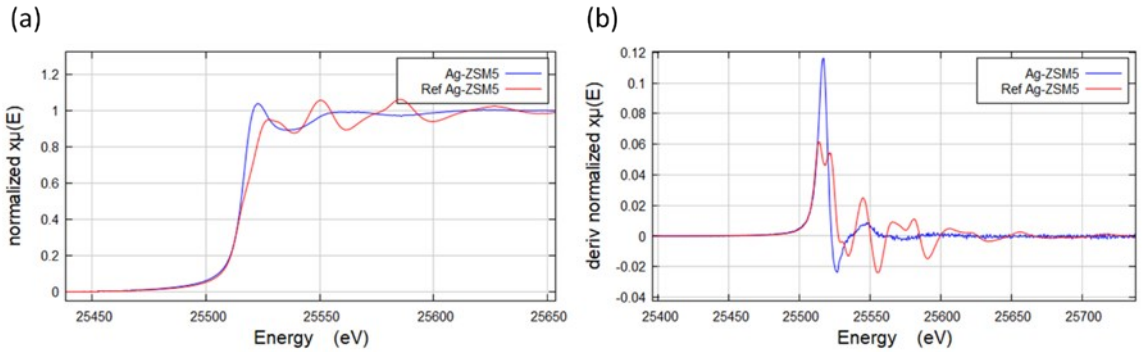


Figure S9. (a) XANES spectra, (b) first derivative of XANES spectra for Ag-ZSM5 and reference Ag foil. The shape of the absorption edge of Ag-ZSM-5 resembles that of typical Ag^{+} residing in zeolites.[3]

2. Synchrotron X-ray powder diffraction

High-resolution SXRD data were collected on Beamline I11, Diamond Light Source, UK. A detailed description of the beamline can be found elsewhere.[4,5] The energy of the incident X-ray beam was set at 15 keV. The wavelength and the 2θ-zero-point correction were refined using a diffraction pattern obtained from a high-quality silicon powder (SRM640c). All the catalysts were loaded in a 0.5 mm borosilicate glass capillary. High-resolution XRD data were obtained from the samples using the multi-analyzer crystal (MAC) detectors.

Using the TOPAS software, the diffraction patterns were analyzed by Rietveld refinement methods to obtain structural details. The quality of the Rietveld refinements of synchrotron XRD data has been assured with a low goodness-of-fit (gof), a low weighted profile factor (R_{wp}) and a well-fitted pattern with acceptable isotropic displacement factor (B_{eq}) within experimental errors. All the errors of the atom-atom distances were calculated from the square root of the $(x_{error})^2+(y_{error})^2+(z_{error})^2$ multiplied by the measure distances. The crystallographic data and refinement details are summarized in Table S7.

Table S7. Crystallographic data and details of Zn-ZSM-5, Fe-ZSM-5 and Ag-ZSM-5

	Zn-ZSM-5	**Fe-ZSM-5**	**Ag-ZSM-5**
Crystal system	Orthorhombic	Orthorhombic	Orthorhombic
Space group	Pnma	Pnma	Pnma
2θ range refinement	3 – 55 °	3 – 55 °	3 – 55 °
Detector	Multi-analyzer crystals	Multi-analyzer crystals	Multi-analyzer crystals
Refinement method	Rietveld	Rietveld	Rietveld
a (Å)	20.12885(3)	20.14434(3)	20.14516(3)
b (Å)	19.95555(3)	19.96015(3)	19.95531(3)
c (Å)	13.43143(3)	13.42903(2)	13.42940(2)
V (Å^3)	5395.172(27)	5399.599(28)	5398.658(27)
R_{wp} / R_p / R_{exp} (%)	7.896/6.086/3.529	7.296/ 5.773/4.378	7.201/ 5.526/ 3.306
Wavelength (Å)	0.825900(2)	0.825838(2)	0.825868(2)
2θ Zero point (°)	-0.004944(10)	0.008791(10)	-0.004293(10)
gof χ^2	2.237	1.667	2.178

First, we have to emphasise that the Rietveld refinement experiments with the pre-adsorption of D_4-methanol on Ag-ZSM-5 and Zn-ZSM-5 with careful selected metal contents was performed at 200 °C (instead of the typical MTA reaction temperature of 400°C) for 5 h in static conditions with no extensive formation of carbonaceous species before the data were collected at room temperature.

Although a preliminary operando synchrotron XRD for methanol activation was carried out over one of the zeolites with no metal modifier by our group (Tsang and co-workers, Appl. Catal. B: Enviro, 237, 245-250, 5, 2018), we have indeed been encountering difficulties for metal-modified zeolites due to low metal loadings for reliable species detections and vigorous carbonaceous deposition during the operando conditions. They clearly affected the accuracy of the refinement so no useful data yet have been resolved. We will continue to improve the signal to noise levels in order to extend the work to more realistic catalysis.

For the present works, we have primarily employed combined synchrotron X-ray and neutron diffraction techniques to directly visualize how organic molecules behave and interact with the BASs and the metal sites within zeolites. By taking advantages of the molecular specificity of Lewis basic species, such as pyridine, methanol, ammonia and D/L-lysine, as chemical probes to the BASs and metal sites in different zeolites, we have elucidated organic adsorbate-

framework interactions at an atomistic level with accepted accuracy. Although the uncertainty errors in atomic positions of adsorbed organic molecules are higher than that of rigid structural elements (O, Si) due to intrinsic higher degrees of freedom and higher isotropic temperature factor, B_{eq}, the generally low but acceptable R_{wp} and χ^2 values with a closely fitted pattern suggest a good quality of refinement indicating the reliability of the atomic positions and angles within experimental errors. For the refinement analysis, there are more than 300 independent *hkl* reflections used for the calculations, which allow a great number of structural variables (less than 160 in the refinements) to be refined in a satisfactory manner.

Table S8. Crystallographic information file data from the SXRD-Rietveld refinement of Fe-ZSM-5.

Atom	x	y	z	SOF	B_{eq} (Å^2)
O1	0.37484	0.06456	0.76019	1	2.620(28)
O2	0.30766	0.05765	0.92189	1	2.620(28)
O3	0.20057	0.06327	0.0213	1	2.620(28)
O4	0.08891	0.06192	0.91246	1	2.620(28)
O5	0.11707	0.04841	0.72735	1	2.620(28)
O6	0.24817	0.05292	0.74948	1	2.620(28)
O7	0.37472	0.85301	0.75909	1	2.620(28)
O8	0.31031	0.84616	0.93167	1	2.620(28)
O9	0.18962	0.84864	0.03094	1	2.620(28)
O10	0.08688	0.83687	0.92893	1	2.620(28)
O11	0.11782	0.84295	0.73818	1	2.620(28)
O12	0.24517	0.83786	0.76504	1	2.620(28)
O13	0.3117	0.94784	0.81867	1	2.620(28)
O14	0.07655	0.95009	0.8307	1	2.620(28)
O15	0.41893	0.13334	0.60855	1	2.620(28)
O16	0.41554	1.01195	0.5772	1	2.620(28)
O17	0.4007	0.87001	0.57872	1	2.620(28)
O18	0.19473	0.12429	0.60641	1	2.620(28)
O19	0.19542	-0.00934	0.60918	1	2.620(28)
O20	0.20483	0.86672	0.58186	1	2.620(28)
O21	0.99639	0.05454	0.79256	1	2.620(28)
O22	0.99639	0.85025	0.79688	1	2.620(28)
O23	0.41976	0.75	0.6393	1	2.620(28)
O24	0.19102	0.75	0.66363	1	2.620(28)
O25	0.28528	0.75	0.06829	1	2.620(28)
O26	0.10132	0.75	0.05902	1	2.620(28)
Si1	0.42213	0.05653	0.66482	1	1.310(14)
Si2	0.31098	0.02971	0.81394	1	1.310(14)
Si3	0.27839	0.05939	0.03343	1	1.310(14)
Si4	0.11894	0.06374	0.02861	1	1.310(14)
Si5	0.07111	0.0291	0.81246	1	1.310(14)
Si6	0.19107	0.05817	0.67351	1	1.310(14)
Si7	0.42687	0.8291	0.67279	1	1.310(14)
Si8	0.30808	0.87029	0.82078	1	1.310(14)
Si9	0.27465	0.8268	0.03215	1	1.310(14)
Si10	0.12256	0.82482	0.02927	1	1.310(14)
Si11	0.07425	0.86938	0.81915	1	1.310(14)
Si12	0.18834	0.82689	0.68637	1	1.310(14)
Fea	0.1549(12)	0.0444(15)	0.8776(16)	0.1200(21)	10
Owb	0.2786(40)	0.3189(36)	0.9377(60)	0.1200(21)	10
Fe1	0.607252	0.200921	0.735797	0.0589(12)	10
Fe1wO1	0.568997	0.182586	0.827671	0.0589(12)	10
Fe1wO2	0.669326	0.173221	0.781744	0.0589(12)	10

Fe1wO3	0.59215	0.133511	0.691928	0.0589(12)	10
Fe1wO4	0.545178	0.22862	0.689849	0.0589(12)	10
Fe1wO5	0.622354	0.26833	0.779666	0.0589(12)	10
Fe1wO6	0.645507	0.219255	0.643922	0.0589(12)	10

All the T-sites (T=Al, Si) of ZSM-5 were refined using the same B_{eq} parameter.

All the O-sites of ZSM-5 were refined using the same B_{eq} parameter.

Table S9. Atomic parameters from the Rietveld refinement of Zn-ZSM-5 at room temperature.[6]

Species	Atom	*x*	*y*	*z*	SOF	B_{eq} (Å^2)	Wyckoff
Zeolite framework	O1	0.37534(41)	0.05998(44)	0.75634(51)	1	3.162(33)	8d
	O2	0.30852(41)	0.06392(34)	0.92286(51)	1	3.162(33)	8d
	O3	0.19936(37)	0.06248(34)	0.02036(36)	1	3.162(33)	8d
	O4	0.09660(32)	0.05942(42)	0.91524(55)	1	3.162(33)	8d
	O5	0.11409(39)	0.04755(49)	0.73157(53)	1	3.162(33)	8d
	O6	0.24562(38)	0.04613(50)	0.75403(52)	1	3.162(33)	8d
	O7	0.37129(43)	0.84717(42)	0.76213(58)	1	3.162(33)	8d
	O8	0.30718(44)	0.84727(30)	0.92797(51)	1	3.162(33)	8d
	O9	0.19298(41)	0.84592(25)	0.02861(41)	1	3.162(33)	8d
	O10	0.08869(36)	0.84006(36)	0.92130(63)	1	3.162(33)	8d
	O11	0.11853(44)	0.84122(40)	0.73403(56)	1	3.162(33)	8d
	O12	0.24445(46)	0.84050(43)	0.76023(62)	1	3.162(33)	8d
	O13	0.31172(38)	0.95176(40)	0.82323(37)	1	3.162(33)	8d
	O14	0.07629(30)	0.95320(44)	0.82288(44)	1	3.162(33)	8d
	O15	0.41756(37)	0.12185(39)	0.59787(57)	1	3.162(33)	8d
	O16	0.40306(40)	0.99571(40)	0.59239(60)	1	3.162(33)	8d
	O17	0.40119(40)	0.86793(37)	0.57318(62)	1	3.162(33)	8d
	O18	0.18991(48)	0.12994(34)	0.61613(47)	1	3.162(33)	8d
	O19	0.20092(49)	0.00283(36)	0.59363(51)	1	3.162(33)	8d
	O20	0.19764(48)	0.87069(35)	0.58273(48)	1	3.162(33)	8d
	O21	0.99607(40)	0.04867(50)	0.79614(47)	1	3.162(33)	8d
	O22	0.99711(44)	0.85163(43)	0.79477(49)	1	3.162(33)	8d
	O23	0.42002(54)	0.7500	0.64499(66)	1	3.162(33)	4c
	O24	0.19445(68)	0.7500	0.65775(59)	1	3.162(33)	4c
	O25	0.28290(48)	0.7500	0.05561(70)	1	3.162(33)	4c
	O26	0.10353(54)	0.7500	0.05963(80)	1	3.162(33)	4c
	Si1	0.42180(20)	0.05861(27)	0.66258(31)	1	1.309(15)	8d
	Si2	0.30903(28)	0.02941(17)	0.81279(32)	1	1.309(15)	8d
	Si3	0.27978(17)	0.06190(22)	0.03485(29)	1	1.309(15)	8d
	Si4	0.12177(18)	0.06289(23)	0.02602(31)	1	1.309(15)	8d
	Si5	0.06889(21)	0.02935(20)	0.81760(34)	1	1.309(15)	8d
	Si6	0.18615(22)	0.05581(23)	0.67469(28)	1	1.309(15)	8d
	Si7	0.42467(22)	0.82990(20)	0.67103(34)	1	1.309(15)	8d
	Si8	0.30720(26)	0.86994(20)	0.81691(29)	1	1.309(15)	8d
	Si9	0.27366(20)	0.82692(19)	0.02870(32)	1	1.309(15)	8d
	Si10	0.11940(21)	0.82681(21)	0.03012(36)	1	1.309(15)	8d
	Si11	0.07193(22)	0.87211(23)	0.81566(33)	1	1.309(15)	8d
	Si12	0.18877(27)	0.82612(17)	0.68528(32)	1	1.309(15)	8d
Zn-1	Translate	0.9290(8)	0.7173(11)	0.1885(10)			
	Zn1	0.9290	0.7173	0.1885	0.104(2)	8.1(12)	4c
	$Zn1O_W1$	0.9060	0.6164	0.1529	0.104(2)	12.1(19)	4c
	$Zn1O_W2$	0.8513	0.7182	0.2951	0.104(2)	12.1(19)	4c
	$Zn1O_W3$	0.9963	0.6840	0.2994	0.104(2)	12.1(19)	4c
	$Zn1O_W4$	1.0066	0.7164	0.0819	0.104(2)	12.1(19)	4c
	$Zn1O_W5$	0.8616	0.7506	0.0777	0.104(2)	12.1(19)	4c
	$Zn1O_W6$	0.9519	0.8181	0.2242	0.104(2)	12.1(19)	4c
Zn-2	Zn2	0.7774(11)	0.1209(12)	0.8225(17)	0.071(3)	16.3(21)	8d
OZn2	$Zn2O_W1$	0.7858(12)	0.3052(17)	0.6895(21)	0.071(3)	24.4 (31)	8d

Table S10. Crystallographic information file data from the SXRD-Rietveld refinement of Ag-ZSM-5.

Atom	x	y	z	SOF	B_{eq} (Å^2)
O1	0.37573	0.05967	0.7588	1	2.131(18)
O2	0.31138	0.05946	0.92214	1	2.131(18)
O3	0.19767	0.06065	0.0222	1	2.131(18)
O4	0.09746	0.06158	0.91601	1	2.131(18)
O5	0.11457	0.05448	0.73287	1	2.131(18)
O6	0.245	0.04709	0.7548	1	2.131(18)
O7	0.37597	0.84744	0.76071	1	2.131(18)
O8	0.30611	0.84756	0.93273	1	2.131(18)
O9	0.19252	0.84883	0.02748	1	2.131(18)
O10	0.08674	0.83659	0.92471	1	2.131(18)
O11	0.12038	0.8428	0.73663	1	2.131(18)
O12	0.24999	0.83988	0.76698	1	2.131(18)
O13	0.31521	0.951	0.82173	1	2.131(18)
O14	0.08128	0.95204	0.82173	1	2.131(18)
O15	0.41958	0.12578	0.60142	1	2.131(18)
O16	0.41087	1.00267	0.58481	1	2.131(18)
O17	0.40186	0.86708	0.57415	1	2.131(18)
O18	0.19043	0.13074	0.61749	1	2.131(18)
O19	0.20396	-0.0031	0.60558	1	2.131(18)
O20	0.20025	0.86941	0.58455	1	2.131(18)
O21	0.99707	0.0493	0.79521	1	2.131(18)
O22	0.99767	0.85033	0.79299	1	2.131(18)
O23	0.41828	0.75	0.64505	1	2.131(18)
O24	0.19283	0.75	0.65617	1	2.131(18)
O25	0.28814	0.75	0.06079	1	2.131(18)
O26	0.10805	0.75	0.06611	1	2.131(18)
Si1	0.42141	0.05626	0.66467	1	1.0653(90)
Si2	0.31088	0.02958	0.81437	1	1.0653(90)
Si3	0.278	0.06081	0.03293	1	1.0653(90)
Si4	0.11821	0.06392	0.03204	1	1.0653(90)
Si5	0.07091	0.02948	0.81579	1	1.0653(90)
Si6	0.18846	0.05709	0.6768	1	1.0653(90)
Si7	0.42471	0.82923	0.67271	1	1.0653(90)
Si8	0.3078	0.87149	0.81978	1	1.0653(90)
Si9	0.2744	0.82653	0.03427	1	1.0653(90)
Si10	0.12114	0.8268	0.02907	1	1.0653(90)
Si11	0.07177	0.86957	0.8193	1	1.0653(90)
Si12	0.188	0.82622	0.68557	1	1.0653(90)
Aga	0.25988(98)	0.82695(99)	0.4353(17)	0.0458(72)	10
Agc	0.44038(86)	-0.20640(83)	0.3174(11)	0.0651(76)	10
Agb	0.2813(24)	0.0942(20)	-0.3336(31)	0.0227(13)	10
Ow2	0.5182(46)	0.2250(60)	-0.4270(62)	0.0651(76)	10
Ow3	0.6174(44)	0.259(15)	-0.2263(61)	0.0651(76)	10

3. Method - Electron Microscopy

High-angle annular dark-field scanning transmission electron microscopy (HAADF-STEM) was carried out using an aberration-corrected JEOL ARM200F. The microscope was operated at 200 kV in HAADF-STEM mode with HAADF detector collection semiangles from 73 to 271 mrad. The probe array sizes of 512 × 512 and a dwell time of 0.3 μs per pixel. The probe current was setting on 15 pA. The unfiltered contrast of the raw HAADF-STEM images cannot be directly interpreted as chemical structure. This effect can be compensated by nonlinear filtering algorithm based on Gaussian low-pass filter adding Wiener filter, the detail information was recorded.[7] STEM image simulations with Dr. Probe apply the multislice method to calculate the quasi-elastic forward scattering of the incident electron probes by the sample.[8] Using supercells of over 1900 atoms, the implementation of frozen-lattice variations is realized with a set of pre-calculated frozen states for each slice of the input structure. Microscope setup is under 0.04 nm probe size, with an electron beam energy of 200 kV, the aperture radius alpha (beam convergence) is 24 mrad and zero defocus. Moreover, the detector was placed on the optical axis in the diffraction plane as an ADF detector from 75 mrad to 270 mrad. The input files for the model-based Rietveld refinement result is the unit cell to extract signal at periodic thickness levels up to maximum object thickness in one simulation. The pixel size in the simulation image is 0.025 nm.

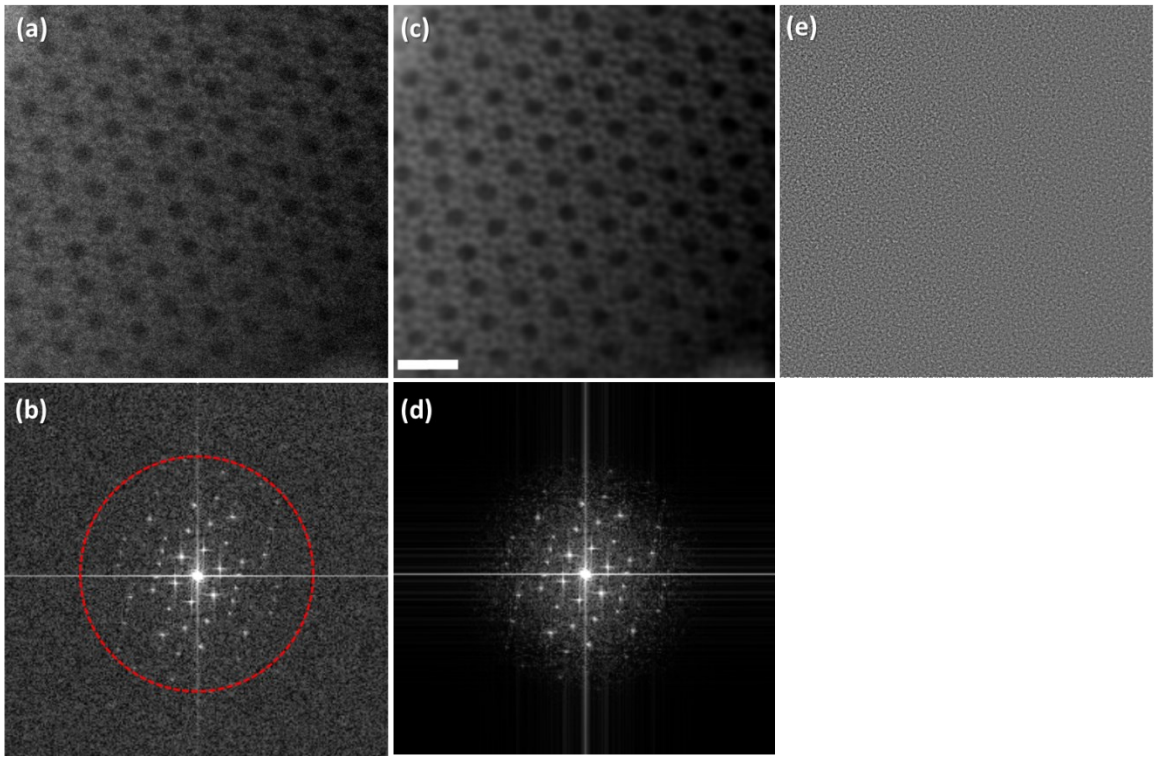


Figure S10. The nonlinear filtering algorithm adding residuals of Wiener filtering and Gaussian low-pass filtering has been used in this work. (a) The experimental HAADF-STEM image of Ag-ZSM-5 along the $[0\bar{1}0]$ axis and (b) the reduced Fast Fourier Transform (FFT), respectively. (c) The denoised image from experimental data has applied on the nonlinear filtering algorithm and (d) the FFT shown the cut frequency. Images by convoluting a Gaussian kernel (σ = 2 pixels and kernel size of 5 x 5 pixels) were calculated for testing the performance of the nonlinear algorithm in a quantitative sense as red circle indicated in (b). (e) Residual error image. (the scare bar is 2 nm)

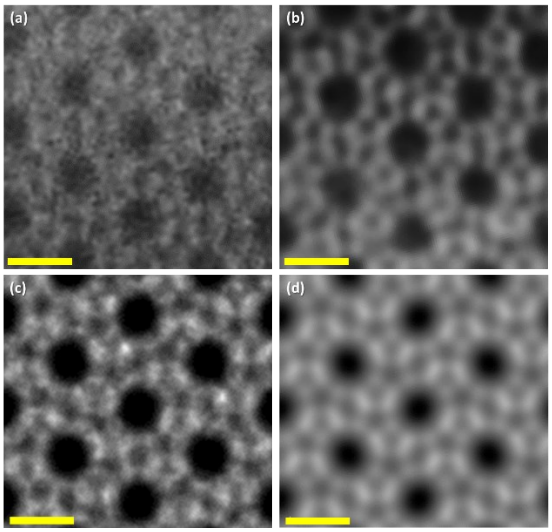


Figure S11. Aberration-corrected High-angle annular dark-field scanning transmission electron microscopy (HAADF-STEM) image of Ag-ZSM-5 (a) The experimental HAADF-STEM image along the $[01\bar{0}]$ axis. This image is cropped from the original drift-corrected image shown in supplementary Fig. (b) The experimental HAADF-STEM image denoised using a nonlinear filtering algorithm. (c) The simulated HAADF-STEM image of Ag-ZSM-5. (d) The simulated projected electrostatic potential map of the model based on the Rietveld refinement result (scale bar: 8Å).

5. Method - Neutron powder diffraction (NPD)

High-resolution neutron powder diffraction (NPD) data were collected at beamline GDDP, China Spallation Neutron Source (CSNS), Dongguang, China using the time-of-flight diffractometer GPPD (the general purpose powder diffractometer). Sample is loaded in 9.1mm vanadium can. The wavelength (λ = 1.4940(1) and 1.8856(1) Å) and the 2θ zero point (2θ = -0.02269^{o}) were determined by fitting the diffraction data of a high-quality $Na_2Al_2Ca_3F_{14}$ sample. ND data were collected for a D_4-methanol @Ag-ZSM5 and D_4-methanol @Zn-ZSM5 samples.

Before data collection, samples were dehydrated under vacuum at 200 °C for 5 h. Adsorbed water should have been removed completely. The adsorption of D_4-methanol on Ag-ZSM-5 and Zn-ZSM-5 were performed at room temperature using a Schlenk line. The samples were treated under vacuum at 200 °C for 5 h beforehand.

All samples were loaded into vanadium cans (7 mm inner diameter, 50 mm height) in a glove box. ND data were collected at 298 K the 2θ range of 0–160^{o} with 0.1^{o} angular step. Each data set was collected for 2 h for good statistics.

Table S11. Crystallographic data and details of D_4-methanol@Ag-ZSM-5, D_4-methanol@Zn-ZSM-5 from NPD.

Samples	**D_4-methanol@Ag-ZSM-5**	**D_4-methanol@Zn-ZSM-5**
Crystal system	Orthorhombic	orthorhombic
Space group	Pnma	Pnma
2θ range refinement	2 – 45 ^{o}	3 – 45 ^{o}
Detector	Multi-analyzer crystals	Multi-analyzer crystals
Refinement method	Rietveld	Rietveld
a (Å)	20.093	20.087
b (Å)	19.90	19.90
c (Å)	13.40	13.40
V (Å^3)	5357.96	5357.87
R_{wp} / R_p / R_{exp} (%)	3.98/3.7/1.57	3.03/2.97/1.50
Wavelength (Å)	0.688160	0.826551
2θ Zero point (°)	-0.00028	0.000339
gof $\chi 2$	2.53	2.02

Table S12. Crystallographic information file data from the NPD-Rietveld refinement of D_4-methanol@Ag-ZSM-5.

Atom	*x*	*y*	*z*	SOF	B_{eq} (Å^2)
O23	0.41828	0.75	0.64505	1	2.130
O24	0.19283	0.75	0.65617	1	2.130
O25	0.28814	0.75	0.06079	1	2.130
O26	0.10805	0.75	0.06611	1	2.130
O1	0.37573	0.05967	0.7588	1	2.130
O2	0.31138	0.05946	0.92214	1	2.130
O3	0.19767	0.06065	0.0222	1	2.130
O4	0.09746	0.06158	0.91601	1	2.130
O5	0.11457	0.05448	0.73287	1	2.130
O6	0.245	0.04709	0.7548	1	2.130
O7	0.37597	0.84744	0.76071	1	2.130
O8	0.30611	0.84756	0.93273	1	2.130
O9	0.19252	0.84883	0.02748	1	2.130
O10	0.08674	0.83659	0.92471	1	2.130
O11	0.12038	0.8428	0.73663	1	2.130
O12	0.24999	0.83988	0.76698	1	2.130
O13	0.31521	0.951	0.82173	1	2.130
O14	0.08128	0.95204	0.82173	1	2.130
O15	0.41958	0.12578	0.60142	1	2.130
O16	0.41087	1.00267	0.58481	1	2.130
O17	0.40186	0.86708	0.57415	1	2.130
O18	0.19043	0.13074	0.61749	1	2.130
O19	0.20396	-0.0031	0.60558	1	2.130
O20	0.20025	0.86941	0.58455	1	2.130
O21	0.99707	0.0493	0.79521	1	2.130
O22	0.99767	0.85033	0.79299	1	2.130
Si1	0.42141	0.05626	0.66467	1	1.0649
Si2	0.31088	0.02958	0.81437	1	1.0649
Si3	0.278	0.06081	0.03293	1	1.0649
Si4	0.11821	0.06392	0.03204	1	1.0649
Si5	0.07091	0.02948	0.81579	1	1.0649
Si6	0.18846	0.05709	0.6768	1	1.0649

Si7	0.42471	0.82923	0.67271	1	1.0649
Si8	0.3078	0.87149	0.81978	1	1.0649
Si9	0.2744	0.82653	0.03427	1	1.0649
Si10	0.12114	0.8268	0.02907	1	1.0649
Si11	0.07177	0.86957	0.8193	1	1.0649
Si12	0.188	0.82622	0.68557	1	1.0649
Aga	0.26488	0.82280	0.42966	0.04597	10
Agc	0.46142	-0.25072	0.31111	0.06557	10
Agb	0.25344	0.08545	-0.34457	0.0227	10
Ow2	0.5210	0.3	-0.4261	0.06557	10
Ow3	0.6270	0.2341	-0.2149	0.06557	10
C-1	0.83798	0.17126	0.69930	0.03000	8
O-2	0.78731	0.14961	0.76701	0.03000	8
D-3	0.80495	0.15031	0.83600	0.03000	8
D-4	0.81839	0.17048	0.62263	0.03000	8
D-5	0.84686	0.22537	0.70927	0.03000	8
D-6	0.87682	0.13246	0.69414	0.03000	8

Table S13. Crystallographic information file data from the NPD-Rietveld refinement of D_4-methanol@Zn-ZSM-5.

Atom	*x*	*y*	*z*	SOF	B_{eq} (Å^2)
O1	0.37453	0.05487	0.76359	1.0	3.16
O2	0.30509	0.06148	0.91646	1.0	3.16
O3	0.19589	0.04304	0.02402	1.0	3.16
O4	0.10135	0.05557	0.91074	1.0	3.16
O5	0.11706	0.06062	0.73029	1.0	3.16
O6	0.24758	0.04477	0.74085	1.0	3.16
O7	0.37926	0.85239	0.76956	1.0	3.16
O8	0.31379	0.83943	0.93433	1.0	3.16
O9	0.19892	0.84228	0.02730	1.0	3.16
O10	0.08577	0.83974	0.91545	1.0	3.16
O11	0.11778	0.84062	0.72682	1.0	3.16
O12	0.24416	0.83851	0.76555	1.0	3.16
O13	0.31463	0.94888	0.81271	1.0	3.16
O14	0.08254	0.95388	0.82881	1.0	3.16
O15	0.40978	0.12161	0.58510	1.0	3.16
O16	0.39723	0.99725	0.59337	1.0	3.16
O17	0.40325	0.87016	0.58749	1.0	3.16
O18	0.19009	0.12957	0.61947	1.0	3.16
O19	0.19221	0.00846	0.57589	1.0	3.16
O20	0.20193	0.87601	0.59741	1.0	3.16
O21	0.99474	0.04448	0.79638	1.0	3.16
O22	0.99445	0.85286	0.79101	1.0	3.16
O23	0.42789	0.73257	0.62264	1.0	3.16
O24	0.19712	0.73811	0.66072	1.0	3.16
O25	0.28604	0.73051	0.05402	1.0	3.16
O26	0.09595	0.73927	0.05845	1.0	3.16
Zn1wO5	0.92701	0.74971	0.03935	0.10478	12.13
Zn1wO4	0.98451	0.68609	0.18697	0.10478	12.13
Zn1wO3	0.98452	0.68648	0.18709	0.10478	12.13
Zn1wO2	0.77846	0.62263	0.29658	0.10478	12.13
Zn1wO1	0.95010	0.67831	0.30539	0.10478	12.13
Zn1wO6	0.94227	0.80658	0.34633	0.10478	12.13

Zn2wO1	0.78834	0.22010	0.53276	0.07059	24.43
Si1	0.42630	0.06877	0.66713	1.0	1.30
Si2	0.31221	0.02805	0.81102	1.0	1.30
Si3	0.28078	0.06363	0.03245	1.0	1.30
Si4	0.11917	0.05390	0.02077	1.0	1.30
Si5	0.06982	0.02880	0.81353	1.0	1.30
Si6	0.18341	0.05707	0.68220	1.0	1.30
Si7	0.42681	0.82636	0.67699	1.0	1.30
Si8	0.31782	0.86958	0.81961	1.0	1.30
Si9	0.27168	0.82731	0.02049	1.0	1.30
Si10	0.12795	0.82459	0.03131	1.0	1.30
Si11	0.07338	0.85814	0.79740	1.0	1.30
Si12	0.19300	0.82916	0.67740	1.0	1.30
Zn1	0.85291	0.69989	0.10658	0.10478	8.08
Zn2	0.70219	0.12028	0.78954	0.07059	16.29
C-1	0.71387	0.18742	0.64555	0.05	8
O-2	0.76131	0.15155	0.70463	0.05	8
D-3	0.79470	0.13030	0.66039	0.05	8
D-4	0.67676	0.21104	0.69468	0.05	8
D-5	0.73766	0.23215	0.61310	0.05	8
D-6	0.68236	0.15149	0.60481	0.05	8

6. *Solid-state nuclear magnetic resonance spectroscopy (ssNMR)*

^{31}P NMR

The Si:Al ratio of the ZSM-5 used is determined to be 19.25 with the same theoretical Si:H^+ ratio.
According to the crystal refinement, the ratio of Si: M (from occupancy value) after ion exchange of each catalyst: Si:Fe(site 1)=407:1 Si:Fe(site 2)=100:1 so overall Si: Fe(total)=80:1

Si:Zn(site 1)=231:1 Si:Zn(site2)= 169:1, overall Si:Zn(total)=98:1
Si:Ag(site 1)=343:1 Si:Ag(site2)= 240:1 Si:Ag(site3)=600:1 so overall Si:Ag(total)=114:1
These ratios suggest that the presence of an excess of BASs in the samples after ion-exchange.

Probe nuclear magnetic resonance (NMR) was used to measure the acidity before and after metal ion has been exchanged.[9]
Trimethylphosphine oxide (TMPO)-adsorbed sample was prepared for ^{31}P MAS NMR. Before loading TMP molecules, about 100 mg of catalysts was placed in a home-made glass tube and activated at 298 K for 2 h under vacuum (10^{-1} Pa) to ensure maximum adsorption of TMPO molecules, which was followed by mixing with CH_2Cl_2 solution containing 0.1 M TMPO under nitrogen and followed by a 1 h ultrasonic treatment (for equilibrium), and then solvent was evacuated completely under vacuum. The sample tube was then sealed for storage and transferred to Bruker 4 mm ZrO_2 rotor with a Kel-F endcap in a glove box under nitrogen atmosphere before NMR measurement. Solid-state magic angle spinning (MAS) NMR measurements were carried out using a Bruker Advance III 400WB spectrometer at room temperature. To remove the effect of proton spins on quantitative ^{31}P spectra, a strong radio frequency field (B) is usually applied in a pulsed at the resonance frequency of the non-observed abundant spins (^{1}H herein) which contribute to the coupling of both spin species. If B is strong such that spins of ^{1}H are flipped rapidly compared with the spin-spin interactions, the interaction is averaged to zero, and consequently, the excess broadening is zeroed. The high-power decoupling (HPDEC) was thus used for the quantitative ^{31}P analysis. Considering the long relaxation time of ^{31}P nuclei in NMR experiment, we used 30° pulse with the width of 1.20 μs, 15 s delay time. The radiofrequency for decoupling was 59 kHz. The spectral width was 400 ppm, from 200 to −200 ppm. The number of scans was 800 and the spinning frequency was 10 kHz. The ^{31}P chemical shifts were reported relative to 85% aqueous solution of H_3PO_4, with $NH_4H_2PO_4$ as a secondary standard (0.81 ppm). The quantitative analysis of adsorbed TMPO molecules was then calculated according to the calibration line established by running standard samples with various adsorbed TMPO concentration.

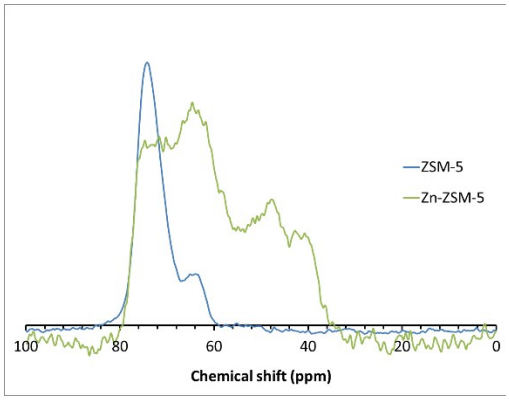


Figure S12. ^{31}P NMR of TMPO adsorbed on Zn-ZSM-5/H-ZSM-5

The TMPO probe NMR indicated most strong acidity (70-80 ppm) of H-ZSM-5 retained after ion-exchange, but Zn^{II} with terminal OH substituted in the framework also created the weak Brønsted acid sites at lower chemical shifts. The integrated area of TMPO molecule adsorbed (0.4 mmol g^{-1}) is consistent with the value from crystal refinement.

^{13}C NMR

Before data collection, samples were pre-treated using the following procedure. They were first placed in glass tubes connected to a vacuum line and dehydrated under vacuum at 400 °C for 10 h. When the samples were cooled to room temperature, a known amount of ^{13}C-methanol was introduced to the activated samples. The adsorption process was quenched by liquid N_2. After that, samples were transferred into a ZrO_2 rotor with a kel-F end-cap under a dry N_2 atmosphere in a glovebox.

^{1}H, ^{13}C magic-angle spinning (MAS) NMR measurements were carried out using a Bruker Avance III 400 W spectrometer at resonance frequencies of 399.33 and 104.22 MHz, respectively. A single-pulse sequence with a $\pi/2$ pulse length of 4.2 μs and a recycle delay of 3 s was used for $^{1}H-^{13}C$ cross-polarization (CP) NMR experiments using a 4 mm rotor at a spinning rate of 10 kHz. Hexamethylbenzene was used as the reference for the ^{13}C chemical shifts (17.35 ppm for methyl carbon).

7. *Computing modelling*

Periodic DFT calculations were performed to optimize the crystal structure of under the Kohn-Sham formulation as implemented in the Vienna *Ab initio* Simulation Package (VASP).[10] The exchange-correlation energy was described by the Perdew, Burke, and Ernzerhof functional (PBE) with the dispersion correction.[11] The semiempirical Grimme's D3 correction was employed to include van der Waals interactions.[12] A 19T cluster model was cut from the optimized structures to explore the reaction mechanism, and the terminal was saturated by hydrogen with the 1.456 Å Si-H bond length. All the cluster model calculation were carried out on Gaussian 09 program[13] and the B3LYP with Grimme D3BJ correction[14], was used to geometry optimization, transition state search and frequency calculation. The light elements (C, H, O, Si and Al) were described by 6-31G (d, p) basis set, but Ag and Zn were described by LanL2DZ with the pseudopotential.

Product Distribution of GVL-to-aromatics over various metal-doped ZSM-5

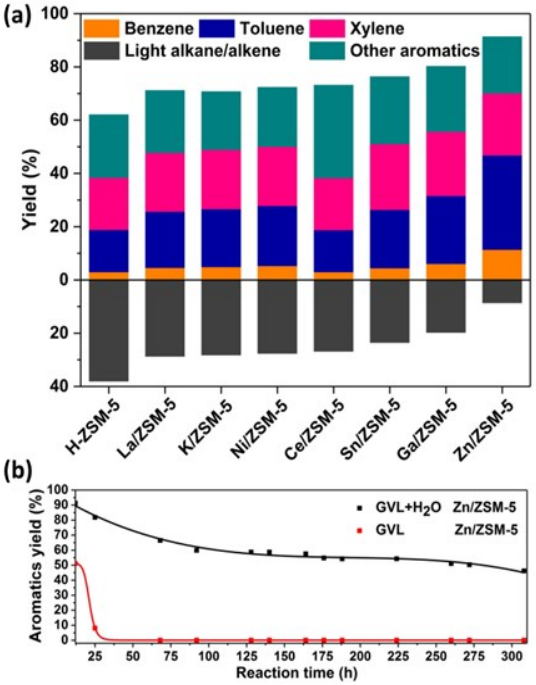


Figure S13. (a) Product distribution over various ZSM-5 based catalysts (5 g) by feeding 40 wt% GVL aqueous solution to the preheated catalyst bed with WHSV 1.0 h^{-1} at 10 bar after 12 h (the time to collect the liquid products for analysis) at complete gamma valerolactone (GVL) conversions. (b) Long-term catalytic performance of Zn-ZSM-5 with water activation using WHSV 1.0 h^{-1} at 450 °C.[6]

It is noted from the lifetime study in the figure below that there was a considerable drop of aromatics yield from the first 50 hours; the performance, however, remained significantly steady thereafter. In addition, the weight ratio of coke in the catalyst even after the first day to the end of the prolonged testing period remained around 13-15% throughout. Thus, it appears that this level of coke has quickly built up due to the nature of the structure as well as the acid sites distribution but somehow reached a steady value afterwards. Nevertheless, there is no rapid catalyst deactivation, and the catalytic activity can be fully regenerated by calcination in air under 600 °C.

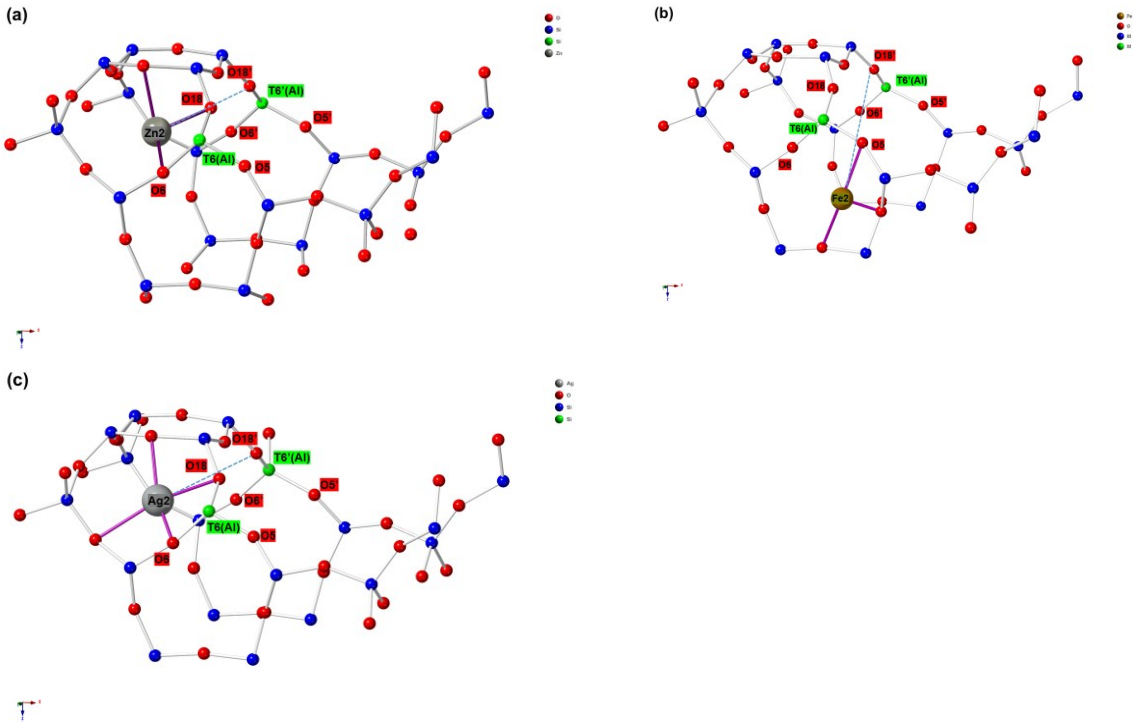


Figure S14. Anchored transition metal ion (Site 2) shown in H-ZSM-5 (**a**) Zn^{2+}; (**b**) Fe^{3+} and (**c**) Ag^{+} creating a range of molecular distances with O^{2-} of BAS of T6 (O5, O6, O18, O19) and T6' (O5', O6', O18', O19') sites in H-ZSM-5 structure. Typically, Zn-O18' is 5.32(6) Å; Fe-O18' is 7.58(7) Å and Ag-O18' is 5.83(6) Å.

From the above studies, we believe the similar methoxy is formed over Zn, Fe or Ag-ZSM-5, which show the importance of methoxy on the Lewis acid metal sites.

Concept of FLP activation:

Base: a lone pair of electrons
Acid: an empty orbital

Classical adduct will be formed if no steric clash otherwise the unquenched reactivity for heterolytic activation of small molecules is resulted.

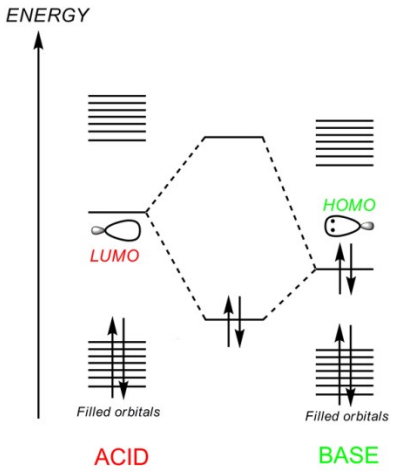


Figure S15. Frontier MO Theory showing a classical adduct formation with free Lewis acid and Lewis base. If a steric hindrance existed between the Lewis acid and base within molecular distance, it could form FLP for heterolytic cleavage of a small molecule such as methanol whereby base will activate proton and acid activate the polar methoxy species.

It is noted that the structure characterization of FLP-like sites is very difficultly verified by experimental techniques. FLP-like sites show some common acid-base properties. If poisoning the active sites by small Lewis acid or base, the catalytic performance might be inhibited. From our careful analysis and DFT modelling of the catalytic performance of methanol conversion (to aliphatic and aromatic products), the synergetic effect between the FLPs is verified.

To gain further information, a poison experiment may implicate the FLP structures. There are many well-known species such highly conjugated alkenes and polar species that can rapidly inhibit the methanol conversions with enhanced carbon deposition although the full poisoning mechanisms could be rather complex. For example in 1997, Jack Lunsford and David Goodman (Appl. Catal. A 1997, 149, 289) demonstrated clearly that water molecule has a strong inhibtation effect on methanol coversions over solid catalysts including zeolites, which was attributed to its strong competitive adsorption to the acid sites.

From our previous studies of W-ZSM-5, we have identified from diffraction that *cis*-stilbene binds strongly onto the Lewis acidic W species, giving molecular poisoning phenomenon (*Chem. Commun.*, 2018, 54, 7014). The above poisoning studies infer consistently to the significance of the FLP structures.

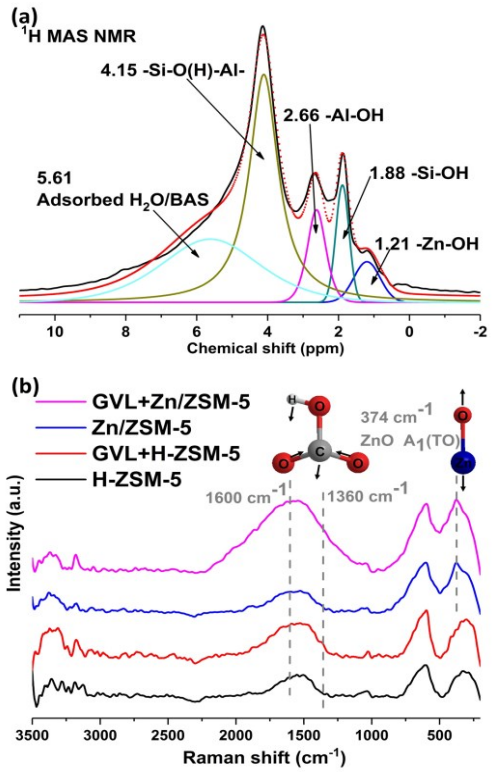
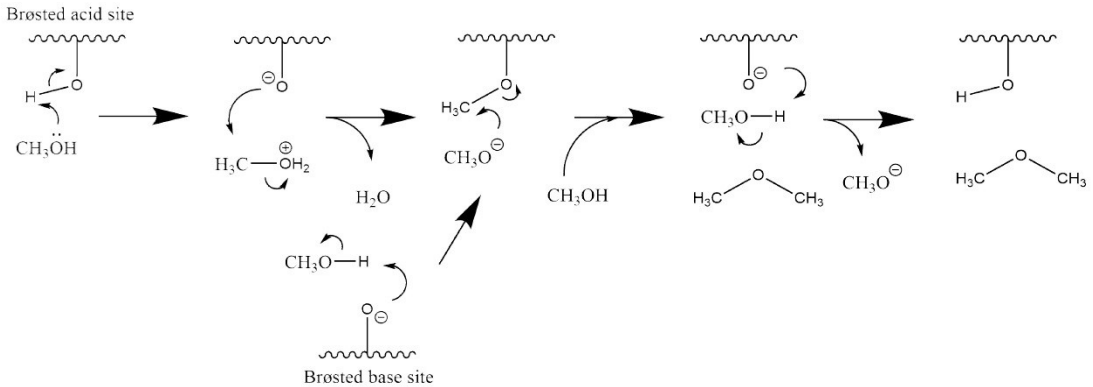


Figure S16. (**a**). ^{1}H MAS NMR of fresh Zn-ZSM-5 at 30 °C, after vacuum pre-treatment at 300 °C for 8 h, experimental data (black line), simulated data (red dot) and partial contributions to the simulated spectrum (blue, green, violet, dark yellow and light blue line). This gives the characteristic Zn-OH peak. (**b**) shows clearly the characteristic large peak and wide broadening of Raman absorption frequencies near 1100-2240 cm^{-1} which encompasses (-C=O) of GVL at ~1600 cm^{-1} peak maxima and symmetrical (O-C-O) at 1360 cm^{-1} peak maxima upon the GVL adsorption on Zn-ZSM-5. In addition, A1 (TO) mode of Zn-O at 374 cm^{-1} can be visible on the terminal Zn-OH in Zn-ZSM-5.

The general perceived mechanism for DME formation from methanol over unmodified H-ZSM-5 is shown below. This acid-base reaction can also be regarded as similar to FLP type of activation whereby the H^+ on BAS acts as an acid and the O^{2-} as a base to interact with CH_3OH.



Scheme S1. The general acid-base mechanism for the formation DME from methanol by H-ZSM-5. The wavy lines represent the wall of zeolites.

All Cartesian coordinates and total energies are shown from theoretical calculations are presented in Table S14; the imaginary frequencies in three transition states are -460 cm^{-1}, -504 cm^{-1}, -502cm^{-1} for H-ZSM-5, Zn-ZSM-5 and Ag-ZSM-5, respectively. Moreover, their vibrational mode is corresponding to the direction of reactant and product formation, which can be observed from their displacement vectors. The used LANL2DZ basis set is the Gaussian build-in version, which includes the d functions, as well as the polarization functions.

Table S14. Cartesian coordinates and energies of species based on theoretical calculations.

ZSM-5-OCH3

E = -7391.937591 a.u.

O	0	6.20949400	-0.41491800	-1.19286900
O	0	-1.08516800	1.01826400	-2.63136500
O	0	-0.54715200	3.56347000	-2.87636100
O	0	-4.76576600	-0.28356800	2.20929800
O	0	-0.43875500	5.79948400	-1.38827300
O	0	-4.26335300	-0.61439300	-0.38873400
O	0	-0.71644400	5.63155000	1.28554600
O	0	-4.64142200	-2.78946300	-1.81131700
O	0	-1.76948200	3.26374300	2.03223000
O	0	6.29449800	1.14869600	0.96886000
O	0	-1.34088800	2.66588000	-0.52387500
O	0	-0.42567300	-1.00171700	3.00077000
O	0	3.76385500	-2.09107300	0.97573500
O	0	-0.33006600	-1.21854300	0.32535100
O	0	0.18538800	-3.79326700	-0.92932200
O	0	-2.96478800	-2.02335200	3.17543800
O	0	-2.52241000	-4.14575700	-0.85374200
O	0	4.54966500	-2.44869300	-1.62101800
O	0	-0.10352600	-1.43805600	-2.61572000
O	0	-2.73213500	-1.07138700	-2.54945500
O	0	4.40095200	-0.03829400	2.46678400
O	0	-0.24610900	1.20063400	1.45550300
O	0	-2.86256400	1.10902400	0.98854700
O	0	1.82972800	-0.34695800	1.65051500
O	0	2.10954900	-1.73674100	-1.07748300
Si	0	6.12788800	-1.97048300	-1.67337700
Si	0	-1.31410700	-0.52430200	-3.15286200
Si	0	6.98546000	0.84228700	-0.47804400
Si	0	-4.54774300	-1.78599200	2.83894400
Si	0	-0.15883600	5.16083300	-2.86284600
Si	0	-4.34053900	0.46231000	0.82517700
Si	0	-0.38372900	6.61349700	0.02289200
Si	0	-4.21043100	-1.22096900	-1.89901800
Si	0	-1.94000000	4.89243400	2.07832700
Si	0	-4.11128300	-4.24346400	-1.26146500
Si	0	5.91800200	0.58561600	2.46395700
Si	0	-1.54902700	2.04968700	0.97358700
Si	0	-1.37491000	-2.28197300	3.46772600
Si	0	3.18997200	-1.07810000	2.16334100

Si	0	3.39784800	-2.68796800	-0.49391100
Si	0	-1.02782000	-4.84853800	-0.69380500
Si	0	0.17388000	-0.37413900	1.59966900
Al	0	0.24558700	-2.08544700	-1.05838700
C	0	2.45175500	-0.39064000	-1.56846700
H	0	3.32724700	-0.02717600	-1.03254000
H	0	2.64233900	-0.46150100	-2.63659000
H	0	1.60005600	0.25654300	-1.37372900
Si	0	-1.54685500	2.49360000	-2.14155000
H	-1	6.85871400	-2.84898400	-0.77429500
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H	-1	5.89333900	1.73768500	3.33080000
H	-1	2.89122900	-1.80923500	3.38207300
H	-1	0.94006700	7.08420800	0.35701300
H	-1	1.26591400	5.34049300	-3.20437600
H	-1	-1.02203200	5.83599800	-3.83816600
H	-1	-1.30197700	7.75745400	-0.10539500
H	-1	-1.85657100	5.27929700	3.48573600
H	-1	-3.18395200	5.31514800	1.41352500
H	-1	-5.37870500	1.45721900	0.59011900
H	-1	-5.35354400	-1.79494100	4.05665700
H	-1	-5.06622200	-2.79240000	1.89363400
H	-1	-4.94016500	-4.70805500	-0.15087800
H	-1	-4.39692700	-5.19702800	-2.31885000
H	-1	-0.89000100	-5.38952000	0.64962300
H	-1	-0.92079700	-5.95677000	-1.64225000
H	-1	3.08587100	-4.10305800	-0.39744200
H	-1	-0.96997300	-3.45479800	2.68501000
H	-1	-1.21281000	-2.53708400	4.93520900
H	-1	6.79881300	1.98739000	-1.35983500
H	-1	-1.34277000	-0.55978600	-4.61726800
H	-1	-5.15402100	-0.51787900	-2.75261100
H	-1	-2.96346200	2.73183200	-2.51451800

ZSM-5-OCH3_MeOH

E = -7507.637322 a.u.

O	0	6.18857400	0.27891000	-0.83619800
O	0	-1.16524500	0.80696500	-2.64395500
O	0	-0.87818400	3.36363300	-3.08725900
O	0	-4.89150900	-0.47948200	2.16714100
O	0	-1.06573000	5.71065700	-1.78916000
O	0	-4.25656400	-0.97431100	-0.37164900
O	0	-1.43974600	5.73418700	0.87772600
O	0	-4.34536000	-3.27989500	-1.62546200
O	0	-2.26988800	3.33589800	1.78571000
O	0	6.00386100	2.01377900	1.19140800
O	0	-1.67280100	2.58443500	-0.69374100
O	0	-0.55576300	-0.66027600	3.18162600
O	0	3.79446400	-1.48710500	1.34366600
O	0	-0.34006500	-1.12403100	0.55923400
O	0	0.49974700	-3.69344400	-0.55418700
O	0	-2.97235400	-1.94483000	3.33937600
O	0	-2.14691400	-4.32251200	-0.47492900
O	0	4.73472900	-1.89963400	-1.17091200
O	0	0.05399400	-1.51907900	-2.37273400
O	0	-2.59242400	-1.43206200	-2.43073400
O	0	4.18099600	0.73127400	2.69904300
O	0	-0.52557900	1.39486100	1.43143900
O	0	-3.09984300	1.00689600	0.88320800
O	0	1.68069800	0.09725200	1.85111600
O	0	2.18856300	-1.40584300	-0.71299100
Si	0	6.26780800	-1.31189000	-1.18039100
Si	0	-1.21752900	-0.78667100	-3.03449700
Si	0	6.78515800	1.66258900	-0.19840900
Si	0	-4.55354700	-1.89657800	2.92885900
Si	0	-0.65654200	4.98959600	-3.19345800
Si	0	-4.49191600	0.19059500	0.73799600
Si	0	-1.15446500	6.63924500	-0.45183300
Si	0	-4.07565200	-1.68494900	-1.82405400
Si	0	-2.61311800	4.93553800	1.68820000
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Si	0	-1.88337700	2.06986400	0.84190900
Si	0	-1.37847800	-2.00071700	3.70977800
Si	0	3.09961300	-0.46033700	2.43993500
Si	0	3.55573000	-2.24287000	-0.10301800
Si	0	-0.60161700	-4.84810600	-0.20841400
Si	0	0.04578100	-0.10559700	1.75116800
Al	0	0.40218000	-1.97633800	-0.74650900
C	0	2.42531200	-0.07473900	-1.28209300
H	0	3.21719100	0.41640400	-0.71896300
H	0	2.70319300	-0.19606900	-2.32673600
H	0	1.50104500	0.49207200	-1.19559200
Si	0	-1.79444800	2.26163100	-2.29570800

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H	-1	6.85943900	-1.47851700	-2.50621500
H	-1	8.22358500	1.52849200	0.07525300
H	-1	6.72674800	0.72786700	3.30922500
H	-1	5.43957200	2.74051100	3.47704400
H	-1	2.81726700	-1.08783300	3.72809600
H	-1	0.09837600	7.27263200	-0.11394800
H	-1	0.75541700	5.28824600	-3.49931800
H	-1	-1.54158300	5.48566200	-4.25214000
H	-1	-2.17865200	7.66503300	-0.70976300
H	-1	-2.63179400	5.44363900	3.05920200
H	-1	-3.86465400	5.16964400	0.94679000
H	-1	-5.61473600	1.04696500	0.38153000
H	-1	-5.40709600	-1.89033000	4.11296400
H	-1	-4.92544600	-3.02503300	2.05464300
H	-1	-4.51517300	-5.07712800	0.18745800
H	-1	-3.83117000	-5.68130900	-1.91049500
H	-1	-0.45512200	-5.25889900	1.18325500
H	-1	-0.32811700	-6.01142300	-1.05120500
H	-1	3.40972200	-3.64907900	0.16819700
H	-1	-0.82114100	-3.18378500	3.04132400
H	-1	-1.25414500	-2.11630500	5.19480200
H	-1	6.51742400	2.70077500	-1.18352100
H	-1	-1.17129100	-0.95033600	-4.49077200
H	-1	-5.04407400	-1.15951100	-2.76966700
H	-1	-3.21037800	2.31209900	-2.73532100
C	0	2.76864300	-3.20507800	-3.48459700
H	0	3.74659000	-2.75157500	-3.66155800
H	0	2.59955300	-3.98029700	-4.24326200
H	0	1.99265800	-2.43762700	-3.57777500
O	0	2.80867900	-3.75889700	-2.17316500
H	0	1.91427900	-4.02508300	-1.89945500

ZSM-5-OCH3_MeOH-to-DME(TS)

E = -7507.559125 a.u.

O	0	6.22233300	0.27313500	-0.82205300
O	0	-1.14353000	0.74007300	-2.65272300
O	0	-0.84118100	3.27201300	-3.20529300
O	0	-4.85222200	-0.31198300	2.23566800
O	0	-1.02264700	5.67770500	-2.01198500
O	0	-4.24438100	-0.94811600	-0.27215000
O	0	-1.39393500	5.82082100	0.65218900
O	0	-4.32815000	-3.29726800	-1.43834800
O	0	-2.25101500	3.46800700	1.66680300
O	0	6.04658600	2.10109900	1.13418400
O	0	-1.63460400	2.61360100	-0.77439300
O	0	-0.52967600	-0.45199500	3.25007000
O	0	3.79325800	-1.35359600	1.44652400
O	0	-0.26950000	-1.03817600	0.66120800
O	0	0.49072500	-3.65444400	-0.37316900
O	0	-2.93969800	-1.73646500	3.46991400
O	0	-2.13598000	-4.29466700	-0.22664600
O	0	4.79788400	-1.98630100	-1.01721700
O	0	0.03613100	-1.60435500	-2.26239000
O	0	-2.59301900	-1.47607700	-2.33521300
O	0	4.22268400	0.90463100	2.72140500
O	0	-0.50505200	1.52227300	1.41898600
O	0	-3.06475800	1.09739700	0.85063700
O	0	1.70986700	0.28341000	1.91953500
O	0	2.25754200	-1.60200700	-0.76375600
Si	0	6.29893500	-1.33467100	-1.07449300
Si	0	-1.21178500	-0.86859800	-2.95075300
Si	0	6.81863100	1.68385100	-0.24154200
Si	0	-4.51878500	-1.69740000	3.05739500
Si	0	-0.61430300	4.89073900	-3.38029100
Si	0	-4.46036400	0.28226900	0.77136100
Si	0	-1.10736600	6.66483200	-0.71672500
Si	0	-4.06225500	-1.71006700	-1.69641000
Si	0	-2.57072200	5.06526300	1.49937200
Si	0	-3.68420300	-4.59772000	-0.67592500
Si	0	5.65643300	1.69180900	2.67577800
Si	0	-1.85126200	2.16381900	0.78144000
Si	0	-1.34311100	-1.76885300	3.83808700
Si	0	3.12391700	-0.27740400	2.50422200
Si	0	3.55226600	-2.17502100	0.04679900
Si	0	-0.58968300	-4.79493500	0.05607400
Si	0	0.08693600	0.04526700	1.80120700
Al	0	0.50507200	-1.90904700	-0.61387800
C	0	2.65511900	-1.72164600	-3.01014400
H	0	3.65288300	-2.13162500	-2.98197200
H	0	1.93745200	-2.06563300	-3.73615900
H	0	2.50464400	-0.72612100	-2.62777600
Si	0	-1.75784400	2.21295000	-2.35722600

H	-1	7.07736900	-2.00561000	-0.05350300
H	-1	6.88937300	-1.55367900	-2.39919500
H	-1	8.26114800	1.56679500	0.03964300
H	-1	6.76486600	0.91963800	3.30803400
H	-1	5.48177000	2.94048100	3.38329000
H	-1	2.85207300	-0.86691800	3.81269900
H	-1	0.14716900	7.31229100	-0.41050600
H	-1	0.79805600	5.17210300	-3.70081600
H	-1	-1.49904200	5.33907900	-4.46066900
H	-1	-2.12948000	7.68127500	-1.02255500
H	-1	-2.58452300	5.63754900	2.84542300
H	-1	-3.81932000	5.26856000	0.74863300
H	-1	-5.57786400	1.12766000	0.37567300
H	-1	-5.37363300	-1.63428700	4.23894000
H	-1	-4.89554400	-2.86394200	2.23502200
H	-1	-4.49056300	-5.00104600	0.46455000
H	-1	-3.80912800	-5.70303200	-1.60361000
H	-1	-0.43021100	-5.14467600	1.46538600
H	-1	-0.30617900	-6.00001700	-0.73195000
H	-1	3.43713700	-3.59128300	0.37474000
H	-1	-0.79091300	-2.98508300	3.22564500
H	-1	-1.22039000	-1.81827200	5.32769900
H	-1	6.55646900	2.68300900	-1.27106600
H	-1	-1.14162700	-1.10179500	-4.40153000
H	-1	-5.01364300	-1.22332700	-2.67035900
H	-1	-3.17310100	2.24242000	-2.79769800
C	0	1.46611500	-4.45312600	-3.42286400
H	0	2.06390900	-4.42450000	-4.33747200
H	0	1.26638600	-5.50018800	-3.17069300
H	0	0.51485600	-3.93217700	-3.58068500
O	0	2.22127800	-3.83813500	-2.38151000
H	0	1.64866100	-3.86185000	-1.56807300

ZSM-5-OH_DME

E=-7507.903198 a.u.

O	0	6.09909600	1.08903100	-0.85252300
O	0	-1.27601900	0.61717400	-2.65342800
O	0	-1.27866200	3.17722600	-3.25069600
O	0	-4.81041500	-0.84523900	2.21009600
O	0	-1.75518000	5.55066100	-2.07281300
O	0	-4.10130700	-1.38212200	-0.29835000
O	0	-2.13947200	5.67489600	0.59052800
O	0	-3.93906100	-3.74345800	-1.42903600
O	0	-2.65309500	3.24129700	1.62795700
O	0	5.70831400	2.90368500	1.07999800
O	0	-1.99135200	2.44308100	-0.81383700
O	0	-0.49879800	-0.43370600	3.23061900
O	0	4.00704900	-0.81530000	1.46996000
O	0	-0.20286500	-1.08468800	0.67245800
O	0	0.91712300	-3.53311800	-0.44969500
O	0	-2.72910200	-2.01229100	3.45414700
O	0	-1.63368400	-4.45548400	-0.22774600
O	0	4.97914500	-1.36163900	-1.04115700
O	0	0.20710100	-1.56600800	-2.28010700
O	0	-2.40908500	-1.77444100	-2.36316400
O	0	4.02852500	1.51777500	2.68121000
O	0	-0.69907700	1.47610500	1.34531800
O	0	-3.21199600	0.79061200	0.85676400
O	0	1.64916700	0.48866200	1.85893900
O	0	2.40260900	-1.19899800	-0.63523600
Si	0	6.37097400	-0.49825100	-1.11223100
Si	0	-1.11504300	-0.98011400	-2.97629200
Si	0	6.52110500	2.56976000	-0.29772000
Si	0	-4.30242100	-2.16524100	3.04560800
Si	0	-1.25183300	4.81192300	-3.43832500
Si	0	-4.48667500	-0.19695600	0.75137000
Si	0	-1.95900700	6.53311900	-0.78751800
Si	0	-3.84312300	-2.13409700	-1.71450200
Si	0	-3.20338500	4.77611400	1.44430600
Si	0	-3.14681000	-4.95391900	-0.68206300
Si	0	5.36950900	2.45981200	2.62246600
Si	0	-2.12103700	1.98142400	0.74598200
Si	0	-1.14201700	-1.83586100	3.82360700
Si	0	3.13520400	0.17090000	2.46654000
Si	0	3.77679100	-1.63375000	0.05473600
Si	0	-0.07207200	-4.80349800	0.05917300
Si	0	0.06042200	0.08698800	1.76534700
Al	0	0.75123500	-1.66587200	-0.64648900
Si	0	-2.05384200	2.01782200	-2.39440600
H	-1	7.24002000	-1.04843700	-0.08498800
H	-1	6.99456500	-0.63772100	-2.43291900
H	-1	7.97054200	2.64392800	-0.01523900
H	-1	6.57012600	1.83575000	3.25978400

H	-1	5.04583200	3.68179100	3.32552100
H	-1	2.91041100	-0.42028300	3.78245100
H	-1	-0.79536600	7.33321900	-0.48386800
H	-1	0.11278200	5.27048300	-3.76268700
H	-1	-2.18813500	5.14593300	-4.51912000
H	-1	-3.10091300	7.41253500	-1.09373100
H	-1	-3.29378000	5.35174000	2.78708600
H	-1	-4.47556800	4.81935300	0.69492200
H	-1	-5.70626200	0.48971100	0.34992100
H	-1	-5.15547700	-2.20169900	4.22888700
H	-1	-4.53058900	-3.37466200	2.23141800
H	-1	-3.86511900	-5.45556200	0.47286400
H	-1	-3.10406400	-6.07993600	-1.59235800
H	-1	0.18278900	-5.08724700	1.46678000
H	-1	0.40962400	-5.93386900	-0.72561600
H	-1	3.82568600	-3.07174300	0.35959700
H	-1	-0.44160500	-2.97853100	3.21500200
H	-1	-1.01038800	-1.86128200	5.31085700
H	-1	6.13880100	3.53150500	-1.32924900
H	-1	-1.03257900	-1.20001700	-4.42248000
H	-1	-4.85748400	-1.79154500	-2.68335100
H	-1	-3.46228600	1.87545200	-2.83470600
C	0	3.65716200	-5.00223000	-1.88593000
H	0	3.97452400	-5.60165000	-2.74619800
H	0	4.48412100	-4.37054700	-1.54614700
H	0	3.34393700	-5.66449200	-1.07717000
O	0	2.52520100	-4.20777600	-2.24378500
H	0	1.60310200	-3.81691200	-1.18455700
C	0	2.80714200	-3.24122200	-3.27592600
H	0	3.08641400	-3.77143400	-4.19237100
H	0	1.89362400	-2.66743200	-3.42106900
H	0	3.61320000	-2.57329700	-2.95822300

Ag-ZSM-5-OCH3

E = -7490.625097 a.u

Ag	0	0.91483600	1.70807100	-0.85468200
O	0	6.08828700	-0.87663800	-1.01694300
O	0	-0.85495000	0.85648500	-2.45087400
O	0	-0.16768900	3.44860000	-2.67630200
O	0	-4.94958700	-0.21299300	2.19106500
O	0	-0.19003900	5.71151400	-1.20575000
O	0	-4.36385300	-0.51354200	-0.39421600
O	0	-0.52983600	5.44734900	1.45426200
O	0	-4.82928300	-2.62432200	-1.87956600
O	0	-1.76262600	3.15142400	2.25767700
O	0	6.22099700	0.63290100	1.18152000
O	0	-1.20718300	2.60860700	-0.29617100
O	0	-0.61969900	-1.21975600	3.01986400
O	0	3.49464300	-2.44776200	1.05192500
O	0	-0.42716900	-1.28185300	0.30870200
O	0	-0.08333500	-3.94562100	-0.85751500
O	0	-3.23220400	-2.05188200	3.14058400
O	0	-2.82211800	-4.12443700	-0.91835900
O	0	4.35508600	-2.83210200	-1.51839200
O	0	-0.26760200	-1.69310200	-2.64848800
O	0	-2.81715900	-0.97312900	-2.53039600
O	0	4.24957100	-0.48741000	2.61875700
O	0	-0.28414100	1.04930100	1.60370000
O	0	-2.90954800	1.06517100	1.11280400
O	0	1.69916300	-0.58493400	1.74399200
O	0	1.94811500	-2.00255400	-1.09776700
Si	0	5.95193500	-2.41923300	-1.52909100
Si	0	-1.33654800	-0.55837500	-3.10682100
Si	0	6.92686400	0.31645100	-0.25746800
Si	0	-4.80356600	-1.73443500	2.78681100
Si	0	0.09899400	5.05142400	-2.68232600
Si	0	-4.42501300	0.53929100	0.84035700
Si	0	-0.12578800	6.46613300	0.22918900
Si	0	-4.31628500	-1.07264800	-1.92734200
Si	0	-1.81447300	4.79596000	2.23396700
Si	0	-4.41128700	-4.12204600	-1.35793800
Si	0	5.79617700	0.05789200	2.66026100
Si	0	-1.57593100	1.97954900	1.14294500
Si	0	-1.67498400	-2.42914800	3.46321800
Si	0	2.98302900	-1.44110000	2.27164200
Si	0	3.15583400	-3.01681500	-0.43313600
Si	0	-1.38091700	-4.92272200	-0.73814100
Al	0	-1.49377000	2.46242800	-2.06117700
H	-1	-4.73188600	-5.04281800	-2.43978200
H	-1	-5.28965400	-4.57111900	-0.27164300
H	-1	-1.29942500	-5.49251000	0.58735600
H	-1	-1.31653300	-6.00789200	-1.71685000
H	-1	-5.22232800	-0.32063700	-2.78188200

H	-1	-5.40346800	1.59160600	0.59958400
H	-1	-1.38351000	-0.53328100	-4.57701000
H	-1	-2.93793900	2.81045300	-2.45136200
H	-1	-0.72746900	5.81679700	-3.64845300
H	-1	-0.97438800	7.67028200	0.12084200
H	-1	1.21787600	6.86431400	0.60898000
H	-1	1.51701900	5.18204400	-2.98416300
H	-1	-1.73419600	5.15015200	3.64458600
H	-1	-3.01688300	5.30376200	1.54970700
H	-1	5.81121600	1.18950500	3.55199500
H	-1	6.76163300	-0.96922800	3.13679600
H	-1	8.33251900	-0.06520400	-0.03418300
H	-1	6.82046200	1.48930600	-1.11446400
H	-1	6.60338400	-3.35442400	-0.63685800
H	-1	6.48255700	-2.52297300	-2.88095000
H	-1	2.76076300	-4.40573000	-0.35747000
H	-1	2.61853700	-2.18626300	3.46846300
H	-1	-1.54882200	-2.71919900	4.92940300
H	-1	-5.62469500	-1.73053500	3.99212600
H	-1	-5.35027600	-2.69569200	1.81279600
H	-1	-1.31281800	-3.60040000	2.66394100
Si	0	0.03651400	-0.55711000	1.67002300
Al	0	0.03964400	-2.25139100	-1.05410700
C	0	2.38371600	-0.73408000	-1.66335600
H	0	2.65426000	-0.06293800	-0.83615400
H	0	3.25471600	-0.89553800	-2.29391000
H	0	1.55693000	-0.36766400	-2.27157800

Ag-ZSM-5-OCH3_CH3OH

E = -7606.351102 a.u.

Ag	0	0.81460800	0.93866400	-0.61566900
O	0	6.00677100	-1.30089500	-0.86301000
O	0	-0.85250200	0.92475000	-2.46209400
O	0	0.03272200	3.50273600	-2.64774300
O	0	-5.06741800	0.05001500	2.14067200
O	0	0.15779400	5.72467800	-1.08658400
O	0	-4.47820100	-0.24337600	-0.44093500
O	0	-0.28459300	5.47121800	1.56858300
O	0	-5.04160000	-2.31287400	-1.95356200
O	0	-1.68590400	3.24375900	2.28984900
O	0	6.19113300	0.17824800	1.36343100
O	0	-1.06292300	2.61006100	-0.24572900
O	0	-0.86127900	-1.27852000	3.04994400
O	0	3.09107800	-2.64858100	1.08916600
O	0	-0.41348400	-1.24473100	0.33878300
O	0	-0.43450200	-3.93803500	-0.83757600
O	0	-3.52503400	-1.93041200	3.11830800
O	0	-3.16955900	-3.97873800	-0.98128400
O	0	4.16042500	-3.15933100	-1.39084700
O	0	-0.47968600	-1.67634800	-2.61950600
O	0	-2.94247000	-0.76233200	-2.57504000
O	0	4.13021800	-0.87241200	2.72966900
O	0	-0.40315100	1.01440600	1.74980200
O	0	-2.96035000	1.25255800	1.09886500
O	0	1.55434000	-0.63828000	1.98702100
O	0	1.78381600	-2.21421800	-1.22726900
Si	0	5.77226000	-2.82412700	-1.40063100
Si	0	-1.42576500	-0.45161300	-3.11364800
Si	0	6.89646000	-0.16402500	-0.07331700
Si	0	-5.05858500	-1.48191300	2.72833500
Si	0	0.41028900	5.08235300	-2.57899300
Si	0	-4.49159600	0.79997300	0.80604500
Si	0	0.22557900	6.46281700	0.36252100
Si	0	-4.44529800	-0.78857100	-1.98120300
Si	0	-1.62046500	4.88409200	2.31741300
Si	0	-4.74270000	-3.84856000	-1.45649200
Si	0	5.69368500	-0.38670100	2.82582100
Si	0	-1.55712700	2.05925700	1.17965300
Si	0	-2.00236800	-2.41112500	3.46502800
Si	0	2.75834100	-1.66560300	2.38146100
Si	0	2.87157200	-3.24499800	-0.40425600
Si	0	-1.77866900	-4.85657600	-0.78367800
Al	0	-1.33916400	2.56834800	-2.00948500
H	-1	-5.09826900	-4.73428200	-2.56203000
H	-1	-5.66939900	-4.25131200	-0.38932800
H	-1	-1.74942500	-5.45001500	0.53716100
H	-1	-1.75447100	-5.93693400	-1.78367300
H	-1	-5.27027700	0.03448300	-2.85040100

H	-1	-5.39310600	1.92091100	0.56718000
H	-1	-1.40224400	-0.41120200	-4.58198600
H	-1	-2.78118200	3.01620300	-2.43209500
H	-1	-0.34378500	5.89666100	-3.55063400
H	-1	-0.54417400	7.72379700	0.25426800
H	-1	1.58920100	6.76471500	0.77543100
H	-1	1.84970200	5.10350200	-2.84927900
H	-1	-1.54262700	5.20558800	3.74322600
H	-1	-2.77562500	5.47044600	1.61744600
H	-1	5.75717500	0.73741400	3.74104000
H	-1	6.57501400	-1.48360900	3.31300400
H	-1	8.27218600	-0.64292600	0.17176900
H	-1	6.88166000	1.02836300	-0.92066700
H	-1	6.33440300	-3.81658500	-0.51128700
H	-1	6.31327500	-2.94778400	-2.75535900
H	-1	2.40937700	-4.61845600	-0.31880200
H	-1	2.33693800	-2.43224700	3.54995700
H	-1	-1.90285200	-2.70771900	4.92955800
H	-1	-5.90234200	-1.43504400	3.92381700
H	-1	-5.64753500	-2.39348900	1.72787500
H	-1	-1.67925800	-3.57842900	2.64754600
Si	0	-0.09176100	-0.58741700	1.78959100
Al	0	-0.12447800	-2.26999000	-1.05251600
C	0	2.35860700	-1.26666200	-2.20380700
H	0	3.09874600	-0.64477200	-1.70171100
H	0	2.81513000	-1.83440200	-3.01123800
H	0	1.53397000	-0.67823400	-2.59038900
C	0	3.13325100	3.08336600	-1.14889500
H	0	2.53398700	3.72667100	-0.49447000
H	0	3.81769700	2.48934800	-0.53867400
H	0	3.71477800	3.70867700	-1.83283900
O	0	2.30852400	2.16680000	-1.88294300
H	0	1.58570100	2.67171500	-2.33662700

Ag-ZSM-5-OCH3_CH3OH-to-OH+DME(TS)

E = -7606.302571 a.u.

Ag	0	1.32906100	2.66928100	-0.20099200
O	0	5.87706500	-1.72396100	-0.88185300
O	0	-0.61512100	0.93726400	-2.53595800
O	0	0.17900300	3.43401300	-2.50745000
O	0	-5.08430100	0.16168100	2.13499300
O	0	0.49522400	5.55386500	-0.93047600
O	0	-4.56793100	-0.16146300	-0.44934300
O	0	-0.00867700	5.21381900	1.66427100
O	0	-5.04754800	-2.11921600	-2.11035200
O	0	-1.55163700	3.08819600	2.35149300
O	0	6.11607700	-0.32240300	1.39197200
O	0	-0.96229900	2.56642100	-0.18184200
O	0	-0.94510200	-1.39064100	3.00821400
O	0	3.11603000	-3.08100300	1.10740500
O	0	-0.74065400	-1.37151300	0.29584100
O	0	-0.66044800	-4.03588000	-0.98352800
O	0	-3.63737000	-1.91410800	3.03416800
O	0	-3.38472700	-3.90346800	-1.06658900
O	0	3.90622100	-3.39862900	-1.48237200
O	0	-0.51654300	-1.70577400	-2.63147900
O	0	-2.89065900	-0.46843800	-2.49999800
O	0	3.97263200	-1.22268800	2.75214100
O	0	-0.29875700	0.85632100	1.70996500
O	0	-2.89624400	1.19945000	1.05971800
O	0	1.46360500	-1.03329300	1.80147000
O	0	1.57257800	-2.39466200	-0.94909100
Si	0	5.53150500	-3.22950500	-1.43743300
Si	0	-1.36758000	-0.42794800	-3.10842200
Si	0	6.81749000	-0.68127600	-0.04172200
Si	0	-5.14426800	-1.39839100	2.65583500
Si	0	0.67919800	4.96406500	-2.45279400
Si	0	-4.47071300	0.86805600	0.80081100
Si	0	0.54704400	6.26681700	0.53110300
Si	0	-4.43601400	-0.60826000	-2.01531700
Si	0	-1.39866800	4.71846900	2.41064200
Si	0	-4.92173100	-3.67064900	-1.57335800
Si	0	5.57495100	-0.89598600	2.83760500
Si	0	-1.45907300	1.90780400	1.22095000
Si	0	-2.13947600	-2.48464700	3.37359400
Si	0	2.63883900	-2.05728200	2.30947400
Si	0	2.64616200	-3.49376500	-0.42470800
Si	0	-2.04145400	-4.85837400	-0.90729900
Al	0	-1.22423200	2.50591200	-1.95474400
H	-1	-5.33050100	-4.50533800	-2.69262700
H	-1	-5.88762500	-4.04379500	-0.52215600
H	-1	-2.06225900	-5.46979800	0.39539200
H	-1	-2.07710000	-5.90048500	-1.92611700
H	-1	-5.24083000	0.25036900	-2.87037200

H	-1	-5.28500500	2.05414300	0.57468200
H	-1	-1.40698600	-0.36373700	-4.58154100
H	-1	-2.60715800	3.06907900	-2.37010300
H	-1	-0.01935800	5.82500700	-3.40244500
H	-1	-0.14667300	7.56523700	0.42631300
H	-1	1.91849300	6.48387000	0.93545700
H	-1	2.11314200	4.90120900	-2.70971100
H	-1	-1.30113000	5.03690500	3.83509000
H	-1	-2.49738800	5.41583600	1.71790800
H	-1	5.71393900	0.19810900	3.77247300
H	-1	6.40951500	-2.04421000	3.29969100
H	-1	8.16503600	-1.22934100	0.20227400
H	-1	6.88110600	0.53251600	-0.85464300
H	-1	6.07099900	-4.26281300	-0.56270400
H	-1	6.11321000	-3.34687200	-2.77647600
H	-1	2.12370700	-4.85047300	-0.41280700
H	-1	2.14268600	-2.76177200	3.48855600
H	-1	-2.09748300	-2.83625500	4.83046800
H	-1	-5.99755800	-1.33048900	3.83522800
H	-1	-5.78056800	-2.24694100	1.62858500
H	-1	-1.90611400	-3.66181700	2.54003400
C	0	2.66414600	1.59979400	-3.30844800
H	0	3.70897400	1.67410800	-3.00384500
H	0	2.29742100	2.56066100	-3.66833000
H	0	2.55525600	0.83626900	-4.08464000
O	0	1.89231900	1.23043800	-2.14854700
H	0	0.88535400	1.15898600	-2.41258300
Al	0	-0.22106300	-2.38300600	-1.05032700
Si	0	-0.17076300	-0.79285800	1.68360600
C	0	2.02269300	-0.55030800	-1.55919800
H	0	1.38102600	-0.26965900	-0.74478500
H	0	3.08883100	-0.59830700	-1.37925700
H	0	1.61879800	-0.91352000	-2.48670300

Zn-ZSM-5-OCH3

E = -7410.428632 a.u.

O	0	6.09665900	-1.02248100	-1.11524800
O	0	-0.83973600	0.83445300	-2.53718000
O	0	-0.06305000	3.45331800	-2.59300000
O	0	-4.83430300	-0.10439600	2.19892700
O	0	-0.01541200	5.70257900	-1.25437600
O	0	-4.40137500	-0.47338100	-0.39765500
O	0	-0.37928700	5.41753400	1.37244700
O	0	-4.88211300	-2.55755900	-1.89526700
O	0	-1.67080100	3.17380800	2.18160400
O	0	6.27833700	0.49573700	1.07819300
O	0	-0.98818500	2.59584800	-0.33042500
O	0	-0.57827500	-1.22537400	3.01065400
O	0	3.49399600	-2.54132700	0.99007100
O	0	-0.46885300	-1.29939500	0.30272300
O	0	-0.14169100	-3.95775200	-0.87532300
O	0	-3.21486700	-2.00553900	3.14041600
O	0	-2.88697700	-4.08040300	-0.92543200
O	0	4.29355400	-2.91651900	-1.59769700
O	0	-0.33454300	-1.74532000	-2.67327900
O	0	-2.84691500	-0.92749600	-2.54534400
O	0	4.28935000	-0.57874200	2.53682500
O	0	-0.25365800	1.02249500	1.64510000
O	0	-2.84926500	1.15803100	0.92874000
O	0	1.72296300	-0.64970600	1.69514800
O	0	1.89932100	-2.03618000	-1.09876400
Si	0	5.90332300	-2.55999800	-1.62298100
Si	0	-1.35395400	-0.57880300	-3.14519700
Si	0	6.95772900	0.15783300	-0.36904900
Si	0	-4.77220100	-1.63916500	2.79050100
Si	0	0.21223000	5.05845000	-2.74609800
Si	0	-4.38025700	0.61233600	0.80452200
Si	0	0.04027600	6.46658400	0.18251300
Si	0	-4.33974200	-1.01836700	-1.93914700
Si	0	-1.67600400	4.81327400	2.18791400
Si	0	-4.47709500	-4.05228100	-1.35191800
Si	0	5.84732900	-0.06762200	2.55855700
Si	0	-1.46900600	1.96551100	1.10483200
Si	0	-1.65851700	-2.40567300	3.44578100
Si	0	3.00644500	-1.51715900	2.20183800
Si	0	3.10313400	-3.08450500	-0.49667200
Si	0	-1.45626500	-4.90602400	-0.75512500
Al	0	-1.43258600	2.39410000	-2.09295200
H	-1	-4.82914400	-4.96383300	-2.42698600
H	-1	-5.35706800	-4.47377800	-0.25544800
H	-1	-1.37914300	-5.47532400	0.57025400
H	-1	-1.42810300	-5.99751300	-1.73196200
H	-1	-5.22442800	-0.23356900	-2.78041700
H	-1	-5.33474100	1.69270200	0.59613600

H	-1	-1.40749300	-0.53175600	-4.60971100
H	-1	-2.87250300	2.85031200	-2.48120300
H	-1	-0.61108800	5.80618900	-3.70843800
H	-1	-0.78482600	7.67630900	0.05672200
H	-1	1.39459500	6.82642100	0.52756900
H	-1	1.62572000	5.12694700	-3.06249500
H	-1	-1.56449800	5.18368700	3.59565900
H	-1	-2.86288100	5.35735000	1.51204700
H	-1	5.89577700	1.06653800	3.44761500
H	-1	6.79726100	-1.11281500	3.03100900
H	-1	8.35744000	-0.25171200	-0.15715500
H	-1	6.86817900	1.33052100	-1.22882000
H	-1	6.55484200	-3.50610700	-0.73303800
H	-1	6.43074100	-2.67941300	-2.97870900
H	-1	2.69392100	-4.47629800	-0.41514600
H	-1	2.63297700	-2.24227700	3.40447000
H	-1	-1.53098100	-2.68372000	4.90508100
H	-1	-5.59384800	-1.61338100	4.00165900
H	-1	-5.35956000	-2.59092000	1.82316400
H	-1	-1.33414400	-3.57679500	2.64052700
Si	0	0.06793800	-0.58598100	1.64102100
Al	0	0.00708700	-2.26107800	-1.07048300
C	0	2.31738800	-0.69321400	-1.53114000
H	0	2.61356700	-0.12303000	-0.65023200
H	0	3.14256900	-0.79968700	-2.23173300
H	0	1.45882300	-0.23898000	-2.02320400
Zn	0	1.01537000	2.93361100	-0.70462200

Zn-ZSM-5-OCH3_MeOH

E = -7526.138734 a.u.

O	0	6.06121300	-1.12151800	-0.81781000
O	0	-0.73359000	0.98995100	-2.43205300
O	0	-0.05458300	3.60741700	-2.64446600
O	0	-4.96184200	-0.03464400	2.15147100
O	0	0.05023600	5.75549400	-0.96409300
O	0	-4.52566500	-0.33585000	-0.43521200
O	0	-0.38968900	5.49898900	1.68783100
O	0	-4.89559000	-2.35622200	-2.04921100
O	0	-1.74964000	3.22433600	2.24375200
O	0	6.20060600	0.32060400	1.44301500
O	0	-0.89338200	2.51849900	-0.24525900
O	0	-0.83546700	-1.31171500	3.07075800
O	0	3.13434100	-2.55810800	1.09430700
O	0	-0.41426100	-1.26274400	0.37332500
O	0	-0.31391800	-3.90730000	-0.88664000
O	0	-3.48985400	-2.04617700	3.10369000
O	0	-3.05303400	-3.99820800	-1.03179200
O	0	4.25875500	-3.01963500	-1.37150300
O	0	-0.44939100	-1.62411600	-2.59731300
O	0	-2.87928400	-0.60213400	-2.53499900
O	0	4.14884500	-0.79977300	2.77125300
O	0	-0.46874800	0.98594300	1.83876200
O	0	-2.95727900	1.27953100	0.92004600
O	0	1.55751400	-0.60689700	2.04646300
O	0	1.85409200	-2.14206000	-1.25389000
Si	0	5.85967700	-2.64439400	-1.37036200
Si	0	-1.35786900	-0.38253000	-3.09375800
Si	0	6.91728700	0.01749300	0.00557100
Si	0	-5.01067700	-1.58883700	2.69716600
Si	0	0.33846900	5.17785600	-2.47438900
Si	0	-4.48325000	0.73578800	0.78921800
Si	0	0.10882100	6.49960200	0.48930800
Si	0	-4.39343900	-0.80140100	-1.99493200
Si	0	-1.71853500	4.85513700	2.39701200
Si	0	-4.61905500	-3.88992400	-1.52495500
Si	0	5.69551300	-0.27561100	2.89112400
Si	0	-1.53770800	2.02270000	1.16821100
Si	0	-1.94908600	-2.47372200	3.44567100
Si	0	2.78644200	-1.60450100	2.40653800
Si	0	2.95564500	-3.14028600	-0.40653200
Si	0	-1.64135300	-4.84587000	-0.84181000
Al	0	-1.35801900	2.60549100	-1.98405200
H	-1	-4.96012800	-4.76188700	-2.64427400
H	-1	-5.55710500	-4.32393100	-0.46898100
H	-1	-1.61982500	-5.45484500	0.46927700
H	-1	-1.59771700	-5.90647200	-1.85858300
H	-1	-5.22961900	0.00610300	-2.86226000
H	-1	-5.41683500	1.83746700	0.58224500

H	-1	-1.34055400	-0.33276700	-4.57077900
H	-1	-2.80649300	3.03220800	-2.38021500
H	-1	-0.42169200	5.97934400	-3.43671300
H	-1	-0.68804300	7.74394500	0.39357500
H	-1	1.46103400	6.82160000	0.91653200
H	-1	1.78269800	5.22138100	-2.73063800
H	-1	-1.65916400	5.15285200	3.83657900
H	-1	-2.88184100	5.42427400	1.70567200
H	-1	5.73222000	0.83788300	3.82295700
H	-1	6.59939500	-1.35891100	3.36784900
H	-1	8.30156800	-0.43554800	0.25264300
H	-1	6.88445600	1.22287700	-0.82513500
H	-1	6.43556500	-3.63805300	-0.49279100
H	-1	6.41270800	-2.73590900	-2.72365100
H	-1	2.52684600	-4.52414400	-0.34233400
H	-1	2.38044400	-2.39890000	3.55817300
H	-1	-1.86264500	-2.78333100	4.90108600
H	-1	-5.88038700	-1.57891900	3.88409100
H	-1	-5.58955200	-2.49841200	1.67600400
H	-1	-1.60421900	-3.61446000	2.60802000
Si	0	-0.07558700	-0.59404200	1.81052000
Al	0	-0.04768200	-2.22140500	-1.03538900
C	0	2.40289400	-1.31324200	-2.34678800
H	0	3.20575500	-0.69656700	-1.94869000
H	0	2.76720500	-1.97445700	-3.13066100
H	0	1.59110300	-0.70320400	-2.71971400
C	0	3.23769000	2.77158000	-1.93220300
H	0	2.98723300	3.51558900	-1.16768800
H	0	3.92343000	2.03869500	-1.50040000
H	0	3.72900400	3.27009400	-2.77258800
O	0	2.07848700	2.05966200	-2.38181300
H	0	1.38867000	2.69377100	-2.71059200
Zn	0	0.83173400	1.13761600	-0.80202400

Zn-ZSM-5-OCH3_MeOH-to-OH_DME(TS)

E = -7526.101653 a.u.

O	0	5.97667400	-1.39172700	-0.90730100
O	0	-0.64768000	1.01942400	-2.58686300
O	0	0.10322700	3.53815100	-2.37347100
O	0	-4.95812400	0.02221500	2.15748900
O	0	0.26088900	5.70587800	-0.91305100
O	0	-4.54732400	-0.28911000	-0.43506300
O	0	-0.19998900	5.29739100	1.68832000
O	0	-4.92586700	-2.24724100	-2.11678400
O	0	-1.64033800	3.09869600	2.31506100
O	0	6.16798300	0.00351000	1.37426900
O	0	-0.84447400	2.51281900	-0.17836700
O	0	-0.82330100	-1.40259400	3.02754700
O	0	3.29098900	-2.88145600	1.08716600
O	0	-0.65079200	-1.31691000	0.30682900
O	0	-0.46260400	-3.97110900	-1.00040600
O	0	-3.50833600	-2.02478100	3.04466400
O	0	-3.18622500	-3.95844600	-1.07542900
O	0	4.07542700	-3.14540300	-1.51085000
O	0	-0.42094600	-1.62047600	-2.61810600
O	0	-2.84799500	-0.49047500	-2.48640700
O	0	4.06934100	-0.99585400	2.73891500
O	0	-0.33197000	0.87671200	1.80432400
O	0	-2.88231200	1.21546800	0.92838400
O	0	1.54846200	-0.91592400	1.79271500
O	0	1.70242100	-2.24280800	-0.94767800
Si	0	5.69335100	-2.90656500	-1.46884000
Si	0	-1.33589900	-0.39816100	-3.11235700
Si	0	6.87542700	-0.31350100	-0.06452500
Si	0	-5.02493200	-1.54646900	2.66446500
Si	0	0.50459100	5.10950100	-2.41399400
Si	0	-4.44511900	0.76242500	0.79764900
Si	0	0.32113100	6.37546000	0.57051000
Si	0	-4.38609400	-0.71226700	-2.00472800
Si	0	-1.55315300	4.72947800	2.43602500
Si	0	-4.73251500	-3.79171900	-1.57721600
Si	0	5.65457300	-0.59477400	2.81806100
Si	0	-1.45229400	1.90077100	1.22296500
Si	0	-1.98587000	-2.52705500	3.37639400
Si	0	2.77374700	-1.88229300	2.29435800
Si	0	2.82884500	-3.29961700	-0.44467200
Si	0	-1.80299400	-4.85710000	-0.92472600
Al	0	-1.29871600	2.52860900	-1.92998900
H	-1	-5.10893600	-4.63465200	-2.69891700
H	-1	-5.67814000	-4.20780400	-0.52448500
H	-1	-1.79313700	-5.47565600	0.37446000
H	-1	-1.79716400	-5.89506200	-1.94915700
H	-1	-5.22050800	0.12142500	-2.85271400
H	-1	-5.32979600	1.90461300	0.60159500

H	-1	-1.36962100	-0.32186200	-4.57833100
H	-1	-2.70650100	3.04623900	-2.34590100
H	-1	-0.24054000	5.91399500	-3.37185600
H	-1	-0.42899700	7.62828600	0.46607200
H	-1	1.68155000	6.63251000	0.96358700
H	-1	1.93121600	5.07758000	-2.69015200
H	-1	-1.46495700	5.03661000	3.86533600
H	-1	-2.68284600	5.37522500	1.75366400
H	-1	5.74774000	0.49850200	3.75731400
H	-1	6.53577700	-1.71009600	3.27106300
H	-1	8.24552500	-0.80651600	0.17265000
H	-1	6.88507400	0.90481600	-0.87147600
H	-1	6.27889000	-3.92181400	-0.60155700
H	-1	6.27540300	-2.99393500	-2.81075200
H	-1	2.36039400	-4.67624900	-0.44296700
H	-1	2.30363100	-2.60799000	3.46890700
H	-1	-1.92534100	-2.86798400	4.82297200
H	-1	-5.88859800	-1.52320700	3.84696300
H	-1	-5.64014800	-2.41872700	1.63505000
H	-1	-1.70658900	-3.67336100	2.52780700
C	0	2.62789900	1.83179000	-3.24023200
H	0	3.63173500	2.01395800	-2.85442600
H	0	2.20452700	2.75004700	-3.64672500
H	0	2.65831200	1.05360900	-4.00852200
O	0	1.80563900	1.39996500	-2.13882000
H	0	0.81971300	1.25551600	-2.45463500
Al	0	-0.08849600	-2.30178600	-1.04344500
Si	0	-0.09266300	-0.75077200	1.70739500
C	0	2.05396800	-0.36628700	-1.52954500
H	0	1.38397300	-0.12766600	-0.72520800
H	0	3.11712800	-0.34092800	-1.32828000
H	0	1.69392200	-0.74865100	-2.46651400
Zn	0	1.21419200	2.91558000	-0.37076600

Zn-ZSM-5-OH_DME

E = -7526.141340 a.u.

O	0	6.06529600	-1.15496000	-0.72472700
O	0	-0.71479900	1.06965800	-2.36243800
O	0	0.04310400	3.65109100	-2.47124900
O	0	-5.01455300	-0.05181400	2.11085000
O	0	0.09851000	5.76489100	-0.72908600
O	0	-4.45919200	-0.24234000	-0.47890500
O	0	-0.37148700	5.41683100	1.89480100
O	0	-4.91278900	-2.23957300	-2.12541100
O	0	-1.76309000	3.14310000	2.44987900
O	0	6.15937800	0.21400700	1.59180200
O	0	-0.95492800	2.65355600	-0.06300000
O	0	-0.90978900	-1.39093500	2.95964400
O	0	3.30160300	-2.72858200	1.18766800
O	0	-0.46314900	-1.04321600	0.22536100
O	0	-0.39501500	-3.84222100	-0.95142700
O	0	-3.55309200	-2.09134400	3.03987200
O	0	-3.09241700	-3.93391400	-1.13702800
O	0	4.20631100	-2.97112200	-1.38382100
O	0	-0.27782300	-1.47036800	-2.59254100
O	0	-2.82157300	-0.58005900	-2.56808100
O	0	4.05605100	-0.86856400	2.89841100
O	0	-0.39851700	0.97209900	1.91417500
O	0	-2.92985000	1.24910700	1.03694600
O	0	1.53334900	-0.79619200	1.96668400
O	0	1.81307900	-2.03800900	-0.90925500
Si	0	5.80633600	-2.66621600	-1.31187500
Si	0	-1.29107100	-0.32245200	-3.07178800
Si	0	6.89952900	-0.06308700	0.15795500
Si	0	-5.06129500	-1.61844100	2.61755500
Si	0	0.44057600	5.28607400	-2.23113300
Si	0	-4.46313000	0.75886700	0.80427100
Si	0	0.15101400	6.46555200	0.76807700
Si	0	-4.35288400	-0.71056000	-2.03650000
Si	0	-1.72369700	4.76912400	2.57452400
Si	0	-4.63535700	-3.79363900	-1.65679000
Si	0	5.62474200	-0.41555700	3.01590700
Si	0	-1.51378500	2.00095800	1.31056300
Si	0	-2.01792700	-2.54533000	3.37290600
Si	0	2.78136400	-1.76697200	2.41312000
Si	0	2.90202600	-3.10895500	-0.38194900
Si	0	-1.68999700	-4.79658100	-0.95597200
Al	0	-1.36035500	2.59213200	-1.75336200
H	-1	-4.95034900	-4.62703500	-2.80491100
H	-1	-5.57697700	-4.24749500	-0.63117100
H	-1	-1.67257900	-5.44121000	0.33383700
H	-1	-1.61740800	-5.82440200	-2.00164800
H	-1	-5.17228200	0.13942400	-2.88752600
H	-1	-5.39744000	1.86856500	0.59987000

H	-1	-1.26616100	-0.18662100	-4.54097500
H	-1	-2.73351700	3.12163500	-2.28004100
H	-1	-0.30911100	6.07013000	-3.21058700
H	-1	-0.62004600	7.72220300	0.65853800
H	-1	1.50822000	6.76588300	1.18718900
H	-1	1.87294600	5.27198400	-2.49355400
H	-1	-1.66829700	5.04597800	4.00291600
H	-1	-2.85212200	5.39055400	1.86544700
H	-1	5.67000500	0.66927500	3.97952600
H	-1	6.52266900	-1.51795800	3.47489700
H	-1	8.28004600	-0.52247600	0.42036600
H	-1	6.89804300	1.17740300	-0.62885600
H	-1	6.39997100	-3.67843300	-0.44631200
H	-1	6.42115100	-2.71316700	-2.64621400
H	-1	2.48790400	-4.52925200	-0.38355100
H	-1	2.29889000	-2.52050900	3.56806000
H	-1	-1.96140000	-2.90217000	4.83001800
H	-1	-5.94438600	-1.63198300	3.78727800
H	-1	-5.62720400	-2.48814100	1.56181700
H	-1	-1.67439400	-3.66737100	2.52184000
Si	0	-0.08676300	-0.62965800	1.76872800
Al	0	0.07793700	-2.20899200	-1.04882900
C	0	3.36940800	2.40225600	-2.33281000
H	0	3.93981300	2.99447100	-3.05719900
H	0	3.23409000	2.96539300	-1.40865100
H	0	3.89732400	1.46839000	-2.11202700
O	0	2.06082100	2.11580700	-2.84516300
C	0	2.06720100	1.31294700	-4.03640200
H	0	1.02980800	1.21501900	-4.35068600
H	0	2.66018400	1.80023400	-4.81823000
H	0	2.47728000	0.32220500	-3.81467600
H	0	0.85807700	3.06282000	-2.64378500
Zn	0	0.91400000	0.52984600	-0.88884300

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