การศึกษากลไกการเปลี่ยนเมทานอลเป็นโพรพิลีนด้วยตัวเร่งปฏิกิริยาเอช-แซดเอสเอ็ม-5 ที่ดัดแปรด้วยฟอสฟอรัสโดยวิธีดีเอฟที

นางสาวตรีรัตน์ ชมพูผุดผ่อง

วิทยานิพนธ์นี้เป็นส่วนหนึ่งของการศึกษาตามหลักสูตรปริญญาวิทยาศาสตรมหาบัณฑิต
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MECHANISTIC STUDY OF METHANOL CONVERSION TO PROPYLENE BY PHOSPHORUS-MODIFIED H-ZSM-5 CATALYSTS USING DFT METHOD

Miss Treerat Chompoopudpong

A Thesis Submitted in Partial Fulfillment of the Requirements
for the Degree of Master of Science Program in Petrochemistry and Polymer Science
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Thesis Title	MECHANISTIC STUDY OF METHANOL CONVERSION TO PROPYLENE BY PHOSPHORUS-MODIFIED H-ZSM-5 CATALYSTS USING DFT METHOD
By	Miss Treerat Chopoopudpong
Field of Study	Petrochemistry and Polymer Science
Thesis Advisor	Associate Professor Vithaya Ruangpornvisuti, Dr.rer.nat.

Accepted by the Faculty of Science, Chulalongkorn University in Partial Fulfillment of the Requirements for the Master's Degree

……..Dean of the Faculty of Science
(Professor Supot Hannongbua, Ph.D.)

THESIS COMMITTEE

……...Chairman
(Associate Professor Supawan Tantayanon, Ph.D.)

……...Thesis Advisor
(Associate Professor Vithaya Ruangpornvisuti, Dr.rer.nat.)

……...Examiner
(Assistant Professor Somsak Pianwanit, Ph.D.)

……...External Examiner
(Nuttawisit Yasarawan, Ph.D.)

ตรีรัตน์ ชมพูผุดผ่อง : การศึกษากลไกการเปลี่ยนเมทานอลเป็นโพรพิลีนด้วยตัวเร่งปฏิกิริยาเอช-แซดเอสเอ็ม-5 ที่ดัดแปรด้วยฟอสฟอรัสโดยวิธีดีเอฟที. (MECHANISTIC STUDY OF METHANOL CONVERSION TO PROPYLENE BY PHOSPHORUS-MODIFIED H-ZSM-5 CATALYSTS USING DFT METHOD) อ. ที่ปรึกษาวิทยานิพนธ์หลัก : รศ.ดร. วิทยา เรืองพรวิสุทธิ์, 152 หน้า.

งานวิจัยนี้เป็นการศึกษากลไกของปฏิกิริยาการเปลี่ยนเมทานอลเป็นโพรพิลีนโดยสร้างแบบจำลองโครงสร้างของตัวเร่งปฏิกิริยาเอช-แซดเอสเอ็ม-5 ที่ดัดแปรด้วยฟอสฟอรัสโดยการคำนวณทางทฤษฎีและใช้วิธี ONIOM(B3LYP/6-31G+(d,p):AM1) ซึ่งการเปลี่ยนเมทานอลเป็นโพรพิลีนประกอบด้วย 3 ปฏิกิริยา ได้แก่ การเปลี่ยนเมทานอลเป็นไดเมทิลอีเทอร์ การเปลี่ยนเอทานอลเป็นเอทิลีน และการเปลี่ยนไดเมทิลอีเทอร์เป็นโพรพิลีน โดยมีการคำนวณพลังงานของปฏิกิริยา ค่าทางเทอร์โมไดนามิกส์ และค่าคงที่สมดุลของปฏิกิริยา

สาขาวิชา ปิโตรเคมีและวิทยาศาสตร์พอลิเมอร์ ลายมือชื่อนิสิต.....

ปีการศึกษา 2555 ลายมือชื่อ อ.ที่ปรึกษาวิทยานิพนธ์หลัก.....

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In this work, reaction mechanism for conversion of methanol to propylene (MTP) over P-H-ZSM-5 catalysts with several models has been theoretically investigated using ONIOM(B3LYP/6-31G+(d,p):AM1) method. The MTP includes three reactions such as methanol conversion to dimethyl ether, ethanol conversion to ethylene, and dimethyl ether conversion to propylene. The reaction energies, thermodynamic properties, rate and equilibrium constants of the MTP reaction over the P-H-ZSM-5 catalysts are reported.

Field of Study: Petrochemistry and Polymer Science Student's Signature.....

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LIST OF ABBREVIATIONS

Å	Angstrom
A	Pre-exponential factor
AO	Atomic orbital
B3LYP	Becke-3-Parameter, Lee, Yang and Parr
DFT	Density functional theory
DME	Dimethyl ether
E	Energy
ECP	Effective core potential
G	Gibbs free energy
GTO	Gaussian-type orbital
H	Enthalpy
h	Planck's constant
$\hat{H}$	Hamiltonian operator
HF	Hartree-Fock
J	Quantum number
k	Force constant
k_B	Boltzmann constant
K_{eq}	Equilibrium constant
KS	Kohn-Sham energy
LCAO	Linear combination of atomic orbitals
LDA	Local density approximation
LSDA	Local spin density approximation
m	Atomic mass
MFI	Mobil-five
MO	Molecular orbital
MTD	Methanol to dimethyl ether
MTO	Methanol to olefin
MTP	Methanol to propylene
ONIOM	Our own N-layered Integrated molecular Orbital and molecular Mechanics

PA	Proton affinity
q	Partition function
q_{REA}	Total partition function of reactant
q_{TS}	Total partition function of transition state
R	Gas constant
S	Entropy
SCF	Self-consistent field
STO	Slater type orbital
T	Absolute temperature
TS	Transition state
TST	Transition state theory
ZPVE	Zero point vibrational energy
ZSM-5	Zeolite Socony Mobil Number 5
Ψ	Wave function
ρ	Electron density function
κ	Temperature-dependent tunneling coefficient
μ	Reduced mass
$\Delta E_{\mathrm{deprot}}$	Deprotonation energy
$\Delta^{\ddagger}E$	Activation energy
$\Delta^{\ddagger}G$	Activation Gibb free energy
$\Delta^{\ddagger}H$	Activation enthalpy
$\Delta^{\ddagger}S$	Activation entropy

CHAPTER I

INTRODUCTION

1.1 Background

Light olefins such as ethylene and propylene are important raw materials in petrochemical industry. The traditional production of light olefins is naphtha cracking process, and ethylene is found as the main product. The methanol to olefin (MTO) process is an alternative process to synthesize light olefins and prevent the reduction of oil resources. Methanol is a raw material of MTO process. Methanol can be synthesized from synthesis gas. Synthesis gas is a mixture of carbon monoxide (CO) and hydrogen gas (H_2), so hydrogen gas can be produced from the gasification of either coal or bio-materials [1-2].

Zeolites have been widely used industry as heterogeneous catalysts. Zeolites are suitable to adsorb hydrocarbon, because the diameters of their pores are almost equal to the molecular diameter of lighter hydrocarbon [3-4]. Zeolites exhibit catalytic activity for methanol-to-olefin synthesis (MTO reaction) with high selectivity above 80% [5]. Zeolites selectively promote cracking of $C_7 – C_{13}$ straight and short branched hydrocarbons of gasoline to $C_3 – C_5$ olefins [6]. Moreover, zeolites are poor hydrothermal stability and resistance to coke formation render. Phosphorus-modified ZSM-5 catalysts were improved catalytic performance and hydrothermal stability after calcinations and steam treatment relative to unmodified zeolites [7-8].

1.2 Zeolites

1.2.1 The zeolite structure

Zeolites are microporous crystalline aluminosilicates. Zeolites consist of SiO_4 and AlO_4 tetrahedral as shown in Figure 1.1 [9]. These SiO_4 and AlO_4 tetrahedral are the primary building units of a zeolite framework [10]. $[SiO_4]^{4-}$ and $[AlO_4]^{5-}$

tetrahedral can be formed a three-dimensional four-connected framework by sharing O-corner atoms in many different ways to build a crystalline lattice.

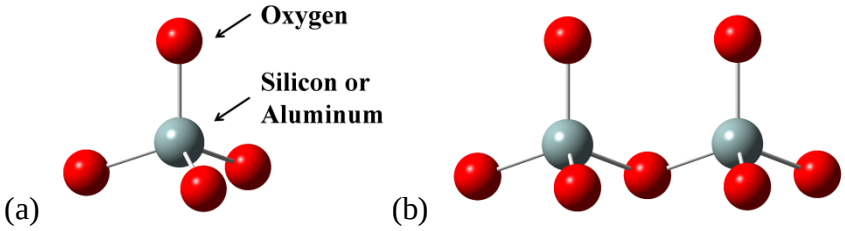
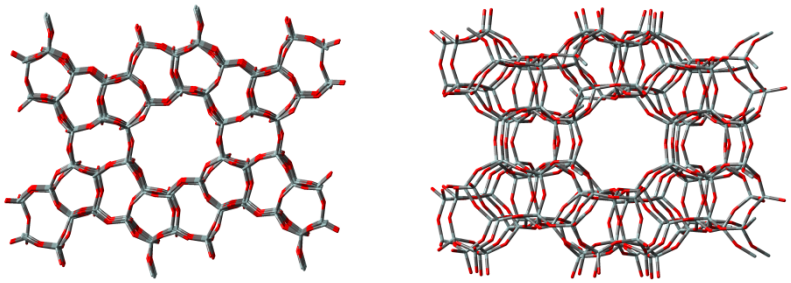


Figure 1.1 (a) SiO_4 and AlO_4 tetrahedral, (b) SiO_4 and AlO_4 tetrahedral shared a common oxygen vertex

The aluminosilicate zeolites construct from $[SiO_4]^{4-}$ and $[AlO_4]^{5-}$ tetrahedral posses an anionic framework, the negative charge of which is compensated by extra-framework cations. The empirical formula of an aluminosilicate zeolite can be expressed as $M_{x/n}[(AlO_2)_x(SiO_2)_y]\cdot wH_2O$, where M is an alkali or alkaline earth cation, n is the valence of the cation, w is the number of water molecules per unit cell, x and y are the total number of tetrahedral per unit cell, and the ratio y/x usually has values of 1 to 5, though for the zeolite, y/x can be ranging from 10 to 100 [11].

1.2.2 ZSM-5 zeolite

ZSM-5 (Zeolite Socony Mobil Number 5) was first synthesized by Argauer and Landolt in Mobil Oil Company in 1972, it is widely used in the petroleum industry as a heterogeneous catalyst for hydrocarbon isomerization. ZSM-5 zeolite is very similar to ZSM-11, but one set of pores is zig-zag channel, or sinusoidal channel (Figure 1.2). ZSM-5 is structure type of MFI framework inverted from mordenite framework. MFI framework contains a characteristic unit with *D2d* symmetry. These units are linked via edge sharing to form a pentasil chain parallel to the *c* axis. These pentasil chains relate by a mirror plane, which are connected oxygen bridges to form corrugated sheet with 10-ring holes.



Straight Channels Sinusoidal Channels

Figure 1.2 Framework structure of zeolite ZSM-5 (MFI) illustrating the straight channel and sinusoidal channels

ZSM-5 chemical formula is $Na_n^+Al_nSi_{96-n}O_{192}\cdot 16H_2O$ ($0<n<27$). The number of Al atoms in the unit cell varies from 0 to 27. The ratios of Si/Al can be changed within a wide range. ZSM-5 typically crystallizes in the Pnma orthorhombic space group with lattice parameters of a = 20.07, b = 19.92, and c = 13.42 Å. The framework density of Si + Al atoms is 17.9T / 1000 $Å^3$. Figure 1.3(a) shows the porous sheet parallel to the (100) plane in ZSM-5, where the 10-membered ring apertures are the entrances to the sinusoisal channels. Figure 1.3(b) shows the channel structure of ZSM-5. There are two channel systems in ZSM-5: a straight channel running parallel to (010) plane of 5.4 x 5.6 Å, and a sinusoidal channel parallel to the (100) plane of dimension 5.1 x 5.5 Å [12].

(a) (b)

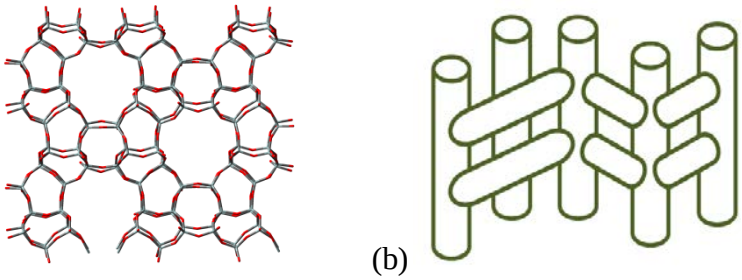


Figure 1.3 (a) Porous sheet parallel to the (100) plane in ZSM-5, (b) the channel structure of ZSM-5

1.2.3 Acidity of H-ZSM-5 zeolite

The H-ZSM-5 zeolite is one of the metal oxides, which is a strong solid acid. The strong acidity in zeolites is generated by the substitution of an aluminum atom with a silicon atom as shown in Figure 1.4.

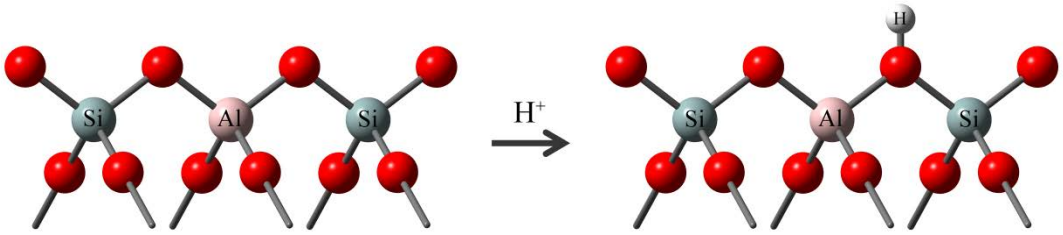


Figure 1.4 Formation of the Brønsted acid sites via linking of the silicon-oxygen and aluminum-oxygen tetrahedral

As a result, negative charge of lattice occurs from the substitution of an aluminum atom with a silicon atom. The negative charge of the lattice is balanced by protons (H^+), generating an acidic hydroxyl group (OH^-) or metal cations (M^+), which can balance the negative charge of the framework. This additional proton gives the zeolite a high level of acidity (H-ZSM-5), which causes its activity. The acidic catalytic activity of H-ZSM-5 strongly depends on the Al component in the framework. However, chemical processes do not require strong acidity always, but the weak acidity may be enough.

The protons are bound covalently to the bridging oxygen atoms of Si–O–Al group and form hydroxyl groups that may act as Brønsted acid site. The Brønsted acid is a molecule or ion that is able to donate H^+. The H-ZSM-5 zeolite is a Brønsted acid because H-ZSM-5 zeolite can donate H^+ to other molecules. The Brønsted acid sites have different acid strengths depending on their environment such as chemical composition and structure of the zeolite. Lewis acid is a molecule or ion that is able to accept an electron lone pair, within the pores of zeolites as shown in Figure 1.5 [13].

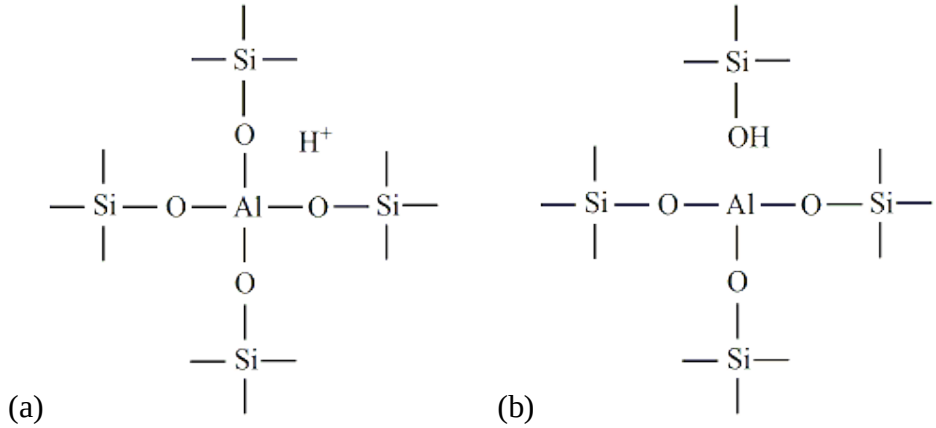


Figure 1.5 Acidity of zeolite (a) the Brønsted acid (b) the Lewis acid

Acidities for H-ZSM-5 (designated HZ) are written as equation (1.1), which can be evaluated in terms of deprotonation energies (ΔE_{deprot}) as defined in equation (1.3).

$$HZ \rightarrow H^{+} + Z^{-} \tag{1.1}$$

$$\Delta E = E_{Z^-} + E_{H^+} - E_{HZ} \tag{1.2}$$

$$\Delta E_{deprot} = E_{Z^-} - E_{HZ} \tag{1.3}$$

where E_{H^+} is zero. E_{Z^-} and E_{HZ} are total energies of Z^- and HZ, respectively. Deprotonation energy can be served as a measure of the acid strength of ZSM-5 zeolite sites while direct experiments related to proton affinity (PA). However, the data can be easily obtained from quantum mechanical calculations in which PA is considered as the energy required remove the acidic proton from the zeolite structure and is calculated by equation (1.3).

1.2.4 P-modified ZSM-5 zeolite

Modification of the ZSM-5 zeolite with phosphorus atom is widely used for improving the catalytic properties of ZSM-5 such as hydrothermal stability, shape-selectivity, control of acidity and increased anti-coking tendency in methanol to olefins reaction. The P-modified ZSM-5 zeolite can operate in two ways; partial pore

blockage and acidity decrease by phosphorus interaction and masking of the aluminum framework by phosphorus to protect against dealumination [14]. The non-modified H-ZSM-5 zeolite is represented by model A. Model B is formed by substituting the framework silicon by phosphorus [15].

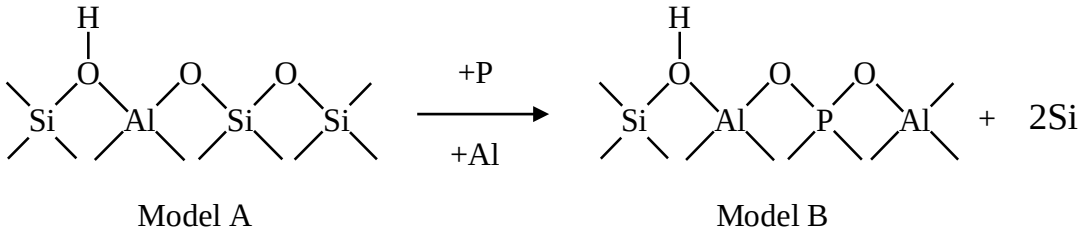


Figure 1.6 Phosphorus substitution of the MFI framework

1.3 Methanol conversion reactions

1.3.1 Methanol to olefin (MTO)

MTO is basically a two-step process. Natural gas or coal is first converted via synthesis gas into methanol, followed by its transformation into light olefins. The conversion of methanol to olefin proceeds through the steps:

$$2CH_3OH \underset{+H_2O}{\overset{-H_2O}{\rightleftharpoons}} CH_3OCH_3 \overset{-H_2O}{\longrightarrow} \text{light olefins} \overset{-H_2O}{\longrightarrow} \text{higher olefins} \qquad (1.4)$$

1.3.2 Methanol to dimethyl ether (MTD)

The initial step of MTO process is the dehydration of methanol to dimethyl ether (DME). The equilibrium mixture is consisting of methanol, DME and water. There are converted to light olefin such as ethylene and propylene. In the last step, the light olefin react to form paraffin, aromatics, naphthenes and higher olefins by alkylation and polycondensation as shown in equation (1.4). The ZSM-5 zeolite has demonstrated high activity and selectivity for the MTO process. The catalytic sites responsible for the catalyst's activity are in the pores and channels of zeolite catalysts [16].

In 1997, the MTD reaction of stepwise mechanism and concerted mechanism over 3T cluster of H-ZSM-5 was studied by density functional theory (DFT) using Hartree-Fock plus MP2 correction as shown in Figure 1.7 and Figure 1.8, respectively [17].

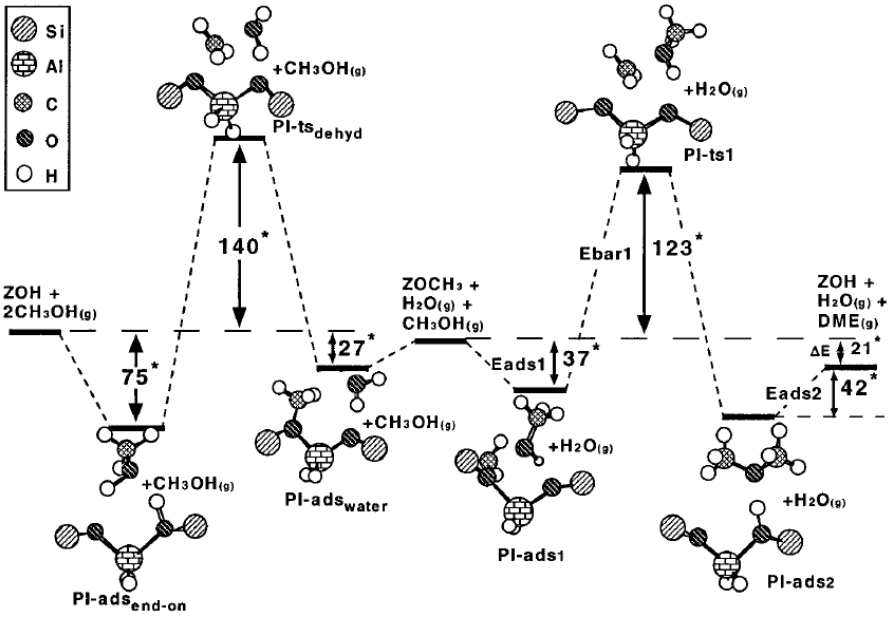


Figure 1.7 Reaction energy diagram for stepwise mechanism of MTD reaction over H-ZSM-5 (kJ/mol)

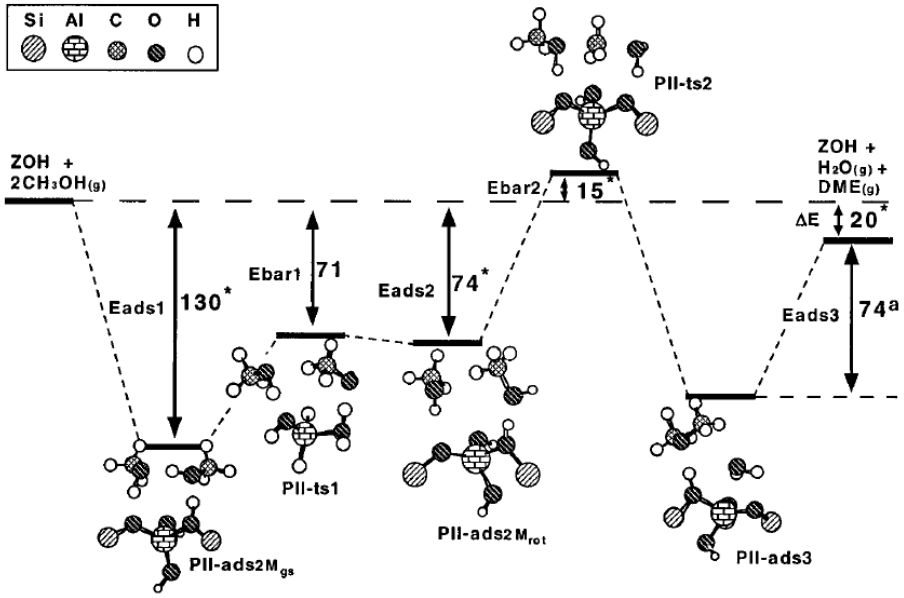


Figure 1.8 Reaction energy diagram for concerted mechanism of MTD reaction over H-ZSM-5 (kJ/mol)

1.3.3 Methanol to propylene (MTP)

Propylene is produced from the direct conversion of dimethyl ether and ethylene over the P-H-ZSM-5 catalysts as follows:

$$2CH_3OH \rightarrow CH_3OCH_3 + H_2O \quad (1.5)$$

$$CH_3CH_2OH \rightarrow CH_2{=}CH_2 + H_2O \quad (1.6)$$

$$CH_3OCH_3 + CH_2{=}CH_2 \rightarrow CH_3CH{=}CH_2 + CH_3OH \quad (1.7)$$

Propylene is the building block of petrochemicals used as feedstock for a variety of polymers and chemical intermediates such as polypropylene, acrylonitrile, propylene oxide, cumene/phenol, oxo alcohols, acrylic acid, isopropyl alcohol, oligomers, and other miscellaneous intermediates.

In 2009, the mechanism of DME conversion to propylene over H-ZSM-5 was studied using the embedded 34T/128T cluster model performed with the ONIOM (M06-2X/6-311+G(2df,2p):UFF) method and its reaction is shown in Figure 1.9 [18].

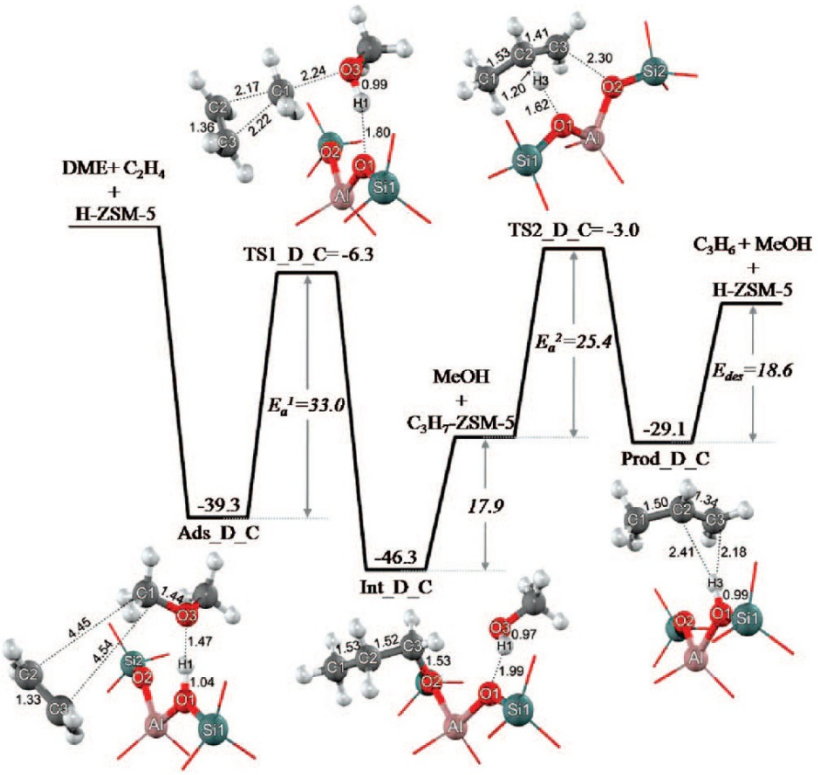


Figure 1.9 Reaction energy diagram for DME conversion to propylene over H-ZSM-5 (kJ/mol)

1.4 Objectives

The aim of this work was studying theoretical mechanisms of the methanol conversion to propylene (MTP) over Phosphorus-modified H-ZSM-5 catalysts with several cluster models ($Si_{49}O_{84}Al_2PH_{41}$). The geometry optimizations for the P-H-ZSM-5 catalysts were modeled using the ONIOM(B3LYP/6-31G+(d,p):AM1) method. The MTP includes three reactions such as methanol conversion to dimethyl ether (MTD), ethanol conversion to ethene, and dimethyl ether conversion to propylene. The reaction energies, thermodynamic properties, rate and equilibrium constants of the MTP reaction over the P-H-ZSM-5 catalysts are reported.

CHAPTER II

THEORETICAL BACKGROUND

Computational chemistry is the field of chemistry that uses principles of computer science to assist in solving chemical problems, alternatively sometimes called theoretical chemistry or molecular modeling. Computational chemistry can be used to calculate structures, molecular properties, reactivity, and spectroscopic quantities. Thus, computational chemistry can assist the experimental chemists for understanding experimental data or predicting the possibility of unknown molecules or exploring reaction mechanism that are not readily studied by experimental means.

2.1 Quantum chemistry

Quantum chemistry is based on the postulates of quantum mechanics. In quantum chemistry, the system is described by a wave function which can be found by solving the Schrödinger equation. The Schrödinger equation is an eigenvalue equation. This equation relates the stationary states of the system and their energies to the Hamiltonian operator, which can be viewed as the recipe for obtaining the energy associated with a wave-function describing the positions of the nuclei and electrons in the system.

2.1.1 The Schrödinger equation

The Schrödinger equation describes the quantum state of a physical system changes with time. The time-independent Schrödinger equation describes stationary states. It is only used when the Hamiltonian is independent on time. The time-independent Schrödinger equation is shown as equation (2.1)

$$E\Psi = \hat{H}\Psi \tag{2.1}$$

where Ψ is the wave function of the quantum system, and $\hat{H}$ is the Hamiltonian operator which in this case gives kinetic and potential energies of a system of atomic nuclei and electrons. The time-dependent Schrödinger equation predicts wave functions can form standing waves also called orbitals, atomic orbitals or molecular orbitals.

2.1.2 The Hamiltonian

The Hamiltonian uses in the energy calculations of quantum chemistry. The Hamiltonian is always the standard non-relativistic, Born-Oppenheimer "electrostatic" Hamiltonian, which is in atomic units. The Hamiltonian is shown in equation (2.2)

$$\hat{H}(\vec{r_1}, \vec{r_2}, \dots, \vec{r_n}) = \sum_{i=1}^{n} \hat{\mathrm{h}}(\vec{r_i}) + \sum_{i=1}^{n} \sum_{j<i} \frac{1}{r_{ij}} \tag{2.2}$$

There are assumed to be *n* electrons in the molecule and their position vectors are ($\vec{r_i}$). Each electron has a *one-electron Hamiltonian* of identical form as equation (2.3)

$$\hat{h}(\vec{r_i}) = -\frac{1}{2}\nabla^2(\vec{r_i}) - \sum_{A=1}^{N} \frac{Z_A}{|\vec{r_i} - \vec{r_A}|} \tag{2.3}$$

where the position vectors of the nuclei are $\vec{r_A}$ and their charges are Z_A, and it is assumed that there are *N* of them [19].

2.2 Semi-empirical methods

Semi-empirical methods are simplified version of Hartree-Fock (HF) theory using empirical corrections in order to improve performance. Semi-empirical methods are derived from experimental data. The most used methods include MNDO, AM1 and PM3. Semi-empirical methods use the molecular orbital (MO) energy levels. Semi-empirical methods are often called empirical methods where the two-electron part of the Hamiltonian is not explicitly included. Semi-empirical methods are closer to the *Ab initio* method in the SCF procedure. *Ab initio* method is used to refine

energy levels and MO coefficients. In *Ab initio* method, each Fock matrix element (F_{rs}) is calculated from a core integral (H_{rs}^{core}), density matrix elements (P_{tu}), and electron repulsion integral (*rs*|*tu*), (*ru*|*ts*). Fock matrix is given by equation (2.4)

$$F_{rs} = H_{rs}^{\text{core}}(1) + \sum_{t=1}^{m}\sum_{i=1}^{m} P_{tu}\left[(rs|tu - \frac{1}{2}(ru|ts)\right] \quad (2.4)$$

Semi-empirical calculations are much faster than *Ab initio* methods. However, their results can be wrong if the molecule being computed is not similar to the molecules in database. Semi-empirical calculations have been most successful in the description of organic chemistry where elements are used extensively and molecules are moderate size [20].

2.3 Density functional theory (DFT) methods

The density functional theory (DFT) is an approach to compute the electronic structure of matter. Its applicability ranges from atoms, molecules and solids to nuclei and quantum. The DFT is not based on the wave function, but rather on the electron probability electron density function, commonly called the electron density or charge density, designated by $\rho(x, y, z)$. This is a probability per unit volume. The electron density function is the basis not only of DFT, but of a whole suite of methods regarding and studying atoms and molecules. The electron density has another property particularly suitable for any method with claims to being an improvement at least a valuable alternative to wave function methods. It is a function of just three variables (*x*, *y*, *z*), while the wave function of an *n*-electron molecule is a function of 4*n* variables (three spatial coordinates and one spin coordinate for each electron). No matter how big the molecule may be, the electron density remains a function of three variables, while the complexity of the wave function increases with the number of electrons.

Hybrid DFT methods, in which part of the energy is calculated using HF, is shown great improvement over conventional HF methods since DFT naturally includes electron correlation. BLYP and B3LYP are the most widely used hybrid

DFT methods which have shown similar or even better performance than high level *Ab initio* methods.

The main advantage of DFT is that this method can be obtained results of the same quality as MP2 calculations. DFT solutions are mostly based on the Kohn-Sham equations. The DFT is one aspect of an ambitious project to recast conventional quantum mechanics i.e. wave mechanics [21].

2.3.1 The Kohn-Sham energy

The Kohn-Sham (KS) energy is regarded the energy of molecule as the deviation from an ideal energy, which latter can be calculated exactly. The relative small discrepancy contains the unknown functional, whose approximation is main problem. The ideal energy is that of an ideal system, a fictitious non-interacting reference system, defined as one in which the electrons do not interact and in which the ground state electron density ρ_r is exactly the same as in our real ground state system ($\rho_r = \rho_0$). The electronic energy of the molecule is the total internal "frozen-nuclei" energy can be found later by adding the internuclear repulsion and the 0 K total internal energy by further adding the zero-point energy [22].

The ground state electronic energy of our real molecule is the sum of the electron kinetic energies $\langle T[\rho_0]\rangle$, the nucleus-electron attraction potential energies $\langle V_{\mathrm{Ne}}[\rho_0]\rangle$, and the electron-electron repulsion potential energies $\langle V_{ee}[\rho_0]\rangle$ and each is a functional of the ground-state electron density. The ground state electronic energy is shown as equation (2.5)

$$E_0 = \langle T[\rho_0]\rangle + \langle V_{\mathrm{Ne}}[\rho_0]\rangle + \langle V_{ee}[\rho_0]\rangle \tag{2.5}$$

$\langle V_{ee}[\rho_0]\rangle$ is the sum over all $2n$ electrons of the potential corresponding to attraction of an electron for all the nuclei A. $\langle V_{\mathrm{Ne}}\rangle$ is shown in equation (2.6)

$$\langle V_{\mathrm{Ne}}\rangle = \sum_{i=1}^{2n}\sum_{\text{nuclei A}} - \frac{Z_{\mathrm{A}}}{r_{\mathrm{iA}}} = \sum_{i=1}^{2n} \upsilon(r_i) \tag{2.6}$$

where $v(r_i)$ is the external potential for the attraction of electron *i* to the nuclei. The density function ρ can be introduced into $\langle V_{\mathrm{Ne}} \rangle$ as shown in equation (2.7)

$$\int \Psi \sum_{i=1}^{2n} f(r_i) \Psi dt = \int \rho(r) f(r) dr \tag{2.7}$$

where $f(r_i)$ is a function of the coordinates of the 2*n* electrons of a system from equation (2.6) and (2.7), invoking the concept of expectation value $\langle V_{\mathrm{Ne}} \rangle \approx \langle \Psi | \tilde{\mathrm{V}}_{\mathrm{Ne}} | \Psi \rangle$, and since $\tilde{V} = V_x$, and given by equation (2.8)

$$E_0 = \int \rho_0(r)\, v(r) dr + \langle T[\rho_0] \rangle + \langle V_{ee}[\rho_0] \rangle \tag{2.8}$$

That cannot known the function in $\langle T[\rho_0] \rangle$ and $\langle V_{ee}[\rho_0] \rangle$. The KS introduced the idea of a reference system of non-interacting electrons. $\Delta\langle T[\rho_0] \rangle$ is the deviation of the real kinetic energy from that of the reference system. $\Delta\langle T[\rho_0] \rangle$ is given by equation (2.9)

$$\Delta\langle T[\rho_0] \rangle \equiv \langle T[\rho_0] \rangle - \langle T_r[\rho_0] \rangle \tag{2.9}$$

$\Delta\langle V_{ee} \rangle$ is the deviation of the real electron-electron repulsion energy from classical charge-cloud coulomb repulsion energy. This classical electrostatic repulsion energy is the summation of the repulsion energies for pairs of infinitesimal volume elements $\rho(r_1)dr_1$ and $\rho(r_2)dr_2$ seperated by distance r_{12}, multiplied by one-half. The sum of infinitesimals is an integral. $\Delta\langle V_{ee}[\rho_0] \rangle$ is given by equation (2.10)

$$\Delta\langle V_{ee}[\rho_0] \rangle \equiv \langle V_{ee}[\rho_0] \rangle - \frac{1}{2} \int \int \frac{\rho_0(r_1)\rho_0(r_2)}{r_{12}} dr_1 r_2 \tag{2.10}$$

The classical charge-cloud repulsion is somewhat inappropriate for electrons in that smearing an electron out into a cloud forces it to repel itself, as any two regions of the cloud interact repulsively. This physically incorrect *electron self-interaction* will be compensated for by a good exchange-correlation functional can be written as equation (2.11)

$$E_0 = \int \rho_0(r) v(r) dr + \langle T_r[\rho_0] \rangle - \frac{1}{2} \int \int \frac{\rho_0(r_1)\rho_0(r_2)}{r_{12}} dr_1 r_2 + \Delta\langle T[\rho_0] \rangle + \Delta\langle V_{ee}[\rho_0] \rangle \tag{2.11}$$

The sum of the kinetic energy deviation from the reference system and the electron-electron repulsion energy deviation from the classical system is called exchange-correlation energy functional or exchange-correlation energy (E_{XC}) as shown in equation (2.12)

$$E_{\mathrm{XC}}[\rho_0] \equiv \Delta\langle T[\rho_0]\rangle + \Delta\langle V_{ee}[\rho_0]\rangle \tag{2.12}$$

The $\Delta\langle T\rangle$ term represents the kinetic correlation energy of the electrons and the $\langle\Delta V_{ee}\rangle$ term the potential correlation energy and the exchange energy, although exchange and correlation energy in DFT do not have exactly.

2.3.2 The Kohn-Sham equations

The KS equations are obtained by utilizing the variation principle, which the second Hohenberg-Kohn theorem assures applies to DFT. The electron density of the reference system is the same as that of our real system is given by equation (2.13)

$$\rho_0 = \rho_r = \sum_{i=1}^{2n} \left|\psi_i^{\mathrm{KS}}(\mathrm{l})\right|^2 \tag{2.13}$$

where the ψ_i^{KS} are the KS spatial orbitals. Substituting the above expression for the orbitals into the energy and varying (E_0) with respect to the ψ_i^{KS} subject to the constraint that these remain orthonormal leads to the KS equations. The procedure is similar to that used in deriving the HF equations as shown in equation (2.14)

$$\left[-\frac{1}{2}\nabla_i^2 - \sum_{\text{nuclei A}} \frac{Z_A}{r_{1A}} + \int \frac{\rho(r_2)}{r_{12}} dr_2 + \upsilon_{\mathrm{XC}}(\mathrm{l})\right]\psi_i^{\mathrm{KS}}(\mathrm{l}) = \epsilon_i^{\mathrm{KS}}\psi_i^{\mathrm{KS}}(\mathrm{l}) \tag{2.14}$$

where ϵ_i^{KS} are the KS energy levels and υ_{XC} (l) is exchange correlation potential, arbitratily designated for electron number l, since the KS equations are a set of one-electron equations with the subscript *i* running from 1 to *n*, over all the 2*n* electrons in the system. Exchange correlation potential is defined as the functional derivative of $E_{\mathrm{XC}}[\rho(r)]$ with respect to $\rho(r)$. $\upsilon_{\mathrm{XC}}(r)$ is shown as equation (2.15).

$$\upsilon_{\mathrm{XC}}(r) = \frac{\delta E_{\mathrm{XC}}[\rho(r)]}{\delta\rho(r)} \tag{2.15}$$

The derivative υ_{XC} for the KS equations and exchange-correlation functional itself for the energy equation are needed. The KS operator is determined using equation (2.16).

$$\hat{h}^{\mathrm{KS}}(\mathrm{l})\psi_i^{\mathrm{KS}}(\mathrm{l}) = \epsilon_i^{\mathrm{KS}}\psi_i^{\mathrm{KS}} \tag{2.16}$$

The difference between DFT method is the choice of the functional from of the exchange-correlation energy. Functional forms are often designed to have a certain limiting behavior, and fitting parameters to known accurate data. Which functional is the better will have to be settled by comparing the performance with experiments or high-level wave mechanics calculations.

2.3.3 Exchange-correlations energy functional

The simple one-dimensional function xe^{-x^2} is a function of the coordinate *x*. One functional of this function is multiply the prescription. The function by *x* and integrated from zero to infinity as shown in equation (2.17).

$$F[f(x)] = F\left[xe^{-x^2}\right] = \int_0^\infty x^2\, e^{-x^2} dx = \frac{\pi^{1/2}}{4} \tag{2.17}$$

The functional derivative of $F\left[xe^{-x^2}\right]$ with respect to the function xe^{-x^2}involves various derivatives of the function $[xe^{-x^2}]$ and given by equation (2.18).

$$\frac{\delta F[f(x)]}{\delta f(x)} = \frac{\delta F\left[xe^{-x^2}\right]}{\delta\left(xe^{-x^2}\right)} = \frac{d\left(x^2e^{-x^2}\right)}{d\left(xe^{-x^2}\right)} + \text{other terms} \tag{2.18}$$

The functional derivative is a function of *x*. Exchange-correlation energy functional $E_{\mathrm{XC}}[\rho(r)]$ is a functional of $\rho(r)$, is a number which depends on the function $\rho(r)$ and on just what mathematical form the functional E_{XC} has while exchange-

correlation potential $v_{\mathrm{XC}}(r)$ is the functional derivative of $E_{\mathrm{XC}}[\rho(r)]$, is a function of the variable *r* [23].

2.3.4 Hybrid functionals

Hybrid functional augments the DFT exchange-correlation energy with a term, which is calculated from HF theory. In KS theory, one expression for the electronic energy (E) is given by equation (2.19)

$$E = 2\sum_{i=1}^{n} H_{ij} + \sum_{i=1}^{n}\sum_{j=1}^{n}\left(2J_{ij} - K_{ij}\right) \tag{2.19}$$

where the sums are over *n* occupies spatial orbitals. If remove the core energy and the coulomb potential energy from this equation. The exchange energy (E_{x}) involves the double sum of the exchange integrals (*J*). E_{x} is shown as equation (2.20).

$$E_{\mathrm{x}} = -\sum_{i=1}^{n}\sum_{j=1}^{n} K_{ij} \tag{2.20}$$

Substituting into equation (2.20), the KS orbitals are quite similar to the HF orbitals, gives an expression based on KS orbitals for the HF exchange energy as shown in equation (2.21).

$$E_{\mathrm{x}}^{\mathrm{HF}} = -\sum_{i=1}^{n}\sum_{j=1}^{n}\left\langle \psi_i^{\mathrm{KS}}(1)\psi_j^{\mathrm{KS}}(2)\left|\frac{1}{r_{ij}}\right|\psi_i^{\mathrm{KS}}(2)\psi_j^{\mathrm{KS}}(1)\right\rangle \tag{2.21}$$

The KS slater determinant is an exact representation of the wave function of the non-interacting electrons reference system, $E_{\mathrm{x}}^{\mathrm{HF}}$ is the exact exchange energy for a system of non-interacting electrons with electron density equal to the real system. $E_{\mathrm{x}}^{\mathrm{HF}}$ gives a HF/DFT exchange-correlation functional, commonly called a hybrid DFT functional.

The most popular hybrid functional is based on an exchange-energy functional, and introduction of the LYP correlation-energy functional. This exchange-correlation functional called the Becke3LYP or B3LYP functional. B3LYP functional is shown in equation (2.22)

$$E_{\mathrm{xc}}^{\mathrm{B3LYP}} = (1 - a_0 - a_x)E_x^{\mathrm{LSDA}} + a_0 E_x^{\mathrm{HF}} + a_0 E_x^{\mathrm{B88}} + (1 - a_c)E_c^{\mathrm{VWN}} + a_c E_c^{\mathrm{LYP}} \quad (2.22)$$

E_x^{LSDA} is LSDA non-gradient-corrected exchange functional, E_x^{HF} is the KS-orbital-based HF exchange energy functional, E_x^{B88} is the Becke 1988 exchange functional, E_c^{VWN} is the Vosko Wilk Nusair function, which forms part of the accurate functional for the homogeneous electron gas of the LDA and the LSDA, and E_c^{LYP} is the LYP correlation functional, E_x and E_c of the last three terms are gradient-corrected. The parameters (a_0, a_x and a_c) are those that give the best fit of the calculated energy to molecular atomization energies [24].

2.4 Basis sets

Basis sets are Gaussian mathematical functions representative of the atomic orbitals (AOs) which are using the linear combination of atomic orbitals (LCAO) approximation to describe MOs and hence model the shape of the electron density and orbitals in a molecule, each basis set is used to determine the wave function. Basis sets are required for *Ab initio* and DFT methods. The general expression for a basis function is given by equation (2.23)

$$\text{Basis function} = N \times e^{(-\propto \times r)} \quad (2.23)$$

where N is the normalization constant, $\propto$ is the orbital exponent, and r is the radius of the orbital in angstroms (Å).

The simplest basis set is the STO-3G in which the Slater-type orbital (STO) is expanded with three Gaussian-type orbitals (GTO). The more complex split-valence basis sets are 3-21G and 6-31G. The 6-31G consists of a core of six GTO's that are not split. The valence orbitals are split into one basis function, which are constructed from three GTO's and another that is a single GTO. The electron density of a nucleus can be polarized. A polarization function can be also included such as the 6-31G* and the 6-31G** [25].

2.4.1 The slater type orbitals (STOs)

STOs are modification of the mathematical functions for hydrogen orbitals could be used to fit many-electron radial data. STOs are the finite collection of functions. STOs use a function that correctly models the form of the variation of the electron density with distance from the nucleus [26]. STOs function is given by equation (2.24).

$$f^{STO}(r) = \left(\frac{\xi^3}{\pi}\right)^{0.5} \exp(-\xi r) \tag{2.24}$$

However, the major problem with slater type orbitals is a computational one. For all but the simplest molecules, the evaluation of electron-electron repulsion integrals is a formidable problem, which is not simplified when the atomic orbitals are approximated using Slater functions. To overcome these problems, GTOs are commonly used instead.

2.4.2 The Gaussian type orbitals (GTOs)

Gaussian functions are used to approximate the radial component of atomic orbitals. The Gaussian approach was applied increasingly to calculations of atomic and molecular electronic structures and properties. GTOs have the advantage that the two electron integrals may be quickly and easily evaluated. The form of GTO is given by equation (2.25)

$$f^{GTO}(r) = \left(\frac{2\propto}{\pi}\right)^{0.75} \exp(-|\propto r^2) \tag{2.25}$$

Assuming that an STO has the correct form for an orbital the GTO is serious deficient at short ranges, has no cusp at the nucleus and also lacks the correct form at long range. In order to overcome these problems it is necessary to use more GTOs to describe the same system to achieve comparable accuracy to that found using STOs [27].

2.4.3 Minimal basis sets

A minimal basis set is a relatively inexpensive one, which can be used for calculations on large molecules. It is minimal in the least number of functions per atom required to describe the occupied atomic orbitals of that atom. This is not accurate. Because the minimal is so small, it is not one which can lead to quantitatively accurate results. However, contains the essentials of chemical bonding and many useful qualitative results can be obtained with it.

The STO-*n*G method uses a contraction of *n* primitive Gaussians for each basis function, where the contraction coefficients and exponents are chosen so that the basis functions approximate Slater functions. In particular, STO-3G basis sets are often used in polyatomic calculations, in preference to evaluating integrals with Slater functions. STO-3G basis sets are used for model calculations on H_2 and HeH^+.

2.4.4 Split valence basis sets

A major problem with minimal basis sets is that they treat all electrons as equal. The outer (valence) electrons are much more important for chemical structure, properties and reactivity than the inner (core) electrons. If a large minimal basis set is used then a wasting a lot of effort calculating the distribution of electrons, that is not really interested in.

The solution to this is to use what are known as split-valence basis sets. In these, we partition our electrons into core and valence types. The valence orbitals are represented by two sets of functions but the core orbitals are represented by a single set of functions. For each of the core electrons, we generally use a single contracted GTO as described above but for the valence electrons we use more than one contracted GTO.

An example of a split-valence basis set is 3-21G: here we use one contracted GTO for each of the core electrons and two contracted GTOs for each of the valence electrons. The 3-21G basis set is known as valence *double-ξ* referring to the fact that it has two contracted GTOs for each electron in the valence space. The 6-31G basis set is a second row atom such as carbon or oxygen the 1*s* function is represented by a

combination of six Gaussians, and the valence orbitals 2*s* and 2*p* are split into two sets of functions, one composed of two Gaussians and the other are composed of a single Gaussian function.

2.4.5 Polarization functions

These types of functions that have high angular momentum are usually called polarization functions. For the hydrogen atom, the *p* orbitals act as polarization functions whereas for the Li-Ne atoms the polarization functions are *d* orbitals. For transition metals, the polarization functions are *f* orbitals. In general, orbitals have higher angular momentum than the occupied ones in the atom.

The polarization functions are generally added to the chosen *sp* basis set to try to model the polarization effect as two atoms are brought close together. The electron cloud on one atom introduces a distortion in the shape of the electron cloud in the neighbouring atom.

6-31G (d) basis set or (6-31G*) contains *d* polarization functions on the heavy atoms of the system whereas 6-31G (d, p) basis set or (6-31G**) also contains 2*p* polarization functions on H and He atom. The 6-31G** basis probably offers advantage over the 6-31G* unless the hydrogens are engaged in some special activity like hydrogen bonding or bridging [28].

2.4.6 Diffuse function

Diffuse functions are basis functions with a larger spatial extent than the normal ones. These functions are particularly important in the modeling of anions or excited stated in which the electrons may be further removed from the nucleus than in ground state, neutral molecules.

Diffuse functions generally designated via the “+” sign should be included in the basis set. Typically a basis set with diffuse functions has one such function, composed of a single Gaussian for each valence atomic orbital of the heavy atoms.

2.4.7 Effective core potentials (ECPs)

For heavy elements calculations, use atomic orbital base basis sets become very time consuming due to the number of electrons involved in the calculation. To overcome this problem, can introduce what are known as effective core potentials (ECPs or pseudopotentials). The theoretical foundation of ECP replaces the inner core electrons in the calculation leading to an increase in speed with a very small loss in accuracy.

An additional benefit of these functions is that they allow for a simple accounting of relativistic effects. The electrons near the very positive nucleus of a heavy element experience a larger relative attraction than for lighter elements. This has the effect of accelerating the electron close to the speed of light where Einstein's theory of general is that the inner core orbital in a lighter element. These effects are taken into account by ECPs [29].

2.5 The ONIOM methods

Another way of performing calculations, use the cluster model, which is used of a hybrid method. The ONIOM method is one of the hybrid methods developed quite recently to facilitate accurate *Ab* initio calculations of large chemical species. The ONIOM method is multi-level extrapolation method, in which the studied molecular system is divided into two or more layers. This method can be used to model a complete system as a small model system (High level) and the real system (Low level). The complete system would be computed with both levels of theory. The energy for the complete system, combining both levels of theory [30] as shown in equation (2.26)

$$E^{\mathrm{ONIOM}} \approx E_{\mathrm{real}}^{\mathrm{High}} = E_{\mathrm{real}}^{\mathrm{low}} + E_{\mathrm{model}}^{\mathrm{high}} - E_{\mathrm{model}}^{\mathrm{low}} \qquad (2.26)$$

2.6 Transition state theory

The Arrhenius equation is used to describe the rate of a chemical reaction. The Arrhenius equation is presented by equation (2.27)

$$k(\mathrm{T}) = \mathrm{A}e^{-\Delta^{\ddagger}E/RT} \tag{2.27}$$

where k(T) is the chemical reaction rate, A is the pre-exponential factor, $\Delta^{\ddagger}E$ is the activation energy.

The transition state theory (TST) is the mechanism of interaction of reactants. The important criterion is that colliding molecules must have sufficient energy to overcome a potential energy barrier to react. TST details a hypothetical transition state that exists between reactants and products during a chemical reaction. The species formed in this hypothetical transition state is called the activated complex. The theory is used to explain how chemical reactions take place, and can be used to determine the standard Gibbs free enegy, enthalpy, and entropy of the reaction. Other names for this theory include abbreviated transition state theory, activated-complex theory and absolute-rate theory.

The TST is applied to the bimolecular reaction of A with B to form AB as shown in equation (2.28)

$$\mathrm{A} + \mathrm{B} \xrightarrow{\mathrm{k}} (\mathrm{A}\cdots\mathrm{B})^{\ddagger} \xrightarrow{\mathrm{k}'} \mathrm{AB} \tag{2.28}$$

where k is the rate constant describing this reaction. Reactants (A and B) reversibly react to form an intermediate complex $(\mathrm{A}\cdots\mathrm{B})^{\ddagger}$, which irreversibly decomposes to form final product (AB). The species $(\mathrm{A}\cdots\mathrm{B})^{\ddagger}$ is called a transition state whose lifetime is less than 10^{-13} sec.

2.6.1 Activation energy

The energy profiles for these elementary reactions share several common features, one of which is particularly important for a discussion of reaction rates. In almost all chemical reactions, the molecules must overcome an energy barrier before starting materials can become products. This energy barrier is called the activation energy $(\Delta^{\ddagger}E)$ of the chemical reaction. Activation energies arise because chemical bonds in reactant molecules must distort or break before new bonds can form in product molecules. The activation energy for any reaction mechanism is independent of both reactant concentrations and temperature. The activation energy diagram is

energy of the molecules along the reaction coordinate which measures the progress of the reaction as shown in figure 2.1

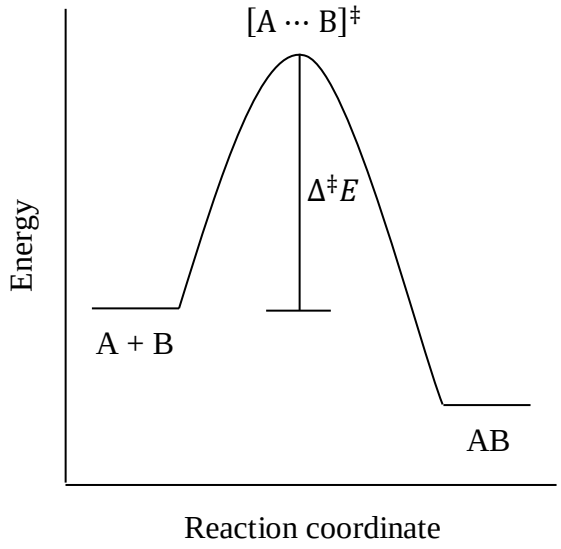


Figure 2.1 The activation energy diagram for the bimolecular reaction

The rate of reaction of A and B to form AB in two ways is written in equation (2.29)

$$\frac{\mathrm{d[AB]}}{\mathrm{dt}} = k[\mathrm{A}][\mathrm{B}] = k'[\mathrm{A} \cdots \mathrm{B}]^{\ddagger} \tag{2.29}$$

In this equation, k is the bimolecular rate constant for conversion of A and B to AB and k′ is the unimolecular rate constant for decomposition of the activated complex $(\mathrm{A}\cdots\mathrm{B})^{\ddagger}$ to form AB. Eyring approach can write an equilibrium constant ($K_{\mathrm{eq}}^{\ddagger}$) and an expression for $\Delta^{\ddagger}G$, is the Gibb free energy change of reaction to form the transition state. These quantities are expressed in equation (2.30) and (2.31).

$$K_{\mathrm{eq}}^{\ddagger} = \frac{[\mathrm{A} \cdots \mathrm{B}]^{\ddagger}}{[\mathrm{A}][\mathrm{B}]} \tag{2.30}$$

$$\Delta^{\ddagger}G = -RT \ln K_{\mathrm{eq}}^{\ddagger} \tag{2.31}$$

$\Delta^{\ddagger}G$ is described by the Legendre transformation of the Gibb's free energy function as shown in equation (2.32)

$$\Delta^{\ddagger}G = \Delta^{\ddagger}H - T \cdot \Delta^{\ddagger}S \quad (2.32)$$

where $\Delta^{\ddagger}H$ is the difference between the enthalpy of the transition state and the sum of the enthalpies of the reactants in the ground state. It is called activation enthalpy. S is the entropy, which is the extent of randomness or disorder in a system. The difference between the entropy of the transition state and the sum of the entropies of the reactants is called activation entropy ($\Delta^{\ddagger}S$).

2.6.2 Principles of the transition state theory:

There is a thermodynamic equilibrium between the transition state and the state of reactants at the top of the energy barrier. The rate of chemical reaction is proportional to the concentration of the particles in the high-energy transition state.

2.6.3 Rate constant and the Boltzmann distribution

The distribution of molecular energies is called the Boltzmann distribution. The specific shape of the Boltzmann distribution depends on the temperature of the sample. Adding thermal energy to the molecules gives them more kinetic energy. Thus as the temperature increases, the Boltzmann distribution broadens and shifts toward higher energy.

The Boltzmann distribution is the energy associated with some state or condition of a system is ε then the frequency with state or condition occurs. The Boltzmann's factor expresses the probability of a state of energy relative to the probability of a state of zero energy. The Boltzmann's factor is equal to $e^{-\varepsilon/k_B T}$. T is the system's absolute temperature and k_B is the Boltzmann constant, which have encountered in the kinetic theory of gases as shown in equation (2.33)

$$k_B = 1.38 \times 10^{-23} \text{ J/K} = 1.38 \times 10^{-16} \text{ erg/K} \quad (2.33)$$

TST assumes an equilibrium energy distribution among all possible quantum states among the reaction coordinate. Assuming that the molecules at the transition are in

equilibrium with the reactant, the rate constant can be expressed in equation (2.34)

$$K_{\mathrm{eq}} = \frac{k_{\mathrm{B}}T}{h} e^{-\Delta^{\ddagger}G/RT} \tag{2.34}$$

$\Delta^{\ddagger}G$ is the Gibbs free energy difference between the transition and reactant [31].

2.6.4 Rate constant with tunneling corrections

Tunneling effect is important when small atoms are involved in the reactions. The tunneling effect is expressed as a temperature-dependent tunneling coefficient (κ). For the calculation of rate constant, the Arrhenius equation was provided by transition state theory that expresses as equation (2.35)

$$k(T) = \kappa \left[\frac{k_{\mathrm{B}}T}{h}\right] \left[\frac{q_{\mathrm{TS}}}{q_{\mathrm{REA}}}\right] \exp\left(-\frac{\Delta^{\ddagger}E}{RT}\right) \tag{2.35}$$

where h is the Planck's constant, T is the absolute temperature, R is the gas constant, q_{TS} and q_{REA} are the partition functions of transition state and reactant of reaction step whose values are computed of translational, rotational and vibrational partition functions.

Tunneling effect accounts for the situation when the reaction can happen for some small atoms even though the reaction system does not have enough energy to overcome the reaction barrier. If the small atoms go through the barrier instead of overcoming it, the actual reaction rate constant is higher than predicted.

Different approximations have been developed, including classical and semi-classical approximations. The most widely used classical approximation is the Wigner tunneling correction which is given as equation (2.36)

$$\kappa = 1 + \frac{1}{24}\left(\frac{h\nu_{\mathrm{i}}}{k_{\mathrm{B}}T}\right)^{2} \tag{2.36}$$

where ν_{i} is the imaginary frequency of the unstable asymmetric stretch along the reaction coordinate. The rate constant becomes equation (2.37).

$$k(T) + \mathrm{w}(T) = \kappa k(T) \tag{2.37}$$

The correction can be derived by treating the motion through the transition state as a vibration on an upside-down potential and expanding the corresponding quantum partition function to second order in T^{-1}. Although an improvement over TST, the Wigner tunneling correction cannot describe a truly multidimensional tunneling.

2.6.5 Partition functions

The Hamiltonian of an atom or a molecule can be rigorously separated in two terms such as a translation term and an internal term. An ensemble of energy levels corresponds to each of these terms such as one for translation energy levels (ε_i) and one for internal energy levels (ε_j). The partition function for each a system can be written as equation (2.38).

$$q = \sum_{\mathrm{i,j\,=levels}} \mathrm{g_i g_j e^{-(\beta\varepsilon_i+\beta\varepsilon_j)}} = \sum_{\mathrm{i}} \mathrm{g_i e^{-\beta\varepsilon_i}} \sum_{\mathrm{j}} \mathrm{g_j e^{-\beta\varepsilon_j}} = q_{\mathrm{trans}} q_{\mathrm{int}} \tag{2.38}$$

The partition function of the system is simply the product of the respective partition functions.

It is often possible to express with a certain degree of approximation. The internal energy of a molecule as a sum of terms each corresponding to one of the degrees of freedom such as translation, rotation, vibration and electronic. Thus, allows the energy of each level (ε) to be separated into trans, rot, vib and elec contribution as shown in equation (2.39)

$$\varepsilon = \varepsilon_{trans} + \varepsilon_{rot} + \varepsilon_{vib} + \varepsilon_{elec} \tag{2.39}$$

The energy can be written as a sum of terms implies that the partition function can be written as a product of terms. As the enthalpy and entropy contributions involve taking the logarithm of q, the product transforms into sums of enthalpy and entropy contributions as shown in equation (2.40), (2.41), and (2.42).

$$q = q_{\text{trans}}\, q_{\text{rot}}\, q_{\text{vib}}\, q_{\text{elec}} \tag{2.40}$$

$$H = H_{trans} + H_{rot} + H_{vib} + H_{elec} \tag{2.41}$$

$$S = S_{trans} + S_{rot} + S_{vib} + S_{elec} \tag{2.42}$$

For each of the partition functions, the sum over allowed quantum states runs to infinity. However, since the energies become larger, the partition functions are finite [32].

2.6.5.1 Translational partition function

The translation partition function is approximation of the sum by an integral is valid if the spacing between energy levels is smaller than *k*(T). In this case, the partition function can be written as equation (2.43)

$$q_{\text{trans}} = \left(\frac{2\pi MkT}{h^2}\right)^{\frac{3}{2}} V \tag{2.43}$$

where *M* is the total molecular mass. The volume depends on the number of particles. The factor $\left(\frac{h^2}{2\pi MkT}\right)^{\frac{1}{2}}$ that occurs in the translational partition function has units of length and is usually denoted by Λ as shown in equation (2.44)

$$q_{\text{trans}} = \frac{V}{\Lambda^3} \tag{2.44}$$

The quantity Λ can be given the following interpretation.

2.6.5.2 Vibrational partition function

The vibrational partition function is the sum of energy levels measuring the energy from the lowest available level as shown in equation (2.45).

$$q_{\text{vib}} = \sum_{n=0}^{\infty} \exp\left(\frac{-nh\nu}{k_{\text{B}}T}\right) \tag{2.45}$$

This is the geometric series ($1 + x + x^2 + x^3 + \ldots$) for which the sum to infinity for $x < 1$ is $(1 - x)^{-1}$. The vibrational partition function is written by equation (2.46).

$$q_{\text{vib}} = \left[1 - \exp\left(\frac{-h\nu}{k_{\text{B}}T}\right)\right]^{-1} \tag{2.46}$$

2.6.5.3 Rotational partition function

In the lowest approximation, the rotation of a molecule is assumed to occur with a geometry that is independent of the rotational quantum number. The energy levels of the rotational motion of a linear molecule are given by equation (2.47).

$$\varepsilon_{\text{rot}} = \frac{J(J+1)h^2}{8\pi^2 I} \tag{2.47}$$

Each rotational level has a degeneracy of $(2J + 1)$ so there are $(2J + 1)$ states at each level. The rotational partition functions are evaluated by integration over J as shown in equation (2.48).

$$q_{\text{rot}} = \int_0^{\infty} (2J + 1) \exp\left[\frac{-J(J+1)h^2}{8\pi^2 I k_{\text{B}} T}\right] \mathrm{d}J \tag{2.48}$$

This is the result for a heteronuclear diatomic molecule. This reduces the number of different terms contribute to the rotational partition function is given by equation (2.49).

$$q_{\text{rot}} = \frac{8\pi^2 I k_{\text{B}} T}{h^2 \sigma} \tag{2.49}$$

σ is called the symmetry number, which is unity for a heteronuclear diatomic and a homonuclear diatomic or symmetrical linear molecule.

2.6.5.4 Electronic partition function

The electronic partition function involves a sum over electronic quantum states. These are the solutions to the electronic Schrödinger equation. The energy

difference between the ground and excited states is usually much larger than $k_B T$. The electronic partition function is given by equation (2.50)

$$q_{elec} = \sum(2J+1)exp(-\varepsilon_{e1}/k_{\mathrm{B}}T) \tag{2.50}$$

where *J* is the quantum number determined the total electronic angular momentum, and the summation is over all the electronic states of the atom. For the ground state, ε_{e1} is zero. The value of *J* is contained in the spectroscopic term symbol for the state.

2.7 Molecular vibrational frequencies

Molecules can be characterized as being in constant vibrational motion. This motion is described for nuclei of a polyatomic system, can utilize the Cartesian coordinates (X_m, Y_m, Z_m) for a nucleus of mass *m* referred to a fixed coordinate system. For *n* nuclei, can generate 3*n* coordinates to describe the motion of all the atoms. Three of these coordinates may be used to locate the center of mass of the system in space. These three coordinates define the translation of the entire system through space. Because translational energies have a small impact on vibrational spectra, the three coordinates of the center of mass can be dropped from the total required to determine the vibrational degrees of freedom.

For a diatomic molecule, the frequency is given by equation (2.51)

$$\tilde{\nu} = \frac{1}{2\pi c}\sqrt{\frac{k}{\mu}} \tag{2.51}$$

where *k* is the force constant, m_1 and m_2 are the atomic masses, and μ is the reduced mass as shown in equation (2.52)

$$\mu = \frac{m_1 m_2}{m_1 + m_2} \tag{2.52}$$

The vibrational states associated with a particular normal mode are not influenced, to a first approximation by the energies of adjacent states. The portion of vibrational

energy (E_{vib}) contributes by a particular normal mode n_i is given by equation (2.53)

$$E_{\text{vib}} = \left(n_i + \frac{1}{2}\right) h\nu_i \qquad n_i = 0, 1, 2, 3,... \tag{2.53}$$

where v is the vibrational frequency and n is a vibrational quantum number running from zero to infinity. Each normal mode will possess a similar energy-quantum number relationship, and the total vibrational energy (E_{vib}) can be obtained by summing over all $3n - 6$ fundamental vibrations as shown in equation (2.54).

$$E_{\text{vib}} = \sum_{i=1}^{3n-6} \left(n_i + \frac{1}{2}\right) h\nu_i \tag{2.54}$$

2.8 Thermochemistry

Thermochemistry is the branch of chemistry which deals with the study of energy changes accompanying chemical reactions. The energy given out during a chemical change appears in the form of heat, which is absorbed may be in the form of thermal, electrical or photo energy. The amount of energy is evolved or absorbed during a chemical change always remains for the same quantities of reacting substances.

Thermochemistry is based on the first law of thermodynamics. The energy changes in chemical reactions are generally due to breaking up of the existing bonds between the atoms and the formation of new bonds.

Calculation of thermochemistry such as enthalpies of reaction is calculated heats of formation as shown in equation (2.55).

$$\Delta_r H^o(298\ K) = \sum_{\text{products}} \Delta_f H^o_{\text{prod}}(298\ K) \ - \ \sum_{\text{reactants}} \Delta_f H^o_{\text{react}}(298\ K) \tag{2.55}$$

The sum of electronic and thermal enthalpies simply takes the difference of the sums of these values for the reactants and the products. The enthalpy of reaction can be calculated by equation (2.56)

$$\Delta_r H^o(298\ K) = \sum_{\text{products}} (\varepsilon_0 + H_{corr})_{\text{prod}} - \sum_{\text{reactants}} (\varepsilon_0 + H_{corr})_{\text{react}} \tag{2.56}$$

The same equation can be used to calculate Gibbs free energies of reaction. Calculating enthalpies of formation is a straight-forward. The first step is to calculate the enthalpies of formation ($\Delta_f H^o(0\ K)$) of the species involved in the reaction. The second step is to calculate the enthalpies of formation of the species at 298 *K*. Calculating the Gibbs free energy of reaction is similar, except to add in the entropy term as shown in equation (2.57).

$$\Delta_f G^o(298\ K) = \Delta_f H^o(298\ K) - T(S^o(M, 298\ K)) - \sum S^o(X, 298\ K) \qquad (2.57)$$

Atomization energy of the molecule is given by equation (2.58).

$$\sum D_0(M) = \sum_{\text{atoms}} \pi\varepsilon_0(X) - \varepsilon_0(M) - \varepsilon_{\text{ZPE}}(M) \qquad (2.58)$$

$\varepsilon_0(M)$ is the total energies of the molecule. $\varepsilon_{\text{ZPE}}(M)$ is the zero-point energy of the molecule. The enthalpy ($\Delta_f H^o(0\ K)$) and Gibbs free energy ($\Delta_f H^o(298\ K)$) for each molecule are shown in equation (2.59) and (2.60)

$$\Delta_f H^o(M, 0\ K) = \sum_{\text{atoms}} x\Delta_f H^o(X, 0\ K) - \sum D_0(M) \qquad (2.59)$$

$$\Delta_f H^o(M, 298\ K) = \Delta_f H^o(M, 0\ K) + (H_M^o(298\ K) - H_M^o(0\ K)) + \sum_{atoms} x(H_x^o(298\ K) - H_x^o(0\ K))$$

$$\Delta_f G^o(M, 298\ K) = \Delta_r H^o(298\ K) - 298.15(S^o(M, 298\ K) - (\sum S^o(X, 298\ K)) \qquad (2.60)$$

($H_x^o(298\ K) - H_x^o(0\ K)$) is enthalpy correction of the molecule, ($H_x^o(298\ K) - H_x^o(0\ K)$) is enthalpy corrections of the atomic elements, $S^o(X, 298\ K)$ is entropy for the atoms and $S^o(M, 298\ K)$ is entropy for the atoms.

CHAPTER III

COMPUTATIONAL DETAILS

The ZSM-5 zeolite models included 12 distinct tetrahedral sites in the unit cell. These models were made of the MFI structure. The T12 site was selected because it was located at the interaction of the sinusoidal and straight channels which is a characteristic of ZSM-5, and allowing significant interaction between the bridging hydroxyl and adsorbed molecules and thus being considered as catalytically active sites.

The phosphorus-modified H-ZSM-5 (P-H-ZSM-5) catalysts were modeled as 52T cluster ($Si_{49}O_{84}Al_2PH_{41}$) which is based on the "O-AlO_2-O-PO_2-O-AlO_2-O" model. As two-layer ONIOM approach was employed in all calculations, the high and low layers for ONIOM were assigned as the 5T cluster ($Si_2O_{16}Al_2PH$) of P-H-ZSM-5 and the rest part ($Si_{47}O_{68}H_{40}$), respectively. The molecular fraction of P-H-ZSM-5 treated with high level of theory is shown in Figure 3.1, as ball & bond atoms.

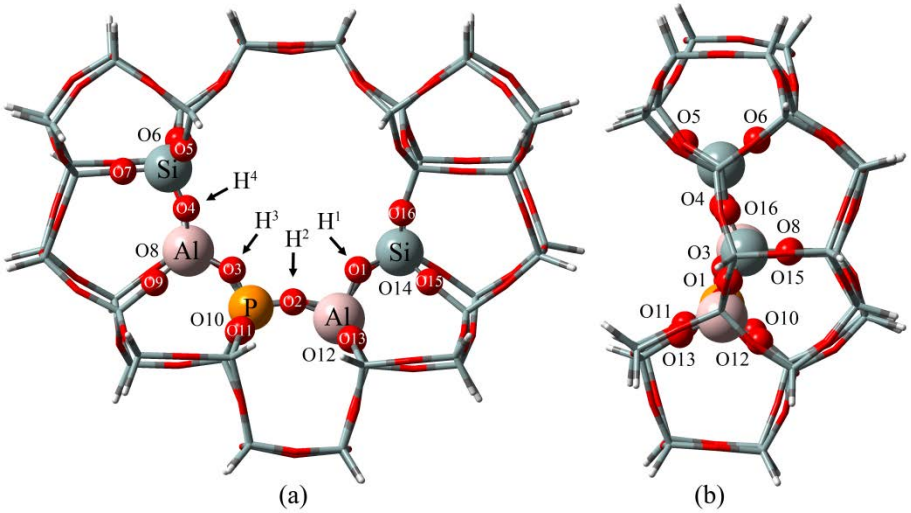


Figure 3.1 P-H-ZSM-5 modeled as a 52T cluster ($Si_{49}O_{84}Al_2PH_{41}$ where acid proton was included). The 5T cluster (O_3Si-O-AlO_2-O-PO_2-O-AlO_2-O-SiO_3) was represented by ball & bond. The 5T cluster included one acid proton (H^1, H^2, H^3 or H^4 atom) and the rest part was represented as tube-type were treated as high and low level of

theories of the two-layer ONIOM approach, respectively; (a) sinusoidal channel view and (b) straight channel view

The geometry optimizations for the P-H-ZSM-5 catalysts modeled as the 52T cluster and configurations of their interactions with reactant, product and their corresponding transition states were carried out using the two-layer ONIOM(MO:MO) method. The high and low layers for the two-layer ONIOM(MO:MO) were the DFT and semi-empirical methods, respectively. The density functional theory (DFT), Becke three-parameter exchange functional [32] with the Lee-Yang-Parr correlation functional [33] (B3LYP) using 6-31G+(d,p) basis sets [33-35] was employed for a high level and the semi-empirical AM1 method [36] was employed for a low level. The calculations were performed with GAUSSIAN 03 program [37]. The zero point vibrational energy (ZPVE) corrections were derived from frequency calculations at the ONIOM(B3LYP/6-31G+(d,p):AM1) level.

3.1 Model selection for the P-H-ZSM-5 catalysts

The structure of 52T cluster of the P-H-ZSM-5 zeolite was constructed from the idealized infinite ZSM-5 crystal lattice structure [38] and it was decorated as follows. The dangling bonds of the 52T cluster of ZSM-5 were saturated with hydrogen atoms, the silicon atoms located at the crystallographic positions T3, T12 and T12′ were substituted by Al, P, and Al, respectively, as shown in Figure 3.1. One hydrogen atom was added to O1, O2, O3 or O4 bridged oxygen atom which are denoted as P-H^1-ZSM-5, P-H^2-ZSM-5, P-H^3-ZSM-5 and P-H^4-ZSM-5, respectively, as defined in Figure 3.2. The P-H-ZSM-5 catalysts were therefore modeled and denoted as P-H^1-ZSM-5, P-H^2-ZSM-5, P-H^3-ZSM-5 and P-H^4-ZSM-5. For the two-layer ONIOM schemes, the high and low zones (Hi:Lo) defined for the P-H^1-ZSM-5, P-H^2-ZSM-5, P-H^3-ZSM-5 and P-H^4-ZSM-5 catalysts are modeled as (O_3Si-O-AlO_2-O-PO_2-O-AlO_2-O<u>H</u>-SiO_3:$Si_{47}O_{68}H_{40}$), (O_3Si-O-AlO_2-O-PO_2-O<u>H</u>-AlO_2-O-SiO_3:$Si_{47}O_{68}H_{40}$), (O_3Si-O-AlO_2-O<u>H</u>-PO_2-O-AlO_2-O-SiO_3:$Si_{47}O_{68}H_{40}$) and (O_3Si-O<u>H</u>-AlO_2-O-PO_2-O-AlO_2-O-SiO_3:$Si_{47}O_{68}H_{40}$); underlined H represents an acidic proton.

The P-H^1-ZSM-5, P-H^2-ZSM-5, P-H^3-ZSM-5 and P-H^4-ZSM-5 catalysts were obtained from full optimizations of the (O_3Si-O-AlO_2-O-PO_2-O-AlO_2-OH-SiO_3:$Si_{47}O_{68}H_{40}$), (O_3Si-O-AlO_2-O-PO_2-OH-AlO_2-O-SiO_3:$Si_{47}O_{68}H_{40}$), (O_3Si-O-AlO_2-OH-PO_2-O-AlO_2-O-SiO_3:$Si_{47}O_{68}H_{40}$) and (O_3Si-OH-AlO_2-O-PO_2-O-AlO_2-O-SiO_3:$Si_{47}O_{68}H_{40}$) clusters at the ONIOM(B3LYP/6-31G+(d,p):AM1) level of theory, as shown in Figure 3.2(a), (b), (c), and (d), respectively. Their geometrical coordinates are shown in Tables A1-A4, in appendices. As the adsorption of methanol in the vicinity of bridged hydroxyl proton of the P-H^1-ZSM-5, P-H^2-ZSM-5, P-H^3-ZSM-5 and P-H^4-ZSM-5 catalysts were examined, methanol can preferably be adsorbed on the P-H^1-ZSM-5 and P-H^4-ZSM-5 catalysts. Optimizations of the adsorption configurations for one methanol molecule adsorbed on the P-H^1-ZSM-5, P-H^2-ZSM-5, P-H^3-ZSM-5 and P-H^4-ZSM-5 catalysts were examined. It was found that the ONIOM(B3LYP/6-31G+(d,p):AM1) optimized structures for initial configurations of methanol located in vicinity of H^2 acid site on P-H^2-ZSM-5 and H^3 acid site on P-H^3-ZSM-5 are MeOH/P-H^1-ZSM-5 and MeOH/P-H^4-ZSM-5, respectively.

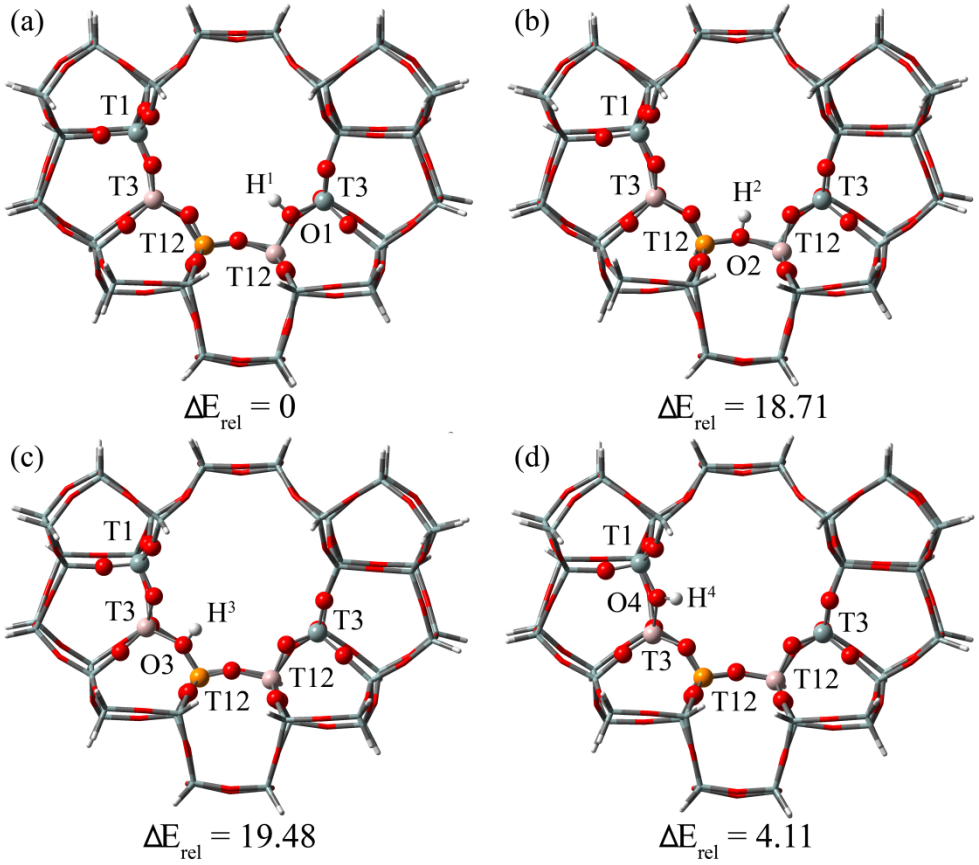


Figure 3.2 The ONIOM(B3LYP/6-31G+(d,p):AM1)-optimized structures of four possible conformations of the P-H-ZSM-5 catalysts. The P-H-ZSM-5 catalysts of which an acidic proton were bonded to bridge (a) O1 (denoted as P-H^1-ZSM-5), (b) O2 (as P-H^2-ZSM-5), (c) O3 (as P-H^3-ZSM-5) and (d) O4 (as P-H^4-ZSM-5). The relative energies (ΔE_{rel}) compared with the most stable configuration (P-H^1-ZSM-5) P-H-ZSM-5 catalysts are in kcal/mol

3.2 Structure optimizations for adsorption configurations of adsorbates on P-H-ZSM-5 catalysts

Full structure optimizations for interaction configurations of reactant, transition states, intermediates and products on the P-H-ZSM-5 catalyst were carried out using the ONIOM(B3LYP/6-31G+(d,p):AM1) approach. In this work, the two-layer ONIOM where the 5T cluster of P-H-ZSM-5 structure was treated using a high level of theory, the 5T clusters $Si_2O_{16}Al_2PH^1$, $Si_2O_{16}Al_2PH^2$, $Si_2O_{16}Al_2PH^3$ and $Si_2O_{16}Al_2PH^4$ were denoted as the P-H^1-ZSM-5, P-H^2-ZSM-5, P-H^3-ZSM-5 and P-H^4-ZSM-5 zeolite catalysts, respectively. The rest part of P-H-ZSM-5 catalysts treated using a low level of theory is the $Si_{47}O_{68}H_{40}$ clusters.

3.3 Thermodynamic properties, rate and equilibrium constants

The standard enthalpy ΔH°_{298} and the Gibb free energy change ΔG°_{298} of all interaction configurations have been derived from the ZPVE computed at the ONIOM(B3LYP/6-31G+(d,p):AM1) level of theory [27]. At 298.15 K and 1 atm, the equilibrium constant (K_{eq}) was computed using a thermodynamic equation $\Delta G^{\circ} = -RTln\,K_{\mathrm{eq}}$. The rate constant $k(T)$ for reaction process derived from the transition-state theory were computed from the activation energy ($\Delta^{\ddagger}E$) using equation (2.36). The tunneling coefficient (κ) can be computed with the Wigner method [39] in equation (2.37). The pre-exponential factor (A) was computed using the equation, $\mathrm{A} = (k_{\mathrm{B}}T/h)(q_{\mathrm{TS}}/q_{\mathrm{REA}})$.

CHAPTER IV

RESULTS AND DISCUSSION

The P-H^1-ZSM-5, P-H^2-ZSM-5, P-H^3-ZSM-5 and P-H^4-ZSM-5 clusters were optimized with the ONIOM(B3LYP/6-31+G(d,p):AM1) level but only the P-H^1-ZSM-5 and P-H^4-ZSM-5 clusters were stable.

Total and relative energies of P-H^1-ZSM-5, P-H^2-ZSM-5, P-H^3-ZSM-5 and P-H^4-ZSM-5 clusters are listed in Table 4.1 and Table 4.2. It shows that their relative stabilities are in order: P-H^1-ZSM-5 > P-H^4-ZSM-5 > P-H^2-ZSM-5 ≈ P-H^3-ZSM-5. The P-H^1-ZSM-5 is more stable than the P-H^4-ZSM-5 by ≈ 4 kcal/mol. Cartesian coordinates for the P-H^1-ZSM-5 and P-H^4-ZSM-5 clusters are shown in Table A1 and A2, in Appendices.

4.1 Acidity of P-H-ZSM-5 zeolite

Table 4.1 ΔE_{deprot} of different acid sites of P-H-ZSM-5, computed with the B3LYP/ 6-31+G(d,p)//ONIOM(B3LYP/6-31+G(d,p):AM1) method

Cluster	E_{total}[a]		E_{rel}[a]		ΔE_{deprot}[b]
	Z^-	HZ	Z^-	HZ	
P-H^1-ZSM-5	-21362.7602693	-21363.2700541	0.000000	0.000000	319.90
P-H^2-ZSM-5	-21362.7477872	-21363.2395063	0.012482	0.030548	308.56
P-H^3-ZSM-5	-21362.7533387	-21363.2409259	0.006931	0.029128	305.97
P-H^4-ZSM-5	-21362.7599708	-21363.2638174	0.000298	0.006237	316.17

[a] Total energies are in a.u.

[b] In kcal/mol.

Table 4.2 ΔE_{deprot} of different acid sites of P-H-ZSM-5, computed with the ONIOM(B3LYP/6-31+G(d,p):AM1) method

Cluster	E_{total}[a]		E_{rel}[a]		ΔE_{deprot}[b]
	Z^-	HZ	Z^-	HZ	
P-H^1-ZSM-5	-2627.384047	-2627.866240	0.000001	0.000000	302.58
P-H^2-ZSM-5	-2627.384048	-2627.836421	0.000000	0.029819	283.87
P-H^3-ZSM-5	-2627.384032	-2627.835192	0.000016	0.031048	283.11
P-H^4-ZSM-5	-2627.384038	-2627.859688	0.000010	0.006552	298.48

[a] Total energies are in a.u.

[b] In kcal/mol.

The MTP included three reactions such as methanol conversion to dimethyl ether (MTD), ethanol conversion to ethylene, and dimethyl ether conversion to propylene, respectively.

4.2 Optimized structures for interaction configurations of the MeOH conversion to DME (MTD) species over P-H-ZSM-5

The ONIOM(B3LYP/6-31+G(d,p):AM1)-optimized structures for the interaction configurations of reactant, intermediates and transition states on the P-H^1-ZSM-5 for the stepwise mechanism and on P-H^1-ZSM-5 and P-H^4-ZSM-5 for the concerted mechanism are shown in Figure 4.1. The ONIOM(B3LYP/ 6-31+G(d,p):AM1)-optimized structures for interaction configurations of reactant, intermediates, transition states on the P-H^4-ZSM-5 for the stepwise mechanism and on P-H^4-ZSM-5 and P-H^1-ZSM-5 for concerted mechanism are shown in Figure 4.2. All the transition states TS, TS1, TS2 over the P-H^1-ZSM-5 and P-H^4-ZSM-5 are confirmed by their single imaginary frequencies which are shown in parentheses.

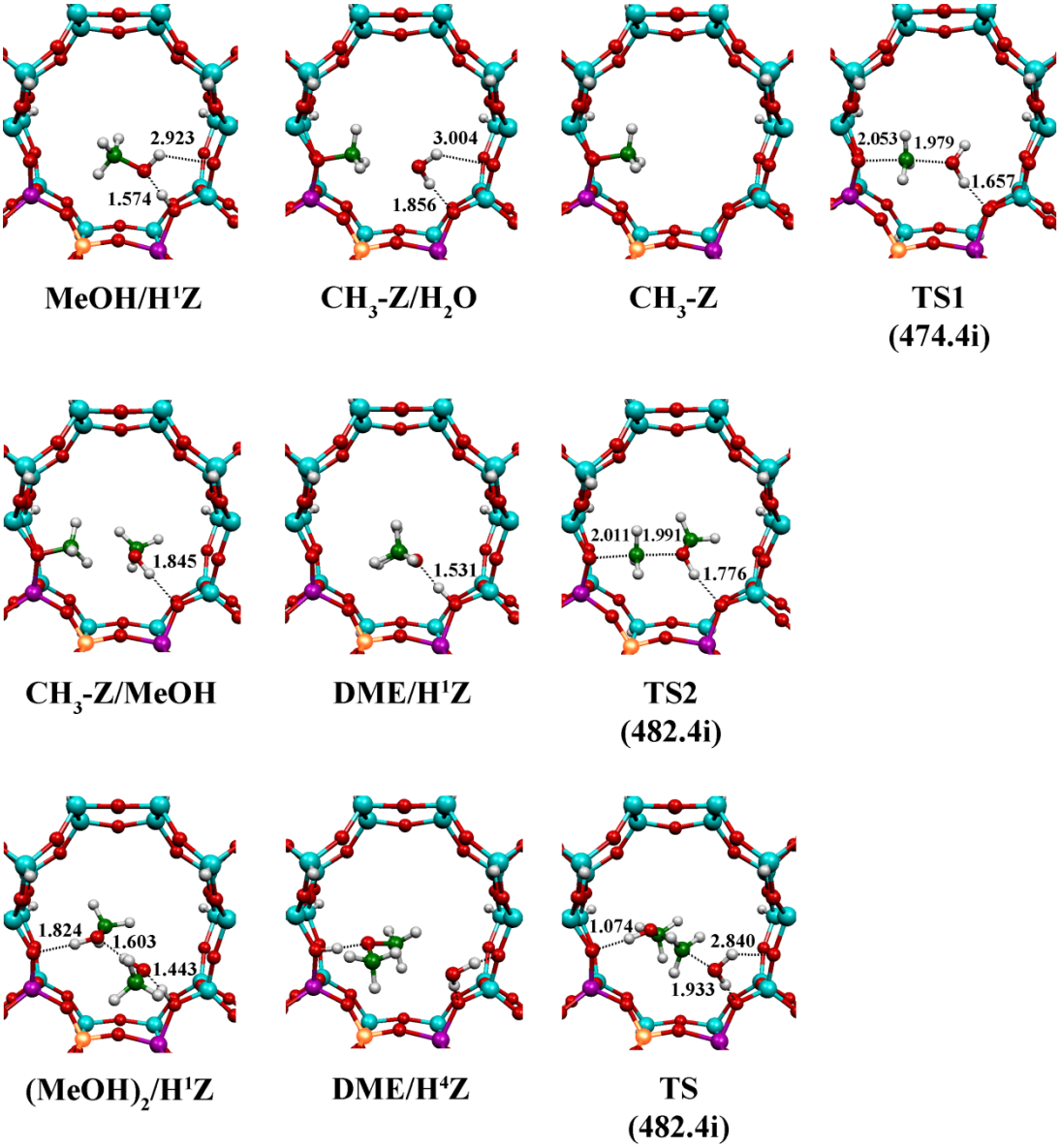


Figure 4.1 Optimized structures for interaction configurations of reactant, intermediates and transition states on the P-H^1-ZSM-5 for stepwise mechanism and on P-H^1-ZSM-5 and P-H^4-ZSM-5 for concerted mechanism. Bond distances are in Å and imaginary frequency for transition states TS, TS1 and TS2 are in cm^{-1}

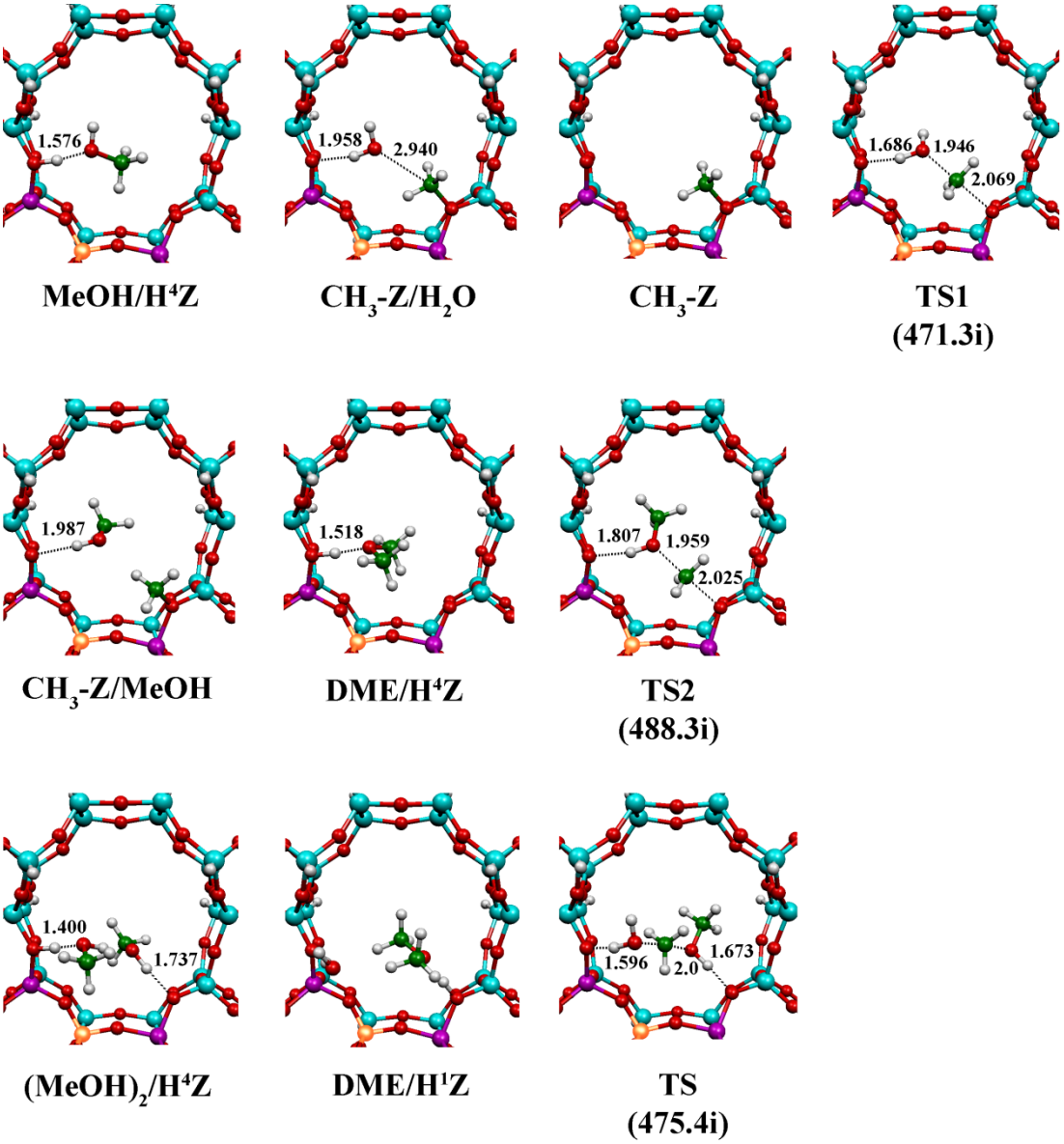


Figure 4.2 Optimized structures for interaction configurations of reactant, intermediates and transition states on the P-H^4-ZSM-5 for stepwise mechanism and on P-H^4-ZSM-5 and P-H^1-ZSM-5 for concerted mechanism. Bond distances are in Å and imaginary frequency for transition states TS, TS1, TS2 are in cm^{-1}

4.3 Investigation of methanol adsorption on the P-H-ZSM-5 catalysts

As possible interaction configurations between MeOH and P-H-ZSM-5 were examined, the ONIOM(B3LYP/6-31G+(d,p):AM1) optimized structures for initial configurations of MeOH located in vicinity of H^2 acid site on P-H^2-ZSM-5 and H^3 acid site on P-H^3-ZSM-5 were found as the MeOH/P-H^1-ZSM-5 and MeOH/P-H^4-ZSM-5, respectively. The potential energies for these initial configurations for MeOH adsorbed on P-H^2-ZSM-5 and on P-H^3-ZSM-5 are shown in Figures A3 and A4, in appendices.

4.4 Mechanism of conversion of MeOH to DME (MTD) over P-H-ZSM-5

Two reaction mechanisms for MTD reaction either over the P-H^1-ZSM-5 and P-H^4-ZSM-5 cluster as (i) stepwise and (ii) concerted mechanisms were found. Nevertheless, the concerted mechanism over the P-H^1-ZSM-5 and the P-H^4-ZSM-5 clusters were similar reactions and the P-H^1-ZSM-5 and the P-H^4-ZSM-5 clusters have become the P-H^4-ZSM-5 and the P-H^1-ZSM-5 clusters while the DME was producing. These concerted mechanisms will be discussed in detail.

4.4.1 Reaction over P-H^1-ZSM-5

The stepwise mechanism of MeOH conversion to DME over the P-H^1-ZSM-5 was composed of six steps as shown in Figure 4.3. The first step, the first MeOH molecule was adsorbed on the P-H^1-ZSM-5 (shorted as H^1Z) to be the MeOH/H^1Z adsorption state. The second step was the dehydration step, which was the MeOH/H^1Z conversion to the methoxide species (CH_3-Z/H_2O) with one water molecule being adsorbed via transition state TS1. The second step was the rate determining step whose rate constant was $k = 1.94 \times 10^{-11}$ s^{-1}. The third step, adsorbed water molecule desorbed from the CH_3-Z/H_2O species. The fourth step was the adsorption of the second MeOH molecule on the CH_3-Z species to form CH_3-Z/MeOH. The fifth step was the step of CH_3-Z/MeOH conversion to DME/H^1Z via transition state TS2. The last step, DME desorbed from the DME/H^1Z adsorption state to afford DME product.

The concerted mechanism for the MTD reaction over the P-H^1-ZSM-5 was composed of three steps as shown in Figure 4.4. The first step was the simultaneous adsorption of two methanol molecules on the P-H^1-ZSM-5 catalyst denoted as $(MeOH)_2/H^1Z$. The second step was the conversion of $(MeOH)_2/H^1Z$ to DME/H^4Z via transition state TS. The last step, DME desorbed from the DME/H^4Z adsorption state to afford the DME product. The second step was the rate determining step of which the rate constant was $k = 1.01 \times 10^{-15}$ s^{-1}. It was found that the reaction rate for the MTD reaction over the P-H^1-ZSM-5 of the stepwise mechanism was much faster than its concerted mechanism.

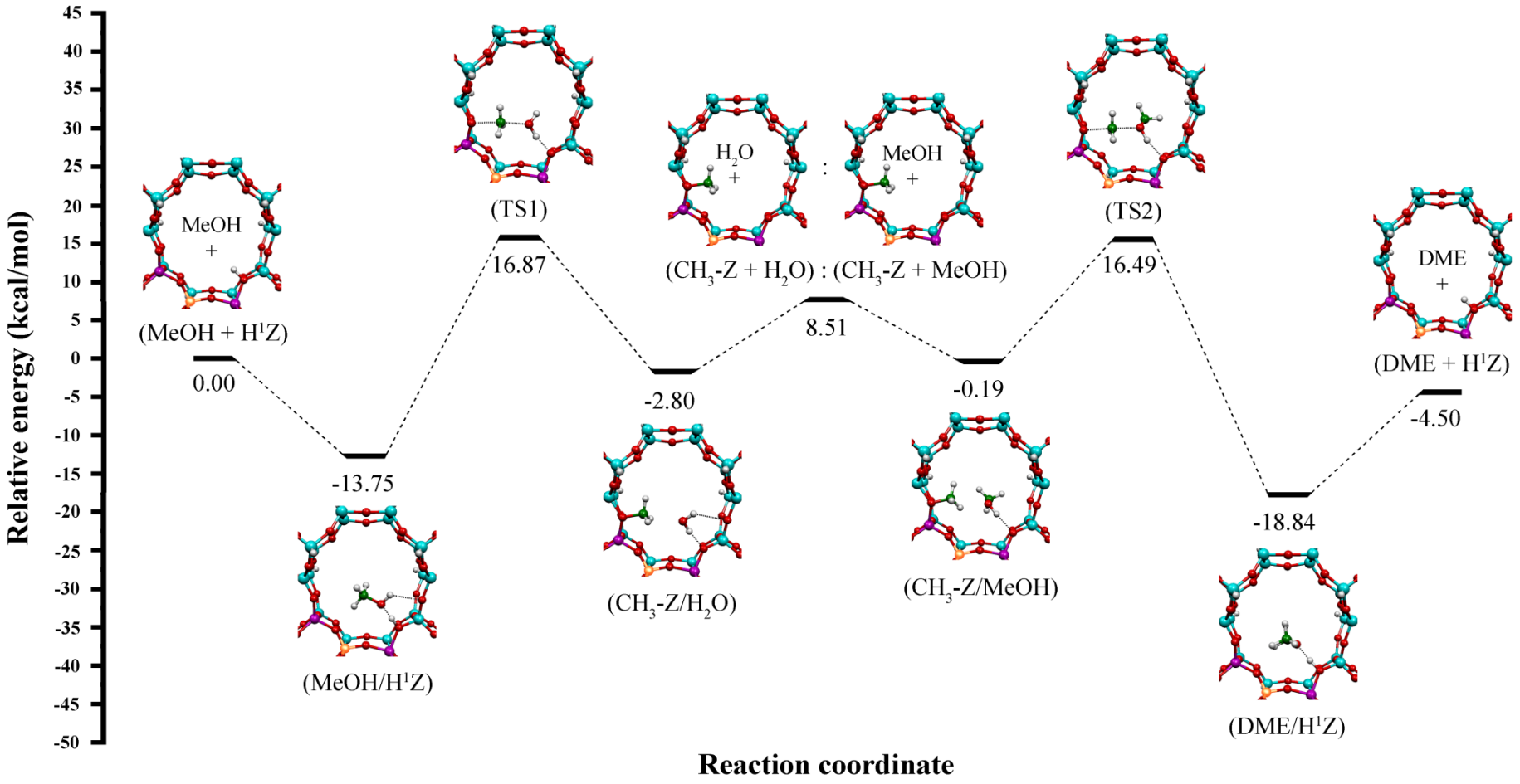


Figure 4.3 Relative energy profile for stepwise reaction of methanol (MeOH) conversion to dimethyl ether (DME) on P-H[1]-ZSM-5

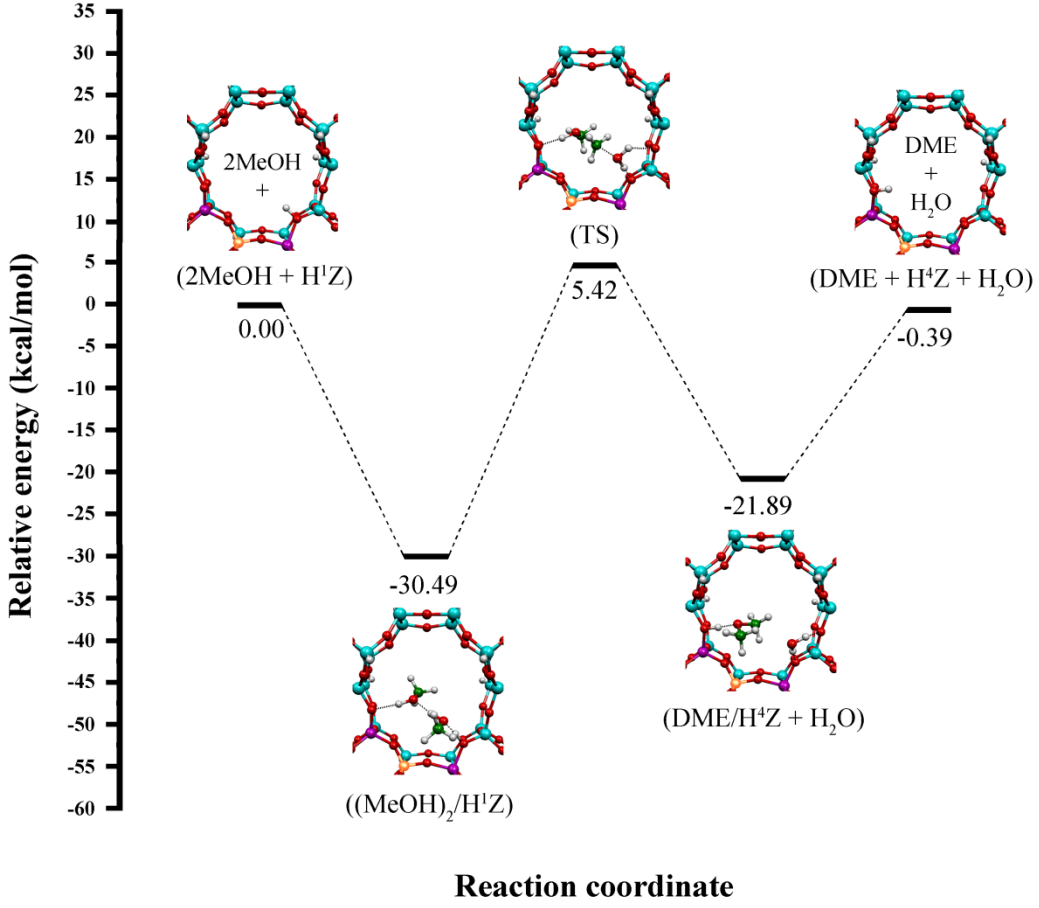


Figure 4.4 Relative energy profile for concerted reaction of methanol (MeOH) conversion to dimethyl ether (DME) on P-H^1-ZSM-5 and P-H^4-ZSM-5

4.4.2 Reaction over P-H^4-ZSM-5

The stepwise and concerted mechanisms occurring over the P-H^4-ZSM-5 are shown in Figures 4.5 and 4.6, respectively. The stepwise mechanism for MTD over the P-H^4-ZSM-5 was composed of six reaction steps. The first and second steps were the adsorption of MeOH on the P-H^4-ZSM-5 (denoted H^4Z) to form MeOH/H^4Z species and the dehydration of MeOH/H^4Z to form CH_3-Z/H_2O species via transition state TS1, respectively. The second step was also the rate determining step of which rate constant was $k = 1.89 \times 10^{-6}$ s^{-1}. The third step, adsorbed water molecule desorbed from the CH_3-Z/H_2O species. The fourth step was the adsorption of the second MeOH molecule on the CH_3-Z species to form CH_3-Z/MeOH. The fifth step was the CH_3-Z/MeOH conversion to DME/H^4Z via transition state TS2. The last step was the DME desorption from the DME/H^4Z and afford DME product.

The concerted mechanism for the MTD reaction over the P-H^4-ZSM-5 comprise of three steps as shown in Figure 4.6. The first step was the simultaneous adsorption of two methanol molecules on the P-H^4-ZSM-5 denoted as $(MeOH)_2H^4Z$. The second step was the $(MeOH)_2H^4Z$ conversion to DME/H^1Z via transition state TS. The last step, DME desorbed from the DME/H^1Z species to afford the DME product. The second step was the rate determining step of the concerted mechanism whose rate constant was $k = 1.73 \times 10^{-16}$ s^{-1}. The reaction rate of the MTD reaction over the P-H^4-ZSM-5 of stepwise mechanism was much faster than its concerted mechanism.

4.5 Thermodynamic properties of the conversion of MeOH to DME over P-H-ZSM-5 and the reaction parameters

The reaction energies, thermodynamic properties, rate and equilibrium constants of the stepwise mechanism for the MeOH conversion to DME over the P-H^1-ZSM-5 (H^1Z) and the concerted mechanism over the H^1Z and H^4Z are listed in Table 4.3. Reaction energies, thermodynamic properties, rate and equilibrium constants of the stepwise mechanism over the P-H^4-ZSM-5 (H^4Z) and the concerted mechanism for the MTD reaction over the H^4Z and H^1Z are listed in Table 4.4.

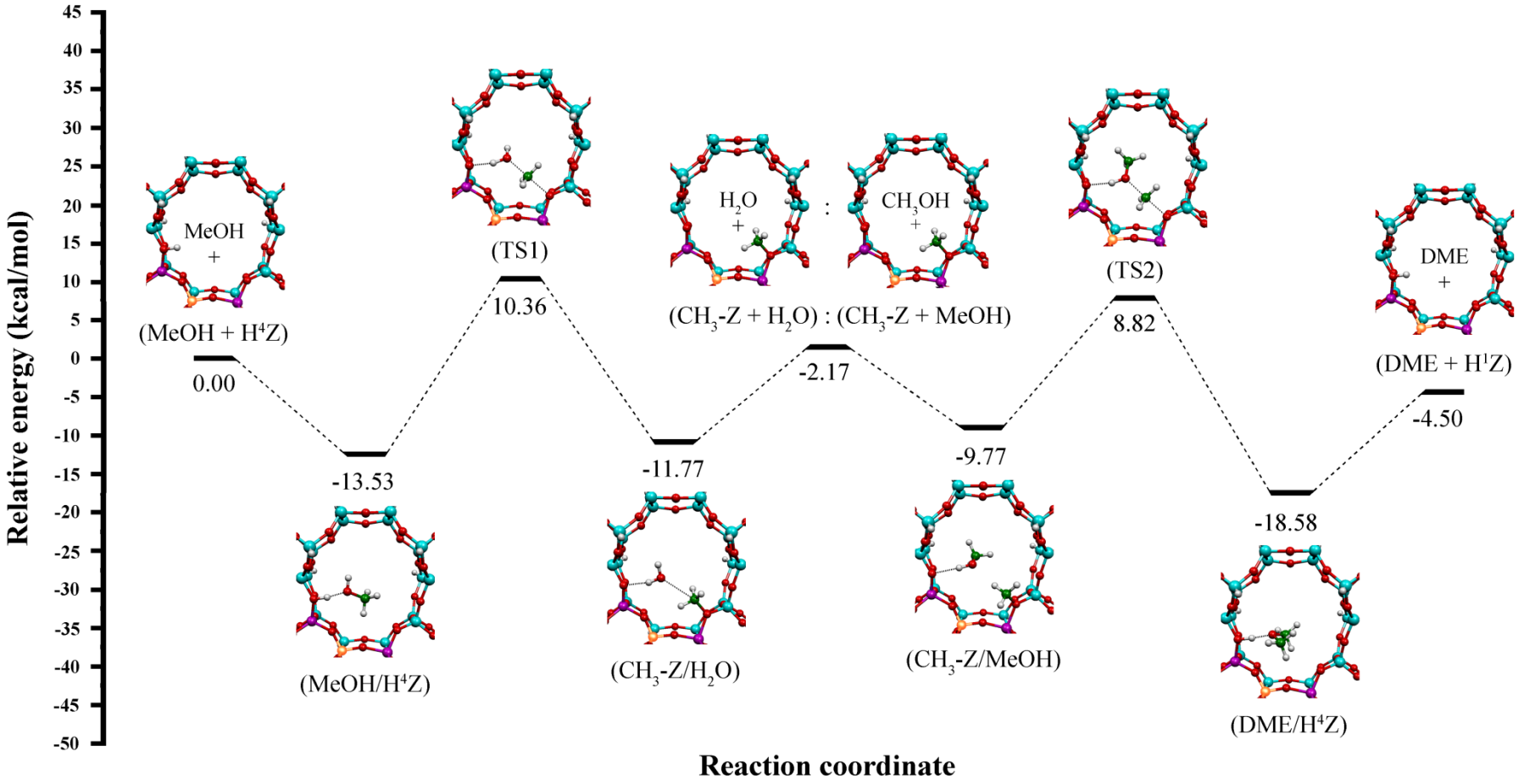


Figure 4.5 Relative energy profile for the stepwise reaction of methanol (MeOH) conversion to dimethyl ether (DME) on P-H^4-ZSM-5

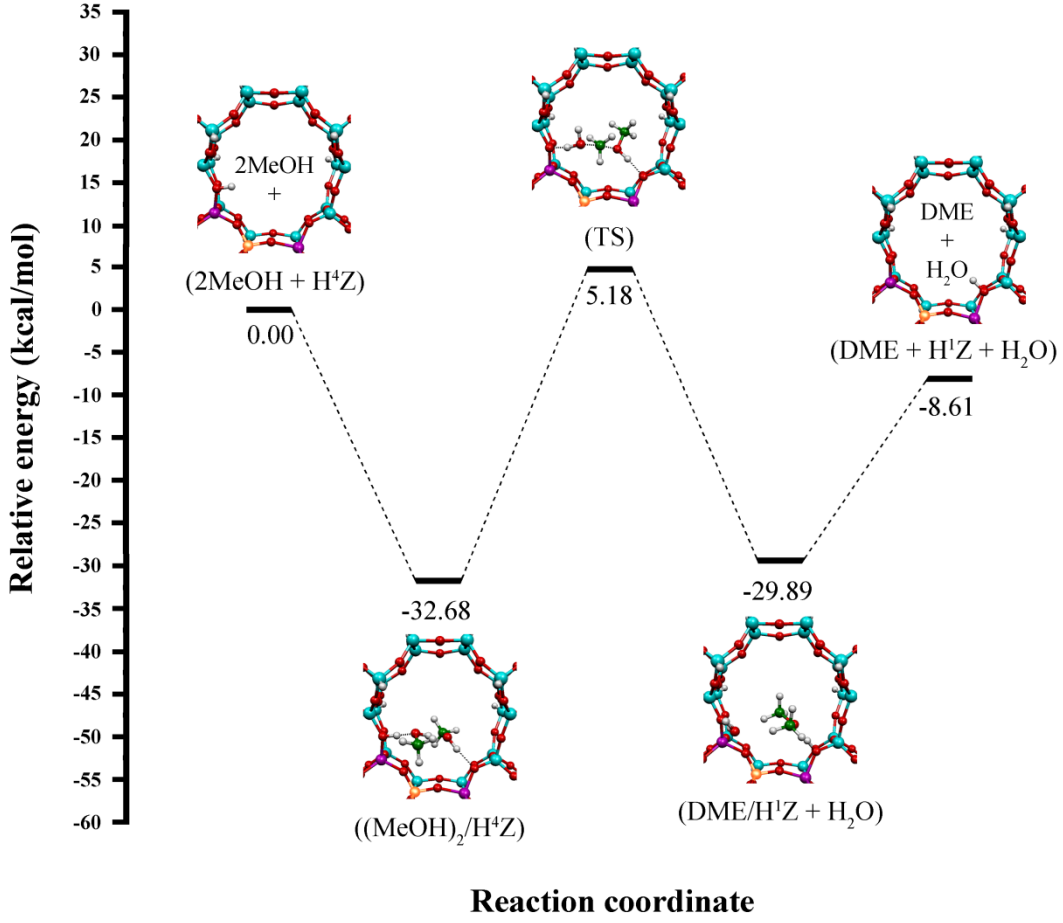


Figure 4.6 Relative energy profile for the concerted reaction of methanol (MeOH) conversion to dimethyl ether (DME) on P-H^4-ZSM-5 and P-H^1-ZSM-5

Table 4.3 Reaction energies, thermodynamic properties, rate and equilibrium constants of stepwise mechanism for the MTD reaction over the P-H^1-ZSM-5 (denoted as H^1Z) and concerted mechanism for the MTD reaction over the H^1Z and H^4Z

Mechanisms/Reactions	$\Delta^{\ddagger}E$ [a,b]	$\Delta^{\ddagger}G^{o}_{298}$ [a,b]	k_{298} [c]	ΔE [a]	ΔH^{o}_{298} [a]	ΔG^{o}_{298} [a]	A^{o}_{298} [c]	K_{298}
Stepwise mechanism:								
$MeOH + H^1Z \rightarrow MeOH/H^1Z$	–	–	–	–13.75	–13.75	–3.11	–	1.91×10^{2}
$MeOH/H^1Z \rightarrow TS1 \rightarrow CH_3–Z/H_2O$	30.62	32.18	1.94×10^{-11}	10.95	11.23	10.96	4.43×10^{11}	9.17×10^{-9}
$CH_3–Z/H_2O \rightarrow CH_3–Z + H_2O$	–	–	–	11.31	11.26	3.11	–	5.27×10^{-3}
$CH_3–Z + MeOH \rightarrow CH_3–Z /MeOH$	–	–	–	–8.70	–8.16	1.05	–	1.71×10^{-1}
$CH_3–Z /MeOH \rightarrow$ TS2 $\rightarrow DME/H^1Z$	16.69	18.91	1.03×10^{-1}	–18.65	–18.87	–18.22	1.44×10^{11}	2.28×10^{13}
$DME/H^1Z \rightarrow DME + H^1Z$	–	–	–	14.34	14.11	3.25	–	4.16×10^{-3}
Concerted mechanism:								
$2\ MeOH + H^1Z \rightarrow MeOH_2/H^1Z$	–	–	–	–30.49	-30.69	-9.34	–	7.04×10^{6}
$MeOH_2/H^1Z \rightarrow TS \rightarrow DME/H^4Z + H_2O$	35.90	38.02	1.02×10^{-15}	8.59	8.83	9.27	1.74×10^{11}	1.61×10^{-7}
$DME/H^4Z+H_2O \rightarrow DME + H^4Z + H_2O$	–	–	–	21.50	21.79	1.15	–	1.44×10^{-1}

[a] Computed at the ONIOM(B3LYP/6–31+G(d,p):AM1) level of theory, in kcal/mol.
[b] At activation state.
[c] In s^{-1}.

Table 4.4 Reaction energies, thermodynamic properties, rate and equilibrium constants of stepwise mechanism for the MTD reaction over the P-H^4-ZSM-5 (denoted as H^4Z) and concerted mechanism for the MTD reaction over the H^4Z and H^1Z

Mechanisms/Reactions	$\Delta^{\ddagger}E$ [a,b]	$\Delta^{\ddagger}G^{o}_{298}$ [a,b]	k_{298} [c]	ΔE [a]	ΔH^{o}_{298} [a]	ΔG^{o}_{298} [a]	A^{o}_{298} [c]	K_{298}
Stepwise mechanism:								
MeOH + H^4Z → MeOH/H^4Z	–	–	–	–13.53	–13.49	–2.89	–	1.31×10^{2}
MeOH/H^4Z → TS1 → CH_3–Z/H_2O	23.89	25.37	1.89×10^{-6}	1.76	2.09	1.44	5.04×10^{11}	8.79×10^{-2}
CH_3–Z/H_2O → CH_3–Z + H_2O	–	–	–	9.60	9.49	1.77	–	5.06×10^{-2}
CH_3–Z + MeOH → CH_3–Z /MeOH	–	–	–	–7.60	–6.98	2.17	–	2.55×10^{-2}
CH_3–Z /MeOH → TS2 → DME/H^4Z	18.58	20.39	8.62×10^{-3}	–8.81	–9.11	2.49	2.95×10^{11}	1.50×10^{-2}
DME/ H^4Z → DME + H^4Z	–	–	–	14.08	13.82	-7.94	–	6.67×10^{5}
Concerted mechanism:								
2 MeOH + H^4Z → $MeOH_2$/H^4Z	–	–	–	–32.68	-33.08	-10.56	–	5.47×10^{7}
$MeOH_2$/H^4Z → TS → DME/H^1Z + H_2O	37.86	39.07	1.73×10^{-16}	2.78	3.44	1.84	8.02×10^{11}	4.46×10^{-2}
DME/H^1Z+H_2O → DME + H^1Z + H_2O	–	–	–	21.28	21.36	1.71	–	5.58×10^{-2}

[a] Computed at the ONIOM(B3LYP/6–31+G(d,p):AM1) level of theory, in kcal/mol.
[b] At activation state.
[c] In s^{-1}.

4.6 Optimized structures for interaction configurations of the ethylene formation from EtOH species over P-H-ZSM-5

The ONIOM(B3LYP/6-31+G(d,p):AM1)-optimized structures for the interaction configurations of reactant, intermediates and transition states on the P-H^1-ZSM-5 for the ethylene formation mechanism are shown in Figure 4.7. The ONIOM(B3LYP/6-31+G(d,p):AM1)-optimized structures for the interaction configurations of reactant, intermediates, transition states on the P-H^4-ZSM-5 for the ethylene formation mechanism are shown in Figure 4.8.

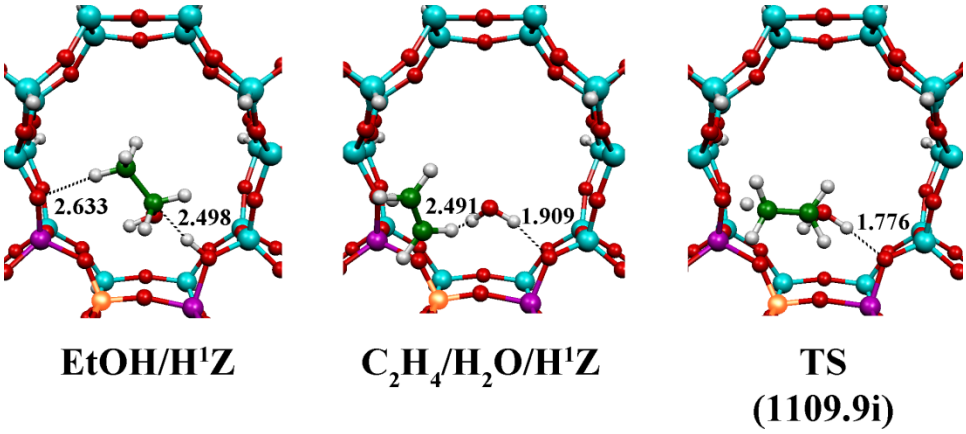


Figure 4.7 Optimized structures for interaction configurations of reactant, intermediates and transition states over the P-H^1-ZSM-5 for the ethylene formation. Bond distances are in Å and imaginary frequency for transition states TS is in cm^{-1}

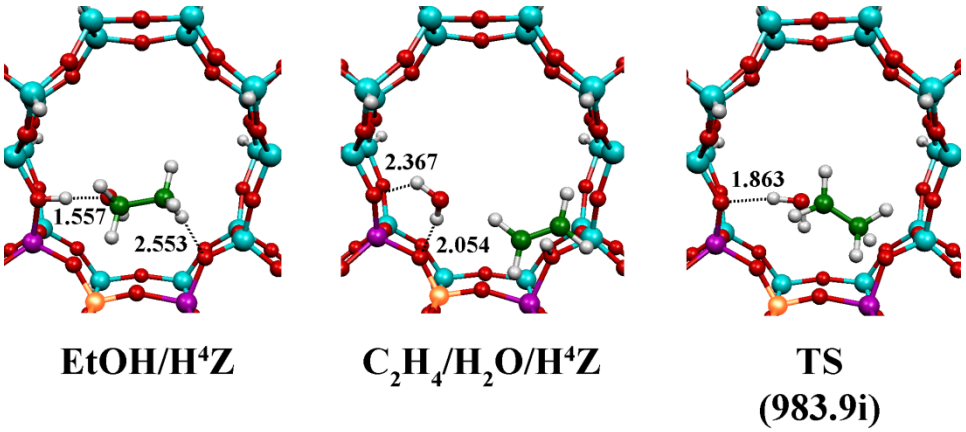


Figure 4.8 Optimized structures for interaction configurations of reactant, intermediates and transition states over the P-H^4-ZSM-5 for the ethylene formation. Bond distances are in Å and imaginary frequency for transition states TS is in cm^{-1}.

4.7 Ethylene formation mechanism from EtOH over P-H-ZSM-5

The ethylene formation mechanism over the P-H^1-ZSM-5 and the P-H^4-ZSM-5 clusters were similar reactions while the ethylene was producing. These mechanisms will be discussed in detail.

4.7.1 Reaction over P-H^1-ZSM-5

The ethylene formation mechanism over the P-H^1-ZSM-5 was composed of three steps as shown in Figure 4.9. The first step, the first EtOH molecule was adsorbed on the P-H^1-ZSM-5 to be the EtOH/H^1Z adsorption state. The second step was the dehydration step, which was the EtOH/H^1Z conversion to the $C_2H_4/H_2O/H^1Z$ via the transition state TS. The second step was the rate determining step whose rate constant was k = 7.64 x 10^{-20} s^{-1}. In the last step, ethylene desorbed from the $C_2H_4/H_2O/H^1Z$ adsorption state to afford the ethylene product.

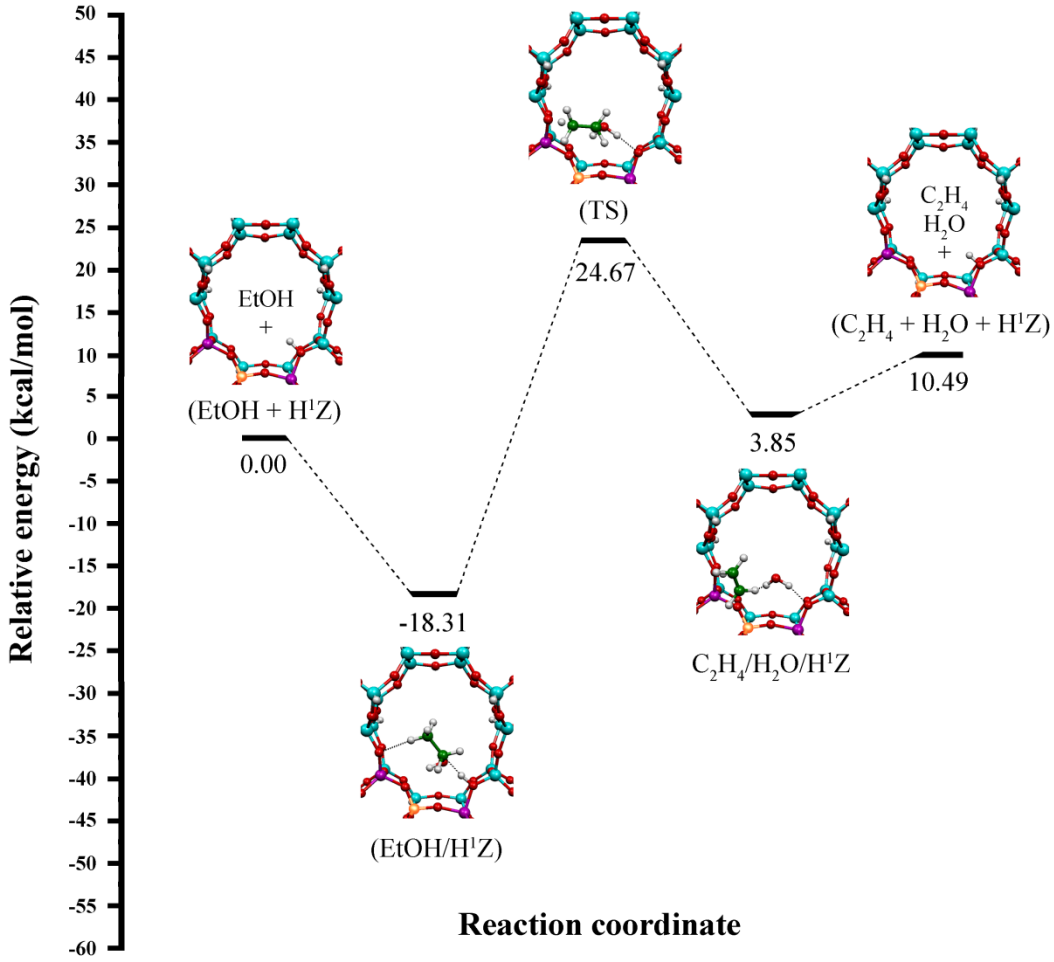


Figure 4.9 Relative energy profile for ethylene formation from ethanol (EtOH) on P-H^{1}-ZSM-5

4.7.2 Reaction over P-H^4-ZSM-5

The ethylene formation mechanism over the P-H^4-ZSM-5 was composed of three steps as shown in Figure 4.10. The first step, the first EtOH molecule was adsorbed on the P-H^4-ZSM-5 to be the EtOH/H^4Z adsorption state. The second step was the dehydration step, which was the EtOH/H^4Z conversion to the C_2H_4/H_2O/H^4Z via transition state TS. The second step was the rate determining step whose rate constant was k = 2.84 x 10^{-15} s^{-1}. The last step, ethylene desorbed from the C_2H_4/H_2O/H^4Z adsorption state to afford ethylene product. It was found that reaction rate for the ethylene formation over the P-H^4-ZSM-5 cluster was much faster than its reaction over the P-H^1-ZSM-5 cluster.

4.8 Thermodynamic properties of the ethylene formation from EtOH over P-H-ZSM-5 and the reaction parameters

Reaction energies, thermodynamic properties, rate and equilibrium constants of the ethylene formation from EtOH over the P-H^1-ZSM-5 (H^1Z) are listed in Table 4.5. The reaction energies, thermodynamic properties, rate and equilibrium constants of the ethylene formation from EtOH over the P-H^4-ZSM-5 (H^4Z) are listed in Table 4.6.

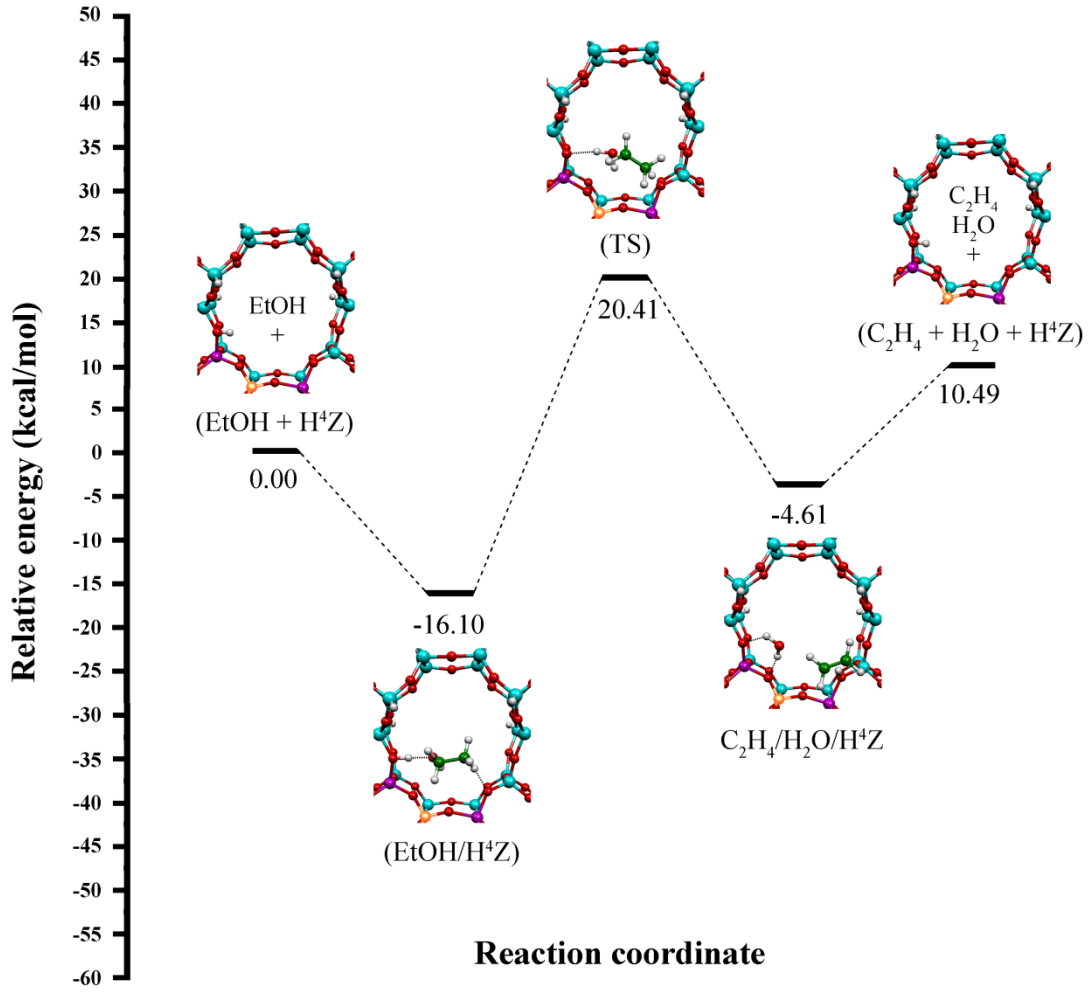


Figure 4.10 Relative energy profile for ethylene formation from ethanol (EtOH) on P-H^4-ZSM-5

Table 4.5 Reaction energies, thermodynamic properties, rate and equilibrium constants of the ethylene formation from EtOH over the P-H^1-ZSM-5 (denoted as H^1Z)

Mechanisms/Reactions	$\Delta^{\ddagger}E$ [a,b]	$\Delta^{\ddagger}G^{o}_{298}$ [a,b]	k_{298} [c]	ΔE [a]	ΔH^{o}_{298} [a]	ΔG^{o}_{298} [a]	A^{o}_{298} [c]	K_{298}
Ethylene formation:								
$EtOH + H^1Z \rightarrow EtOH/H^1Z$	–	–	–	–18.31	–18.44	–6.63	–	7.28×10^{4}
$EtOH/H^1Z \rightarrow TS \rightarrow C_2H_4/H_2O/H^1Z$	42.98	43.99	7.64×10^{-20}	22.16	23.74	19.23	1.12×10^{12}	8.00×10^{-15}
$C_2H_4/H_2O/H^1Z \rightarrow C_2H_4 + H_2O + H^1Z$	–	–	–	6.63	6.77	-10.75	–	7.65×10^{7}

[a] Computed at the ONIOM(B3LYP/6–31+G(d,p):AM1) level of theory, in kcal/mol.
[b] At activation state.
[c] In s^{-1}.

Table 4.6 Reaction energies, thermodynamic properties, rate and equilibrium constants of the ethylene formation from EtOH over the P-H^4-ZSM-5 (denoted as H^4Z)

Mechanisms/Reactions	$\Delta^{\ddagger}E$ [a,b]	$\Delta^{\ddagger}G^{o}_{298}$ [a,b]	k_{298} [c]	ΔE [a]	ΔH^{o}_{298} [a]	ΔG^{o}_{298} [a]	A^{o}_{298} [c]	K_{298}
Ethylene formation:								
$EtOH + H^4Z \rightarrow EtOH/H^4Z$	–	–	–	–16.10	–16.03	–4.85	–	3.59×10^{3}
$EtOH/H^4Z \rightarrow TS \rightarrow C_2H_4/H_2O/H^4Z$	36.51	37.68	2.84×10^{-15}	11.49	12.82	10.05	8.52×10^{11}	4.26×10^{-8}
$C_2H_4/H_2O/H^4Z \rightarrow C_2H_4 + H_2O + H^4Z$	–	–	–	15.10	15.27	-3.36	–	2.92×10^{2}

[a] Computed at the ONIOM(B3LYP/6–31+G(d,p):AM1) level of theory, in kcal/mol.
[b] At activation state.
[c] In s^{-1}.

4.9 Optimized structures for interaction configurations of the DME conversion to propylene species over P-H-ZSM-5

ONIOM(B3LYP/6-31+G(d,p):AM1)-optimized structures for interaction configurations of reactant, intermediates and transition states on the P-H^1-ZSM-5 for the DME conversion to propylene mechanism are shown in Figure 4.11. ONIOM(B3LYP/6-31+G(d,p):AM1)-optimized structures for interaction configurations of reactant, intermediates, transition states on the P-H^4-ZSM-5 for the DME conversion to propylene mechanism are shown in Figure 4.12.

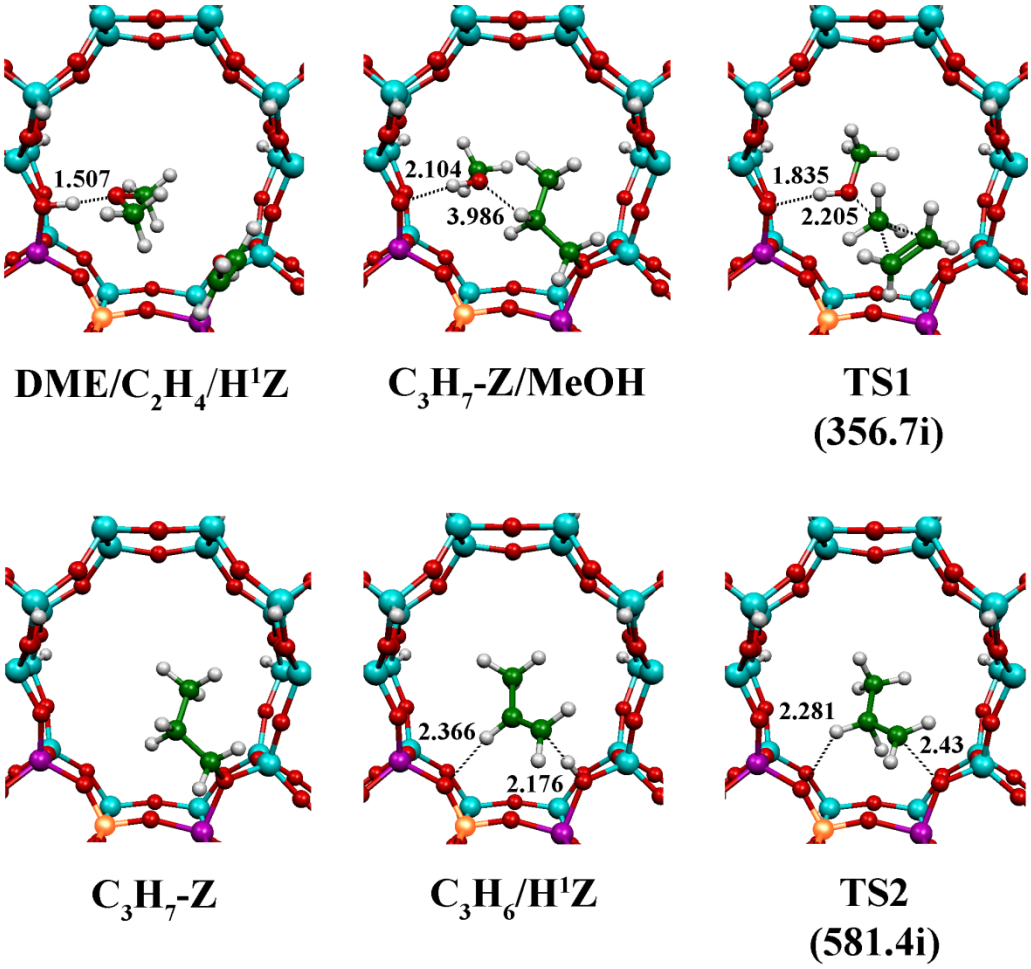


Figure 4.11 Optimized structures for interaction configurations of reactant, intermediates and transition states over the P-H^1-ZSM-5 for the DME conversion to propylene. Bond distances are in Å and imaginary frequency for transition states TS1 and TS2 are in cm^{-1}

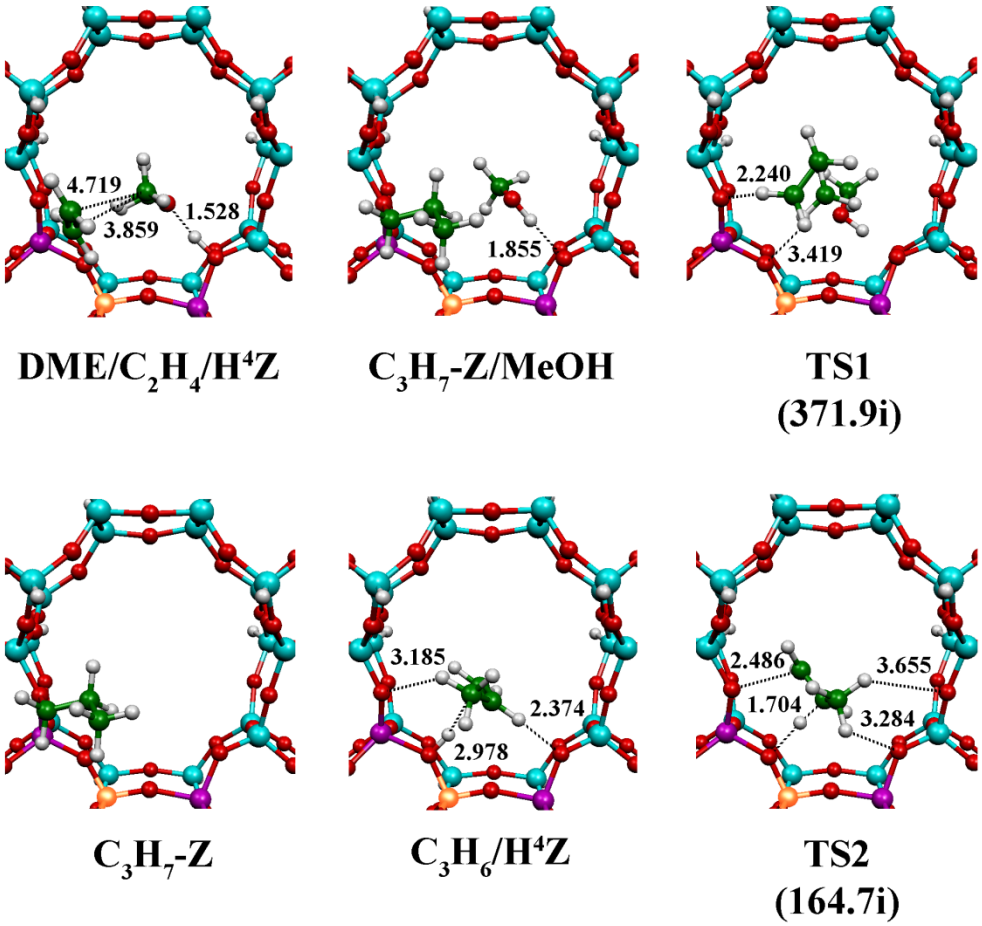


Figure 4.12 Optimized structures for interaction configurations of reactant, intermediates and transition states over the P-H^4-ZSM-5 for for the DME conversion to propylene. Bond distances are in Å and imaginary frequency for transition states TS1 and TS2 are in cm^{-1}

4.10 Mechanism of conversion of DME to propylene over P-H-ZSM-5

The ethylene formation mechanism over the P-H^1-ZSM-5 and the P-H^4-ZSM-5 clusters were similar reactions while the ethylene was producing. These mechanisms will be discussed in detail.

4.10.1 Reaction over P-H^1-ZSM-5

The mechanism of DME conversion to propylene over the P-H^1-ZSM-5 was composed of five steps as shown in Figure 4.13. The first step, the first DME molecule and ethylene were adsorbed on the P-H^1-ZSM-5 to be the DME/C_2H_4/H^1Z adsorption state. The second step was the DME/C_2H_4/H^1Z conversion to the C_3H_7-Z/MeOH species with one MeOH molecule being adsorbed via transition state TS1. The second step was the rate determining step whose rate constant was k = 5.13 x 10^{-29} s^{-1}. In the third step, an adsorbed MeOH molecule on the C_3H_7-Z/MeOH species desorbed from its adsorption state to become dry C_3H_7-Z species. The fourth step was the step of C_3H_7-Z conversion to C_3H_6/H^1Z via transition state TS2. The last step, propylene desorbed from the C_3H_6/H^1Z state to afford propylene product.

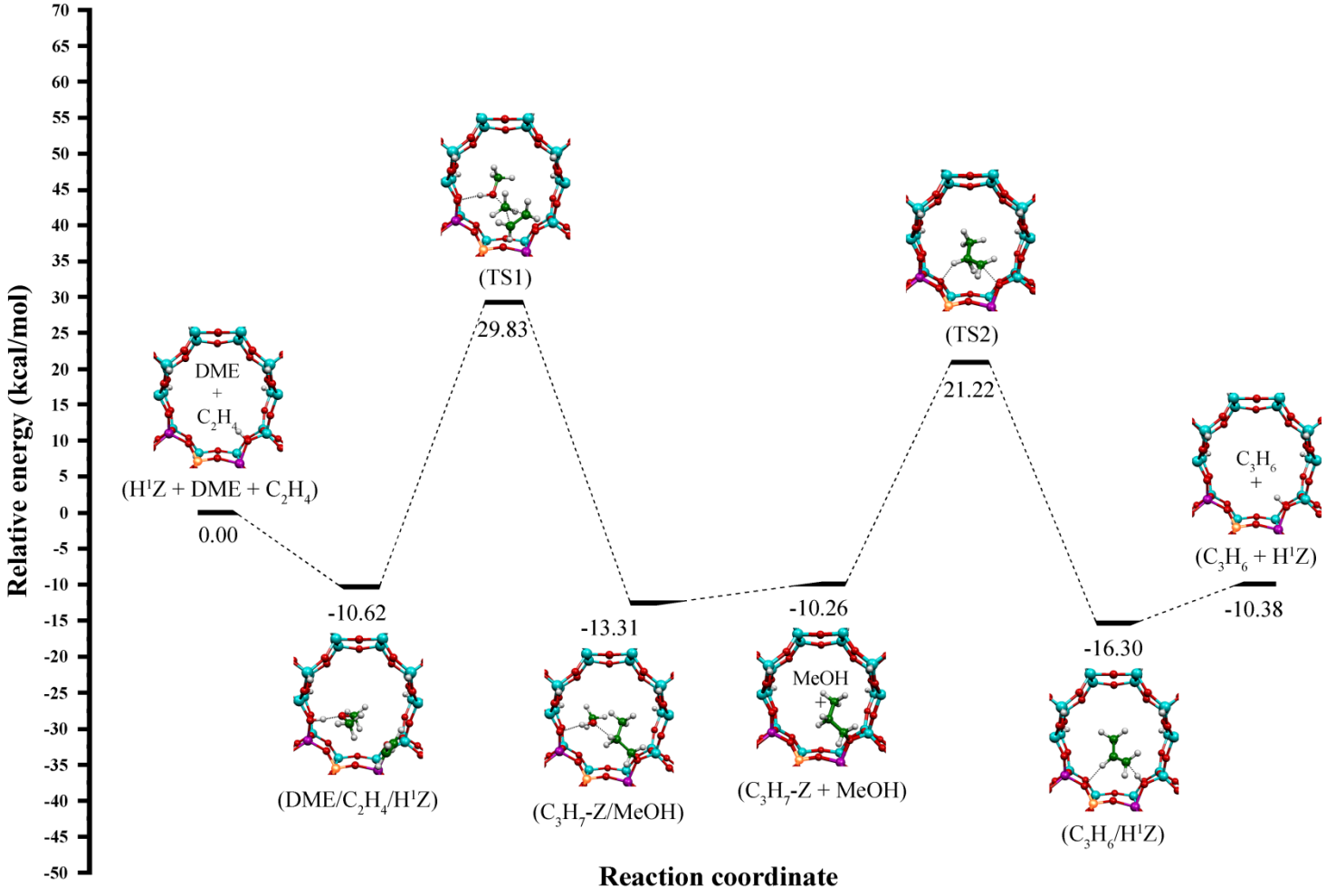


Figure 4.13 Relative energy profile for dimethyl ether (DME) conversion to propylene on P-H^1-ZSM-5

4.10.2 Reaction over P-H^4-ZSM-5

The mechanism of DME conversion to propylene over the P-H^4-ZSM-5 was composed of five steps as shown in Figure 4.14. The first step, the first DME molecule and ethylene were adsorbed on the P-H^4-ZSM-5 to be the DME/C_2H_4/H^4Z adsorption state. The second step was the DME/C_2H_4/H^4Z conversion to the C_3H_7-Z/MeOH species with one MeOH molecule being adsorbed via transition state TS1. The second step was the rate determining step whose rate constant was k = 1.01 x 10^{-21} s^{-1}. The third step, an adsorbed MeOH molecule on the C_3H_7-Z/MeOH species desorbed from its adsorption state to become dry C_3H_7-Z species. The fourth step was the step of C_3H_7-Z conversion to C_3H_6/H^4Z via transition state TS2. In the last step, propylene desorbed from the C_3H_6/H^4Z state to afford propylene product. It was found that reaction rate for the conversion DME to propylene over the P-H^4-ZSM-5 cluster was much faster than its reaction over the P-H^1-ZSM-5 cluster.

4.11 Thermodynamic properties of conversion of DME to propylene over P-H-ZSM-5 and the reaction parameters

Reaction energies, thermodynamic properties, rate and equilibrium constants of the DME conversion to propylene over the P-H^1-ZSM-5 (H^1Z) are listed in Table 4.7. Reaction energies, thermodynamic properties, rate and equilibrium constants of the DME conversion to propylene over the P-H^4-ZSM-5 (H^4Z) are listed in Table 4.8.

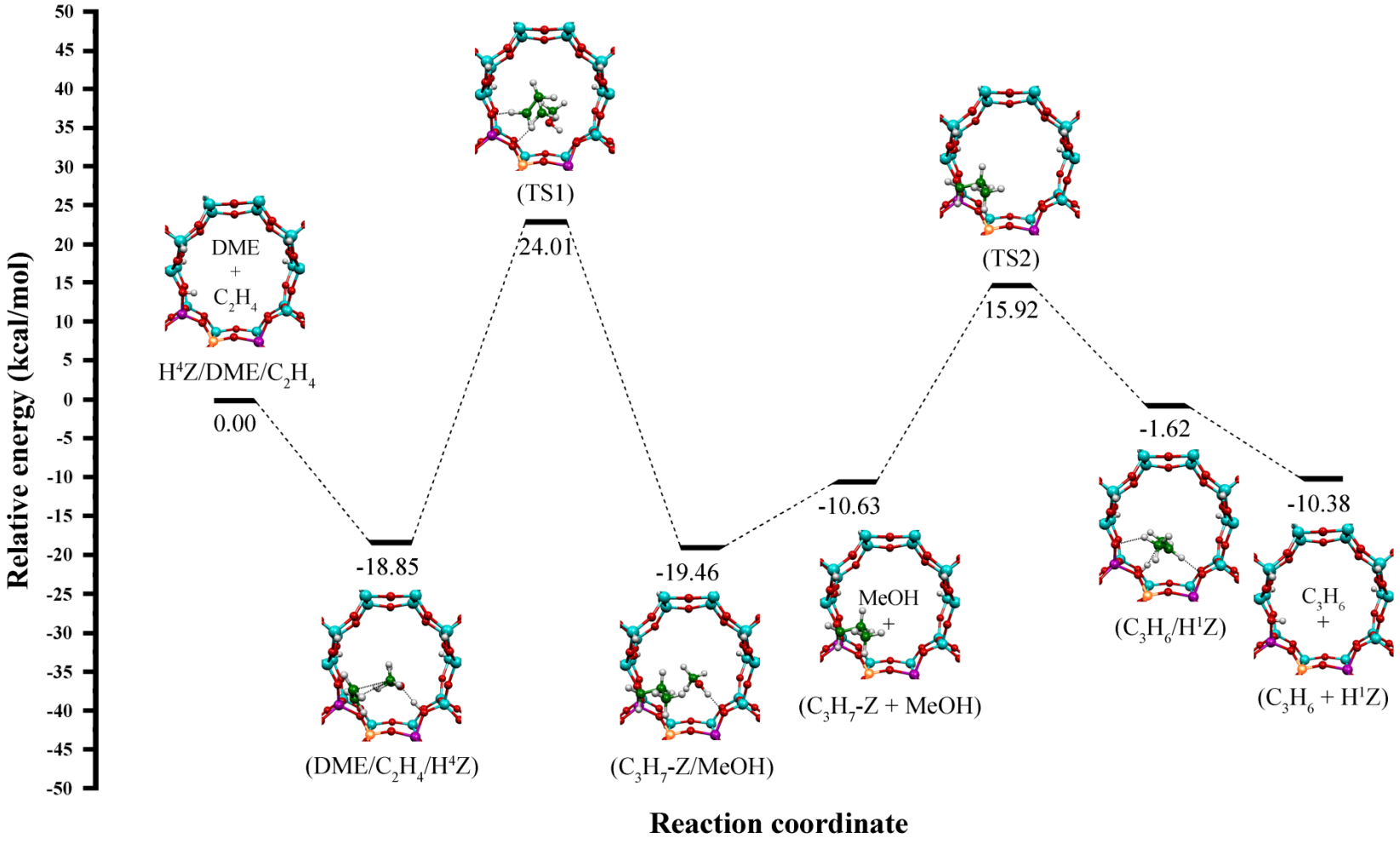


Figure 4.14 Relative energy profile for dimethyl ether (DME) conversion to propylene on P-H^4-ZSM-5

Table 4.7 Reaction energies, thermodynamic properties, rate and equilibrium constants of the DME conversion to propylene over the P-H^1-ZSM-5 (denoted as H^1Z)

Mechanisms/Reactions	$\Delta^{\ddagger}E$ [a,b]	$\Delta^{\ddagger}G^{o}_{298}$ [a,b]	k_{298} [c]	ΔE [a]	ΔH^{o}_{298} [a]	ΔG^{o}_{298} [a]	A^{o}_{298} [c]	K_{298}
DME conversion to propylene:								
DME + C_2H_4 + H^1Z → DME/C_2H_4/H^1Z	–	–	–	–10.62	–9.63	7.80	–	1.92×10^{-6}
DME/C_2H_4/H^1Z → TS1 → C_3H_7–Z/MeOH	40.44	43.51	8.77×10^{-20}	-2.69	-4.35	2.67	3.48×10^{10}	1.10×10^{-2}
C_3H_7–Z/MeOH → C_3H_7–Z + MeOH	–	–	–	3.05	3.09	-8.51	–	1.72×10^{6}
C_3H_7–Z → TS2 → C_3H_6/H^1Z	–	–	–	–6.05	–4.98	-8.21	–	1.04×10^{6}
C_3H_6/H^1Z → C_3H_6 + H^1Z	31.48	30.24	5.55×10^{-10}	5.92	5.50	-4.65	4.99×10^{13}	2.55×10^{3}

[a] Computed at the ONIOM(B3LYP/6–31+G(d,p):AM1) level of theory, in kcal/mol.
[b] At activation state.
[c] In s^{-1}.

Table 4.8 Reaction energies, thermodynamic properties, rate and equilibrium constants of the DME conversion to propylene over the P-H^4-ZSM-5 (denoted as H^4Z)

Mechanisms/Reactions	$\Delta^{\ddagger}E$ [a,b]	$\Delta^{\ddagger}G^{o}_{298}$ [a,b]	k_{298} [c]	ΔE [a]	ΔH^{o}_{298} [a]	ΔG^{o}_{298} [a]	A^{o}_{298} [c]	K_{298}
DME conversion to propylene:								
DME + C_2H_4 + H^4Z → DME/C_2H_4/H^4Z	–	–	–	–18.85	–17.93	0.24	–	6.63×10^{-1}
DME/C_2H_4/H^4Z → TS1 → C_3H_7–Z/MeOH	42.86	46.16	1.01×10^{-21}	-0.61	-1.81	2.33	2.34×10^{10}	1.96×10^{-2}
C_3H_7–Z/MeOH → C_3H_7–Z + MeOH	–	–	–	8.83	8.60	-1.34	–	9.59
C_3H_7–Z → TS2 → C_3H_6/H^4Z	–	–	–	9.02	9.90	7.27	–	4.70×10^{-6}
C_3H_6/H^4Z → C_3H_6 + H^4Z	26.55	26.51	2.31×10^{-7}	-8.76	-9.12	-19.40	6.55×10^{12}	1.66×10^{14}

[a] Computed at the ONIOM(B3LYP/6–31+G(d,p):AM1) level of theory, in kcal/mol.
[b] At activation state.
[c] In s^{-1}.

CHAPTER V

CONCLUSIONS

The structures of P-H-ZSM-5 as the P-H^1-ZSM-5, P-H^2-ZSM-5, P-H^3-ZSM-5, P-H^4-ZSM-5 catalysts and the interaction configurations for reactant, intermediates, transition states, products and involved species of reaction mechanisms over the P-H^1-ZSM-5 and P-H^4-ZSM-5 were obtained using the ONIOM (B3LYP/ 6-31+G(d,p):AM1) method. Their reaction energies, thermodynamic properties, rate and equilibrium constants of the reaction over the P-H-ZSM-5 catalysts are reported.

The rate constants for the methanol conversion to DME reaction of the stepwise mechanism over the P-H^1-ZSM-5 were more than the concerted mechanism.

The rate constants for the methanol conversion to DME reaction of the stepwise mechanism over the P-H^4-ZSM-5 were more than the concerted mechanism.

The rate constants for the ethylene formation from ethanol over the P-H^1-ZSM-5 were less than P-H^4-ZSM-5.

The rate constants for the DME conversion to propylene reaction over the P-H^1-ZSM-5 were less than P-H^4-ZSM-5.

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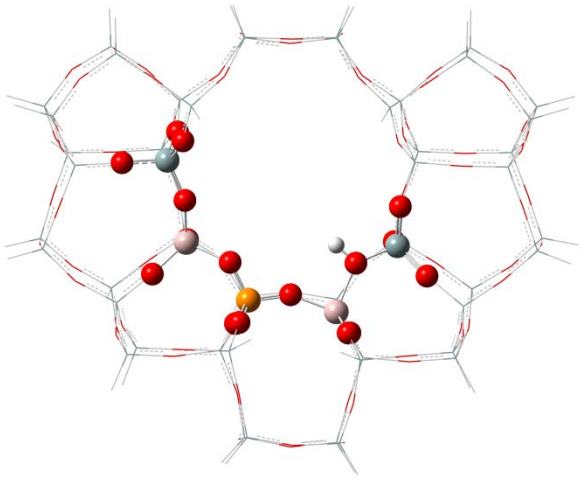
APPENDICES

APPENDIX A

Table A1 Coordinates of 52T cluster for the P-H[1]-ZSM-5, in Å

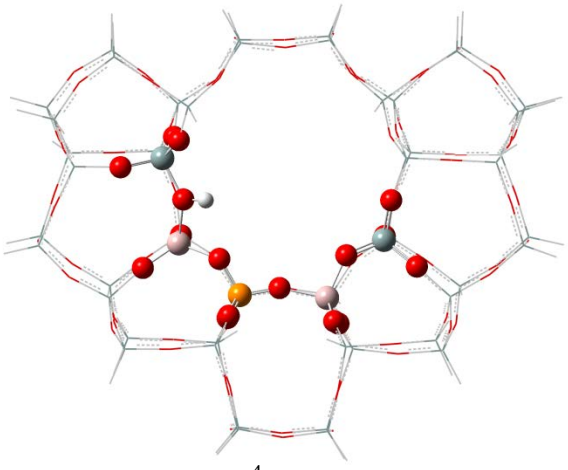


P-H[1]-ZSM-5

Atoms	X	Y	Z
Si	-1.36439	8.05668	0.13357
Si	-1.3159	7.73689	-3.21579
O	-4.02243	-3.12215	-2.50804
O	-4.04765	-0.60243	-0.96881
O	-3.67285	1.08939	1.33929
O	-4.02327	-0.44682	3.68755
O	-4.33885	-3.13839	2.92175
O	-4.23899	-3.1349	0.15829
O	-8.58414	-2.65901	-2.71751
O	-8.46464	-0.27332	-1.24648
O	-9.04177	1.29205	0.92621
O	-8.60605	-0.23097	3.25759
O	-8.64514	-2.86739	2.72195
O	-8.6741	-2.68574	-0.01387
O	-6.29272	-2.10073	-1.34705
O	-6.40736	-1.79364	4.0329
O	-2.70069	-5.6209	-2.71634
O	-5.29387	-5.4567	-3.19083
O	-7.99925	-5.27433	-3.25283
O	-2.84744	-5.11351	1.62501
O	-5.49586	-5.2045	1.35262
O	-8.20566	-5.09455	1.13031
Si	-3.85567	-4.55775	-3.39558
Si	-4.59216	-2.1772	-1.20441
Si	-3.77929	1.09873	3.02222
Si	-4.70883	-1.95134	4.08422
Si	-4.21133	-4.09739	1.53306
Si	-8.94485	-3.94463	-3.77881
Si	-7.9609	-1.88687	-1.33307
Si	-8.94719	1.28856	-0.77816
Si	-9.0238	1.29234	2.62545
Si	-8.09817	-1.7356	3.86825
Si	-9.12367	-3.66644	1.29459
O	-7.82231	2.34051	3.21446
O	-5.07973	2.08175	3.53872
O	-2.43153	1.94523	3.66594
O	-7.75521	2.40813	-1.24003
O	-4.97167	2.16263	-0.97734
O	-2.17073	1.58263	-1.08613
Si	-6.84538	-6.05689	0.77234
Si	-6.71486	-6.20618	-2.62944
Si	-1.95368	-6.52952	1.35753
Si	-1.96962	-6.96946	-1.98828
O	-6.17306	4.42553	2.59387
O	-6.05273	3.9042	-2.87314
O	-6.22896	4.4769	-0.19821
O	-1.8612	4.39677	2.66618
O	-1.70639	6.51556	0.77061
O	-1.60795	7.97395	-1.55498
O	-1.68714	6.12483	-3.63996
O	-1.78661	3.62033	-2.55647
O	-1.88286	3.90443	-0.06698
O	-4.04087	5.30371	1.18312
O	-3.8001	4.54322	-4.30449
Si	-6.39595	3.13632	3.6931
Si	-5.75511	5.30689	1.20133
Si	-5.52223	4.55658	-4.34322
Si	-6.25497	3.2002	-1.3341
Si	-1.52553	3.34177	3.97744
Si	-2.38407	5.03072	1.20001
Si	-2.13784	4.53884	-4.02252
O	0.16265	3.09456	3.96353
O	0.06971	2.67867	-1.13555
O	0.29921	8.35134	0.33653
O	0.36353	7.93213	-3.40867
O	-6.74466	-6.20271	-0.92722
O	-2.12923	-6.9285	-0.29279
O	-0.2682	-6.32764	1.56629
O	-0.28179	-6.94293	-2.2538
O	6.66191	3.99438	2.63016
O	6.30044	3.43082	-2.81406
O	6.42365	4.01463	-0.09904
O	2.31533	4.44932	2.87928
O	2.36142	6.68969	1.03678
O	2.26284	7.9376	-1.47612
O	2.48569	6.29144	-3.79348
O	2.20308	3.80678	-2.75722
O	2.31024	4.09106	0.14609
O	4.54186	5.18688	1.44798
O	4.3321	4.38083	-4.46409
O	8.09114	1.7443	3.27201

O	5.3513	1.72151	3.37261	Si	8.44725	-4.40048	-3.9148
O	2.68791	1.86662	3.59979	Si	7.74423	-2.36806	-1.34678
O	7.73843	1.82045	-1.08315	Si	7.95407	-2.35981	3.83493
O	4.99158	1.77596	-0.93429	Si	8.74925	-4.33615	1.21002
O	2.38648	1.4225	-0.98772	H	-6.52839	3.64665	5.03115
Si	6.7281	2.66922	3.69581	H	-1.86951	3.95838	5.23056
Si	6.21494	4.96606	1.30275	H	2.22676	3.6924	5.36812
Si	6.01823	4.17575	-4.32962	H	6.80271	3.09035	5.0663
Si	6.36564	2.78974	-1.25895	H	-8.70191	-1.98923	5.15049
Si	1.84636	3.29184	4.04066	H	-4.26724	-2.36857	5.38714
Si	2.84485	5.106	1.40653	H	4.08446	-2.51827	5.39991
Si	1.98408	8.11932	0.20096	H	8.53657	-2.71052	5.10214
Si	2.05137	7.80777	-3.16523	H	10.5193	0.83559	3.12671
Si	2.6691	4.63591	-4.17488	H	10.11862	-4.76672	1.22697
Si	3.8734	0.77995	-0.35639	H	10.20681	1.05793	-1.36748
Si	3.92432	0.8981	2.97737	H	9.81934	-4.85731	-3.87785
Si	8.97123	0.70559	-0.72822	H	-10.3211	1.69106	3.10632
Si	9.18036	0.58975	2.66487	H	-10.2174	1.63606	-1.35498
O	6.11124	-6.50239	-1.0754	H	-10.3457	-4.30302	-3.70396
O	1.60351	-6.94115	-0.30584	H	-10.529	-3.96406	1.33363
Si	6.22898	-6.45191	0.62751	Al	1.76278	3.2121	-1.21176
Si	6.0577	-6.49363	-2.77776	H	-6.81705	-7.55697	-3.1141
Si	1.39799	-6.57432	1.34864	H	-6.95755	-7.36012	1.3682
Si	1.3962	-6.96565	-1.99702	H	-2.51841	-8.19001	-2.51827
O	2.15129	-5.59611	-2.68676	H	1.97892	-8.15538	-2.56039
O	4.71749	-5.5743	-3.28449	H	1.84692	-7.64962	2.1926
O	7.41106	-5.66147	-3.39758	H	-2.39275	-7.60179	2.21042
O	2.36531	-5.19088	1.61321	H	6.02545	-7.83527	-3.28987
O	4.99521	-5.45535	1.23717	H	6.1964	-7.77741	1.17751
O	7.68339	-5.65031	1.01484	H	8.10023	-3.95611	-5.24678
O	3.68621	-3.21705	-2.45165	H	2.98599	-4.20451	-4.73735
O	3.90205	-0.71739	-0.95479	H	-3.546	-4.29339	-4.77249
O	3.77849	0.80252	1.25076	H	-8.60451	-3.58884	-5.14033
O	4.04664	-0.67209	3.58636	H	6.48745	3.3088	-5.38815
O	4.05497	-3.38295	2.94843	H	1.92005	4.26392	-5.34105
O	3.90687	-3.20051	0.24975	H	-1.39794	3.97752	-5.11095
O	8.19282	-3.13852	-2.78892	H	-5.95154	3.75933	-5.47095
O	8.39981	-0.81594	-1.22452	H	-5.96592	5.9247	-4.5022
O	9.14596	0.63851	0.9642	H	-6.27165	6.64562	1.25006
O	8.60264	-0.89795	3.25283	H	6.70417	5.44833	-4.38069
O	8.35775	-3.5061	2.64536	H	6.97076	6.18312	1.25223
O	8.3849	-3.28919	-0.0789	H	2.76808	8.85525	-3.83935
O	6.05247	-2.32113	-1.26935	H	2.71301	9.24	0.72581
O	6.26607	-2.23404	4.00978	H	-2.1598	9.08714	0.7373
Si	3.32516	-4.59326	-3.40028	H	-2.06429	8.65407	-4.02795
Si	4.36514	-2.37726	-1.14968	P	-1.45638	2.92954	-1.19672
Si	4.56315	-2.22168	4.08051	Al	-3.78516	1.01846	-0.40619
Si	3.79473	-4.28932	1.54333	H	1.63771	0.80634	-0.99269

Table A2 Coordinates of 52T cluster for the P-H^4-ZSM-5, in Å

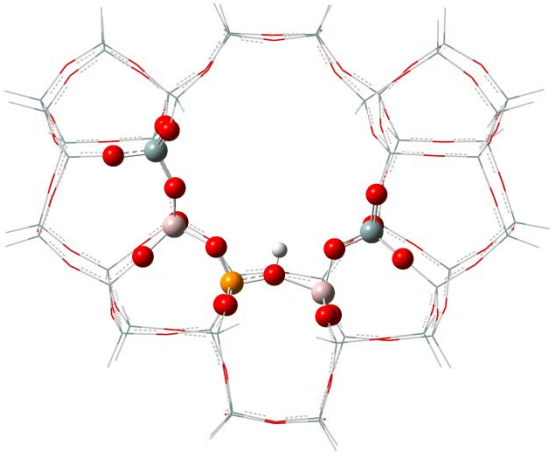


P-H^4-ZSM-5

Atoms	X	Y	Z
Si	-1.4783	7.99802	0.1182
Si	-1.42881	7.65181	-3.22923
O	-4.05519	-3.02648	-2.42956
O	-3.90712	-0.71692	-1.08804
O	-3.74837	0.9634	1.32815
O	-4.07042	-0.51541	3.73152
O	-4.32886	-3.16721	2.99716
O	-4.22966	-3.07561	0.1908
O	-8.50186	-2.68449	-2.69798
O	-8.49836	-0.31625	-1.21763
O	-9.11789	1.22575	0.95214
O	-8.65593	-0.32345	3.26927
O	-8.65014	-2.96675	2.72336
O	-8.66314	-2.74423	-0.00208
O	-6.23502	-2.0443	-1.21254
O	-6.45777	-1.87145	4.08202
O	-2.6093	-5.45602	-2.76325
O	-5.19617	-5.37511	-3.25027
O	-7.8872	-5.27311	-3.29771
O	-2.77436	-5.0547	1.63333
O	-5.41621	-5.20663	1.3546
O	-8.12265	-5.15737	1.09601
Si	-3.79494	-4.40934	-3.41894
Si	-4.59421	-2.16976	-1.13008
Si	-3.82806	1.0043	3.01252
Si	-4.75936	-2.00589	4.16478
Si	-4.16329	-4.07045	1.57987
Si	-8.83218	-3.93751	-3.80736
Si	-7.94108	-1.90848	-1.29231
Si	-9.02535	1.23083	-0.75189
Si	-9.08074	1.20467	2.6514
Si	-8.146	-1.82703	3.88108
Si	-9.08973	-3.76555	1.28295
O	-7.87202	2.25271	3.22277
O	-5.12616	1.99633	3.51914
O	-2.48215	1.86381	3.64291
O	-7.81694	2.31707	-1.24367
O	-5.01361	2.01615	-0.979
O	-2.19696	1.50192	-1.06192
Si	-6.7344	-6.07571	0.72835
Si	-6.58202	-6.1786	-2.67647
Si	-1.87952	-6.45992	1.30618
Si	-1.89644	-6.8246	-2.05235
O	-6.2324	4.33149	2.56528
O	-6.08325	3.73594	-2.90505
O	-6.26785	4.34141	-0.23129
O	-1.92747	4.32789	2.66104
O	-1.78717	6.4543	0.76598
O	-1.7217	7.89474	-1.56919
O	-1.76968	6.03412	-3.65704
O	-1.8296	3.53356	-2.54965
O	-1.93223	3.83515	-0.06415
O	-4.10752	5.21878	1.15961
O	-3.83699	4.39625	-4.33166
Si	-6.44	3.05264	3.67871
Si	-5.8212	5.19736	1.16025
Si	-5.55808	4.37022	-4.38505
Si	-6.29061	3.05467	-1.35711
Si	-1.58809	3.26603	3.96532
Si	-2.44874	4.96231	1.19445
Si	-2.17909	4.43318	-4.02707
O	0.10337	3.04134	3.95491
O	0.03279	2.62034	-1.12155
O	0.17917	8.32358	0.32451
O	0.24702	7.87908	-3.41958
O	-6.61551	-6.18285	-0.97341
O	-2.05142	-6.80833	-0.35547
O	-0.19371	-6.27578	1.52462
O	-0.20802	-6.83637	-2.31429
O	6.59316	4.06369	2.65053
O	6.2598	3.49529	-2.79803
O	6.36878	4.08772	-0.08076
O	2.23519	4.44557	2.88289
O	2.25839	6.68697	1.03517
O	2.14703	7.9241	-1.48456
O	2.39438	6.27383	-3.79521
O	2.14763	3.78974	-2.74857
O	2.24324	4.08457	0.15329
O	4.4558	5.21792	1.45949
O	4.27231	4.39744	-4.45394
O	8.06054	1.83858	3.29689
O	5.32157	1.76889	3.39308
O	2.65423	1.86879	3.60464
O	7.72468	1.91576	-1.06078
O	4.979	1.82445	-0.91819
O	2.37831	1.41797	-0.97876
Si	6.68115	2.74066	3.71723
Si	6.13358	5.02981	1.32331
Si	5.96208	4.22844	-4.31647
Si	6.33569	2.86158	-1.24047
Si	1.78222	3.27711	4.03981
Si	2.76029	5.1105	1.4118
Si	1.86671	8.10861	0.19186

Si	1.93623	7.78547	-3.17322	H	2.14625	3.6855	5.36958
Si	2.6036	4.61971	-4.16892	H	6.74634	3.16422	5.08748
Si	3.87724	0.80806	-0.34482	H	-8.77273	-2.09081	5.15017
Si	3.91081	0.92208	2.98931	H	-4.33941	-2.40976	5.47786
Si	8.97525	0.82198	-0.70238	H	4.11537	-2.49959	5.40271
Si	9.16936	0.7018	2.69157	H	8.57196	-2.61044	5.12226
O	6.22601	-6.43565	-1.06757	H	10.50251	0.9672	3.15942
O	1.66949	-6.89446	-0.35503	H	10.20041	-4.64636	1.25735
Si	6.33913	-6.38593	0.63564	H	10.20766	1.19875	-1.33384
Si	6.18221	-6.42366	-2.77021	H	9.93574	-4.74652	-3.83488
Si	1.46958	-6.54057	1.30287	H	-10.3733	1.59499	3.15138
Si	1.46742	-6.90451	-2.04711	H	-10.2995	1.56822	-1.32333
O	2.25835	-5.5517	-2.72688	H	-10.2317	-4.30638	-3.7705
O	4.83809	-5.51659	-3.28777	H	-10.4843	-4.11088	1.3067
O	7.53237	-5.57693	-3.3775	Al	1.71335	3.19139	-1.20246
O	2.44608	-5.16851	1.58572	H	-6.64651	-7.53028	-3.16412
O	5.08679	-5.41202	1.24407	H	-6.82137	-7.39548	1.2915
O	7.77839	-5.56029	1.02903	H	-2.46934	-8.02788	-2.59719
O	3.77654	-3.17277	-2.46474	H	2.02245	-8.10545	-2.61456
O	3.93876	-0.6863	-0.94692	H	1.90734	-7.62955	2.13499
O	3.77771	0.82729	1.26193	H	-2.32443	-7.55946	2.12123
O	4.05423	-0.64753	3.59532	H	6.16614	-7.76494	-3.28418
O	4.10884	-3.35488	2.94773	H	6.3272	-7.71286	1.18311
O	3.98274	-3.17044	0.24409	H	8.2205	-3.8674	-5.2228
O	8.2811	-3.04183	-2.76688	H	3.11982	-4.16093	-4.76641
O	8.43794	-0.71031	-1.2044	H	-3.49041	-4.06918	-4.77831
O	9.14136	0.75407	0.99096	H	-8.46749	-3.53696	-5.14971
O	8.61267	-0.79592	3.27456	H	6.45107	3.36769	-5.37117
O	8.41478	-3.40883	2.66511	H	1.86454	4.22952	-5.33542
O	8.4589	-3.18759	-0.0581	H	-1.41222	3.88232	-5.10218
O	6.11998	-2.25387	-1.26093	H	-5.96259	3.54264	-5.49988
O	6.29722	-2.17366	4.02227	H	-6.03118	5.72483	-4.57284
Si	3.43948	-4.5472	-3.42389	H	-6.3588	6.52845	1.18712
Si	4.4332	-2.33527	-1.15043	H	6.62138	5.51489	-4.37162
Si	4.59407	-2.19006	4.08628	H	6.86609	6.26139	1.28056
Si	3.87076	-4.25906	1.53728	H	2.63585	8.84256	-3.85034
Si	8.55916	-4.30469	-3.88631	H	2.5831	9.23919	0.7128
Si	7.81236	-2.27467	-1.32919	H	-2.294	9.01765	0.71311
Si	7.98775	-2.26944	3.85314	H	-2.19387	8.55397	-4.04293
Si	8.82599	-4.23256	1.23161	P	-1.49689	2.8532	-1.18477
H	-6.55964	3.57228	5.0144	Al	-3.80822	0.88439	-0.41854
H	-1.94303	3.86877	5.22229	H	-3.21805	-0.74932	-1.75567

Table A3 Coordinates of 52T cluster for the P-H^2-ZSM-5, in Å

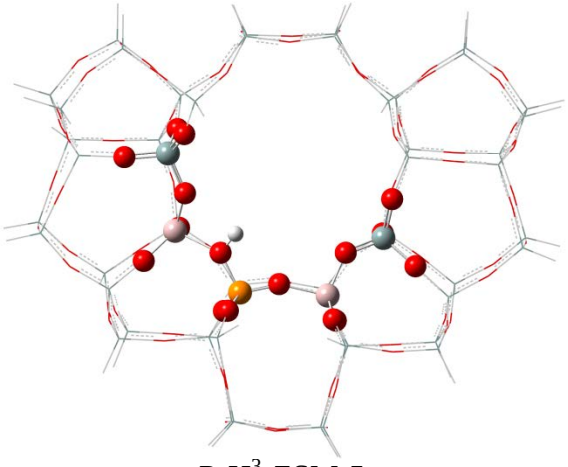


P-H^2-ZSM-5

Atoms	X	Y	Z
Si	-1.92537	7.91453	0.13582
Si	-1.89442	7.61343	-3.21268
O	-3.81458	-3.11318	-2.38521
O	-3.75418	-0.76692	-1.10709
O	-3.93454	0.77064	1.41034
O	-4.11346	-0.70586	3.79688
O	-4.16101	-3.3714	3.0064
O	-4.03228	-3.04888	0.26517
O	-8.1912	-2.94282	-2.78628
O	-8.49493	-0.67508	-1.19261
O	-9.23197	0.76482	1.01252
O	-8.64782	-0.80293	3.27619
O	-8.46479	-3.41478	2.63182
O	-8.40862	-3.14429	-0.08855
O	-6.04184	-2.12484	-1.23064
O	-6.37961	-2.23774	4.08593
O	-2.2266	-5.45422	-2.76193
O	-4.79867	-5.46268	-3.33936
O	-7.49318	-5.48887	-3.42344
O	-2.45385	-5.0753	1.57099
O	-5.07415	-5.3698	1.2142
O	-7.7645	-5.53757	0.97425
Si	-3.43075	-4.44214	-3.41975
Si	-4.40667	-2.26358	-1.11817
Si	-3.95968	0.83451	3.11089
Si	-4.67721	-2.26353	4.18977
Si	-3.8973	-4.18435	1.54721
Si	-8.48319	-4.1838	-3.92319
Si	-7.75649	-2.18973	-1.32805
Si	-9.16292	0.80368	-0.68999
Si	-9.18747	0.70799	2.71258
Si	-8.06225	-2.29636	3.84801
Si	-8.81712	-4.21175	1.16745
O	-8.05102	1.82896	3.29673
O	-5.3048	1.76141	3.60215
O	-2.63141	1.74953	3.66402
O	-8.05661	2.0103	-1.15802
O	-5.2842	1.80529	-0.91463
O	-2.40243	1.47358	-1.03279
Si	-6.3137	-6.34466	0.58397
Si	-6.1524	-6.35517	-2.82183
Si	-1.49515	-6.4549	1.28068
Si	-1.48037	-6.82346	-2.0709
O	-6.55122	4.01356	2.6403
O	-6.38516	3.50415	-2.83504
O	-6.56645	4.10628	-0.14916
O	-2.20707	4.21192	2.70512
O	-2.20046	6.35471	0.78145
O	-2.19962	7.78682	-1.54604
O	-2.21437	5.98398	-3.64992
O	-2.13493	3.5098	-2.53115
O	-2.2473	3.75536	-0.02636
O	-4.45515	5.01422	1.26808
O	-4.19596	4.22695	-4.29554
Si	-6.68596	2.73134	3.76212
Si	-6.16701	4.94363	1.27236
Si	-5.91554	4.13734	-4.33765
Si	-6.58479	2.83896	-1.28588
Si	-1.74984	3.16509	3.99513
Si	-2.78537	4.86146	1.27752
Si	-2.53866	4.38005	-4.03929
O	-0.06751	2.99235	3.92704
O	-0.19575	2.62891	-1.13347
O	-0.28466	8.29207	0.31866
O	-0.23503	7.87487	-3.42359
O	-6.19334	-6.38918	-1.11934
O	-1.67943	-6.80832	-0.37879
O	0.17735	-6.22559	1.50456
O	0.20303	-6.80746	-2.32039
O	6.30446	4.37171	2.61813
O	6.03231	3.74547	-2.81047
O	6.13799	4.3281	-0.12289
O	1.95206	4.4916	2.82197
O	1.82598	6.70348	0.98644
O	1.66467	7.97715	-1.51523
O	1.92874	6.30228	-3.81862
O	1.83966	3.79001	-2.78339
O	1.95968	4.10493	0.0907
O	4.12589	5.39385	1.37506
O	3.9584	4.57671	-4.44912
O	7.91653	2.25046	3.2752
O	5.17764	1.99366	3.35683
O	2.53378	1.91884	3.54734
O	7.67125	2.28078	-1.11947
O	4.92366	1.94858	-0.93714
O	2.30164	1.44468	-1.05024
Si	6.46823	3.04959	3.67843
Si	5.81564	5.27292	1.25466
Si	5.65744	4.47795	-4.30486
Si	6.17709	3.07234	-1.26388
Si	1.61812	3.28755	3.97868

Si	2.44456	5.15187	1.33044	H	-2.12999	3.74211	5.25594
Si	1.41536	8.12554	0.16851	H	1.93831	3.72365	5.31201
Si	1.46775	7.80614	-3.20122	H	6.50184	3.48175	5.04878
Si	2.27607	4.65889	-4.17532	H	-8.70216	-2.64488	5.08872
Si	3.72101	0.93741	-0.45116	H	-4.23892	-2.65238	5.49998
Si	3.84341	1.04479	2.89872	H	4.26029	-2.32698	5.39238
Si	8.9612	1.25606	-0.71651	H	8.71946	-2.11118	5.16618
Si	9.10667	1.19319	2.68201	H	10.41192	1.55835	3.16511
O	6.69312	-6.22488	-0.96615	H	10.50791	-4.11028	1.35138
O	2.04691	-6.85311	-0.34803	H	10.18817	1.68923	-1.32534
Si	6.78358	-6.11134	0.73577	H	10.32383	-4.34004	-3.70795
Si	6.66729	-6.21743	-2.66852	H	-10.5	0.9976	3.22596
Si	1.85397	-6.47111	1.30421	H	-10.4606	1.04335	-1.25509
Si	1.88406	-6.87358	-2.04381	H	-9.86956	-4.59797	-3.89725
O	2.6634	-5.53161	-2.74125	H	-10.1908	-4.63005	1.14096
O	5.26395	-5.42581	-3.21608	Al	1.62919	3.04034	-1.23313
O	7.96491	-5.29206	-3.27378	H	-6.15305	-7.6921	-3.34874
O	2.79425	-5.08375	1.58682	H	-6.29374	-7.67681	1.12006
O	5.44524	-5.2357	1.30826	H	-2.04981	-8.01891	-2.63609
O	8.15493	-5.17516	1.11923	H	2.42166	-8.09237	-2.58926
O	4.07723	-3.09483	-2.46835	H	2.27313	-7.55598	2.15116
O	4.03189	-0.57636	-0.98652	H	-1.93591	-7.54805	2.10657
O	3.72039	0.92227	1.19515	H	6.74768	-7.56263	-3.16967
O	4.07876	-0.48948	3.5816	H	6.86561	-7.42286	1.31635
O	4.34485	-3.19389	2.95132	H	8.59031	-3.58818	-5.1398
O	4.25885	-3.0679	0.21959	H	3.5483	-4.17207	-4.77019
O	8.56905	-2.69725	-2.70408	H	-3.10396	-4.00087	-4.74361
O	8.55199	-0.3237	-1.19862	H	-8.12306	-3.73869	-5.25201
O	9.10738	1.22103	0.98235	H	6.17506	3.6738	-5.39182
O	8.6604	-0.33454	3.28592	H	1.56332	4.26181	-5.35937
O	8.63938	-2.96902	2.72948	H	-1.76046	3.80912	-5.09169
O	8.69789	-2.77499	-0.00129	H	-6.29614	3.26418	-5.42429
O	6.32913	-2.03596	-1.26993	H	-6.44971	5.46606	-4.53436
O	6.43044	-1.85551	4.04588	H	-6.75638	6.25001	1.32543
Si	3.84498	-4.49467	-3.40424	H	6.2343	5.80529	-4.36025
Si	4.63993	-2.16506	-1.16203	H	6.46745	6.55096	1.20811
Si	4.72976	-1.98	4.08012	H	2.11729	8.88542	-3.89299
Si	4.18616	-4.11284	1.54003	H	2.08299	9.28412	0.69181
Si	8.92683	-3.96929	-3.7849	H	-2.78681	8.88713	0.74466
Si	8.013	-1.92154	-1.29762	H	-2.71269	8.48668	-4.00489
Si	8.12354	-1.83266	3.88608	P	-1.66169	2.94974	-1.18056
Si	9.11157	-3.77618	1.30548	Al	-4.10464	0.7254	-0.29712
H	-6.84242	3.24671	5.09403	H	-0.19084	1.6867	-0.94958

Table A4 Coordinates of 52T cluster for the P-H^3-ZSM-5, in Å



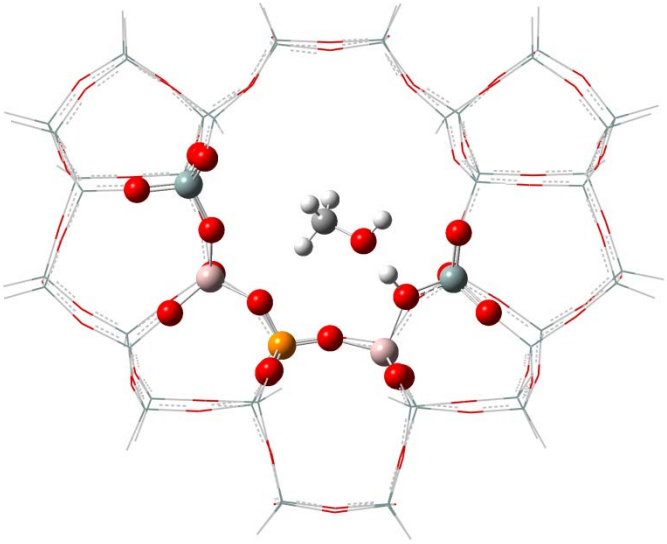
P-H^3-ZSM-5

Atoms	X	Y	Z
Si	-1.36439	8.05668	0.13357
Si	-1.3159	7.73689	-3.21579
O	-4.02243	-3.12215	-2.50804
O	-4.04765	-0.60243	-0.96881
O	-3.67285	1.08939	1.33929
O	-4.02327	-0.44682	3.68755
O	-4.33885	-3.13839	2.92175
O	-4.23899	-3.1349	0.15829
O	-8.58414	-2.65901	-2.71751
O	-8.46464	-0.27332	-1.24648
O	-9.04177	1.29205	0.92621
O	-8.60605	-0.23097	3.25759
O	-8.64514	-2.86739	2.72195
O	-8.6741	-2.68574	-0.01387
O	-6.29272	-2.10073	-1.34705
O	-6.40736	-1.79364	4.0329
O	-2.70069	-5.6209	-2.71634
O	-5.29387	-5.4567	-3.19083
O	-7.99925	-5.27433	-3.25283
O	-2.84744	-5.11351	1.62501
O	-5.49586	-5.2045	1.35262
O	-8.20566	-5.09455	1.13031
Si	-3.85567	-4.55775	-3.39558
Si	-4.59216	-2.1772	-1.20441
Si	-3.77929	1.09873	3.02222
Si	-4.70883	-1.95134	4.08422
Si	-4.21133	-4.09739	1.53306
Si	-8.94485	-3.94463	-3.77881
Si	-7.9609	-1.88687	-1.33307
Si	-8.94719	1.28856	-0.77816
Si	-9.0238	1.29234	2.62545
Si	-8.09817	-1.7356	3.86825
Si	-9.12367	-3.66644	1.29459
O	-7.82231	2.34051	3.21446
O	-5.07973	2.08175	3.53872
O	-2.43153	1.94523	3.66594
O	-7.75521	2.40813	-1.24003
O	-4.97167	2.16263	-0.97734
O	-2.17073	1.58263	-1.08613
Si	-6.84538	-6.05689	0.77234
Si	-6.71486	-6.20618	-2.62944
Si	-1.95368	-6.52952	1.35753
Si	-1.96962	-6.96946	-1.98828
O	-6.17306	4.42553	2.59387
O	-6.05273	3.9042	-2.87314
O	-6.22896	4.4769	-0.19821
O	-1.8612	4.39677	2.66618
O	-1.70639	6.51556	0.77061
O	-1.60795	7.97395	-1.55498
O	-1.68714	6.12483	-3.63996
O	-1.78661	3.62033	-2.55647
O	-1.88286	3.90443	-0.06698
O	-4.04087	5.30371	1.18312
O	-3.8001	4.54322	-4.30449
Si	-6.39595	3.13632	3.6931
Si	-5.75511	5.30689	1.20133
Si	-5.52223	4.55658	-4.34322
Si	-6.25497	3.2002	-1.3341
Si	-1.52553	3.34177	3.97744
Si	-2.38407	5.03072	1.20001
Si	-2.13784	4.53884	-4.02252
O	0.16265	3.09456	3.96353
O	0.06971	2.67867	-1.13555
O	0.29921	8.35134	0.33653
O	0.36353	7.93213	-3.40867
O	-6.74466	-6.20271	-0.92722
O	-2.12923	-6.9285	-0.29279
O	-0.2682	-6.32764	1.56629
O	-0.28179	-6.94293	-2.2538
O	6.66191	3.99438	2.63016
O	6.30044	3.43082	-2.81406
O	6.42365	4.01463	-0.09904
O	2.31533	4.44932	2.87928
O	2.36142	6.68969	1.03678
O	2.26284	7.9376	-1.47612
O	2.48569	6.29144	-3.79348
O	2.20308	3.80678	-2.75722
O	2.31024	4.09106	0.14609
O	4.54186	5.18688	1.44798
O	4.3321	4.38083	-4.46409
O	8.09114	1.7443	3.27201
O	5.3513	1.72151	3.37261
O	2.68791	1.86662	3.59979
O	7.73843	1.82045	-1.08315
O	4.99158	1.77596	-0.93429
O	2.38648	1.4225	-0.98772
Si	6.7281	2.66922	3.69581
Si	6.21494	4.96606	1.30275
Si	6.01823	4.17575	-4.32962
Si	6.36564	2.78974	-1.25895
Si	1.84636	3.29184	4.04066

Si	2.84485	5.106	1.40653	H	-1.86951	3.95838	5.23056
Si	1.98408	8.11932	0.20096	H	2.22676	3.6924	5.36812
Si	2.05137	7.80777	-3.16523	H	6.80271	3.09035	5.0663
Si	2.6691	4.63591	-4.17488	H	-8.70191	-1.98923	5.15049
Si	3.8734	0.77995	-0.35639	H	-4.26724	-2.36857	5.38714
Si	3.92432	0.8981	2.97737	H	4.08446	-2.51827	5.39991
Si	8.97123	0.70559	-0.72822	H	8.53657	-2.71052	5.10214
Si	9.18036	0.58975	2.66487	H	10.5193	0.83559	3.12671
O	6.11124	-6.50239	-1.0754	H	10.11862	-4.76672	1.22697
O	1.60351	-6.94115	-0.30584	H	10.20681	1.05793	-1.36748
Si	6.22898	-6.45191	0.62751	H	9.81934	-4.85731	-3.87785
Si	6.0577	-6.49363	-2.77776	H	-10.3211	1.69106	3.10632
Si	1.39799	-6.57432	1.34864	H	-10.2174	1.63606	-1.35498
Si	1.3962	-6.96565	-1.99702	H	-10.3457	-4.30302	-3.70396
O	2.15129	-5.59611	-2.68676	H	-10.529	-3.96406	1.33363
O	4.71749	-5.5743	-3.28449	Al	1.76278	3.2121	-1.21176
O	7.41106	-5.66147	-3.39758	H	-6.81705	-7.55697	-3.1141
O	2.36531	-5.19088	1.61321	H	-6.95755	-7.36012	1.3682
O	4.99521	-5.45535	1.23717	H	-2.51841	-8.19001	-2.51827
O	7.68339	-5.65031	1.01484	H	1.97892	-8.15538	-2.56039
O	3.68621	-3.21705	-2.45165	H	1.84692	-7.64962	2.1926
O	3.90205	-0.71739	-0.95479	H	-2.39275	-7.60179	2.21042
O	3.77849	0.80252	1.25076	H	6.02545	-7.83527	-3.28987
O	4.04664	-0.67209	3.58636	H	6.1964	-7.77741	1.17751
O	4.05497	-3.38295	2.94843	H	8.10023	-3.95611	-5.24678
O	3.90687	-3.20051	0.24975	H	2.98599	-4.20451	-4.73735
O	8.19282	-3.13852	-2.78892	H	-3.546	-4.29339	-4.77249
O	8.39981	-0.81594	-1.22452	H	-8.60451	-3.58884	-5.14033
O	9.14596	0.63851	0.9642	H	6.48745	3.3088	-5.38815
O	8.60264	-0.89795	3.25283	H	1.92005	4.26392	-5.34105
O	8.35775	-3.5061	2.64536	H	-1.39794	3.97752	-5.11095
O	8.3849	-3.28919	-0.0789	H	-5.95154	3.75933	-5.47095
O	6.05247	-2.32113	-1.26935	H	-5.96592	5.9247	-4.5022
O	6.26607	-2.23404	4.00978	H	-6.27165	6.64562	1.25006
Si	3.32516	-4.59326	-3.40028	H	6.70417	5.44833	-4.38069
Si	4.36514	-2.37726	-1.14968	H	6.97076	6.18312	1.25223
Si	4.56315	-2.22168	4.08051	H	2.76808	8.85525	-3.83935
Si	3.79473	-4.28932	1.54333	H	2.71301	9.24	0.72581
Si	8.44725	-4.40048	-3.9148	H	-2.1598	9.08714	0.7373
Si	7.74423	-2.36806	-1.34678	H	-2.06429	8.65407	-4.02795
Si	7.95407	-2.35981	3.83493	P	-1.45638	2.92954	-1.19672
Si	8.74925	-4.33615	1.21002	Al	-3.78516	1.01846	-0.40619
H	-6.52839	3.64665	5.03115	H	-1.65686	0.86234	-1.45858

APPENDIX B

Table B1 Coordinates of MeOH/H^{1}Z on P-H^1-ZSM-5, in Å

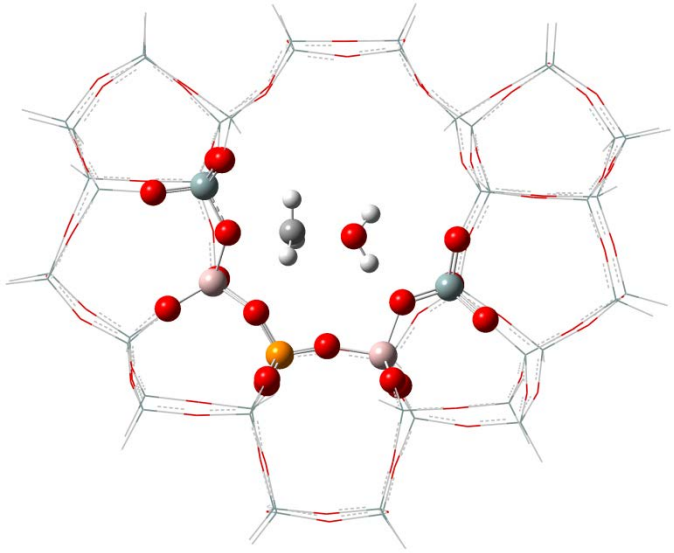


MeOH/H^{1}Z

Atoms	X	Y	Z
Si	–1.62154	8.00576	0.14047
Si	–1.59384	7.68618	–3.21371
O	–4.02775	–3.1062	–2.37582
O	–3.82624	–0.74173	–1.15195
O	–3.79695	0.84773	1.31501
O	–4.07076	–0.57778	3.74432
O	–4.26959	–3.25952	3.03619
O	–4.19381	–2.99005	0.26864
O	–8.40516	–2.77194	–2.68445
O	–8.57469	–0.4454	–1.15121
O	–9.19035	1.06536	1.0417
O	–8.64971	–0.48978	3.33135
O	–8.57489	–3.11929	2.74111
O	–8.56506	–2.89666	0.00948
O	–6.18559	–2.0205	–1.20722
O	–6.41346	–1.99651	4.12512
O	–2.50563	–5.47285	–2.77039
O	–5.10812	–5.46838	–3.24096
O	–7.80803	–5.36392	–3.27468
O	–2.65881	–5.02667	1.57855
O	–5.28843	–5.26218	1.30612
O	–7.99864	–5.29551	1.11565
Si	–3.73719	–4.46071	–3.39446
Si	–4.55018	–2.18134	–1.11568
Si	–3.86996	0.93701	2.99885
Si	–4.71079	–2.08593	4.19033
Si	–4.08117	–4.08926	1.57571
Si	–8.76096	–4.03065	–3.77839
Si	–7.89841	–1.98919	–1.2613
Si	–9.11564	1.09094	–0.66278
Si	–9.12545	1.03399	2.7401
Si	–8.10133	–1.98852	3.9209
Si	–8.98935	–3.91843	1.29455
O	–7.93786	2.10954	3.30444
O	–5.18523	1.90327	3.5089
O	–2.53862	1.82926	3.61176
O	–7.94063	2.21596	–1.14789
O	–5.15451	1.89961	–0.96937
O	–2.30952	1.56548	–1.07519
Si	–6.59499	–6.17945	0.72665
Si	–6.49708	–6.27617	–2.67864
Si	–1.74289	–6.42658	1.28846
Si	–1.74898	–6.82082	–2.06375
O	–6.35109	4.22534	2.60862
O	–6.24607	3.64922	–2.85098
O	–6.36811	4.25139	–0.17968
O	–2.04388	4.33545	2.71987
O	–1.9455	6.48148	0.82765
O	–1.87565	7.8851	–1.54465
O	–1.96346	6.08862	–3.68809
O	–1.95103	3.64789	–2.49207
O	–2.04665	3.8605	–0.0039
O	–4.2406	5.18506	1.22865
O	–4.00968	4.38751	–4.27101
Si	–6.50902	2.93765	3.71939
Si	–5.95215	5.11643	1.21571
Si	–5.72935	4.31961	–4.31919
Si	–6.42243	2.96369	–1.30118
Si	–1.67521	3.23812	3.98693
Si	–2.57376	4.97624	1.25849
Si	–2.34645	4.4695	–4.00042
O	0.01887	3.04376	3.97363
O	–0.08156	2.68583	–1.10014
O	0.04001	8.31849	0.32835
O	0.08284	7.89263	–3.41326
O	–6.50497	–6.29086	–0.976
O	–1.91242	–6.7985	–0.36853
O	–0.05937	–6.21693	1.5004
O	–0.06049	–6.77233	–2.32279
O	6.49361	4.17777	2.66898
O	6.18035	3.5889	–2.7809
O	6.30136	4.18162	–0.06772
O	2.13829	4.45145	2.87404
O	2.11442	6.65962	1.00521
O	1.99521	7.91516	–1.4978
O	2.22081	6.25904	–3.80153
O	2.04126	3.76031	–2.74623
O	2.17126	4.03324	0.15285
O	4.3453	5.26472	1.44508

O	4.15392	4.43059	–4.43475	Si	8.03381	–2.09911	3.90595
O	7.99541	1.98918	3.33677	Si	8.94516	–4.06569	1.31141
O	5.25406	1.8549	3.38916	H	–6.59953	3.44731	5.06108
O	2.58854	1.89307	3.61971	H	–2.04701	3.79048	5.26199
O	7.68457	2.03243	–1.0505	H	2.05856	3.71604	5.36995
O	4.93872	1.89345	–0.90288	H	6.62208	3.27616	5.10818
O	2.32707	1.38649	–1.01825	H	–8.72503	–2.29053	5.18289
Si	6.58635	2.85537	3.73583	H	–4.26571	–2.46918	5.50158
Si	6.02864	5.12415	1.32885	H	4.15975	–2.39865	5.43667
Si	5.84724	4.30793	–4.29902	H	8.61768	–2.41922	5.18072
Si	6.27492	2.95183	–1.22453	H	10.46691	1.20132	3.20482
Si	1.69714	3.29286	4.04372	H	10.32618	–4.45439	1.36331
Si	2.65455	5.09688	1.39004	H	10.20126	1.42781	–1.28066
Si	1.7254	8.09142	0.1806	H	10.10776	–4.62046	–3.73693
Si	1.77287	7.7747	–3.18438	H	–10.42	1.38386	3.26421
Si	2.47641	4.6072	–4.16007	H	–10.4024	1.40635	–1.21871
Si	3.82415	0.868	–0.35552	H	–10.1591	–4.40096	–3.71685
Si	3.85956	0.9812	2.98044	H	–10.3782	–4.28661	1.30425
Si	8.97732	1.00062	–0.66453	Al	1.63799	3.1253	–1.19854
Si	9.14439	0.8939	2.73232	H	–6.56387	–7.62171	–3.18177
O	6.40444	–6.33781	–0.99474	H	–6.62838	–7.4965	1.3008
O	1.81534	–6.82778	–0.36542	H	–2.27918	–8.04249	–2.60985
Si	6.51421	–6.28357	0.70922	H	2.17534	–8.03361	–2.62954
Si	6.36284	–6.32145	–2.69659	H	2.03489	–7.57904	2.12136
Si	1.60655	–6.48321	1.29377	H	–2.17371	–7.51819	2.12107
Si	1.61605	–6.83727	–2.05728	H	6.35488	–7.66098	–3.21522
O	2.40044	–5.47683	–2.73059	H	6.53826	–7.61027	1.25684
O	5.00834	–5.4264	–3.21186	H	8.4032	–3.76495	–5.15375
O	7.70297	–5.46027	–3.30324	H	3.31726	–4.0787	–4.73142
O	2.5776	–5.11158	1.59078	H	–3.44547	–4.08103	–4.74642
O	5.22722	–5.34979	1.3087	H	–8.41608	–3.64095	–5.12902
O	7.92722	–5.41619	1.10381	H	6.3571	3.45778	–5.35301
O	3.87482	–3.09021	–2.40904	H	1.75926	4.20125	–5.33545
O	3.99256	–0.63493	–0.94051	H	–1.5935	3.89633	–5.07354
O	3.72376	0.8859	1.25553	H	–6.1159	3.49702	–5.44431
O	4.05102	–0.58302	3.59227	H	–6.23835	5.66368	–4.48792
O	4.19891	–3.29766	2.99897	H	–6.52896	6.43072	1.24593
O	4.13855	–3.10886	0.29432	H	6.47064	5.612	–4.36294
O	8.4288	–2.91513	–2.7057	H	6.73119	6.37316	1.28885
O	8.53033	–0.56398	–1.16076	H	2.47404	8.82575	–3.86982
O	9.1229	0.94299	1.03138	H	2.44967	9.21629	0.70338
O	8.63453	–0.62102	3.3154	H	–2.42452	9.04174	0.72518
O	8.49079	–3.24104	2.73052	H	–2.35137	8.62279	–3.99533
O	8.58252	–3.04117	0.00412	P	–1.60053	2.91963	–1.15515
O	6.24543	–2.15686	–1.22861	Al	–3.87332	0.8493	–0.43237
O	6.34085	–2.0368	4.06537	H	1.551	–1.17389	–2.48255
Si	3.6063	–4.4706	–3.38288	H	–0.74503	–1.65685	–2.57673
Si	4.56365	–2.25991	–1.09916	C	–0.30474	–1.10701	–1.74224
Si	4.63797	–2.09457	4.1187	H	–0.14269	–1.77567	–0.8925
Si	4.0034	–4.20064	1.58263	H	–0.9795	–0.30345	–1.45683
Si	8.72983	–4.18618	–3.80916	O	0.94236	–0.49546	–2.1613
Si	7.93966	–2.14122	–1.27797	H	1.74645	0.64616	–1.39956

Table B2 Coordinates of TS1 on P–H[1]–ZSM–5, in Å

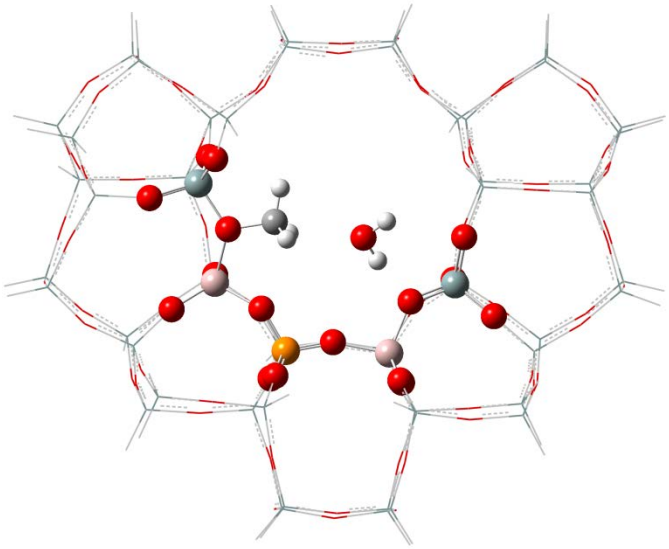


TS1

Atoms	X	Y	Z
Si	–1.59936	8.02397	0.16232
Si	–1.58022	7.69471	–3.18849
O	–4.02384	–3.10561	–2.36854
O	–3.82428	–0.74167	–1.14029
O	–3.80242	0.85381	1.32473
O	–4.08383	–0.56976	3.75265
O	–4.28169	–3.25236	3.04344
O	–4.20259	–2.98926	0.27556
O	–8.40573	–2.77	–2.69058
O	–8.57116	–0.43872	–1.1648
O	–9.18382	1.08122	1.02271
O	–8.65666	–0.4733	3.31548
O	–8.58819	–3.10519	2.73421
O	–8.56939	–2.88689	0.00246
O	–6.18531	–2.01808	–1.2129
O	–6.4286	–1.98548	4.12295
O	–2.51268	–5.47876	–2.7598
O	–5.1128	–5.46464	–3.23499
O	–7.81255	–5.36427	–3.27301
O	–2.67322	–5.02619	1.58872
O	–5.30372	–5.25591	1.31687
O	–8.01299	–5.2858	1.11357
Si	–3.73829	–4.46152	–3.38668
Si	–4.55021	–2.18015	–1.11055
Si	–3.87887	0.94426	3.00753
Si	–4.72639	–2.07783	4.19535
Si	–4.09363	–4.08568	1.58495
Si	–8.76544	–4.03195	–3.77926
Si	–7.89813	–1.98428	–1.26947
Si	–9.10677	1.10119	–0.68185
Si	–9.12765	1.05087	2.72137
Si	–8.11567	–1.97193	3.91209
Si	–9.00036	–3.90562	1.28768
O	–7.9422	2.12594	3.29152
O	–5.19217	1.91497	3.51319
O	–2.54569	1.83616	3.61602
O	–7.92627	2.21946	–1.16854
O	–5.14025	1.90444	–0.97138
O	–2.29414	1.55905	–1.04833
Si	–6.60864	–6.17209	0.73202
Si	–6.50137	–6.2734	–2.67288
Si	–1.75838	–6.42729	1.30087
Si	–1.76045	–6.82789	–2.05083
O	–6.34649	4.23778	2.5989
O	–6.22992	3.65934	–2.85875
O	–6.35964	4.25425	–0.18877
O	–2.03745	4.33228	2.69657
O	–1.93403	6.49312	0.82852
O	–1.85763	7.91876	–1.52274
O	–1.95786	6.09077	–3.63405
O	–1.95655	3.59563	–2.52349
O	–2.04133	3.88154	–0.03542
O	–4.23266	5.19233	1.21554
O	–4.00251	4.40954	–4.27937
Si	–6.51447	2.95337	3.71203
Si	–5.94423	5.12373	1.2037
Si	–5.72188	4.34129	–4.32432
Si	–6.40722	2.9677	–1.31202
Si	–1.6747	3.24449	3.97328
Si	–2.56584	4.98449	1.23994
Si	–2.34076	4.48265	–3.99846
O	0.01832	3.04013	3.96058
O	–0.07385	2.69151	–1.11249
O	0.0645	8.32564	0.34686
O	0.0969	7.88989	–3.39739
O	–6.51192	–6.28501	–0.97019
O	–1.92547	–6.80225	–0.35574
O	–0.07473	–6.21894	1.51322
O	–0.07223	–6.78061	–2.31095
O	6.50743	4.16671	2.67453
O	6.19387	3.58409	–2.77515
O	6.3175	4.17457	–0.06132
O	2.14458	4.44469	2.8765
O	2.12906	6.65298	1.01101
O	2.01385	7.92033	–1.48647
O	2.23817	6.26267	–3.79245
O	2.05524	3.76074	–2.74815
O	2.18404	4.03028	0.15161
O	4.35701	5.25134	1.45377
O	4.17163	4.43324	–4.4301
O	8.00006	1.96973	3.33424
O	5.25775	1.84687	3.38948
O	2.59001	1.88628	3.62236
O	7.69161	2.02078	–1.04654
O	4.94327	1.89581	–0.89632

O	2.33355	1.38577	–1.01981	H	–2.04195	3.81162	5.24334
Si	6.59488	2.84059	3.73718	H	2.05024	3.70695	5.37205
Si	6.04059	5.11464	1.33612	H	6.63341	3.25748	5.11068
Si	5.8644	4.30474	–4.29307	H	–8.7454	–2.26771	5.17257
Si	6.28573	2.94561	–1.21931	H	–4.28684	–2.46162	5.50824
Si	1.6966	3.28573	4.0432	H	4.1563	–2.40985	5.43208
Si	2.66592	5.08876	1.39379	H	8.61358	–2.44068	5.17771
Si	1.74827	8.09052	0.19339	H	10.47046	1.17737	3.2056
Si	1.7884	7.7766	–3.17254	H	10.31471	–4.47967	1.35663
Si	2.49395	4.61208	–4.15781	H	10.20488	1.40355	–1.28357
Si	3.82754	0.86804	–0.35397	H	10.0874	–4.63505	–3.75397
Si	3.86139	0.97606	2.98115	H	–10.4244	1.40243	3.23878
Si	8.98015	0.98222	–0.6651	H	–10.3916	1.41983	–1.24045
Si	9.14799	0.87266	2.73114	H	–10.1638	–4.40086	–3.71349
O	6.38524	–6.34589	–1.00468	H	–10.3902	–4.27004	1.29386
O	1.79958	–6.83592	–0.35239	Al	1.6479	3.12536	–1.20189
Si	6.49564	–6.29291	0.69918	H	–6.56592	–7.62009	–3.17316
Si	6.34045	–6.32728	–2.70635	H	–6.6459	–7.48852	1.30729
Si	1.5907	–6.4877	1.30602	H	–2.2925	–8.04956	–2.59506
Si	1.60417	–6.84078	–2.04465	H	2.16854	–8.03351	–2.61949
O	2.38379	–5.47521	–2.71428	H	2.01853	–7.58173	2.13631
O	4.98576	–5.42975	–3.21684	H	–2.19121	–7.51725	2.13463
O	7.68121	–5.46797	–3.3141	H	6.32926	–7.66594	–3.2271
O	2.56379	–5.11646	1.5979	H	6.51585	–7.62	1.24591
O	5.21201	–5.35522	1.29978	H	8.38025	–3.76747	–5.16042
O	7.9117	–5.43058	1.09438	H	3.28605	–4.08358	–4.72778
O	3.86206	–3.08605	–2.41493	H	–3.44311	–4.0836	–4.73838
O	3.99614	–0.63562	–0.93871	H	–8.42321	–3.64724	–5.132
O	3.72412	0.88496	1.25656	H	6.37183	3.45323	–5.34717
O	4.05229	–0.58807	3.59349	H	1.77873	4.21244	–5.33652
O	4.19235	–3.2996	2.99057	H	–1.58223	3.94701	–5.08718
O	4.11712	–3.11818	0.28459	H	–6.11165	3.52743	–5.45468
O	8.41862	–2.92892	–2.70838	H	–6.23239	5.6863	–4.48105
O	8.52278	–0.5787	–1.16334	H	–6.51977	6.43876	1.22938
O	9.12914	0.92288	1.0303	H	6.49244	5.60666	–4.35627
O	8.6354	–0.64182	3.31284	H	6.74014	6.36542	1.29834
O	8.48455	–3.26213	2.72763	H	2.48528	8.82931	–3.85989
O	8.57589	–3.05434	0.00311	H	2.48019	9.20907	0.71923
O	6.23794	–2.17134	–1.2273	H	–2.39463	9.05837	0.75981
O	6.33822	–2.05063	4.06145	H	–2.33712	8.6221	–3.98149
Si	3.58467	–4.47128	–3.38015	P	–1.59465	2.91507	–1.1657
Si	4.55553	–2.26399	–1.10155	Al	–3.86651	0.84984	–0.42165
Si	4.63523	–2.10265	4.1151	H	1.58953	–1.17024	–2.51012
Si	3.98938	–4.20565	1.57745	H	–0.70882	–1.65868	–2.53092
Si	8.71073	–4.19575	–3.819	C	–0.25192	–1.06182	–1.73831
Si	7.9322	–2.1559	–1.27944	H	–0.07096	–1.682	–0.85491
Si	8.03103	–2.11855	3.90286	H	–0.91643	–0.23981	–1.485
Si	8.93532	–4.08516	1.30641	O	0.9871	–0.47425	–2.21562
H	–6.61225	3.46766	5.05146	H	1.77338	0.65131	–1.44647

Table B3 Coordinates of CH_3–Z/H_2O on P–H^1–ZSM–5, in Å

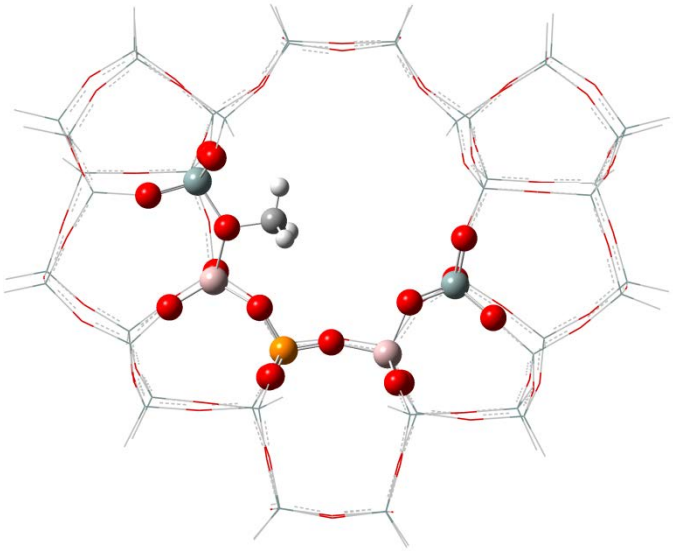


CH_3–Z/H_2O

Atoms	X	Y	Z
Si	–1.59936	8.02397	0.16232
Si	–1.58022	7.69471	–3.18849
O	–4.02384	–3.10561	–2.36854
O	–3.82428	–0.74167	–1.14029
O	–3.80242	0.85381	1.32473
O	–4.08383	–0.56976	3.75265
O	–4.28169	–3.25236	3.04344
O	–4.20259	–2.98926	0.27556
O	–8.40573	–2.77	–2.69058
O	–8.57116	–0.43872	–1.1648
O	–9.18382	1.08122	1.02271
O	–8.65666	–0.4733	3.31548
O	–8.58819	–3.10519	2.73421
O	–8.56939	–2.88689	0.00246
O	–6.18531	–2.01808	–1.2129
O	–6.4286	–1.98548	4.12295
O	–2.51268	–5.47876	–2.7598
O	–5.1128	–5.46464	–3.23499
O	–7.81255	–5.36427	–3.27301
O	–2.67322	–5.02619	1.58872
O	–5.30372	–5.25591	1.31687
O	–8.01299	–5.2858	1.11357
Si	–3.73829	–4.46152	–3.38668
Si	–4.55021	–2.18015	–1.11055
Si	–3.87887	0.94426	3.00753
Si	–4.72639	–2.07783	4.19535
Si	–4.09363	–4.08568	1.58495
Si	–8.76544	–4.03195	–3.77926
Si	–7.89813	–1.98428	–1.26947
Si	–9.10677	1.10119	–0.68185
Si	–9.12765	1.05087	2.72137
Si	–8.11567	–1.97193	3.91209
Si	–9.00036	–3.90562	1.28768
O	–7.9422	2.12594	3.29152
O	–5.19217	1.91497	3.51319
O	–2.54569	1.83616	3.61602
O	–7.92627	2.21946	–1.16854
O	–5.14025	1.90444	–0.97138
O	–2.29414	1.55905	–1.04833
Si	–6.60864	–6.17209	0.73202
Si	–6.50137	–6.2734	–2.67288
Si	–1.75838	–6.42729	1.30087
Si	–1.76045	–6.82789	–2.05083
O	–6.34649	4.23778	2.5989
O	–6.22992	3.65934	–2.85875
O	–6.35964	4.25425	–0.18877
O	–2.03745	4.33228	2.69657
O	–1.93403	6.49312	0.82852
O	–1.85763	7.91876	–1.52274
O	–1.95786	6.09077	–3.63405
O	–1.95655	3.59563	–2.52349
O	–2.04133	3.88154	–0.03542
O	–4.23266	5.19233	1.21554
O	–4.00251	4.40954	–4.27937
Si	–6.51447	2.95337	3.71203
Si	–5.94423	5.12373	1.2037
Si	–5.72188	4.34129	–4.32432
Si	–6.40722	2.9677	–1.31202
Si	–1.6747	3.24449	3.97328
Si	–2.56584	4.98449	1.23994
Si	–2.34076	4.48265	–3.99846
O	0.01832	3.04013	3.96058
O	–0.07385	2.69151	–1.11249
O	0.0645	8.32564	0.34686
O	0.0969	7.88989	–3.39739
O	–6.51192	–6.28501	–0.97019
O	–1.92547	–6.80225	–0.35574
O	–0.07473	–6.21894	1.51322
O	–0.07223	–6.78061	–2.31095
O	6.50743	4.16671	2.67453
O	6.19387	3.58409	–2.77515
O	6.3175	4.17457	–0.06132
O	2.14458	4.44469	2.8765
O	2.12906	6.65298	1.01101
O	2.01385	7.92033	–1.48647
O	2.23817	6.26267	–3.79245
O	2.05524	3.76074	–2.74815
O	2.18404	4.03028	0.15161
O	4.35701	5.25134	1.45377
O	4.17163	4.43324	–4.4301
O	8.00006	1.96973	3.33424
O	5.25775	1.84687	3.38948
O	2.59001	1.88628	3.62236
O	7.69161	2.02078	–1.04654
O	4.94327	1.89581	–0.89632

O	2.33355	1.38577	–1.01981	H	–2.04195	3.81162	5.24334
Si	6.59488	2.84059	3.73718	H	2.05024	3.70695	5.37205
Si	6.04059	5.11464	1.33612	H	6.63341	3.25748	5.11068
Si	5.8644	4.30474	–4.29307	H	–8.7454	–2.26771	5.17257
Si	6.28573	2.94561	–1.21931	H	–4.28684	–2.46162	5.50824
Si	1.6966	3.28573	4.0432	H	4.1563	–2.40985	5.43208
Si	2.66592	5.08876	1.39379	H	8.61358	–2.44068	5.17771
Si	1.74827	8.09052	0.19339	H	10.47046	1.17737	3.2056
Si	1.7884	7.7766	–3.17254	H	10.31471	–4.47967	1.35663
Si	2.49395	4.61208	–4.15781	H	10.20488	1.40355	–1.28357
Si	3.82754	0.86804	–0.35397	H	10.0874	–4.63505	–3.75397
Si	3.86139	0.97606	2.98115	H	–10.4244	1.40243	3.23878
Si	8.98015	0.98222	–0.6651	H	–10.3916	1.41983	–1.24045
Si	9.14799	0.87266	2.73114	H	–10.1638	–4.40086	–3.71349
O	6.38524	–6.34589	–1.00468	H	–10.3902	–4.27004	1.29386
O	1.79958	–6.83592	–0.35239	Al	1.6479	3.12536	–1.20189
Si	6.49564	–6.29291	0.69918	H	–6.56592	–7.62009	–3.17316
Si	6.34045	–6.32728	–2.70635	H	–6.6459	–7.48852	1.30729
Si	1.5907	–6.4877	1.30602	H	–2.2925	–8.04956	–2.59506
Si	1.60417	–6.84078	–2.04465	H	2.16854	–8.03351	–2.61949
O	2.38379	–5.47521	–2.71428	H	2.01853	–7.58173	2.13631
O	4.98576	–5.42975	–3.21684	H	–2.19121	–7.51725	2.13463
O	7.68121	–5.46797	–3.3141	H	6.32926	–7.66594	–3.2271
O	2.56379	–5.11646	1.5979	H	6.51585	–7.62	1.24591
O	5.21201	–5.35522	1.29978	H	8.38025	–3.76747	–5.16042
O	7.9117	–5.43058	1.09438	H	3.28605	–4.08358	–4.72778
O	3.86206	–3.08605	–2.41493	H	–3.44311	–4.0836	–4.73838
O	3.99614	–0.63562	–0.93871	H	–8.42321	–3.64724	–5.132
O	3.72412	0.88496	1.25656	H	6.37183	3.45323	–5.34717
O	4.05229	–0.58807	3.59349	H	1.77873	4.21244	–5.33652
O	4.19235	–3.2996	2.99057	H	–1.58223	3.94701	–5.08718
O	4.11712	–3.11818	0.28459	H	–6.11165	3.52743	–5.45468
O	8.41862	–2.92892	–2.70838	H	–6.23239	5.6863	–4.48105
O	8.52278	–0.5787	–1.16334	H	–6.51977	6.43876	1.22938
O	9.12914	0.92288	1.0303	H	6.49244	5.60666	–4.35627
O	8.6354	–0.64182	3.31284	H	6.74014	6.36542	1.29834
O	8.48455	–3.26213	2.72763	H	2.48528	8.82931	–3.85989
O	8.57589	–3.05434	0.00311	H	2.48019	9.20907	0.71923
O	6.23794	–2.17134	–1.2273	H	–2.39463	9.05837	0.75981
O	6.33822	–2.05063	4.06145	H	–2.33712	8.6221	–3.98149
Si	3.58467	–4.47128	–3.38015	P	–1.59465	2.91507	–1.1657
Si	4.55553	–2.26399	–1.10155	Al	–3.86651	0.84984	–0.42165
Si	4.63523	–2.10265	4.1151	H	1.58953	–1.17024	–2.51012
Si	3.98938	–4.20565	1.57745	H	–2.23021	–1.50452	–2.25196
Si	8.71073	–4.19575	–3.819	C	–2.3978	–0.86951	–1.37908
Si	7.9322	–2.1559	–1.27944	H	–1.94917	–1.48095	–0.59
Si	8.03103	–2.11855	3.90286	H	–1.92357	0.10236	–1.26946
Si	8.93532	–4.08516	1.30641	O	0.9871	–0.47425	–2.21562
H	–6.61225	3.46766	5.05146	H	1.46997	0.21698	–1.74327

Table B4 Coordinates of CH_3–Z on P–H^1–ZSM–5, in Å

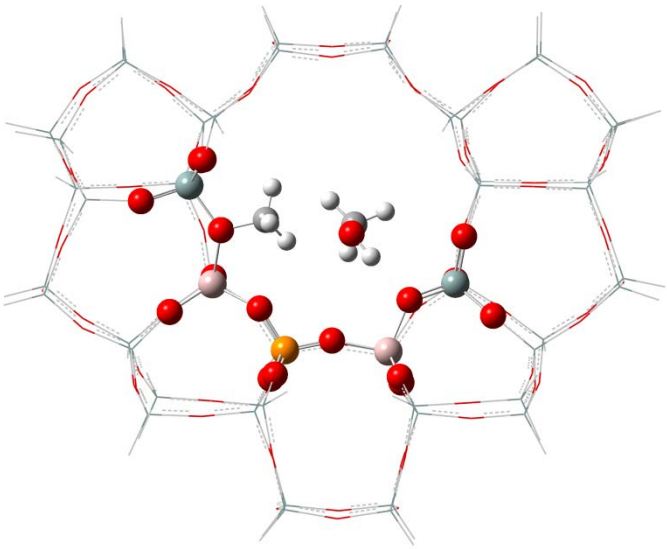


CH_3–Z

Atoms	X	Y	Z
Si	–1.78625	8.0662	0.25361
Si	–1.79549	7.77691	–3.098
O	–3.91328	–3.20273	–2.34806
O	–3.48211	–0.89456	–1.08609
O	–3.83847	0.7126	1.31501
O	–4.07252	–0.68325	3.72702
O	–4.20216	–3.36531	3.05545
O	–4.0472	–3.0931	0.31424
O	–8.05355	–2.78678	–2.71775
O	–8.53074	–0.55507	–1.12664
O	–9.25416	0.8938	1.06366
O	–8.64914	–0.67769	3.31716
O	–8.48218	–3.28281	2.68336
O	–8.27873	–3.00893	–0.02653
O	–5.96389	–1.90167	–1.15398
O	–6.37943	–2.14204	4.11282
O	–2.35115	–5.5284	–2.72777
O	–4.94122	–5.52638	–3.27475
O	–7.61004	–5.38788	–3.31924
O	–2.51708	–5.12185	1.62232
O	–5.15163	–5.36333	1.26803
O	–7.84097	–5.43531	1.04377
Si	–3.55797	–4.54111	–3.40266
Si	–4.4169	–2.34835	–1.06672
Si	–3.89895	0.84639	3.01058
Si	–4.67765	–2.19448	4.20518
Si	–3.94746	–4.21995	1.62764
Si	–8.47409	–4.00377	–3.84292
Si	–7.69658	–2.00598	–1.25662
Si	–9.19256	0.93883	–0.63686
Si	–9.17138	0.8465	2.76483
Si	–8.06659	–2.16551	3.90002
Si	–8.82179	–4.05026	1.20448
O	–7.99836	1.94058	3.31478
O	–5.25502	1.76905	3.47651
O	–2.59472	1.7735	3.5884
O	–8.04062	2.06512	–1.16647
O	–5.281	1.634	–1.01899
O	–2.44008	1.62798	–1.08124
Si	–6.42956	–6.31218	0.66911
Si	–6.33124	–6.35356	–2.73735
Si	–1.55758	–6.50272	1.31979
Si	–1.56824	–6.87934	–2.03119
O	–6.46044	4.0554	2.53126
O	–6.31147	3.41127	–2.91972
O	–6.40161	4.03854	–0.24026
O	–2.16646	4.28524	2.71688
O	–2.12161	6.52918	0.91798
O	–2.07757	7.95794	–1.42639
O	–2.18203	6.18158	–3.58134
O	–2.04397	3.6597	–2.5196
O	–2.13456	3.90932	–0.02521
O	–4.34986	5.07641	1.20689
O	–4.09894	4.35818	–4.25425
Si	–6.57868	2.80782	3.68652
Si	–6.04926	4.95496	1.14528
Si	–5.80125	4.18181	–4.35036
Si	–6.50727	2.76599	–1.3644
Si	–1.73197	3.1946	3.96832
Si	–2.66777	4.98006	1.27145
Si	–2.43931	4.56135	–3.98124
O	–0.04858	3.01116	3.95089
O	–0.18098	2.70349	–1.10652
O	–0.12959	8.38179	0.42799
O	–0.12668	7.98078	–3.32041
O	–6.32586	–6.37245	–1.03507
O	–1.76812	–6.84129	–0.3399
O	0.11208	–6.26643	1.52874
O	0.10869	–6.82822	–2.29529
O	6.37044	4.29639	2.65067
O	6.07656	3.70892	–2.78695
O	6.19142	4.2755	–0.08904
O	2.01814	4.48016	2.86702
O	1.93287	6.69953	1.04554
O	1.79774	8.02224	–1.4302
O	2.01451	6.35691	–3.74374
O	1.90606	3.82361	–2.73234
O	2.0299	4.08024	0.13764
O	4.20125	5.35107	1.42602
O	4.01487	4.61382	–4.40057
O	7.93199	2.14336	3.30966
O	5.18946	1.93297	3.37148
O	2.5384	1.896	3.5819
O	7.66537	2.2022	–1.0936
O	4.92028	1.92227	–0.92103
O	2.28283	1.43428	–1.04834

Si	6.49456	2.96768	3.70562	H	–6.65701	3.34156	5.01807
Si	5.88585	5.21638	1.29616	H	–2.14571	3.71148	5.24561
Si	5.7086	4.4813	–4.26542	H	1.95996	3.69367	5.35185
Si	6.19011	3.03175	–1.24199	H	6.52882	3.38667	5.08018
Si	1.63958	3.28071	4.0107	H	–8.69793	–2.51125	5.145
Si	2.51471	5.12988	1.36918	H	–4.23389	–2.56119	5.51916
Si	1.55936	8.14843	0.2564	H	4.21748	–2.35292	5.40602
Si	1.57342	7.86205	–3.11473	H	8.67526	–2.23232	5.1706
Si	2.33145	4.70908	–4.11237	H	10.42185	1.42863	3.17923
Si	3.70778	0.93325	–0.43579	H	10.43835	–4.23136	1.34762
Si	3.83162	1.01937	2.91134	H	10.18146	1.59599	–1.30529
Si	8.95058	1.17297	–0.69709	H	10.23026	–4.44037	–3.72356
Si	9.10961	1.08326	2.70039	H	–10.47	1.15234	3.30235
O	6.57924	–6.27553	–0.97905	H	–10.4928	1.175	–1.19449
O	1.95973	–6.87271	–0.34077	H	–9.89251	–4.28389	–3.80619
Si	6.6859	–6.17525	0.72315	H	–10.2137	–4.38612	1.10159
Si	6.54433	–6.25196	–2.68093	Al	1.59443	3.05978	–1.20012
Si	1.79246	–6.49625	1.3154	H	–6.41728	–7.68699	–3.26196
Si	1.79654	–6.87543	–2.0361	H	–6.44548	–7.63458	1.22544
O	2.55532	–5.51802	–2.72248	H	–2.13165	–8.08256	–2.5843
O	5.15002	–5.42862	–3.20774	H	2.33357	–8.08643	–2.59823
O	7.85414	–5.34892	–3.29055	H	2.21662	–7.58528	2.15382
O	2.72277	–5.10337	1.59121	H	–2.00426	–7.5932	2.14476
O	5.36241	–5.28447	1.30854	H	6.58894	–7.59427	–3.19419
O	8.0729	–5.26425	1.1064	H	6.74693	–7.49311	1.29198
O	3.98372	–3.08675	–2.43728	H	8.50648	–3.6452	–5.1454
O	3.98967	–0.58859	–0.98411	H	3.43297	–4.14576	–4.74153
O	3.70502	0.90407	1.20637	H	–3.25805	–4.09026	–4.72713
O	4.05352	–0.52624	3.57889	H	–8.06691	–3.61227	–5.17397
O	4.28681	–3.2371	2.97385	H	6.21405	3.68534	–5.36489
O	4.20983	–3.08734	0.24332	H	1.62695	4.33936	–5.31056
O	8.50746	–2.77328	–2.70165	H	–1.66949	4.08811	–5.08922
O	8.53273	–0.4044	–1.18601	H	–6.12014	3.36152	–5.49825
O	9.10278	1.1195	1.00092	H	–6.41834	5.48397	–4.47479
O	8.65277	–0.44586	3.29591	H	–6.69576	6.23554	1.13217
O	8.57879	–3.07552	2.73039	H	6.32107	5.79359	–4.29623
O	8.64534	–2.86703	–0.0002	H	6.56301	6.48145	1.25824
O	6.28659	–2.08565	–1.25514	H	2.24236	8.93191	–3.80494
O	6.39217	–1.92518	4.05194	H	2.27588	9.27139	0.79495
Si	3.74222	–4.47975	–3.38125	H	–2.59982	9.07753	0.86724
Si	4.59825	–2.18021	–1.13337	H	–2.57895	8.70777	–3.86172
Si	4.6897	–2.01577	4.09206	P	–1.67641	2.96417	–1.17197
Si	4.12486	–4.14152	1.55567	Al	–3.89241	0.84212	–0.39925
Si	8.84107	–4.04081	–3.79436	H	–1.65057	–0.63572	–2.09466
Si	7.97343	–1.99283	–1.28927	C	–2.00859	–1.12559	–1.1975
Si	8.0857	–1.93302	3.89224	H	–1.8267	–2.19597	–1.24539
Si	9.04697	–3.87754	1.30297	H	–1.53194	–0.70605	–0.31616

Table B5 Coordinates of CH_3–Z/MeOH on P–H^1–ZSM–5, in Å

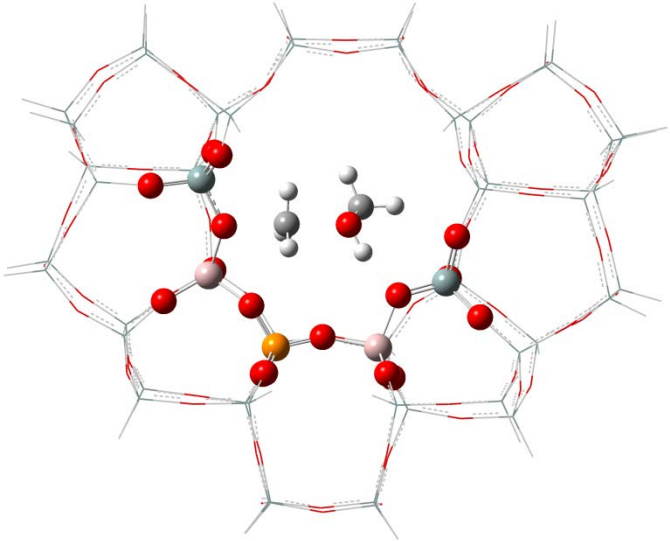


CH_3–Z/MeOH

Atoms	X	Y	Z
Si	–1.78767	8.07133	0.26864
Si	–1.79516	7.77267	–3.08251
O	–3.89021	–3.19857	–2.31893
O	–3.45959	–0.89908	–1.03983
O	–3.83629	0.7174	1.34095
O	–4.08509	–0.67724	3.74976
O	–4.22055	–3.36399	3.07972
O	–4.05577	–3.09901	0.34196
O	–8.03219	–2.77831	–2.71717
O	–8.52229	–0.55133	–1.12485
O	–9.25585	0.89783	1.06278
O	–8.66575	–0.67118	3.32085
O	–8.49268	–3.27322	2.68183
O	–8.26658	–3.00082	–0.02573
O	–5.94859	–1.89135	–1.14542
O	–6.39703	–2.13257	4.12321
O	–2.34178	–5.53313	–2.69823
O	–4.92853	–5.51592	–3.25094
O	–7.59661	–5.38107	–3.31419
O	–2.53567	–5.12964	1.65501
O	–5.16902	–5.36757	1.2929
O	–7.8554	–5.43027	1.04666
Si	–3.54006	–4.53746	–3.37498
Si	–4.40562	–2.34742	–1.04024
Si	–3.90918	0.85371	3.03596
Si	–4.69588	–2.18774	4.22428
Si	–3.96475	–4.22579	1.65631
Si	–8.45226	–3.99404	–3.844
Si	–7.6811	–1.99808	–1.25445
Si	–9.18661	0.94209	–0.63742
Si	–9.18378	0.85287	2.7645
Si	–8.08333	–2.15909	3.90345
Si	–8.82747	–4.03826	1.20059
O	–8.01234	1.94611	3.31959
O	–5.26947	1.7743	3.49321
O	–2.60902	1.78453	3.61715
O	–8.02837	2.06405	–1.16165
O	–5.26575	1.63382	–1.00427
O	–2.42197	1.62644	–1.04794
Si	–6.44452	–6.31173	0.68091
Si	–6.32078	–6.34638	–2.72489
Si	–1.57908	–6.51301	1.35205
Si	–1.57296	–6.89095	–1.99863
O	–6.47244	4.0591	2.53918
O	–6.29634	3.4035	–2.91231
O	–6.39766	4.03749	–0.23322
O	–2.18644	4.29643	2.73879
O	–2.12913	6.53784	0.93822
O	–2.07709	7.95638	–1.41125
O	–2.17638	6.17514	–3.5628
O	–2.04184	3.65646	–2.49443
O	–2.15187	3.91608	–0.00163
O	–4.36456	5.09293	1.22109
O	–4.08495	4.34693	–4.24699
Si	–6.59408	2.81348	3.69607
Si	–6.06262	4.95911	1.15314
Si	–5.78661	4.16734	–4.34663
Si	–6.49371	2.76274	–1.3555
Si	–1.7489	3.209	3.99183
Si	–2.68319	4.99151	1.29185
Si	–2.42803	4.55356	–3.9612
O	–0.06518	3.02991	3.97118
O	–0.17624	2.73423	–1.06332
O	–0.13088	8.38519	0.44405
O	–0.12696	7.98156	–3.30528
O	–6.32835	–6.369	–1.0226
O	–1.78468	–6.84896	–0.30874
O	0.08975	–6.27807	1.56554
O	0.10486	–6.85088	–2.25445
O	6.36476	4.29561	2.689
O	6.08132	3.71811	–2.74915
O	6.19373	4.27568	–0.05159
O	2.01137	4.49383	2.88807
O	1.93764	6.71104	1.06606
O	1.79649	8.0297	–1.41335
O	2.01751	6.36368	–3.72662
O	1.9069	3.83042	–2.71211
O	2.0427	4.09373	0.1594
O	4.20689	5.36315	1.45841
O	4.02468	4.62132	–4.36974
O	7.91225	2.13477	3.34721
O	5.16727	1.93614	3.39472
O	2.51543	1.90719	3.59822
O	7.66078	2.19776	–1.05723
O	4.91394	1.9282	–0.89544
O	2.28062	1.44279	–1.04377

Si	6.47612	2.96239	3.73993	H	6.50452	3.37633	5.11616
Si	5.8913	5.21855	1.33284	H	–8.71887	–2.50861	5.14518
Si	5.71856	4.49599	–4.22562	H	–4.25796	–2.5538	5.54043
Si	6.18936	3.03364	–1.20653	H	4.17553	–2.3453	5.42623
Si	1.62381	3.29536	4.02995	H	8.63254	–2.23869	5.21508
Si	2.52094	5.14269	1.39416	H	10.40177	1.41771	3.22271
Si	1.55882	8.15648	0.27341	H	10.40808	–4.23815	1.39289
Si	1.57321	7.8682	–3.09778	H	10.17232	1.575	–1.26284
Si	2.33993	4.71608	–4.08993	H	10.21803	–4.44128	–3.67522
Si	3.69985	0.93579	–0.4183	H	–10.485	1.16084	3.29424
Si	3.80769	1.02743	2.92948	H	–10.4838	1.1804	–1.20092
Si	8.93781	1.15949	–0.65666	H	–9.87201	–4.26805	–3.81435
Si	9.09029	1.07309	2.74122	H	–10.2208	–4.36447	1.08752
O	6.56	–6.28581	–0.93896	Al	1.59919	3.07368	–1.17471
O	1.94699	–6.88882	–0.29527	H	–6.4013	–7.67884	–3.25281
Si	6.65373	–6.17748	0.76328	H	–6.46868	–7.63513	1.23447
Si	6.53749	–6.27044	–2.64128	H	–2.14332	–8.08948	–2.55467
Si	1.77161	–6.50326	1.35794	H	2.32926	–8.11252	–2.54577
Si	1.79242	–6.89784	–1.99145	H	2.19701	–7.58484	2.20519
O	2.55158	–5.5443	–2.68377	H	–2.03117	–7.60345	2.17405
O	5.14083	–5.45967	–3.18049	H	6.59471	–7.61501	–3.1476
O	7.84656	–5.36295	–3.24626	H	6.70456	–7.49272	1.33939
O	2.69202	–5.10239	1.62487	H	8.49344	–3.6569	–5.10102
O	5.32967	–5.27891	1.33519	H	3.42026	–4.18433	–4.715
O	8.04274	–5.27155	1.15147	H	–3.23545	–4.08566	–4.69807
O	3.99241	–3.10884	–2.42413	H	–8.03631	–3.6051	–5.17307
O	3.98722	–0.58365	–0.95961	H	6.23208	3.7075	–5.32679
O	3.68324	0.91243	1.22457	H	1.6432	4.33947	–5.29074
O	4.02313	–0.51787	3.59993	H	–1.64902	4.07931	–5.0624
O	4.25386	–3.2286	2.99423	H	–6.10165	3.34046	–5.49083
O	4.1659	–3.08678	0.26156	H	–6.40619	5.4675	–4.47909
O	8.48431	–2.78221	–2.65837	H	–6.71944	6.23429	1.13463
O	8.51052	–0.4154	–1.14378	H	6.32528	5.81112	–4.24779
O	9.08731	1.10749	1.0418	H	6.5757	6.47973	1.29673
O	8.62914	–0.45388	3.33859	H	2.24015	8.93908	–3.78831
O	8.54794	–3.08245	2.77428	H	2.27214	9.28253	0.80985
O	8.61476	–2.87503	0.04324	H	–2.59973	9.08699	0.87718
O	6.25845	–2.09321	–1.21772	H	–2.58141	8.69952	–3.84824
O	6.35768	–1.92266	4.08343	P	–1.6738	2.97158	–1.14125
Si	3.73456	–4.50758	–3.35307	Al	–3.87981	0.84569	–0.37401
Si	4.56694	–2.18474	–1.11615	H	–1.52764	–0.57373	–1.82748
Si	4.65481	–2.00894	4.1145	C	–1.98741	–1.15348	–1.03418
Si	4.09111	–4.136	1.57784	H	–1.8201	–2.21596	–1.19362
Si	8.82677	–4.04918	–3.74858	H	–1.60167	–0.85573	–0.06077
Si	7.94433	–2.00184	–1.24777	H	1.08231	–0.03224	1.33887
Si	8.05207	–1.93807	3.93284	C	1.4846	–0.88907	0.77936
Si	9.01667	–3.88446	1.34678	H	1.17344	–1.80976	1.28462
H	–6.67715	3.34916	5.02653	H	2.58202	–0.83412	0.80281
H	–2.16262	3.72723	5.26855	O	0.98509	–0.93866	–0.54715
H	1.94479	3.70649	5.37153	H	1.32892	–0.1389	–1.00131

Table B6 Coordinates of TS2 on P–H[1]–ZSM–5, in Å

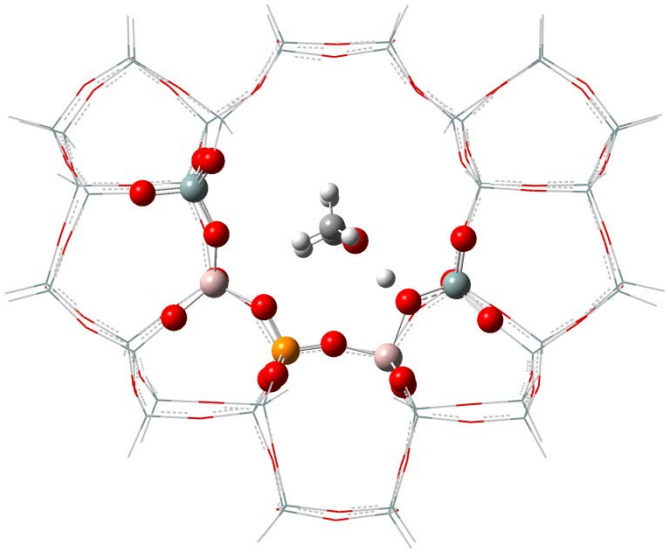


TS2

Atoms	X	Y	Z
Si	–1.60661	8.06173	0.19899
Si	–1.62387	7.7605	–3.15065
O	–4.1587	–3.16977	–2.39133
O	–3.60325	–0.86819	–1.18616
O	–3.81293	0.74016	1.26787
O	–4.07472	–0.61469	3.70336
O	–4.30482	–3.28022	3.03053
O	–4.20997	–3.01702	0.27547
O	–8.27062	–2.65982	–2.66384
O	–8.64311	–0.3767	–1.10273
O	–9.23473	1.12238	1.08818
O	–8.66142	–0.46781	3.34077
O	–8.58455	–3.08669	2.74551
O	–8.45013	–2.83598	0.03015
O	–6.13345	–1.79812	–1.15621
O	–6.42731	–1.99279	4.12658
O	–2.57918	–5.48197	–2.77317
O	–5.20178	–5.50945	–3.24938
O	–7.86597	–5.27782	–3.24503
O	–2.6626	–5.0421	1.56886
O	–5.31625	–5.26312	1.27505
O	–8.01431	–5.26213	1.11472
Si	–3.82257	–4.52775	–3.42747
Si	–4.59893	–2.28518	–1.10704
Si	–3.85675	0.89699	2.96216
Si	–4.727	–2.10225	4.1928
Si	–4.088	–4.1339	1.59623
Si	–8.7176	–3.88627	–3.76844
Si	–7.87003	–1.8619	–1.22343
Si	–9.19917	1.16033	–0.61323
Si	–9.1386	1.07116	2.7886
Si	–8.11729	–1.96424	3.93853
Si	–8.97214	–3.86238	1.28302
O	–7.92277	2.12376	3.32609
O	–5.1816	1.86456	3.42754
O	–2.52275	1.78892	3.5295
O	–7.99314	2.21652	–1.16539
O	–5.23894	1.71788	–1.04955
O	–2.39497	1.62222	–1.12552
Si	–6.63599	–6.1848	0.72769
Si	–6.61009	–6.28159	–2.6781
Si	–1.70441	–6.42394	1.26716
Si	–1.74363	–6.80521	–2.0824
O	–6.33789	4.18588	2.50877
O	–6.24167	3.50834	–2.94148
O	–6.30058	4.15018	–0.26382
O	–2.04559	4.29315	2.67439
O	–1.95194	6.52642	0.86286
O	–1.90315	7.95506	–1.48024
O	–2.04358	6.17018	–3.62403
O	–1.94217	3.64491	–2.55614
O	–2.04109	3.89582	–0.06178
O	–4.21401	5.14044	1.16636
O	–3.99703	4.38036	–4.27833
Si	–6.46764	2.94309	3.66797
Si	–5.91633	5.06595	1.11363
Si	–5.70303	4.24414	–4.37985
Si	–6.44388	2.8756	–1.38133
Si	–1.63284	3.19001	3.92257
Si	–2.53563	4.99376	1.22797
Si	–2.33239	4.55368	–4.01501
O	0.04839	2.98168	3.91375
O	–0.10752	2.64944	–1.13306
O	0.05271	8.3654	0.36816
O	0.04855	7.92825	–3.3746
O	–6.5745	–6.28078	–0.97679
O	–1.92957	–6.76759	–0.38971
O	–0.03263	–6.19349	1.46853
O	–0.07022	–6.71296	–2.35892
O	6.50017	4.21382	2.64804
O	6.20562	3.65012	–2.79636
O	6.3277	4.2112	–0.09351
O	2.1217	4.45544	2.85612
O	2.09487	6.67325	1.01826
O	1.97379	7.94857	–1.48559
O	2.14805	6.24743	–3.77922
O	2.00955	3.73109	–2.73404
O	2.09971	4.05334	0.13043
O	4.32163	5.26417	1.41796
O	4.12939	4.48699	–4.42064
O	8.04571	2.03006	3.28481
O	5.30869	1.87953	3.43766
O	2.64391	1.87447	3.59502
O	7.75062	2.09405	–1.11124
O	4.99937	1.90466	–0.92153
O	2.35663	1.38742	–0.95269

Si	6.64233	2.89549	3.71359	H	6.7286	3.33222	5.08024
Si	6.0078	5.13751	1.29853	H	–8.74126	–2.27091	5.19738
Si	5.82562	4.38207	–4.29194	H	–4.27729	–2.48592	5.49981
Si	6.3028	2.97156	–1.25115	H	4.22183	–2.43927	5.38624
Si	1.73549	3.25958	4.00098	H	8.68623	–2.38307	5.12761
Si	2.62967	5.08957	1.35482	H	10.503	1.22142	3.14274
Si	1.73873	8.10966	0.19858	H	10.37367	–4.44535	1.30286
Si	1.74553	7.77047	–3.16798	H	10.24594	1.41964	–1.33986
Si	2.4481	4.59137	–4.12584	H	10.1372	–4.63311	–3.78383
Si	3.81407	0.90531	–0.39978	H	–10.4213	1.42088	3.33748
Si	3.94624	0.98887	2.95185	H	–10.4915	1.47144	–1.15224
Si	9.00741	1.02449	–0.72812	H	–10.1391	–4.14672	–3.71125
Si	9.17731	0.92391	2.66832	H	–10.3703	–4.18075	1.21683
O	6.44598	–6.36062	–1.02144	Al	1.67382	3.00367	–1.18886
O	1.79037	–6.8159	–0.41397	H	–6.74957	–7.61625	–3.18752
Si	6.56523	–6.27151	0.68042	H	–6.67654	–7.49534	1.31016
Si	6.4063	–6.33592	–2.72365	H	–2.28095	–8.02356	–2.62887
Si	1.64287	–6.45993	1.24831	H	2.11204	–8.03183	–2.67664
Si	1.61897	–6.80445	–2.10861	H	2.03493	–7.57707	2.06584
O	2.42482	–5.47442	–2.79287	H	–2.15098	–7.51037	2.09784
O	5.02834	–5.48929	–3.25524	H	6.42424	–7.68013	–3.23428
O	7.73608	–5.4623	–3.33374	H	6.60562	–7.59373	1.24148
O	2.62037	–5.10619	1.55492	H	8.4302	–3.77437	–5.18752
O	5.26025	–5.3638	1.28206	H	3.37525	–4.12552	–4.79
O	7.97296	–5.39181	1.06162	H	–3.55972	–4.09491	–4.76638
O	3.97368	–3.11511	–2.47046	H	–8.32107	–3.514	–5.1083
O	4.09271	–0.61303	–0.93845	H	6.33768	3.5694	–5.37583
O	3.84097	0.89053	1.24461	H	1.73801	4.20922	–5.31699
O	4.11116	–0.57308	3.59757	H	–1.5788	4.05935	–5.12519
O	4.23996	–3.28669	2.94359	H	–6.035	3.41451	–5.51741
O	4.17302	–3.13841	0.2132	H	–6.28717	5.55897	–4.52754
O	8.48582	–2.90898	–2.74202	H	–6.52936	6.36272	1.09574
O	8.55287	–0.54162	–1.21944	H	6.42032	5.70141	–4.35324
O	9.16425	0.96422	0.96942	H	6.67748	6.40713	1.27286
O	8.67119	–0.59101	3.2604	H	2.43918	8.81532	–3.87203
O	8.56113	–3.22375	2.6881	H	2.46966	9.23375	0.71487
O	8.6335	–3.01225	–0.0415	H	–2.41101	9.07929	0.81439
O	6.28427	–2.19547	–1.28323	H	–2.38859	8.70205	–3.92014
O	6.39983	–2.05082	4.02359	P	–1.59799	2.94106	–1.20589
Si	3.66175	–4.48024	–3.43003	Al	–3.87165	0.8758	–0.44537
Si	4.5924	–2.23181	–1.15608	H	–2.07382	–1.14705	–2.59028
Si	4.69627	–2.09621	4.0744	C	–2.18505	–1.20161	–1.50891
Si	4.0526	–4.18784	1.52481	H	–1.97361	–2.2059	–1.14666
Si	8.76185	–4.18567	–3.84031	H	–1.52307	–0.50107	–1.01422
Si	7.97014	–2.12257	–1.32543	H	0.45843	0.00513	1.61796
Si	8.09209	–2.07521	3.8533	C	0.64792	–0.91186	1.04232
Si	8.99599	–4.04099	1.25837	H	–0.10863	–1.65512	1.31734
H	–6.50008	3.47813	5.00086	H	1.63556	–1.30345	1.3221
H	–2.04407	3.70736	5.20066	O	0.54357	–0.69424	–0.35613
H	2.03212	3.6821	5.34459	H	1.152	0.03075	–0.61573

Table B7 Coordinates of DME/H[1]Z on P–H[1]–ZSM–5, in Å

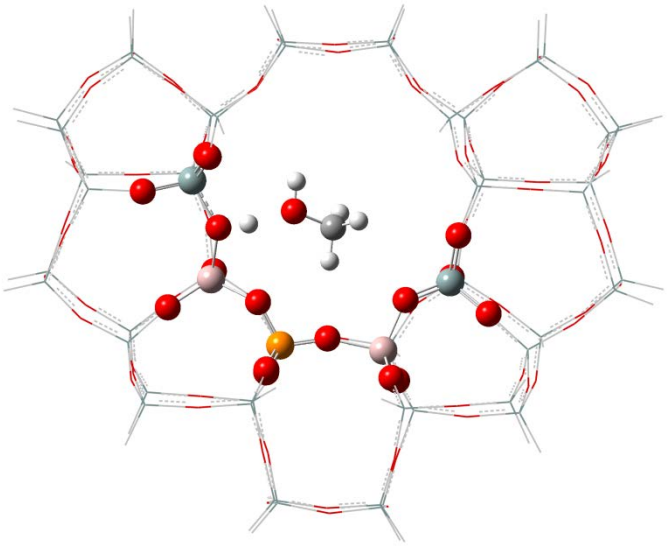


DME/H[1]Z

Atoms	X	Y	Z
Si	–1.64607	8.06907	0.21476
Si	–1.65756	7.7776	–3.13545
O	–4.12275	–3.1714	–2.38172
O	–3.60849	–0.86843	–1.16926
O	–3.82101	0.74692	1.27683
O	–4.07884	–0.61696	3.70637
O	–4.28972	–3.28471	3.04115
O	–4.20655	–3.02503	0.28461
O	–8.26395	–2.69648	–2.67391
O	–8.63563	–0.4082	–1.11572
O	–9.25012	1.07922	1.07776
O	–8.66297	–0.49926	3.33405
O	–8.5723	–3.11631	2.7351
O	–8.4478	–2.86842	0.01957
O	–6.13029	–1.82898	–1.16371
O	–6.42423	–2.01168	4.12574
O	–2.54235	–5.48538	–2.76186
O	–5.16201	–5.50331	–3.25449
O	–7.82888	–5.31095	–3.25462
O	–2.64482	–5.03828	1.57804
O	–5.29882	–5.27561	1.28927
O	–7.99422	–5.29163	1.10548
Si	–3.77859	–4.52511	–3.42079
Si	–4.59059	–2.29604	–1.10097
Si	–3.86534	0.89854	2.97184
Si	–4.72329	–2.10665	4.19926
Si	–4.07625	–4.13928	1.60682
Si	–8.69601	–3.92899	–3.77808
Si	–7.86663	–1.89555	–1.2345
Si	–9.21449	1.11957	–0.62354
Si	–9.14926	1.0354	2.77813
Si	–8.11354	–1.99386	3.93137
Si	–8.9593	–3.89688	1.27515
O	–7.93804	2.09626	3.30954
O	–5.19362	1.85964	3.44072
O	–2.53097	1.78965	3.53838
O	–8.02359	2.19705	–1.16868
O	–5.27109	1.69957	–1.03801
O	–2.434	1.63992	–1.13428
Si	–6.60689	–6.20284	0.72303
Si	–6.55933	–6.29486	–2.68307
Si	–1.67896	–6.41584	1.28067
Si	–1.71393	–6.81099	–2.0671
O	–6.36337	4.1694	2.50578
O	–6.26316	3.48466	–2.94095
O	–6.32799	4.13352	–0.26484
O	–2.05401	4.29104	2.67784
O	–1.99258	6.53275	0.8756
O	–1.9413	7.96659	–1.46502
O	–2.06587	6.18609	–3.61466
O	–1.93199	3.65721	–2.55464
O	–2.03489	3.90343	–0.05974
O	–4.23115	5.10913	1.16873
O	–4.01121	4.38412	–4.25206
Si	–6.49248	2.9266	3.66504
Si	–5.93391	5.04704	1.11136
Si	–5.7136	4.22253	–4.37419
Si	–6.47383	2.85668	–1.37982
Si	–1.64002	3.19113	3.92851
Si	–2.55084	4.98887	1.23255
Si	–2.34495	4.5681	–4.006
O	0.04054	2.97836	3.91791
O	–0.12581	2.61501	–1.12807
O	0.01296	8.37342	0.38654
O	0.01428	7.95618	–3.35617
O	–6.52976	–6.28646	–0.98146
O	–1.90312	–6.76547	–0.37491
O	–0.0083	–6.17295	1.47782
O	–0.03912	–6.73342	–2.3388
O	6.47428	4.23489	2.63187
O	6.16486	3.65335	–2.80878
O	6.29308	4.23025	–0.10852
O	2.10633	4.45653	2.86129
O	2.04487	6.6667	1.02003
O	1.93831	7.97018	–1.46735
O	2.10829	6.26705	–3.75817
O	1.9694	3.74122	–2.73187
O	2.06985	4.04715	0.13295
O	4.28833	5.27911	1.40702
O	4.08549	4.51201	–4.41858
O	8.04452	2.07236	3.28758
O	5.31163	1.883	3.41225
O	2.64677	1.88301	3.60882
O	7.7448	2.12977	–1.12575
O	5.00403	1.89377	–0.91791
O	2.3589	1.39184	–0.97394

Si	6.62556	2.92057	3.70112	H	6.69373	3.36178	5.06735
Si	5.97458	5.15645	1.28378	H	–8.74024	–2.30626	5.18746
Si	5.7821	4.40573	–4.29341	H	–4.27596	–2.48294	5.50917
Si	6.2828	2.98526	–1.26049	H	4.24284	–2.42742	5.39085
Si	1.72688	3.26144	4.00896	H	8.70755	–2.33788	5.12418
Si	2.59748	5.0888	1.35383	H	10.50179	1.27009	3.13023
Si	1.69877	8.11513	0.21762	H	10.39768	–4.39609	1.30427
Si	1.71077	7.79251	–3.14983	H	10.24249	1.46599	–1.3427
Si	2.40508	4.61326	–4.11745	H	10.15888	–4.59749	–3.77906
Si	3.80603	0.90559	–0.40176	H	–10.4327	1.38004	3.32839
Si	3.9393	0.99507	2.94971	H	–10.5097	1.41244	–1.16569
Si	9.0036	1.06558	–0.73486	H	–10.1144	–4.20553	–3.7198
Si	9.17448	0.96891	2.66237	H	–10.3557	–4.22376	1.21306
O	6.47992	–6.34037	–1.01432	Al	1.65068	2.99904	–1.18993
O	1.81455	–6.82428	–0.3897	H	–6.67797	–7.63311	–3.18821
Si	6.6031	–6.25077	0.6871	H	–6.64363	–7.51751	1.29638
Si	6.43925	–6.32167	–2.71664	H	–2.2587	–8.02687	–2.61173
Si	1.66702	–6.45116	1.26862	H	2.14897	–8.04464	–2.64915
Si	1.64996	–6.81791	–2.0852	H	2.05194	–7.56076	2.09955
O	2.45327	–5.48659	–2.76954	H	–2.11774	–7.50209	2.11567
O	5.0542	–5.48806	–3.24998	H	6.46787	–7.66709	–3.22364
O	7.76334	–5.4398	–3.32754	H	6.65718	–7.57173	1.25005
O	2.6477	–5.09764	1.56536	H	8.44709	–3.75174	–5.18517
O	5.28833	–5.35707	1.28893	H	3.3812	–4.13913	–4.77703
O	8.0043	–5.3586	1.06295	H	–3.50579	–4.08946	–4.75669
O	3.99948	–3.11907	–2.46606	H	–8.30459	–3.55199	–5.11807
O	4.08357	–0.61679	–0.9287	H	6.29238	3.60715	–5.38853
O	3.81921	0.89807	1.24349	H	1.68961	4.24073	–5.30843
O	4.11194	–0.56454	3.59902	H	–1.59877	4.08348	–5.1254
O	4.26529	–3.27693	2.94904	H	–6.0198	3.38393	–5.51244
O	4.19812	–3.13263	0.21899	H	–6.31314	5.52895	–4.53445
O	8.49941	–2.87877	–2.7428	H	–6.53692	6.34848	1.0921
O	8.56405	–0.50582	–1.22461	H	6.37578	5.72616	–4.33924
O	9.15269	1.00839	0.96351	H	6.6399	6.42834	1.25549
O	8.67828	–0.54919	3.25517	H	2.40902	8.83384	–3.8544
O	8.57584	–3.18536	2.68781	H	2.43197	9.23143	0.74717
O	8.65002	–2.97479	–0.04215	H	–2.4521	9.08432	0.83183
O	6.29962	–2.16694	–1.28252	H	–2.42678	8.71671	–3.90344
O	6.41529	–2.01964	4.02711	P	–1.60991	2.94246	–1.20502
Si	3.68022	–4.48741	–3.41811	Al	–3.89258	0.8753	–0.43609
Si	4.60899	–2.22668	–1.15398	H	–0.47823	–0.92184	–2.31912
Si	4.71225	–2.08131	4.07798	C	–0.62678	–0.92655	–1.24131
Si	4.08082	–4.18092	1.53159	H	–1.02819	–1.92775	–1.09764
Si	8.78099	–4.15793	–3.837	H	–1.1779	–0.00464	–1.11342
Si	7.9856	–2.08842	–1.32793	H	0.34475	–0.31545	1.42601
Si	8.10713	–2.03498	3.85155	C	0.73938	–1.12423	0.79315
Si	9.01751	–4.00019	1.25877	H	0.15194	–2.02976	0.98117
H	–6.54207	3.46218	4.99723	H	1.77931	–1.31774	1.088
H	–2.05025	3.71231	5.20528	O	0.62973	–0.82177	–0.58936
H	2.01875	3.6876	5.35244	H	1.74901	0.64428	–0.87577

Table B8 Coordinates of MeOH/H^{4}Z on P–H^4–ZSM–5, in Å

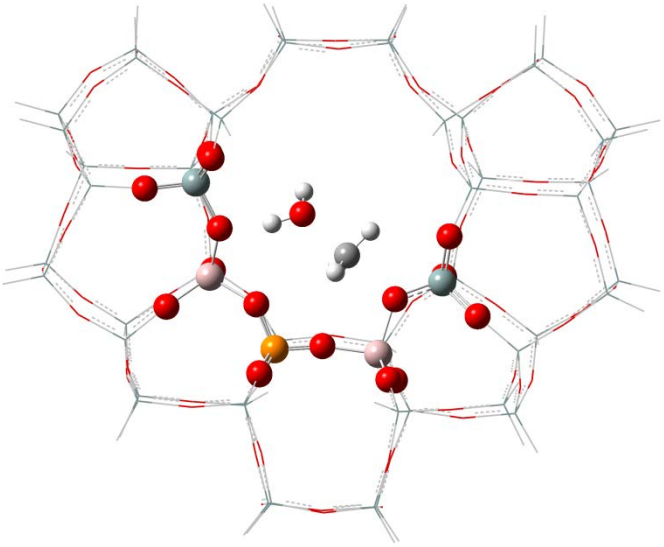


MeOH/H^{4}Z

Atoms	X	Y	Z
Si	–1.9223	7.94803	0.16243
Si	–1.91579	7.63258	–3.18429
O	–3.83216	–3.12316	–2.37829
O	–3.74214	–0.80853	–1.14993
O	–3.91064	0.71731	1.3794
O	–4.10109	–0.7317	3.77231
O	–4.16637	–3.39013	3.03429
O	–4.05301	–3.05945	0.28792
O	–8.1538	–2.91239	–2.77289
O	–8.56668	–0.66789	–1.15957
O	–9.27593	0.75628	1.0519
O	–8.65493	–0.81611	3.29242
O	–8.45056	–3.42431	2.64591
O	–8.38499	–3.15203	–0.0716
O	–6.06313	–2.08171	–1.20281
O	–6.37927	–2.25285	4.101
O	–2.22898	–5.43782	–2.76287
O	–4.80888	–5.44418	–3.34261
O	–7.48909	–5.44997	–3.42599
O	–2.44214	–5.06986	1.56441
O	–5.06766	–5.36607	1.20105
O	–7.75234	–5.541	0.97664
Si	–3.43034	–4.44885	–3.4394
Si	–4.48461	–2.37493	–1.09928
Si	–3.94452	0.8097	3.08068
Si	–4.67814	–2.26469	4.21313
Si	–3.8914	–4.20096	1.58666
Si	–8.45845	–4.13143	–3.93297
Si	–7.7972	–2.15387	–1.30118
Si	–9.223	0.82253	–0.648
Si	–9.19662	0.70615	2.75275
Si	–8.06313	–2.30251	3.86854
Si	–8.80758	–4.21837	1.18557
O	–8.04768	1.81998	3.31429
O	–5.31071	1.70934	3.56043
O	–2.63619	1.7355	3.64664
O	–8.09939	1.99175	–1.14453
O	–5.33172	1.73487	–0.93167
O	–2.45103	1.45991	–1.08095
Si	–6.30689	–6.34849	0.57683
Si	–6.16541	–6.34256	–2.83056
Si	–1.4719	–6.44705	1.27
Si	–1.4618	–6.80832	–2.08014
O	–6.53035	3.98668	2.60735
O	–6.42276	3.43232	–2.86031
O	–6.56792	4.05959	–0.16437
O	–2.20955	4.20698	2.68578
O	–2.21227	6.39963	0.82267
O	–2.2121	7.82804	–1.51704
O	–2.26194	6.01708	–3.63495
O	–2.13058	3.49646	–2.54281
O	–2.22123	3.75697	–0.04901
O	–4.42308	4.96595	1.225
O	–4.19383	4.21063	–4.26937
Si	–6.66195	2.71825	3.7387
Si	–6.1272	4.9149	1.23787
Si	–5.90352	4.10804	–4.3351
Si	–6.61328	2.79623	–1.30154
Si	–1.75983	3.16347	3.97179
Si	–2.7396	4.85824	1.2316
Si	–2.5294	4.39382	–4.0083
O	–0.07752	2.9839	3.94208
O	–0.22366	2.6069	–1.1402
O	–0.27754	8.31597	0.33986
O	–0.25436	7.88396	–3.40471
O	–6.1869	–6.35773	–1.12825
O	–1.67913	–6.78151	–0.39143
O	0.19605	–6.21697	1.48685
O	0.21507	–6.77986	–2.33571
O	6.29482	4.37773	2.62096
O	6.04008	3.75823	–2.81105
O	6.1455	4.33777	–0.11912
O	1.93998	4.48643	2.82122
O	1.82429	6.69899	0.98872
O	1.6623	7.98673	–1.50826
O	1.91775	6.30707	–3.81194
O	1.82018	3.78461	–2.77516
O	1.92903	4.08349	0.09024
O	4.10552	5.36961	1.37039
O	3.94339	4.58271	–4.43378
O	7.91053	2.25926	3.28179
O	5.17454	1.99248	3.36641
O	2.52673	1.91457	3.55276
O	7.67997	2.29612	–1.12278
O	4.94397	1.94872	–0.93247
O	2.31344	1.44881	–1.05956

Si	6.45905	3.05754	3.68141	H	1.93105	3.71811	5.31224
Si	5.79453	5.2754	1.25689	H	6.49629	3.48808	5.05255
Si	5.64067	4.495	–4.29854	H	–8.7032	–2.66491	5.10437
Si	6.18179	3.08631	–1.26472	H	–4.23888	–2.65374	5.5217
Si	1.60793	3.28542	3.97774	H	4.26024	–2.32575	5.38603
Si	2.42063	5.13455	1.31659	H	8.71967	–2.09902	5.16995
Si	1.41852	8.12568	0.17666	H	10.40766	1.57335	3.17151
Si	1.44833	7.80652	–3.19198	H	10.52059	–4.09791	1.3627
Si	2.25713	4.6581	–4.15817	H	10.1991	1.70293	–1.31609
Si	3.72633	0.95086	–0.45687	H	10.34879	–4.33927	–3.6934
Si	3.83806	1.05251	2.8946	H	–10.5018	0.98659	3.2886
Si	8.96721	1.27411	–0.71353	H	–10.5262	1.05113	–1.20267
Si	9.1031	1.20847	2.6854	H	–9.84974	–4.52525	–3.92306
O	6.71096	–6.22378	–0.962	H	–10.1799	–4.63659	1.1425
O	2.0476	–6.84519	–0.36784	Al	1.55409	3.01442	–1.23299
Si	6.80324	–6.10353	0.73981	H	–6.17125	–7.677	–3.35917
Si	6.69091	–6.21096	–2.66423	H	–6.27437	–7.68572	1.09568
Si	1.87753	–6.46165	1.28665	H	–2.04524	–7.99293	–2.65241
Si	1.90204	–6.85493	–2.06456	H	2.41782	–8.08123	–2.61313
O	2.67848	–5.51577	–2.76227	H	2.28266	–7.55492	2.12887
O	5.28253	–5.42786	–3.21409	H	–1.92768	–7.5373	2.09053
O	7.98615	–5.28381	–3.26876	H	6.77082	–7.55625	–3.16615
O	2.81138	–5.07514	1.56936	H	6.88548	–7.41517	1.32088
O	5.45712	–5.23665	1.30911	H	8.62216	–3.58477	–5.13221
O	8.17067	–5.16404	1.12398	H	3.5825	–4.16631	–4.78055
O	4.10048	–3.08655	–2.47285	H	–3.11157	–3.96075	–4.74608
O	4.04931	–0.56786	–0.98706	H	–8.06523	–3.6758	–5.24761
O	3.72995	0.9262	1.19209	H	6.16184	3.69769	–5.38991
O	4.07429	–0.48635	3.57467	H	1.56485	4.26948	–5.35818
O	4.35263	–3.19056	2.94929	H	–1.77585	3.88862	–5.11334
O	4.27877	–3.06905	0.20667	H	–6.27283	3.24549	–5.43606
O	8.59514	–2.6895	–2.69685	H	–6.4682	5.42713	–4.51442
O	8.56803	–0.3102	–1.19586	H	–6.72532	6.21765	1.28872
O	9.10977	1.23347	0.98601	H	6.21648	5.82328	–4.35394
O	8.66385	–0.32356	3.28726	H	6.43542	6.55966	1.21961
O	8.64438	–2.95912	2.7352	H	2.09352	8.88685	–3.88843
O	8.71387	–2.76479	0.00258	H	2.10199	9.27499	0.70234
O	6.35042	–2.03598	–1.27452	H	–2.76957	8.93256	0.77427
O	6.43275	–1.85007	4.0458	H	–2.72464	8.52474	–3.96751
Si	3.87578	–4.48169	–3.41214	P	–1.72009	2.82847	–1.19329
Si	4.6603	–2.15043	–1.1666	Al	–3.97193	0.89556	–0.32175
Si	4.73179	–1.9698	4.0765	H	–2.89351	–0.788	–1.62115
Si	4.20713	–4.10209	1.53394	C	–0.0809	–0.00633	–2.15966
Si	8.95379	–3.96198	–3.775	H	–0.13479	1.0579	–2.06254
Si	8.03341	–1.90789	–1.29469	H	0.32425	–0.25698	–3.11775
Si	8.12606	–1.81944	3.88879	H	0.54901	–0.40317	–1.39114
Si	9.12476	–3.76204	1.3123	O	–1.39219	–0.56325	–2.03612
H	–6.79381	3.23324	5.07337	H	–1.34455	–1.51795	–2.12493
H	–2.16509	3.72093	5.23466				

Table B9 Coordinates of TS1 on P–H^4–ZSM–5, in Å

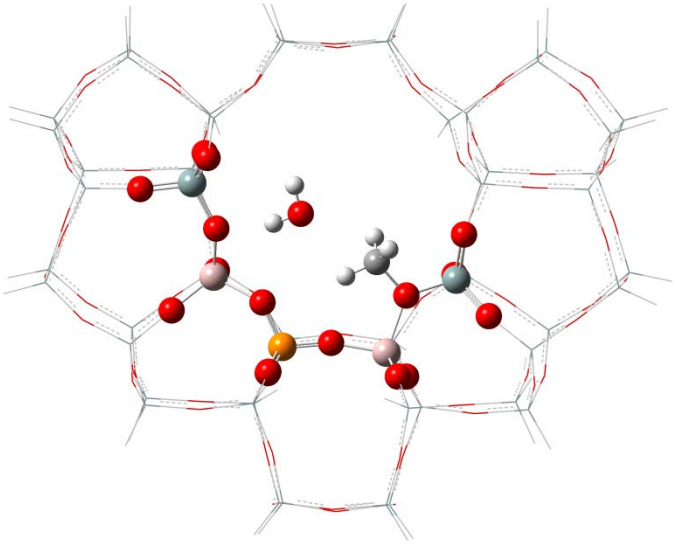


TS1

Atoms	X	Y	Z
Si	–1.76884	8.03403	0.18983
Si	–1.76689	7.71115	–3.15758
O	–3.9164	–3.15727	–2.34809
O	–3.63466	–0.82041	–1.15219
O	–3.84379	0.74519	1.33112
O	–4.07129	–0.64997	3.74832
O	–4.19524	–3.32085	3.06071
O	–4.07058	–3.02732	0.3103
O	–8.16993	–2.82374	–2.69263
O	–8.55693	–0.54972	–1.12087
O	–9.23225	0.92039	1.06901
O	–8.63833	–0.63849	3.33241
O	–8.49498	–3.25209	2.72365
O	–8.37203	–3.0123	0.00259
O	–6.04894	–1.96228	–1.16312
O	–6.37652	–2.11326	4.1314
O	–2.3694	–5.45667	–2.76976
O	–4.98922	–5.49598	–3.23755
O	–7.6636	–5.41521	–3.28113
O	–2.52373	–5.05859	1.58255
O	–5.16096	–5.30397	1.27814
O	–7.85644	–5.41158	1.09742
Si	–3.62037	–4.50057	–3.41357
Si	–4.4761	–2.31129	–1.07706
Si	–3.89503	0.87691	3.02642
Si	–4.67463	–2.16236	4.22186
Si	–3.95503	–4.15641	1.61999
Si	–8.57622	–4.06057	–3.80063
Si	–7.78173	–2.03437	–1.24368
Si	–9.17474	0.96379	–0.632
Si	–9.15729	0.88361	2.7703
Si	–8.06476	–2.12491	3.92631
Si	–8.86067	–4.04361	1.26417
O	–7.98747	1.97984	3.32295
O	–5.24733	1.80311	3.49674
O	–2.58251	1.79438	3.60171
O	–8.01407	2.08414	–1.15272
O	–5.24514	1.73677	–0.99048
O	–2.36965	1.55108	–1.06284
Si	–6.43869	–6.27261	0.71255
Si	–6.36342	–6.34682	–2.69367
Si	–1.58232	–6.45017	1.27348
Si	–1.58833	–6.81415	–2.07946
O	–6.44227	4.09936	2.55742
O	–6.32165	3.47129	–2.90034
O	–6.42606	4.10609	–0.21661
O	–2.13944	4.28601	2.69566
O	–2.09121	6.49583	0.85777
O	–2.05679	7.91214	–1.48973
O	–2.14401	6.1058	–3.61615
O	–2.05538	3.58724	–2.53131
O	–2.13024	3.85984	–0.03982
O	–4.32846	5.08033	1.20154
O	–4.09896	4.32383	–4.27254
Si	–6.56875	2.84485	3.70452
Si	–6.03141	5.00068	1.1724
Si	–5.80696	4.19976	–4.35069
Si	–6.50125	2.83136	–1.34072
Si	–1.7074	3.21283	3.96289
Si	–2.64746	4.95784	1.24232
Si	–2.43544	4.48758	–3.99904
O	–0.02476	3.02441	3.94118
O	–0.15143	2.69184	–1.13315
O	–0.11671	8.36894	0.36923
O	–0.09998	7.93192	–3.37469
O	–6.35272	–6.35156	–0.99226
O	–1.79294	–6.7772	–0.38917
O	0.08949	–6.22958	1.48048
O	0.08865	–6.7514	–2.33947
O	6.38441	4.28978	2.65734
O	6.12668	3.68984	–2.77543
O	6.22744	4.25819	–0.08044
O	2.03262	4.49867	2.84602
O	1.96575	6.72398	1.02177
O	1.81927	8.01241	–1.47735
O	2.06435	6.34053	–3.78699
O	1.93449	3.8185	–2.75455
O	2.03584	4.1111	0.11459
O	4.22295	5.34876	1.41333
O	4.06891	4.58696	–4.40461
O	7.94937	2.13462	3.32038
O	5.20883	1.92719	3.38766
O	2.55716	1.9112	3.56907
O	7.71793	2.18694	–1.08034
O	4.97445	1.8979	–0.91041
O	2.32879	1.46273	–1.03583

Si	6.51394	2.96387	3.71488	H	1.98717	3.71921	5.33203
Si	5.90801	5.20573	1.29673	H	6.55229	3.38757	5.08797
Si	5.76204	4.45883	–4.25614	H	–8.69241	–2.45477	5.17753
Si	6.23919	3.01104	–1.23041	H	–4.22868	–2.53917	5.53211
Si	1.66327	3.29995	3.99355	H	4.19218	–2.37421	5.39446
Si	2.53356	5.14971	1.34959	H	8.65206	–2.25028	5.19208
Si	1.5759	8.15461	0.20735	H	10.43163	1.39381	3.21299
Si	1.60116	7.84025	–3.16164	H	10.4286	–4.26059	1.37649
Si	2.38248	4.68856	–4.13664	H	10.22841	1.55271	–1.27578
Si	3.7337	0.93232	–0.43576	H	10.25364	–4.47716	–3.68072
Si	3.85029	1.02125	2.91471	H	–10.4584	1.19164	3.30081
Si	8.9889	1.14375	–0.67541	H	–10.472	1.22189	–1.18782
Si	9.12025	1.06031	2.72317	H	–9.98526	–4.38009	–3.73853
O	6.57848	–6.30035	–0.96196	H	–10.2478	–4.40742	1.2025
O	1.93352	–6.84729	–0.38439	Al	1.63032	3.06362	–1.21389
Si	6.67214	–6.19036	0.74052	H	–6.41786	–7.68531	–3.20944
Si	6.55885	–6.2814	–2.66394	H	–6.43115	–7.58949	1.2822
Si	1.76825	–6.47938	1.27435	H	–2.14869	–8.01539	–2.63938
Si	1.77583	–6.84199	–2.07996	H	2.28467	–8.06342	–2.64526
O	2.55644	–5.49567	–2.76314	H	2.17766	–7.57883	2.10605
O	5.16729	–5.4633	–3.20723	H	–2.04043	–7.54204	2.09007
O	7.87196	–5.37857	–3.26583	H	6.60743	–7.62554	–3.17219
O	2.70368	–5.09319	1.56162	H	6.72145	–7.50555	1.31676
O	5.34635	–5.29183	1.30902	H	8.54386	–3.68349	–5.12017
O	8.05976	–5.28374	1.13028	H	3.49782	–4.15941	–4.77397
O	4.02198	–3.10073	–2.45967	H	–3.36516	–4.05657	–4.74998
O	4.00641	–0.596	–0.97483	H	–8.20025	–3.67068	–5.14133
O	3.73415	0.89634	1.21133	H	6.2761	3.66368	–5.35242
O	4.04981	–0.52635	3.58709	H	1.6916	4.30885	–5.33995
O	4.26879	–3.23388	2.95554	H	–1.67711	3.98365	–5.10156
O	4.19797	–3.09809	0.21728	H	–6.16163	3.36972	–5.48099
O	8.52654	–2.80105	–2.68025	H	–6.38543	5.51769	–4.49247
O	8.55935	–0.43028	–1.16619	H	–6.6488	6.29553	1.18113
O	9.13	1.0908	1.02374	H	6.37068	5.77307	–4.28597
O	8.64502	–0.46396	3.31762	H	6.58775	6.46969	1.2601
O	8.56996	–3.09464	2.75177	H	2.25583	8.91763	–3.85404
O	8.64477	–2.89178	0.0203	H	2.27636	9.29365	0.73328
O	6.2996	–2.09921	–1.25345	H	–2.59489	9.04012	0.79555
O	6.37709	–1.94343	4.05734	H	–2.55564	8.6236	–3.93809
Si	3.78095	–4.48909	–3.40685	P	–1.6533	2.91711	–1.1805
Si	4.60864	–2.18385	–1.15055	Al	–3.88733	0.87958	–0.38371
Si	4.67406	–2.02484	4.0871	H	–2.66255	–0.96298	–1.43485
Si	4.11361	–4.14016	1.53815	C	0.02555	–0.85886	–1.33383
Si	8.86629	–4.07366	–3.76454	H	–0.08435	0.22014	–1.30496
Si	7.98647	–2.01351	–1.27347	H	0.85856	–1.11418	–1.99127
Si	8.07169	–1.95022	3.90966	H	0.20884	–1.23763	–0.32413
Si	9.03904	–3.90024	1.32681	O	–1.21263	–1.40422	–1.86752
H	–6.65262	3.37302	5.03801	H	–1.13139	–2.36212	–1.96164
H	–2.11508	3.74842	5.2344				

Table B10 Coordinates of CH_3–Z/H_2O on P–H^4–ZSM–5, in Å

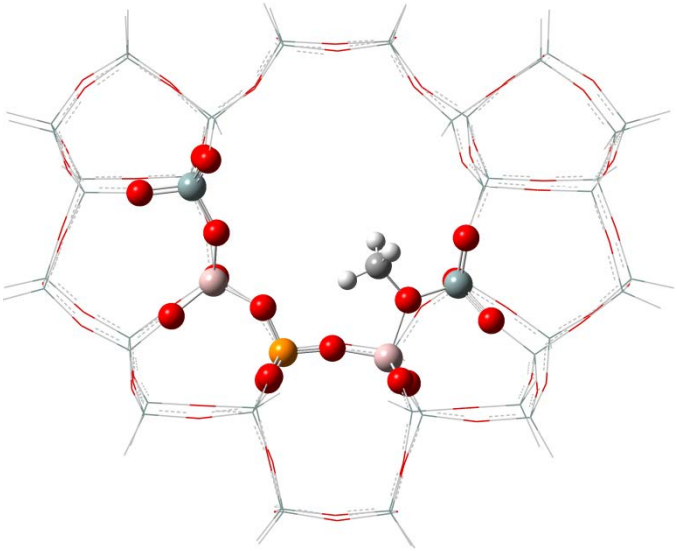


CH_3–Z/H_2O

Atoms	X	Y	Z
Si	–1.76884	8.03403	0.18983
Si	–1.76689	7.71115	–3.15758
O	–3.9164	–3.15727	–2.34809
O	–3.63466	–0.82041	–1.15219
O	–3.84379	0.74519	1.33112
O	–4.07129	–0.64997	3.74832
O	–4.19524	–3.32085	3.06071
O	–4.07058	–3.02732	0.3103
O	–8.16993	–2.82374	–2.69263
O	–8.55693	–0.54972	–1.12087
O	–9.23225	0.92039	1.06901
O	–8.63833	–0.63849	3.33241
O	–8.49498	–3.25209	2.72365
O	–8.37203	–3.0123	0.00259
O	–6.04894	–1.96228	–1.16312
O	–6.37652	–2.11326	4.1314
O	–2.3694	–5.45667	–2.76976
O	–4.98922	–5.49598	–3.23755
O	–7.6636	–5.41521	–3.28113
O	–2.52373	–5.05859	1.58255
O	–5.16096	–5.30397	1.27814
O	–7.85644	–5.41158	1.09742
Si	–3.62037	–4.50057	–3.41357
Si	–4.4761	–2.31129	–1.07706
Si	–3.89503	0.87691	3.02642
Si	–4.67463	–2.16236	4.22186
Si	–3.95503	–4.15641	1.61999
Si	–8.57622	–4.06057	–3.80063
Si	–7.78173	–2.03437	–1.24368
Si	–9.17474	0.96379	–0.632
Si	–9.15729	0.88361	2.7703
Si	–8.06476	–2.12491	3.92631
Si	–8.86067	–4.04361	1.26417
O	–7.98747	1.97984	3.32295
O	–5.24733	1.80311	3.49674
O	–2.58251	1.79438	3.60171
O	–8.01407	2.08414	–1.15272
O	–5.24514	1.73677	–0.99048
O	–2.36965	1.55108	–1.06284
Si	–6.43869	–6.27261	0.71255
Si	–6.36342	–6.34682	–2.69367
Si	–1.58232	–6.45017	1.27348
Si	–1.58833	–6.81415	–2.07946
O	–6.44227	4.09936	2.55742
O	–6.32165	3.47129	–2.90034
O	–6.42606	4.10609	–0.21661
O	–2.13944	4.28601	2.69566
O	–2.09121	6.49583	0.85777
O	–2.05679	7.91214	–1.48973
O	–2.14401	6.1058	–3.61615
O	–2.05538	3.58724	–2.53131
O	–2.13024	3.85984	–0.03982
O	–4.32846	5.08033	1.20154
O	–4.09896	4.32383	–4.27254
Si	–6.56875	2.84485	3.70452
Si	–6.03141	5.00068	1.1724
Si	–5.80696	4.19976	–4.35069
Si	–6.50125	2.83136	–1.34072
Si	–1.7074	3.21283	3.96289
Si	–2.64746	4.95784	1.24232
Si	–2.43544	4.48758	–3.99904
O	–0.02476	3.02441	3.94118
O	–0.15143	2.69184	–1.13315
O	–0.11671	8.36894	0.36923
O	–0.09998	7.93192	–3.37469
O	–6.35272	–6.35156	–0.99226
O	–1.79294	–6.7772	–0.38917
O	0.08949	–6.22958	1.48048
O	0.08865	–6.7514	–2.33947
O	6.38441	4.28978	2.65734
O	6.12668	3.68984	–2.77543
O	6.22744	4.25819	–0.08044
O	2.03262	4.49867	2.84602
O	1.96575	6.72398	1.02177
O	1.81927	8.01241	–1.47735
O	2.06435	6.34053	–3.78699
O	1.93449	3.8185	–2.75455
O	2.03584	4.1111	0.11459
O	4.22295	5.34876	1.41333
O	4.06891	4.58696	–4.40461
O	7.94937	2.13462	3.32038
O	5.20883	1.92719	3.38766
O	2.55716	1.9112	3.56907
O	7.71793	2.18694	–1.08034
O	4.97445	1.8979	–0.91041
O	2.32879	1.46273	–1.03583
Si	6.51394	2.96387	3.71488

Si	5.90801	5.20573	1.29673	H	1.98717	3.71921	5.33203
Si	5.76204	4.45883	–4.25614	H	6.55229	3.38757	5.08797
Si	6.23919	3.01104	–1.23041	H	–8.69241	–2.45477	5.17753
Si	1.66327	3.29995	3.99355	H	–4.22868	–2.53917	5.53211
Si	2.53356	5.14971	1.34959	H	4.19218	–2.37421	5.39446
Si	1.5759	8.15461	0.20735	H	8.65206	–2.25028	5.19208
Si	1.60116	7.84025	–3.16164	H	10.43163	1.39381	3.21299
Si	2.38248	4.68856	–4.13664	H	10.4286	–4.26059	1.37649
Si	3.7337	0.93232	–0.43576	H	10.22841	1.55271	–1.27578
Si	3.85029	1.02125	2.91471	H	10.25364	–4.47716	–3.68072
Si	8.9889	1.14375	–0.67541	H	–10.4584	1.19164	3.30081
Si	9.12025	1.06031	2.72317	H	–10.472	1.22189	–1.18782
O	6.57848	–6.30035	–0.96196	H	–9.98526	–4.38009	–3.73853
O	1.93352	–6.84729	–0.38439	H	–10.2478	–4.40742	1.2025
Si	6.67214	–6.19036	0.74052	Al	1.63032	3.06362	–1.21389
Si	6.55885	–6.2814	–2.66394	H	–6.41786	–7.68531	–3.20944
Si	1.76825	–6.47938	1.27435	H	–6.43115	–7.58949	1.2822
Si	1.77583	–6.84199	–2.07996	H	–2.14869	–8.01539	–2.63938
O	2.55644	–5.49567	–2.76314	H	2.28467	–8.06342	–2.64526
O	5.16729	–5.4633	–3.20723	H	2.17766	–7.57883	2.10605
O	7.87196	–5.37857	–3.26583	H	–2.04043	–7.54204	2.09007
O	2.70368	–5.09319	1.56162	H	6.60743	–7.62554	–3.17219
O	5.34635	–5.29183	1.30902	H	6.72145	–7.50555	1.31676
O	8.05976	–5.28374	1.13028	H	8.54386	–3.68349	–5.12017
O	4.02198	–3.10073	–2.45967	H	3.49782	–4.15941	–4.77397
O	4.00641	–0.596	–0.97483	H	–3.36516	–4.05657	–4.74998
O	3.73415	0.89634	1.21133	H	–8.20025	–3.67068	–5.14133
O	4.04981	–0.52635	3.58709	H	6.2761	3.66368	–5.35242
O	4.26879	–3.23388	2.95554	H	1.6916	4.30885	–5.33995
O	4.19797	–3.09809	0.21728	H	–1.67711	3.98365	–5.10156
O	8.52654	–2.80105	–2.68025	H	–6.16163	3.36972	–5.48099
O	8.55935	–0.43028	–1.16619	H	–6.38543	5.51769	–4.49247
O	9.13	1.0908	1.02374	H	–6.6488	6.29553	1.18113
O	8.64502	–0.46396	3.31762	H	6.37068	5.77307	–4.28597
O	8.56996	–3.09464	2.75177	H	6.58775	6.46969	1.2601
O	8.64477	–2.89178	0.0203	H	2.25583	8.91763	–3.85404
O	6.2996	–2.09921	–1.25345	H	2.27636	9.29365	0.73328
O	6.37709	–1.94343	4.05734	H	–2.59489	9.04012	0.79555
Si	3.78095	–4.48909	–3.40685	H	–2.55564	8.6236	–3.93809
Si	4.60864	–2.18385	–1.15055	P	–1.6533	2.91711	–1.1805
Si	4.67406	–2.02484	4.0871	Al	–3.88733	0.87958	–0.38371
Si	4.11361	–4.14016	1.53815	H	–2.10122	–1.1338	–1.60236
Si	8.86629	–4.07366	–3.76454	C	1.30867	0.43449	–1.16781
Si	7.98647	–2.01351	–1.27347	H	0.33182	0.90082	–1.24165
Si	8.07169	–1.95022	3.90966	H	1.64082	–0.31834	–1.88493
Si	9.03904	–3.90024	1.32681	H	1.257	–0.14929	–0.24419
H	–6.65262	3.37302	5.03801	O	–1.21263	–1.40422	–1.86752
H	–2.11508	3.74842	5.2344	H	–1.13139	–2.36212	–1.96164

Table B11 Coordinates of CH_3–Z on P–H^4–ZSM–5, in Å

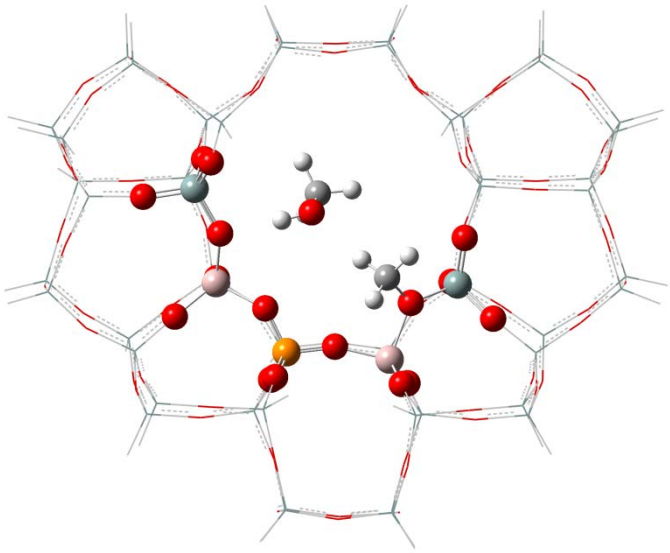


CH_3–Z

Atoms	X	Y	Z
Si	–1.64289	8.03483	0.13066
Si	–1.62568	7.683	–3.21945
O	–3.95904	–3.12148	–2.3724
O	–3.71824	–0.76178	–1.16366
O	–3.79179	0.82351	1.3188
O	–4.06879	–0.58006	3.75468
O	–4.22949	–3.26194	3.03922
O	–4.14648	–2.99199	0.27256
O	–8.33014	–2.81569	–2.67536
O	–8.54555	–0.48989	–1.15353
O	–9.18453	1.0148	1.03846
O	–8.63944	–0.53055	3.3353
O	–8.54618	–3.15356	2.74599
O	–8.46965	–2.93007	0.01512
O	–6.11261	–1.99785	–1.22122
O	–6.3909	–2.02486	4.13122
O	–2.47895	–5.48638	–2.79492
O	–5.09567	–5.48779	–3.20965
O	–7.78834	–5.42173	–3.23508
O	–2.61625	–5.03583	1.57339
O	–5.24411	–5.26197	1.31576
O	–7.95234	–5.33163	1.13507
Si	–3.72734	–4.486	–3.39945
Si	–4.48554	–2.19272	–1.11561
Si	–3.88118	0.93121	3.00053
Si	–4.68736	–2.098	4.19691
Si	–4.03292	–4.09265	1.5809
Si	–8.73376	–4.08401	–3.74156
Si	–7.82836	–2.01401	–1.26167
Si	–9.10077	1.04143	–0.6653
Si	–9.13354	0.98476	2.7378
Si	–8.07905	–2.02332	3.92885
Si	–8.93629	–3.94695	1.29006
O	–7.96317	2.07622	3.30714
O	–5.20992	1.88787	3.49161
O	–2.569	1.85163	3.61005
O	–7.91823	2.15669	–1.15097
O	–5.11901	1.85843	–0.98455
O	–2.26208	1.57738	–1.02863
Si	–6.53986	–6.20736	0.75894
Si	–6.46722	–6.32316	–2.64483
Si	–1.70426	–6.43694	1.26956
Si	–1.70077	–6.82206	–2.08456
O	–6.39872	4.19834	2.5892
O	–6.25031	3.59047	–2.86672
O	–6.36987	4.19896	–0.198
O	–2.09456	4.35983	2.69822
O	–2.00144	6.52226	0.82582
O	–1.90031	7.90707	–1.55306
O	–2.0162	6.08326	–3.6676
O	–2.00949	3.61358	–2.51857
O	–2.12677	3.91559	–0.03161
O	–4.30433	5.21872	1.23235
O	–4.05354	4.38657	–4.29832
Si	–6.53718	2.9161	3.70853
Si	–6.01198	5.09244	1.19502
Si	–5.77149	4.29217	–4.33302
Si	–6.40274	2.90672	–1.31452
Si	–1.71288	3.26895	3.96723
Si	–2.63674	5.01848	1.2492
Si	–2.39333	4.46961	–4.01218
O	–0.01944	3.07216	3.95006
O	–0.09822	2.83268	–1.08091
O	0.02497	8.3171	0.3074
O	0.05324	7.85711	–3.43275
O	–6.46114	–6.33782	–0.94299
O	–1.87639	–6.79423	–0.39051
O	–0.02183	–6.24095	1.48909
O	–0.0143	–6.75843	–2.34136
O	6.47682	4.19586	2.67815
O	6.1483	3.61617	–2.77901
O	6.26826	4.22107	–0.06248
O	2.12018	4.45449	2.87166
O	2.08416	6.64055	0.98193
O	1.9702	7.88233	–1.52663
O	2.18164	6.20222	–3.81752
O	2.06836	3.70508	–2.75392
O	2.21481	4.0105	0.15263
O	4.33672	5.30072	1.47114
O	4.14382	4.41311	–4.47017
O	7.96055	2.008	3.35337
O	5.21358	1.88017	3.39934
O	2.54954	1.89709	3.62847
O	7.6039	2.04898	–1.02419
O	4.84758	1.96357	–0.89926
O	2.25871	1.32293	–1.00316

Si	6.55082	2.87397	3.74748	H	–6.62176	3.43165	5.04824
Si	6.01916	5.15414	1.34493	H	–2.08174	3.82867	5.2401
Si	5.83712	4.31227	–4.31209	H	2.00927	3.72592	5.36994
Si	6.21169	2.99017	–1.21721	H	6.57949	3.29679	5.11944
Si	1.66062	3.30221	4.04058	H	–8.70079	–2.32864	5.19078
Si	2.65207	5.09409	1.3913	H	–4.23855	–2.47976	5.50706
Si	1.707	8.07156	0.15162	H	4.14876	–2.40301	5.42561
Si	1.74373	7.72536	–3.2114	H	8.60331	–2.38521	5.19548
Si	2.46657	4.5553	–4.17757	H	10.44006	1.24375	3.20825
Si	3.80181	0.87369	–0.3427	H	10.35298	–4.41573	1.39416
Si	3.82765	0.99191	2.99147	H	10.1364	1.52708	–1.27117
Si	8.93004	1.05343	–0.65397	H	10.15985	–4.58162	–3.72701
Si	9.11817	0.92611	2.7408	H	–10.4367	1.31752	3.25091
O	6.45	–6.31384	–1.00126	H	–10.3856	1.35269	–1.22726
O	1.85274	–6.83437	–0.38316	H	–10.1354	–4.43192	–3.64268
Si	6.55013	–6.253	0.70239	H	–10.3283	–4.30171	1.26648
Si	6.41942	–6.30345	–2.70405	Al	1.65094	3.11635	–1.19408
Si	1.64603	–6.4942	1.27664	H	–6.51904	–7.66796	–3.15037
Si	1.66368	–6.82914	–2.07653	H	–6.55503	–7.51605	1.35164
O	2.4605	–5.47587	–2.74442	H	–2.22201	–8.04845	–2.62927
O	5.05797	–5.43206	–3.23681	H	2.21148	–8.03008	–2.65094
O	7.75762	–5.43008	–3.29914	H	2.07958	–7.59087	2.10067
O	2.6076	–5.1186	1.58083	H	–2.14805	–7.53183	2.09127
O	5.25622	–5.32534	1.29654	H	6.4363	–7.64582	–3.21575
O	7.95819	–5.37962	1.10319	H	6.57868	–7.57801	1.25439
O	3.96914	–3.09428	–2.4336	H	8.4554	–3.72269	–5.14023
O	4.05833	–0.61298	–0.91722	H	3.37138	–4.08205	–4.75399
O	3.68515	0.89733	1.26667	H	–3.47605	–4.10736	–4.75944
O	4.03483	–0.5697	3.60296	H	–8.41212	–3.72017	–5.1049
O	4.20179	–3.27917	2.97945	H	6.37189	3.45601	–5.3483
O	4.14719	–3.09793	0.27416	H	1.74215	4.13004	–5.34121
O	8.47981	–2.88468	–2.68784	H	–1.62785	3.91973	–5.08865
O	8.53563	–0.52115	–1.15965	H	–6.1587	3.47856	–5.46429
O	9.08569	0.98583	1.04075	H	–6.30614	5.62922	–4.4756
O	8.62244	–0.59267	3.3245	H	–6.63445	6.38585	1.20436
O	8.49895	–3.21407	2.74655	H	6.44608	5.6228	–4.38163
O	8.62505	–2.99465	0.02366	H	6.73047	6.39804	1.30906
O	6.28172	–2.14283	–1.21417	H	2.44952	8.7654	–3.90898
O	6.33219	–2.01627	4.06535	H	2.44366	9.1935	0.66362
Si	3.66058	–4.46539	–3.40356	H	–2.42392	9.08971	0.71099
Si	4.59736	–2.24544	–1.11061	H	–2.37441	8.61932	–4.00956
Si	4.62954	–2.08518	4.11166	P	–1.62689	2.96526	–1.1519
Si	4.01999	–4.18735	1.56367	Al	–3.8249	0.83623	–0.4252
Si	8.78062	–4.15058	–3.79729	C	1.33941	0.22849	–1.40535
Si	7.97393	–2.11084	–1.26615	H	0.37653	0.66585	–1.62917
Si	8.02639	–2.07254	3.91563	H	1.75281	–0.26348	–2.28205
Si	8.97197	–4.02911	1.32727	H	1.2354	–0.46708	–0.57562

Table B12 Coordinates of CH_3–Z/MeOH on P–H^4–ZSM–5, in Å

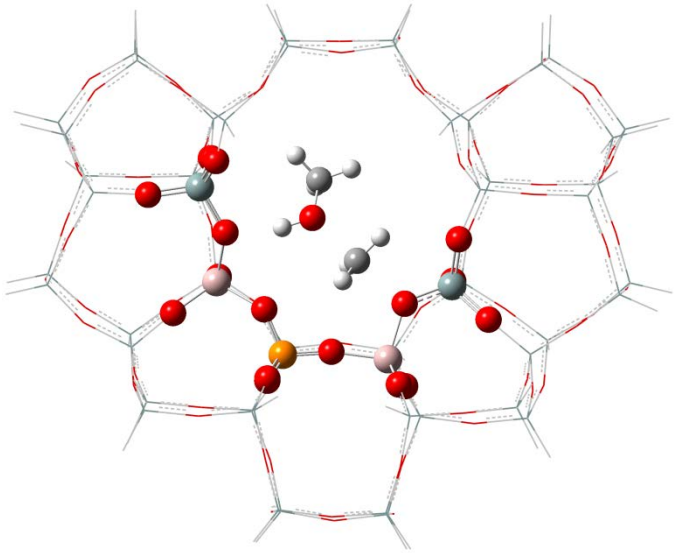


CH_3–Z/MeOH

Atoms	X	Y	Z
Si	–1.68039	7.99411	0.15301
Si	–1.66484	7.65618	–3.19737
O	–3.9103	–3.06699	–2.3763
O	–3.82564	–0.73775	–1.10748
O	–3.81713	0.8407	1.37673
O	–4.08162	–0.60209	3.78978
O	–4.23365	–3.28097	3.03579
O	–4.16316	–3.02012	0.27025
O	–8.36242	–2.84479	–2.71359
O	–8.54097	–0.52154	–1.17346
O	–9.18895	0.97258	1.02524
O	–8.64862	–0.57487	3.31869
O	–8.54405	–3.19829	2.71472
O	–8.51835	–2.97174	–0.01745
O	–6.14446	–2.08146	–1.23936
O	–6.40269	–2.06161	4.12108
O	–2.42994	–5.47178	–2.75548
O	–5.02087	–5.43492	–3.23117
O	–7.7205	–5.42431	–3.298
O	–2.60791	–5.04588	1.58661
O	–5.23452	–5.29495	1.30896
O	–7.9406	–5.36652	1.09006
Si	–3.64024	–4.4404	–3.38362
Si	–4.51044	–2.19853	–1.10395
Si	–3.89655	0.92159	3.06087
Si	–4.69964	–2.12981	4.20195
Si	–4.03355	–4.11598	1.57973
Si	–8.70034	–4.11211	–3.8043
Si	–7.85884	–2.06241	–1.29013
Si	–9.10444	1.0046	–0.67862
Si	–9.14175	0.94178	2.72434
Si	–8.08906	–2.07094	3.90483
Si	–8.94345	–3.99807	1.26433
O	–7.97738	2.03571	3.30245
O	–5.22687	1.87196	3.55995
O	–2.57952	1.83456	3.67128
O	–7.93977	2.14709	–1.14748
O	–5.14915	1.89547	–0.92183
O	–2.29451	1.52821	–1.01509
Si	–6.52052	–6.22917	0.71101
Si	–6.38601	–6.29679	–2.69361
Si	–1.68368	–6.4416	1.29499
Si	–1.66892	–6.82192	–2.05782
O	–6.41373	4.17617	2.63347
O	–6.26082	3.61238	–2.82761
O	–6.42433	4.21613	–0.15433
O	–2.10689	4.33002	2.72752
O	–2.01634	6.46906	0.83199
O	–1.94038	7.87818	–1.53102
O	–2.01685	6.04444	–3.63522
O	–1.99484	3.57004	–2.48938
O	–2.11826	3.85546	0.00012
O	–4.31339	5.17107	1.25585
O	–4.04399	4.34454	–4.26594
Si	–6.56993	2.88676	3.74282
Si	–6.02421	5.08013	1.24667
Si	–5.76264	4.26112	–4.31166
Si	–6.43752	2.92951	–1.27771
Si	–1.72029	3.25519	4.00828
Si	–2.6465	4.9667	1.2684
Si	–2.38388	4.42898	–3.98167
O	–0.0259	3.06825	3.97739
O	–0.10338	2.73016	–1.05189
O	–0.01582	8.29597	0.32999
O	0.0093	7.8699	–3.41375
O	–6.41288	–6.32541	–0.99137
O	–1.84614	–6.80875	–0.3634
O	–0.00205	–6.23627	1.51839
O	0.01926	–6.78043	–2.31117
O	6.4605	4.2184	2.66556
O	6.14173	3.63368	–2.78801
O	6.27895	4.22902	–0.07493
O	2.10566	4.45564	2.8692
O	2.06018	6.63281	0.9804
O	1.9307	7.90086	–1.51108
O	2.14677	6.23694	–3.81021
O	1.99828	3.73391	–2.75817
O	2.18929	4.00051	0.15042
O	4.31879	5.29512	1.44452
O	4.09737	4.42668	–4.44694
O	7.95048	2.03516	3.3383
O	5.2015	1.89346	3.35189
O	2.54028	1.90538	3.61859
O	7.64817	2.07399	–1.05278
O	4.89789	1.94996	–0.91014
O	2.31204	1.34137	–1.10968

Si	6.53124	2.8884	3.72533	H	6.54331	3.29953	5.10107
Si	6.00358	5.16627	1.32483	H	–8.7185	–2.38581	5.16072
Si	5.79328	4.32939	–4.31347	H	–4.26032	–2.52472	5.51152
Si	6.24362	2.99859	–1.23129	H	4.15115	–2.34416	5.42315
Si	1.65351	3.30695	4.0453	H	8.60156	–2.33671	5.2077
Si	2.63397	5.08769	1.38476	H	10.43719	1.28914	3.21255
Si	1.66844	8.07081	0.16931	H	10.37493	–4.38841	1.42484
Si	1.70143	7.75522	–3.19623	H	10.17542	1.5243	–1.27337
Si	2.41884	4.58925	–4.17324	H	10.18554	–4.56888	–3.70776
Si	3.82131	0.87923	–0.3747	H	–10.4469	1.27202	3.23444
Si	3.8096	1.00968	2.95326	H	–10.3909	1.30723	–1.24212
Si	8.96064	1.06764	–0.66017	H	–10.0915	–4.50664	–3.73545
Si	9.12092	0.96075	2.73694	H	–10.3299	–4.37513	1.26417
O	6.48187	–6.30725	–0.97233	Al	1.62786	3.11423	–1.19896
O	1.8808	–6.84405	–0.34649	H	–6.40468	–7.63962	–3.20763
Si	6.58055	–6.24202	0.73111	H	–6.54193	–7.5497	1.27718
Si	6.45266	–6.30357	–2.67526	H	–2.20291	–8.03816	–2.61293
Si	1.66529	–6.49545	1.31022	H	2.25026	–8.04643	–2.60904
Si	1.69565	–6.84575	–2.04058	H	2.09597	–7.58676	2.14285
O	2.49417	–5.493	–2.70858	H	–2.12184	–7.5343	2.12272
O	5.08858	–5.43894	–3.21175	H	6.47649	–7.64758	–3.18222
O	7.78796	–5.42639	–3.27176	H	6.61484	–7.56527	1.28683
O	2.62992	–5.11982	1.60658	H	8.47426	–3.72124	–5.11979
O	5.28402	–5.31683	1.32335	H	3.39228	–4.10446	–4.731
O	7.98444	–5.36065	1.12991	H	–3.34932	–4.0643	–4.73657
O	3.99243	–3.10181	–2.41869	H	–8.36834	–3.71819	–5.15679
O	4.07462	–0.61818	–0.91984	H	6.31139	3.47497	–5.35972
O	3.65168	0.93123	1.22787	H	1.69964	4.17392	–5.3435
O	4.03069	–0.55173	3.55934	H	–1.61368	3.88388	–5.0568
O	4.21779	–3.26838	2.99338	H	–6.1465	3.41667	–5.42107
O	4.16649	–3.10135	0.28928	H	–6.28399	5.59789	–4.49901
O	8.5008	–2.87583	–2.67039	H	–6.61769	6.38669	1.28275
O	8.55358	–0.50819	–1.15143	H	6.39604	5.64224	–4.39305
O	9.10095	1.01615	1.03633	H	6.69926	6.41892	1.28762
O	8.62967	–0.55851	3.32266	H	2.3983	8.80361	–3.88965
O	8.51358	–3.18397	2.76482	H	2.39536	9.19341	0.69317
O	8.6487	–2.97666	0.04306	H	–2.47354	9.03326	0.745
O	6.30295	–2.13811	–1.19522	H	–2.43664	8.57117	–3.98997
O	6.33677	–1.97542	4.06261	P	–1.62838	2.90887	–1.12589
Si	3.68517	–4.48085	–3.37949	Al	–3.8807	0.84327	–0.36457
Si	4.61923	–2.25202	–1.09557	H	1.13558	–0.39982	–1.17739
Si	4.63415	–2.05119	4.10431	C	1.53883	0.33557	–1.86971
Si	4.03972	–4.18633	1.58341	H	0.72251	0.84615	–2.36598
Si	8.80423	–4.14432	–3.77649	H	2.19265	–0.12824	–2.60419
Si	7.99518	–2.09971	–1.25002	H	–2.25086	–2.32303	1.16925
Si	8.03172	–2.03447	3.92219	C	–1.37435	–1.86189	0.7643
Si	8.99305	–4.00609	1.35164	H	–0.50378	–2.3468	1.154
H	–6.69168	3.3975	5.08157	H	–1.3579	–0.82706	1.03591
H	–2.08043	3.82744	5.27785	O	–1.3884	–1.98052	–0.6607
H	2.01735	3.73306	5.36966	H	–2.16943	–1.54574	–1.01077

Table B13 Coordinates of TS2 on P–H[4]–ZSM–5, in Å

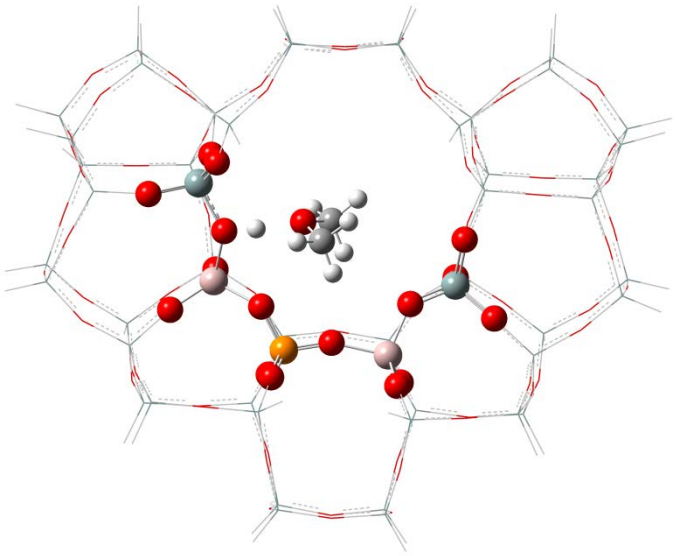


TS2

Atoms	X	Y	Z
Si	–1.60562	8.05237	0.21308
Si	–1.59267	7.74208	–3.14034
O	–3.97857	–3.11209	–2.35707
O	–3.67452	–0.77062	–1.11585
O	–3.77181	0.83926	1.3251
O	–4.09726	–0.58102	3.74543
O	–4.30136	–3.27001	3.04218
O	–4.18241	–2.99097	0.28626
O	–8.28618	–2.72653	–2.74997
O	–8.54404	–0.42643	–1.2029
O	–9.192	1.07911	0.98711
O	–8.68182	–0.49186	3.27301
O	–8.58576	–3.11587	2.66496
O	–8.49292	–2.87581	–0.06091
O	–6.10601	–1.93318	–1.22306
O	–6.45188	–1.99206	4.09247
O	–2.4701	–5.50422	–2.74772
O	–5.04542	–5.43934	–3.27799
O	–7.74048	–5.32672	–3.3411
O	–2.67304	–5.03639	1.5963
O	–5.30396	–5.27032	1.28814
O	–8.00274	–5.29222	1.03726
Si	–3.65424	–4.45134	–3.38793
Si	–4.48601	–2.1791	–1.10612
Si	–3.88355	0.93486	3.00611
Si	–4.75073	–2.08665	4.1836
Si	–4.09842	–4.10402	1.58558
Si	–8.65953	–3.97318	–3.85221
Si	–7.81962	–1.94737	–1.31229
Si	–9.09463	1.10606	–0.71596
Si	–9.14669	1.03668	2.68626
Si	–8.13646	–1.99253	3.86112
Si	–8.97372	–3.89957	1.20242
O	–7.96112	2.10609	3.26643
O	–5.2092	1.90028	3.48829
O	–2.56563	1.8383	3.63136
O	–7.89433	2.20675	–1.19277
O	–5.09942	1.85885	–0.99048
O	–2.25108	1.59289	–1.02796
Si	–6.59675	–6.18182	0.66801
Si	–6.44001	–6.24945	–2.73631
Si	–1.75975	–6.44291	1.31645
Si	–1.734	–6.85829	–2.03246
O	–6.37411	4.21579	2.56575
O	–6.17797	3.60851	–2.88758
O	–6.32271	4.21849	–0.22159
O	–2.08205	4.34927	2.72566
O	–1.95095	6.52182	0.87417
O	–1.86535	7.95175	–1.4722
O	–1.95053	6.13636	–3.59614
O	–1.94185	3.63484	–2.49827
O	–2.06177	3.9167	–0.00909
O	–4.25989	5.21883	1.22324
O	–3.96747	4.43397	–4.28376
Si	–6.5343	2.93572	3.6848
Si	–5.96831	5.10697	1.17508
Si	–5.68355	4.31319	–4.34672
Si	–6.36271	2.926	–1.33789
Si	–1.70541	3.25319	3.99075
Si	–2.59354	5.01303	1.26835
Si	–2.31234	4.52658	–3.97406
O	–0.01034	3.07001	3.96047
O	–0.05454	2.79078	–1.06293
O	0.0599	8.34473	0.39715
O	0.08211	7.95518	–3.3534
O	–6.47202	–6.27306	–1.03305
O	–1.91894	–6.82456	–0.3386
O	–0.07787	–6.24027	1.54208
O	–0.04523	–6.84343	–2.28366
O	6.50455	4.16969	2.66666
O	6.19206	3.62003	–2.78303
O	6.31275	4.18624	–0.06969
O	2.14411	4.46578	2.88406
O	2.13262	6.66561	1.02581
O	2.0043	7.9746	–1.44665
O	2.23203	6.34428	–3.76616
O	2.0492	3.82515	–2.74868
O	2.2391	4.04101	0.16256
O	4.37795	5.29154	1.46667
O	4.16679	4.51443	–4.41556
O	7.95415	1.95769	3.33131
O	5.20223	1.85521	3.29212
O	2.54292	1.8985	3.58446
O	7.68406	2.03316	–1.05608
O	4.93234	1.91365	–0.94167

O	2.33631	1.39934	–1.18469	H	6.53374	3.2121	5.08978
Si	6.53948	2.82322	3.70752	H	–8.77907	–2.3061	5.11062
Si	6.05894	5.12908	1.33021	H	–4.32506	–2.46588	5.50238
Si	5.86001	4.37231	–4.2847	H	4.10097	–2.33467	5.39227
Si	6.28325	2.96305	–1.23393	H	8.55027	–2.42347	5.19027
Si	1.66982	3.30059	4.03563	H	10.43862	1.20064	3.21218
Si	2.69008	5.1094	1.41063	H	10.30068	–4.47042	1.39279
Si	1.7438	8.11648	0.23673	H	10.19435	1.41273	–1.28009
Si	1.77457	7.85141	–3.13326	H	10.10252	–4.62472	–3.74258
Si	2.48989	4.69869	–4.14629	H	–10.4456	1.38804	3.19796
Si	3.81108	0.87525	–0.42953	H	–10.3716	1.43188	–1.28719
Si	3.79426	0.99552	2.89621	H	–10.0659	–4.31347	–3.80546
Si	8.96806	0.98985	–0.66556	H	–10.3685	–4.24308	1.17143
Si	9.12231	0.88005	2.73152	Al	1.66986	3.18023	–1.19879
O	6.39466	–6.35467	–1.00144	H	–6.50976	–7.59212	–3.24629
O	1.80822	–6.87773	–0.31439	H	–6.64635	–7.50352	1.22943
Si	6.48873	–6.28939	0.70214	H	–2.28322	–8.07336	–2.57506
Si	6.36485	–6.34612	–2.70439	H	2.19716	–8.09156	–2.5673
Si	1.58927	–6.50447	1.3363	H	2.01803	–7.58227	2.1873
Si	1.63086	–6.89139	–2.00936	H	–2.20624	–7.525	2.15354
O	2.42137	–5.53831	–2.68643	H	6.38366	–7.68857	–3.21571
O	5.00242	–5.47462	–3.23397	H	6.50553	–7.61261	1.25877
O	7.70277	–5.47295	–3.30091	H	8.39033	–3.76374	–5.14491
O	2.55547	–5.12429	1.60747	H	3.27531	–4.14604	–4.72465
O	5.20194	–5.34818	1.29037	H	–3.33087	–4.05443	–4.72699
O	7.90196	–5.42466	1.10437	H	–8.2938	–3.5847	–5.19762
O	3.9217	–3.13409	–2.43276	H	6.3564	3.5381	–5.35762
O	4.03086	–0.63068	–0.96907	H	1.77241	4.30303	–5.32509
O	3.62296	0.93123	1.17147	H	–1.52667	4.00296	–5.0496
O	4.00376	–0.56793	3.502	H	–6.03768	3.49173	–5.48313
O	4.16934	–3.28898	2.97338	H	–6.233	5.6427	–4.50281
O	4.10185	–3.11415	0.27323	H	–6.57867	6.40624	1.18122
O	8.4296	–2.92787	–2.69242	H	6.49354	5.6724	–4.32567
O	8.51391	–0.57214	–1.15919	H	6.7768	6.36906	1.28966
O	9.10951	0.93692	1.03078	H	2.4645	8.91336	–3.81283
O	8.62014	–0.63692	3.31391	H	2.47363	9.22863	0.77854
O	8.45232	–3.25624	2.74254	H	–2.39413	9.09015	0.81359
O	8.57829	–3.04359	0.02092	H	–2.36211	8.66629	–3.92465
O	6.2396	–2.17501	–1.21537	P	–1.58036	2.96159	–1.13566
O	6.2968	–2.00893	4.03966	Al	–3.80384	0.84407	–0.42086
Si	3.5944	–4.51932	–3.37791	H	0.7907	0.01255	–1.57362
Si	4.55412	–2.27488	–1.11822	C	1.58603	0.52428	–2.11578
Si	4.59313	–2.06346	4.07208	H	1.17299	1.16799	–2.89059
Si	3.97358	–4.20358	1.5636	H	2.28045	–0.18185	–2.56246
Si	8.72293	–4.1935	–3.80431	H	–1.06683	–2.8986	0.40621
Si	7.93195	–2.15456	–1.2675	C	–0.59609	–1.91777	0.25416
Si	7.99071	–2.10322	3.90464	H	0.48378	–2.02598	0.40355
Si	8.9213	–4.07808	1.32572	H	–0.98755	–1.22039	1.00633
H	–6.63167	3.45353	5.02284	O	–0.79435	–1.43567	–1.06912
H	–2.06942	3.80532	5.26815	H	–1.73475	–1.19372	–1.17748
H	2.03261	3.69975	5.36866				

Table B14 Coordinates of DME/H^{4}Z onP–H^4–ZSM–5, in Å

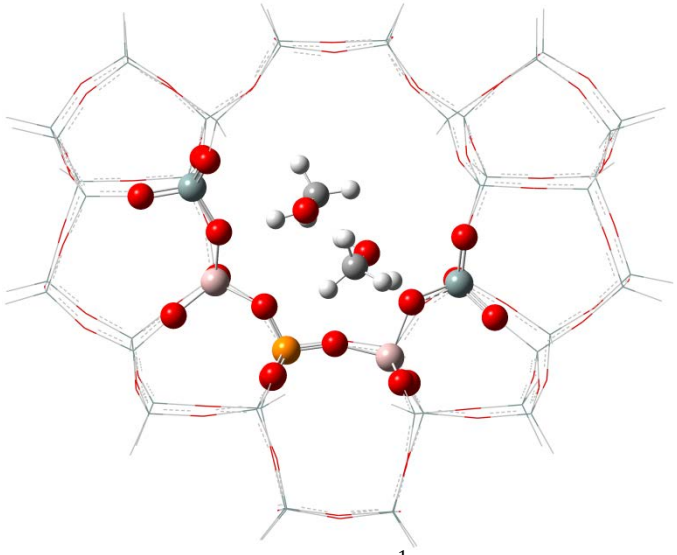


DME/H^{4}Z

Atoms	X	Y	Z
Si	–1.60642	8.05062	0.20987
Si	–1.59612	7.73781	–3.1434
O	–3.98344	–3.11031	–2.35745
O	–3.67906	–0.76929	–1.11587
O	–3.77321	0.83986	1.32576
O	–4.0972	–0.58072	3.74601
O	–4.30202	–3.26919	3.04197
O	–4.18773	–2.98981	0.28603
O	–8.29194	–2.72809	–2.74779
O	–8.54873	–0.42628	–1.20233
O	–9.19028	1.08185	0.9874
O	–8.68205	–0.49086	3.27269
O	–8.5875	–3.11569	2.66739
O	–8.49586	–2.87482	–0.05824
O	–6.11074	–1.93179	–1.2235
O	–6.45242	–1.99114	4.09291
O	–2.47199	–5.50118	–2.74975
O	–5.04824	–5.43847	–3.27707
O	–7.7441	–5.3282	–3.33854
O	–2.6728	–5.03275	1.59298
O	–5.30412	–5.271	1.28957
O	–8.00351	–5.29134	1.03934
Si	–3.65795	–4.44934	–3.38824
Si	–4.49081	–2.17752	–1.1062
Si	–3.88399	0.93536	3.00687
Si	–4.75129	–2.0862	4.18382
Si	–4.09983	–4.10285	1.58507
Si	–8.66628	–3.97622	–3.84808
Si	–7.82441	–1.94733	–1.31131
Si	–9.09518	1.10784	–0.71582
Si	–9.14636	1.0381	2.68652
Si	–8.13709	–1.99117	3.86206
Si	–8.97546	–3.89945	1.20486
O	–7.96106	2.10671	3.26874
O	–5.20918	1.90083	3.49008
O	–2.56552	1.83853	3.63134
O	–7.89333	2.20606	–1.19415
O	–5.09679	1.86408	–0.99043
O	–2.24971	1.59075	–1.02656
Si	–6.59789	–6.18135	0.66975
Si	–6.44207	–6.24931	–2.7346
Si	–1.75941	–6.43944	1.31405
Si	–1.73373	–6.85433	–2.0349
O	–6.37354	4.2171	2.56979
O	–6.17779	3.61408	–2.88455
O	–6.32691	4.21846	–0.21713
O	–2.08218	4.34904	2.72494
O	–1.95174	6.5208	0.87258
O	–1.86726	7.94861	–1.47516
O	–1.95504	6.1321	–3.59835
O	–1.93924	3.63177	–2.4984
O	–2.062	3.91543	–0.0095
O	–4.2605	5.21809	1.22356
O	–3.96425	4.41924	–4.28853
Si	–6.53427	2.93611	3.68771
Si	–5.96908	5.10755	1.17822
Si	–5.68027	4.29813	–4.35246
Si	–6.36294	2.92844	–1.33629
Si	–1.70491	3.25336	3.99016
Si	–2.59416	5.01211	1.26746
Si	–2.31025	4.52071	–3.97572
O	–0.00984	3.07025	3.95929
O	–0.05346	2.78913	–1.0606
O	0.05929	8.34268	0.39266
O	0.07862	7.9499	–3.35791
O	–6.47304	–6.27199	–1.03132
O	–1.91787	–6.82159	–0.34096
O	–0.07755	–6.23693	1.54008
O	–0.04503	–6.83733	–2.28663
O	6.50422	4.17132	2.67034
O	6.19327	3.6246	–2.78017
O	6.31666	4.18498	–0.06601
O	2.14428	4.46657	2.88205
O	2.13395	6.66585	1.0226
O	2.00206	7.97154	–1.45205
O	2.22942	6.34035	–3.77095
O	2.04866	3.82265	–2.75005
O	2.24047	4.04094	0.16106
O	4.37898	5.29176	1.46536
O	4.16659	4.51072	–4.41639
O	7.95448	1.95933	3.33243
O	5.20258	1.85578	3.29263
O	2.54336	1.89931	3.58391
O	7.68254	2.03025	–1.05783
O	4.93203	1.91575	–0.94126

O	2.33722	1.3983	–1.18448	H	6.53314	3.2109	5.09242
Si	6.53937	2.82367	3.70972	H	–8.77931	–2.30329	5.11214
Si	6.06025	5.12939	1.33239	H	–4.32562	–2.46607	5.50243
Si	5.85968	4.36637	–4.2867	H	4.10118	–2.33512	5.39237
Si	6.28395	2.96414	–1.23255	H	8.5506	–2.42156	5.19172
Si	1.67023	3.30172	4.03408	H	10.43886	1.2021	3.2125
Si	2.69114	5.10984	1.40878	H	10.30238	–4.47035	1.39637
Si	1.74318	8.11507	0.23144	H	10.19507	1.41752	–1.27802
Si	1.77124	7.84744	–3.13845	H	10.1062	–4.62643	–3.74016
Si	2.48942	4.69454	–4.14864	H	–10.4456	1.38928	3.19744
Si	3.81233	0.87564	–0.42922	H	–10.3721	1.43571	–1.28605
Si	3.79482	0.99579	2.89657	H	–10.072	–4.31841	–3.7973
Si	8.96927	0.99124	–0.66487	H	–10.37	–4.24398	1.17419
Si	9.12235	0.88153	2.73236	Al	1.67064	3.1791	–1.19934
O	6.39701	–6.35416	–0.99972	H	–6.51105	–7.59215	–3.24422
O	1.80791	–6.87473	–0.31707	H	–6.64822	–7.50315	1.23091
Si	6.49068	–6.28893	0.70389	H	–2.28169	–8.06986	–2.57777
Si	6.36753	–6.34603	–2.70266	H	2.19593	–8.08775	–2.57067
Si	1.58945	–6.50178	1.33376	H	2.01782	–7.58003	2.18438
Si	1.63099	–6.88723	–2.01208	H	–2.20631	–7.5213	2.15123
O	2.42365	–5.53481	–2.68795	H	6.38586	–7.68858	–3.21373
O	5.00559	–5.474	–3.23255	H	6.50796	–7.61215	1.26049
O	7.70597	–5.47355	–3.29906	H	8.39478	–3.76506	–5.1432
O	2.55647	–5.12216	1.60476	H	3.28144	–4.1441	–4.72552
O	5.20318	–5.34841	1.29167	H	–3.33613	–4.05172	–4.72749
O	7.90343	–5.42364	1.10652	H	–8.30458	–3.58818	–5.19469
O	3.92652	–3.13229	–2.43317	H	6.35304	3.52394	–5.35461
O	4.03397	–0.62996	–0.9689	H	1.77305	4.29689	–5.32745
O	3.62407	0.93108	1.1718	H	–1.52053	3.99945	–5.04946
O	4.00401	–0.56748	3.5029	H	–6.03274	3.46227	–5.47884
O	4.17021	–3.28823	2.97304	H	–6.22924	5.62563	–4.52642
O	4.10609	–3.11322	0.27289	H	–6.57846	6.40727	1.18491
O	8.4337	–2.92856	–2.69096	H	6.49526	5.6651	–4.33754
O	8.52041	–0.57234	–1.15841	H	6.7779	6.36949	1.2919
O	9.10893	0.93832	1.03162	H	2.46001	8.90962	–3.81886
O	8.62019	–0.63527	3.31519	H	2.47279	9.22838	0.77121
O	8.45336	–3.25499	2.74423	H	–2.39421	9.08919	0.80997
O	8.58172	–3.04323	0.02268	H	–2.36587	8.66193	–3.9275
O	6.24432	–2.17344	–1.2145	P	–1.57927	2.95957	–1.13491
O	6.29722	–2.00797	4.04046	Al	–3.80454	0.8453	–0.4202
Si	3.59867	–4.51737	–3.37834	H	0.42607	0.19613	–0.78192
Si	4.55887	–2.27363	–1.1182	C	0.24281	–0.58142	–1.5236
Si	4.59356	–2.06317	4.07241	H	–0.14086	0.07323	–2.30434
Si	3.97542	–4.20266	1.56299	H	1.01871	–1.17552	–1.99828
Si	8.72681	–4.19463	–3.8024	H	–1.06149	–2.89901	0.41035
Si	7.93677	–2.15416	–1.26641	C	–0.59909	–1.91439	0.25748
Si	7.9912	–2.10177	3.90591	H	0.48123	–2.01282	0.41027
Si	8.92322	–4.07745	1.32806	H	–0.99878	–1.21885	1.0069
H	–6.63172	3.45271	5.0262	O	–0.79787	–1.43687	–1.06742
H	–2.06835	3.80572	5.26764	H	–1.73873	–1.19766	–1.17698
H	2.03301	3.70176	5.36686				

Table B15 Coordinates of $(MeOH)_2/H^1Z$ on P–H^1–ZSM–5, in Å

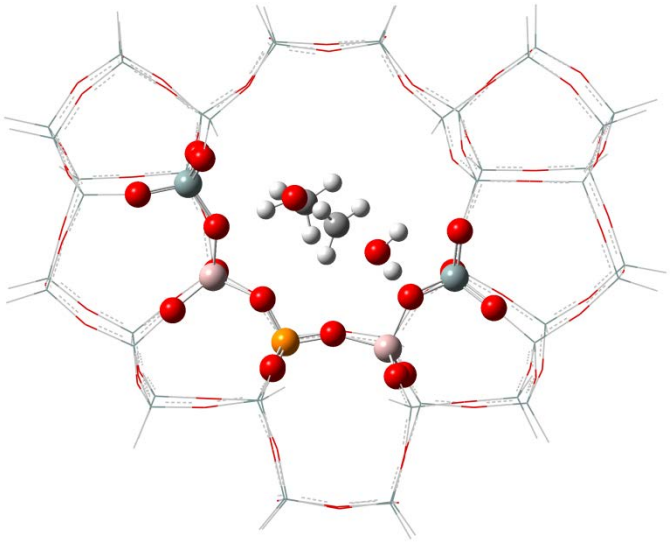


$(MeOH)_2/H^1Z$

Atoms	X	Y	Z
Si	–1.49325	8.02695	0.21529
Si	–1.48345	7.70468	–3.13313
O	–4.10782	–3.06658	–2.32705
O	–3.69606	–0.77979	–1.03064
O	–3.78505	0.87932	1.33959
O	–4.13544	–0.53893	3.73442
O	–4.41024	–3.22742	3.06408
O	–4.32533	–2.98393	0.32207
O	–8.36899	–2.59929	–2.71797
O	–8.60916	–0.27875	–1.19074
O	–9.193	1.25878	0.98719
O	–8.71741	–0.32197	3.27163
O	–8.69382	–2.95388	2.69204
O	–8.58842	–2.72955	–0.03118
O	–6.19245	–1.8159	–1.18648
O	–6.52862	–1.87989	4.09826
O	–2.61012	–5.43375	–2.76327
O	–5.22222	–5.39521	–3.21541
O	–7.9058	–5.21823	–3.2843
O	–2.82152	–5.0283	1.62041
O	–5.47247	–5.24259	1.34282
O	–8.16908	–5.15476	1.07932
Si	–3.83607	–4.41214	–3.37039
Si	–4.59661	–2.14978	–1.0592
Si	–3.89291	0.98793	3.02417
Si	–4.83174	–2.0192	4.19317
Si	–4.24577	–4.09875	1.62536
Si	–8.78877	–3.84433	–3.80624
Si	–7.90991	–1.80988	–1.2845
Si	–9.10691	1.27767	–0.71589
Si	–9.14663	1.21856	2.68694
Si	–8.21425	–1.82988	3.87667
Si	–9.10228	–3.73517	1.23487
O	–7.93312	2.25686	3.26325
O	–5.19335	1.98225	3.50701
O	–2.53174	1.82864	3.63354
O	–7.86956	2.32525	–1.21413
O	–5.09369	1.8936	–1.00451
O	–2.23058	1.53475	–1.02293
Si	–6.80103	–6.10504	0.72435
Si	–6.63525	–6.17939	–2.67847
Si	–1.86183	–6.39513	1.29945
Si	–1.84531	–6.77867	–2.05444
O	–6.28954	4.30976	2.52745
O	–6.10663	3.64796	–2.92972
O	–6.23777	4.29417	–0.25921
O	–1.98953	4.31021	2.71771
O	–1.82245	6.48506	0.86455
O	–1.76789	7.92262	–1.46749
O	–1.84261	6.09369	–3.57934
O	–1.87123	3.56888	–2.50097
O	–1.94329	3.85344	–0.01282
O	–4.12796	5.19597	1.18327
O	–3.84999	4.39827	–4.30176
Si	–6.48955	3.06205	3.67347
Si	–5.83633	5.17368	1.13263
Si	–5.56423	4.31443	–4.39326
Si	–6.32012	3.00264	–1.37095
Si	–1.62326	3.22066	3.9905
Si	–2.46172	4.97573	1.24867
Si	–2.19535	4.48773	–3.97237
O	0.06181	2.99219	3.95186
O	0.00694	2.62556	–1.10032
O	0.16447	8.34275	0.4062
O	0.18639	7.93558	–3.34179
O	–6.6682	–6.20104	–0.97605
O	–2.03168	–6.74907	–0.3613
O	–0.1846	–6.14212	1.50705
O	–0.16015	–6.71627	–2.31526
O	6.56156	4.10804	2.70693
O	6.3214	3.57121	–2.73388
O	6.43416	4.11886	–0.0275
O	2.18381	4.43318	2.87674
O	2.2265	6.66276	1.05174
O	2.10766	7.97792	–1.43118
O	2.34285	6.34282	–3.75669
O	2.08292	3.82636	–2.73633
O	2.21888	4.04381	0.15065
O	4.42471	5.20262	1.46422
O	4.26627	4.49003	–4.35141
O	8.02991	1.87992	3.34998
O	5.28447	1.79037	3.38085
O	2.61577	1.84644	3.56985
O	7.86099	1.99096	–1.04376
O	5.12088	1.81258	–0.88805
O	2.47924	1.4372	–1.14085

Si	6.62932	2.76403	3.74715	H	–4.41315	–2.39904	5.51362
Si	6.10916	5.0546	1.35986	H	4.11361	–2.42453	5.40768
Si	5.95871	4.35395	–4.21102	H	8.57229	–2.53692	5.19876
Si	6.42939	2.88992	–1.19234	H	10.4921	1.06371	3.26315
Si	1.74627	3.24829	4.01777	H	10.25649	–4.63155	1.39827
Si	2.72905	5.07386	1.39466	H	10.33535	1.22974	–1.234
Si	1.85187	8.10932	0.25315	H	10.0554	–4.76972	–3.74138
Si	1.88255	7.84188	–3.11773	H	–10.4365	1.59933	3.19946
Si	2.58286	4.68418	–4.11384	H	–10.3757	1.63728	–1.28387
Si	3.8607	0.88622	–0.43529	H	–10.2038	–4.14203	–3.74795
Si	3.89009	0.94475	2.90951	H	–10.5052	–4.04139	1.19784
Si	9.07669	0.88081	–0.63742	Al	1.75598	3.07871	–1.20631
Si	9.17563	0.77421	2.76137	H	–6.72921	–7.51853	–3.19174
O	6.30999	–6.40775	–1.00501	H	–6.90296	–7.42113	1.29012
O	1.68319	–6.80043	–0.3485	H	–2.37593	–7.99916	–2.60226
Si	6.40938	–6.35132	0.69978	H	2.06436	–7.99441	–2.61766
Si	6.27419	–6.37362	–2.70612	H	1.88111	–7.53004	2.14826
Si	1.48252	–6.4336	1.30677	H	–2.27092	–7.50525	2.11849
Si	1.51789	–6.7933	–2.04341	H	6.24408	–7.70861	–3.23649
O	2.31611	–5.43524	–2.70353	H	6.40522	–7.67945	1.24536
O	4.92401	–5.46443	–3.21193	H	8.37545	–3.84046	–5.14001
O	7.62539	–5.53017	–3.3093	H	3.24697	–4.08903	–4.72295
O	2.47547	–5.0753	1.57965	H	–3.55189	–4.00283	–4.7147
O	5.12435	–5.40567	1.2864	H	–8.41295	–3.48067	–5.15544
O	7.83257	–5.51002	1.10861	H	6.46153	3.55173	–5.30691
O	3.84978	–3.07368	–2.43124	H	1.89501	4.32104	–5.32256
O	4.04408	–0.6481	–0.99422	H	–1.41159	3.96039	–5.04678
O	3.76721	0.85887	1.19507	H	–5.91982	3.47165	–5.51382
O	4.04336	–0.62007	3.54528	H	–6.09148	5.64804	–4.58445
O	4.15226	–3.32659	2.97543	H	–6.39269	6.49669	1.12979
O	4.08545	–3.14249	0.2559	H	6.58264	5.66028	–4.23172
O	8.44513	–3.01597	–2.6827	H	6.80464	6.30935	1.34229
O	8.5656	–0.66736	–1.13427	H	2.55579	8.91676	–3.79496
O	9.19765	0.8156	1.06123	H	2.57512	9.22511	0.79712
O	8.64352	–0.73841	3.3354	H	–2.30277	9.04462	0.82315
O	8.44829	–3.36172	2.75215	H	–2.26545	8.61234	–3.92524
O	8.57807	–3.15108	0.0278	P	–1.50252	2.88662	–1.14666
O	6.26358	–2.26679	–1.22442	Al	–3.82247	0.88247	–0.40281
O	6.31427	–2.11206	4.06156	H	1.93855	0.51445	–2.2467
Si	3.55063	–4.46842	–3.37293	C	0.4939	–0.7059	–2.01324
Si	4.57774	–2.27695	–1.10996	H	–0.05801	0.11367	–1.58187
Si	4.61014	–2.12624	4.09436	H	1.01389	–1.27655	–1.26076
Si	3.93846	–4.21634	1.55558	H	–0.14437	–1.33436	–2.61242
Si	8.69414	–4.28359	–3.80029	O	1.47808	–0.14743	–2.88061
Si	7.9574	–2.23571	–1.25572	H	2.15261	–0.80555	–3.10657
Si	8.00727	–2.20285	3.91866	H	–0.06189	–1.97981	1.15795
Si	8.89109	–4.19219	1.33354	C	–0.93825	–1.38577	0.88535
H	–6.58031	3.60333	5.00209	H	–1.79005	–1.68907	1.49662
H	–1.98626	3.7787	5.26559	H	–0.73591	–0.3222	1.05033
H	2.09053	3.64647	5.35688	O	–1.22414	–1.65148	–0.49661
H	6.66724	3.16015	5.1276	H	–2.1292	–1.28882	–0.73311
H	–8.86039	–2.11412	5.1308				

Table B16 Coordinates of TS on P–H[1]–ZSM–5, in Å

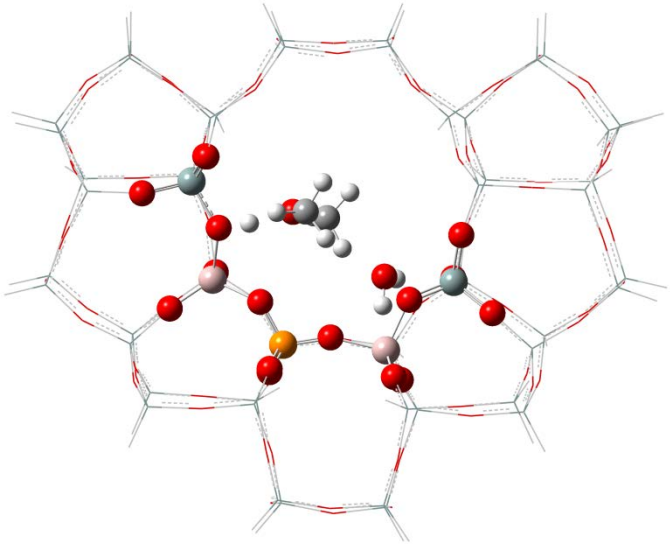


TS

Atoms	X	Y	Z
Si	–1.52801	7.94344	0.08315
Si	–1.46533	7.56408	–3.26053
O	–4.27233	–3.00025	–2.3911
O	–4.13789	–0.7413	–1.01617
O	–3.84116	0.97454	1.38252
O	–4.22936	–0.494	3.75567
O	–4.51044	–3.16859	3.0022
O	–4.55071	–3.1093	0.21103
O	–8.72738	–2.6554	–2.71558
O	–8.69874	–0.26636	–1.21618
O	–9.24634	1.29034	0.95888
O	–8.80214	–0.27809	3.26234
O	–8.82357	–2.94007	2.71398
O	–8.88868	–2.72246	–0.00267
O	–6.49511	–2.02284	–1.22714
O	–6.62618	–1.84995	4.07234
O	–2.65766	–5.31784	–2.7871
O	–5.32183	–5.32275	–3.249
O	–8.02003	–5.23733	–3.30089
O	–2.89502	–4.98037	1.60083
O	–5.59935	–5.24583	1.38523
O	–8.30304	–5.15062	1.09141
Si	–3.9249	–4.3464	–3.40629
Si	–4.87971	–2.19517	–1.09898
Si	–3.95101	1.03979	3.07157
Si	–4.92934	–1.992	4.16505
Si	–4.3591	–4.09889	1.59516
Si	–9.00661	–3.93183	–3.81492
Si	–8.19812	–1.87578	–1.30145
Si	–9.16748	1.29888	–0.74491
Si	–9.1997	1.26438	2.658
Si	–8.31375	–1.79386	3.86564
Si	–9.27345	–3.75796	1.28619
O	–7.97963	2.30356	3.2252
O	–5.24383	2.04149	3.55817
O	–2.57006	1.86035	3.67271
O	–7.93097	2.35859	–1.23283
O	–5.12179	2.03189	–0.95679
O	–2.28939	1.45499	–1.02397
Si	–6.9207	–6.08428	0.72423
Si	–6.70732	–6.13708	–2.68134
Si	–1.85358	–6.28323	1.25605
Si	–1.82066	–6.63151	–2.10666
O	–6.30187	4.36845	2.56113
O	–6.1603	3.72672	–2.90762
O	–6.33301	4.36597	–0.23619
O	–1.95841	4.28766	2.65493
O	–1.82503	6.40389	0.7469
O	–1.7657	7.82081	–1.60367
O	–1.80163	5.9408	–3.67224
O	–1.86563	3.44737	–2.54183
O	–1.95954	3.77588	–0.06087
O	–4.14153	5.18627	1.15221
O	–3.87874	4.32474	–4.32392
Si	–6.55146	3.10933	3.68739
Si	–5.85552	5.21252	1.15189
Si	–5.59871	4.32585	–4.39056
Si	–6.39226	3.07498	–1.35275
Si	–1.62053	3.23679	3.96746
Si	–2.48173	4.91421	1.18552
Si	–2.21752	4.33785	–4.02399
O	0.06831	2.98987	3.93034
O	0.01304	2.54216	–1.12344
O	0.12347	8.28674	0.29292
O	0.20631	7.81423	–3.44807
O	–6.77055	–6.16229	–0.97799
O	–1.9845	–6.62519	–0.41072
O	–0.16723	–6.05397	1.49424
O	–0.1271	–6.62291	–2.3858
O	6.57533	4.15449	2.66221
O	6.37735	3.56367	–2.7927
O	6.42762	4.1706	–0.07633
O	2.19806	4.41934	2.85078
O	2.21102	6.6683	1.01296
O	2.09875	7.89684	–1.50866
O	2.38961	6.24432	–3.80704
O	2.18038	3.7526	–2.76375
O	2.2254	4.06123	0.12621
O	4.42313	5.23409	1.43776
O	4.31999	4.4176	–4.43775
O	8.08815	1.95918	3.34816
O	5.34627	1.83828	3.37949
O	2.66778	1.85919	3.55611
O	7.8902	2.02837	–1.01112
O	5.13253	1.88681	–0.93396
O	2.51367	1.43401	–1.02765
Si	6.67895	2.83489	3.73104

Si	6.10895	5.09958	1.32108	H	–4.51099	–2.39787	5.47764
Si	6.01533	4.29291	–4.30055	H	4.20065	–2.42575	5.39045
Si	6.47565	2.9391	–1.23141	H	8.65846	–2.46593	5.2185
Si	1.75169	3.23758	3.99488	H	10.55446	1.1528	3.28703
Si	2.72653	5.09286	1.3828	H	10.41373	–4.59399	1.47659
Si	1.81297	8.08427	0.16591	H	10.40294	1.39717	–1.20944
Si	1.89676	7.74778	–3.19697	H	10.30661	–4.7907	–3.63753
Si	2.63809	4.59299	–4.17434	H	–10.4841	1.67638	3.16106
Si	4.02301	0.86219	–0.39472	H	–10.435	1.6684	–1.31046
Si	3.96353	0.96086	2.94224	H	–10.3938	–4.34423	–3.78261
Si	9.16634	0.97076	–0.61909	H	–10.6647	–4.11363	1.32755
Si	9.24353	0.85017	2.78014	Al	1.73342	3.1242	–1.22537
O	6.48281	–6.36456	–0.97931	H	–6.76579	–7.48413	–3.1815
O	1.71207	–6.66629	–0.40607	H	–7.02426	–7.41228	1.26351
Si	6.55519	–6.30132	0.72574	H	–2.34459	–7.85766	–2.65124
Si	6.48005	–6.36705	–2.68191	H	2.08238	–7.90249	–2.64711
Si	1.50231	–6.31554	1.25083	H	1.9036	–7.42271	2.07859
Si	1.55304	–6.67923	–2.10151	H	–2.23585	–7.41924	2.05357
O	2.47184	–5.39277	–2.76243	H	6.47207	–7.71214	–3.18522
O	5.1496	–5.4599	–3.24064	H	6.52918	–7.62458	1.28118
O	7.86105	–5.5368	–3.24842	H	8.66236	–3.88566	–5.09304
O	2.57364	–5.01377	1.53695	H	3.49012	–4.09598	–4.77324
O	5.27604	–5.33591	1.291	H	–3.63624	–3.96862	–4.75892
O	7.98496	–5.46882	1.15242	H	–8.64697	–3.52639	–5.15703
O	4.16487	–3.12939	–2.46066	H	6.52265	3.45398	–5.36462
O	4.2518	–0.67726	–0.96959	H	1.92794	4.19133	–5.35533
O	3.88612	0.87151	1.2136	H	–1.46572	3.76645	–5.09879
O	4.14599	–0.59665	3.56432	H	–6.00817	3.48592	–5.49433
O	4.24724	–3.27885	2.93339	H	–6.04855	5.6844	–4.60464
O	4.29397	–3.1178	0.21767	H	–6.35851	6.5571	1.1703
O	8.68995	–2.99888	–2.66079	H	6.63279	5.6002	–4.35876
O	8.74227	–0.59897	–1.12524	H	6.79823	6.35665	1.29348
O	9.27374	0.90519	1.07912	H	2.57878	8.8153	–3.87632
O	8.71549	–0.66339	3.35432	H	2.51571	9.22468	0.68467
O	8.58075	–3.30029	2.77469	H	–2.35643	8.95996	0.66631
O	8.79082	–3.10481	0.06486	H	–2.23848	8.45081	–4.08398
O	6.52655	–2.20769	–1.22162	P	–1.52104	2.77969	–1.17177
O	6.40982	–2.07902	4.05549	Al	–3.93919	0.90718	–0.37111
Si	3.75857	–4.48577	–3.42075	H	1.78678	0.65714	–1.07583
Si	4.85418	–2.30896	–1.15293	C	0.00366	–2.28635	–1.17909
Si	4.70564	–2.11667	4.08342	H	–0.06799	–1.20601	–1.19189
Si	4.05003	–4.17993	1.51949	H	0.05428	–2.98603	–0.33172
Si	8.94827	–4.30394	–3.73822	H	–0.07409	–2.85534	–2.12062
Si	8.21399	–2.19925	–1.2432	O	1.72931	–0.922	–1.15293
Si	8.10537	–2.14491	3.9303	H	2.65184	–1.30338	–1.18626
Si	9.05081	–4.15433	1.3782	H	–1.10932	–1.62862	1.71573
H	–6.68463	3.64406	5.01539	C	–2.02398	–1.37839	1.15332
H	–1.95102	3.85543	5.22316	H	–2.86659	–1.93358	1.58551
H	2.10463	3.64394	5.32896	H	–2.29969	–0.30252	1.21656
H	6.70903	3.25914	5.10259	O	–1.82408	–1.73483	–0.20594
H	–8.94256	–2.05468	5.13398	H	–2.59559	–1.39313	–0.76022

Table B17 Coordinates of DME/H[1]Z on P–H[1]–ZSM–5, in Å

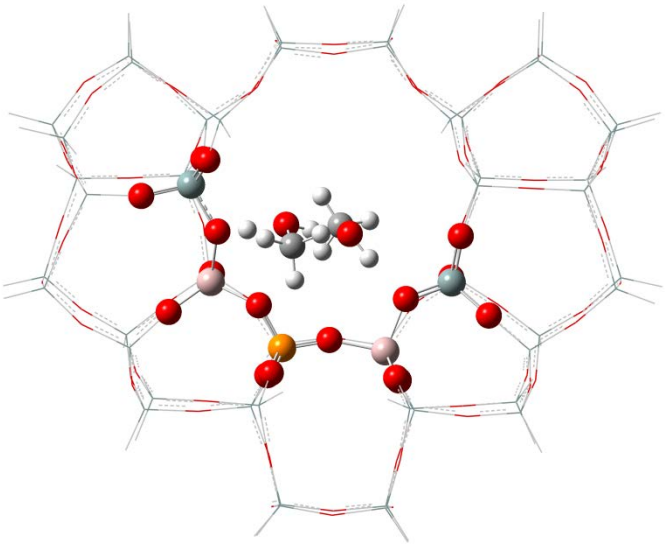


DME/H[1]Z

Atoms	X	Y	Z
Si	–1.57609	7.92934	0.09204
Si	–1.52756	7.54166	–3.24818
O	–4.20428	–2.99454	–2.34752
O	–3.98038	–0.74253	–0.97239
O	–3.88053	0.96399	1.40058
O	–4.20324	–0.53612	3.77123
O	–4.4148	–3.2157	3.03539
O	–4.50746	–3.01786	0.29566
O	–8.62846	–2.70916	–2.70405
O	–8.67685	–0.29863	–1.23711
O	–9.24559	1.20611	0.96854
O	–8.74782	–0.36093	3.25637
O	–8.74594	–3.00466	2.70059
O	–8.79246	–2.76185	–0.02063
O	–6.4001	–1.93664	–1.24033
O	–6.56665	–1.9271	4.08253
O	–2.54075	–5.2387	–2.83297
O	–5.19878	–5.32053	–3.26288
O	–7.88696	–5.27346	–3.30472
O	–2.8316	–4.97972	1.55464
O	–5.50177	–5.28225	1.38431
O	–8.18924	–5.17806	1.05265
Si	–3.84118	–4.29637	–3.41778
Si	–4.79509	–2.16187	–1.066
Si	–3.97364	1.00674	3.09146
Si	–4.86997	–2.04251	4.18936
Si	–4.29136	–4.10753	1.60469
Si	–8.89586	–3.98319	–3.8093
Si	–8.11846	–1.88675	–1.30818
Si	–9.17473	1.25014	–0.73478
Si	–9.19281	1.17411	2.66775
Si	–8.25355	–1.86855	3.86844
Si	–9.17999	–3.80528	1.26128
O	–7.99268	2.23154	3.23697
O	–5.26655	1.99181	3.60695
O	–2.58465	1.81495	3.67917
O	–7.94235	2.31286	–1.21222
O	–5.13481	2.01866	–0.9344
O	–2.28785	1.41371	–0.99473
Si	–6.81586	–6.12082	0.70012
Si	–6.56664	–6.16515	–2.69974
Si	–1.80906	–6.28819	1.1786
Si	–1.7194	–6.58562	–2.18978
O	–6.32136	4.30583	2.56761
O	–6.20894	3.67319	–2.91189
O	–6.36434	4.33811	–0.2276
O	–1.98276	4.24727	2.65921
O	–1.87416	6.38296	0.74434
O	–1.83242	7.80319	–1.5922
O	–1.85573	5.91266	–3.65425
O	–1.90018	3.40169	–2.53338
O	–1.95455	3.74538	–0.05214
O	–4.15891	5.11285	1.16683
O	–3.91556	4.27073	–4.29816
Si	–6.58054	3.06144	3.70381
Si	–5.86763	5.16509	1.16859
Si	–5.6299	4.24824	–4.40113
Si	–6.417	3.04797	–1.3452
Si	–1.63831	3.1999	3.97169
Si	–2.49196	4.88194	1.18825
Si	–2.25117	4.30733	–4.00649
O	0.04099	2.93224	3.9284
O	–0.01826	2.47424	–1.13655
O	0.07266	8.27364	0.30967
O	0.13935	7.79608	–3.44867
O	–6.61952	–6.17302	–0.99659
O	–1.90551	–6.59129	–0.49654
O	–0.14297	–6.00667	1.44314
O	–0.03387	–6.52478	–2.4576
O	6.51983	4.17427	2.64872
O	6.3583	3.56204	–2.80542
O	6.42565	4.23151	–0.10502
O	2.13873	4.40219	2.84571
O	2.14997	6.61629	0.99841
O	2.02789	7.87116	–1.50522
O	2.31645	6.21886	–3.79578
O	2.14056	3.70121	–2.7404
O	2.13166	3.97274	0.13017
O	4.35166	5.18767	1.39812
O	4.23796	4.39033	–4.4275
O	8.04667	1.98774	3.35174
O	5.30719	1.84602	3.40431
O	2.62301	1.8282	3.55522
O	7.90348	2.08551	–1.02454
O	5.14936	1.91485	–0.86647

O	2.52522	1.36481	–1.10878	H	–8.89184	–2.13735	5.13
Si	6.63209	2.86212	3.72375	H	–4.44487	–2.44619	5.50036
Si	6.04135	5.113	1.30385	H	4.19209	–2.40506	5.43785
Si	5.93325	4.27748	–4.30279	H	8.65685	–2.41141	5.22633
Si	6.46433	2.9636	–1.2298	H	10.51006	1.16592	3.32706
Si	1.72385	3.21456	3.99177	H	10.32933	–4.65601	1.5112
Si	2.65671	5.02817	1.34581	H	10.41347	1.44718	–1.18351
Si	1.7629	8.04446	0.17321	H	10.38134	–4.79392	–3.43328
Si	1.83301	7.72435	–3.19402	H	–10.4858	1.54212	3.18228
Si	2.55742	4.55773	–4.14381	H	–10.4481	1.61312	–1.28971
Si	3.95177	0.90834	–0.42974	H	–10.2753	–4.41888	–3.76202
Si	3.93868	0.96639	2.91888	H	–10.5657	–4.18261	1.29005
Si	9.1659	1.03458	–0.60505	Al	1.72937	2.96703	–1.222
Si	9.2055	0.8813	2.79188	H	–6.59098	–7.51344	–3.19685
O	6.30442	–6.28254	–0.98555	H	–6.93604	–7.45233	1.22492
O	1.73942	–6.58345	–0.44262	H	–2.24266	–7.79437	–2.77109
Si	6.46176	–6.25936	0.7172	H	2.15892	–7.85238	–2.67313
Si	6.49713	–6.29033	–2.67979	H	1.93697	–7.38228	2.03362
Si	1.5286	–6.26828	1.21966	H	–2.20748	–7.44454	1.93808
Si	1.64051	–6.61938	–2.14098	H	6.53991	–7.63706	–3.17929
O	2.53302	–5.31669	–2.7858	H	6.46438	–7.59711	1.23853
O	5.19206	–5.39387	–3.31622	H	8.84931	–3.88477	–5.00453
O	7.9075	–5.46595	–3.15939	H	3.5171	–3.99842	–4.78423
O	2.51987	–4.91361	1.51992	H	–3.58407	–3.86121	–4.75905
O	5.19712	–5.31129	1.34035	H	–8.55112	–3.56559	–5.15102
O	7.89019	–5.42399	1.1246	H	6.43165	3.4405	–5.37467
O	4.17511	–3.05323	–2.44553	H	1.83367	4.18037	–5.32681
O	4.22266	–0.61633	–0.99925	H	–1.51136	3.73703	–5.09003
O	3.84261	0.89536	1.20287	H	–6.01416	3.37055	–5.48473
O	4.10807	–0.58411	3.58025	H	–6.10583	5.59095	–4.65322
O	4.19445	–3.24513	2.97721	H	–6.36571	6.51094	1.20671
O	4.2614	–3.03892	0.24464	H	6.53706	5.59124	–4.38723
O	8.74906	–2.94511	–2.58929	H	6.68681	6.39492	1.31539
O	8.74947	–0.54456	–1.09814	H	2.50306	8.80035	–3.87207
O	9.26336	0.95173	1.0938	H	2.47105	9.17928	0.69744
O	8.6736	–0.64276	3.33788	H	–2.41484	8.93468	0.68034
O	8.53619	–3.2989	2.80521	H	–2.31724	8.41446	–4.07154
O	8.7877	–3.06749	0.10683	P	–1.52723	2.74694	–1.16473
O	6.52186	–2.17953	–1.18096	Al	–3.93336	0.92093	–0.34706
O	6.38441	–2.06696	4.08967	H	1.81602	0.07908	–1.55929
Si	3.81368	–4.3923	–3.43764	C	–0.47463	–1.41834	–0.82773
Si	4.83867	–2.21761	–1.12151	H	–0.63436	–0.5221	–1.4084
Si	4.68075	–2.08742	4.12657	H	0.35318	–1.36934	–0.14529
Si	4.01373	–4.10455	1.53497	H	–0.3096	–2.2263	–1.52586
Si	9.04562	–4.27174	–3.62494	O	1.53883	–0.81494	–1.95135
Si	8.21587	–2.14029	–1.19169	H	2.31152	–1.38812	–1.81562
Si	8.07857	–2.11652	3.94221	H	–0.59298	–1.43431	1.66514
Si	8.99001	–4.14978	1.40189	C	–1.63248	–1.39273	1.32903
H	–6.73923	3.60619	5.02453	H	–2.21592	–2.14853	1.86677
H	–1.98304	3.80994	5.22802	H	–2.05218	–0.39462	1.48066
H	2.05614	3.62706	5.33	O	–1.67402	–1.68933	–0.07907
H	6.67519	3.30096	5.09143	H	–2.51664	–1.31665	–0.48352

Table B18 Coordinates of $(MeOH)_2/H^4Z$ on P–H^4–ZSM–5, in Å

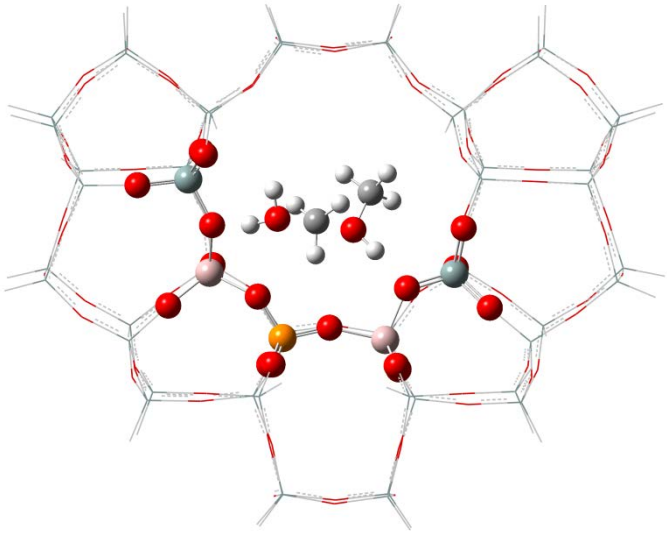


$(MeOH)_2/H^4Z$

Atoms	X	Y	Z
Si	–1.72993	8.03443	0.21874
Si	–1.74045	7.72354	–3.12979
O	–3.99826	–3.1668	–2.33318
O	–3.67846	–0.80246	–1.19054
O	–3.83889	0.73659	1.33745
O	–4.07489	–0.63954	3.7746
O	–4.22029	–3.29983	3.07934
O	–4.10076	–2.97843	0.32976
O	–8.21785	–2.78892	–2.6684
O	–8.58305	–0.51511	–1.09201
O	–9.23575	0.96043	1.10421
O	–8.64842	–0.61186	3.36177
O	–8.50975	–3.23129	2.74925
O	–8.42471	–2.98262	0.02964
O	–6.0929	–1.94341	–1.13309
O	–6.39411	–2.08774	4.16368
O	–2.39939	–5.5049	–2.68609
O	–4.98432	–5.50056	–3.24621
O	–7.66648	–5.37294	–3.28131
O	–2.53438	–5.01125	1.62322
O	–5.16818	–5.27204	1.27792
O	–7.86394	–5.38269	1.10993
Si	–3.60109	–4.51017	–3.35968
Si	–4.51116	–2.28476	–1.07226
Si	–3.88682	0.87451	3.03119
Si	–4.69211	–2.14808	4.24682
Si	–3.97101	–4.11604	1.62703
Si	–8.58165	–4.01981	–3.79694
Si	–7.82236	–2.00963	–1.21557
Si	–9.18184	1.00243	–0.59732
Si	–9.15204	0.91648	2.80442
Si	–8.08132	–2.10332	3.9509
Si	–8.88069	–4.02665	1.29198
O	–7.96733	2.00042	3.35206
O	–5.22236	1.82084	3.50993
O	–2.55661	1.77929	3.59342
O	–8.01443	2.12037	–1.11242
O	–5.24294	1.75935	–0.96284
O	–2.37894	1.55987	–1.04984
Si	–6.44603	–6.23882	0.71101
Si	–6.37413	–6.31843	–2.69609
Si	–1.58751	–6.4078	1.35994
Si	–1.60873	–6.8452	–1.98152
O	–6.41726	4.12213	2.59653
O	–6.31439	3.50369	–2.85756
O	–6.40819	4.13541	–0.17792
O	–2.10475	4.28169	2.71703
O	–2.05665	6.49544	0.88148
O	–2.02229	7.92474	–1.46122
O	–2.13175	6.12059	–3.58564
O	–2.02478	3.59353	–2.50691
O	–2.11248	3.86386	–0.0142
O	–4.30268	5.09827	1.23913
O	–4.08638	4.33321	–4.2335
Si	–6.5447	2.85759	3.73349
Si	–6.00731	5.02403	1.21241
Si	–5.79784	4.23008	–4.30621
Si	–6.49713	2.85771	–1.29874
Si	–1.68	3.19061	3.97203
Si	–2.62367	4.96189	1.27129
Si	–2.4238	4.50265	–3.96501
O	0.004	2.99587	3.94635
O	–0.1449	2.6722	–1.09575
O	–0.07372	8.3576	0.38636
O	–0.07122	7.91796	–3.35741
O	–6.36819	–6.31712	–0.99352
O	–1.79824	–6.79216	–0.28946
O	0.08592	–6.18484	1.56438
O	0.06829	–6.79997	–2.25394
O	6.43625	4.29848	2.64742
O	6.11392	3.69326	–2.79017
O	6.23861	4.27695	–0.09227
O	2.06551	4.47993	2.87333
O	1.99258	6.69276	1.0326
O	1.85317	7.96849	–1.46798
O	2.05665	6.27653	–3.76547
O	1.95106	3.75633	–2.72284
O	2.06515	4.07174	0.14727
O	4.25056	5.33502	1.43083
O	4.04865	4.52816	–4.42356
O	8.00361	2.14144	3.29474
O	5.2645	1.94439	3.40342
O	2.60336	1.90615	3.61016
O	7.68052	2.17533	–1.09493
O	4.92839	1.94633	–0.90552
O	2.29605	1.39874	–0.96561

Si	6.57869	2.97716	3.70952	H	–4.2462	–2.52573	5.55708
Si	5.93601	5.21454	1.29627	H	4.27766	–2.36005	5.42686
Si	5.74517	4.4288	–4.28655	H	8.73688	–2.2444	5.15739
Si	6.2198	3.02858	–1.23954	H	10.48312	1.39929	3.14592
Si	1.68823	3.28533	4.0233	H	10.4495	–4.27207	1.32548
Si	2.56328	5.12324	1.37371	H	10.19304	1.56733	–1.33798
Si	1.61513	8.12601	0.21647	H	10.207	–4.48777	–3.7454
Si	1.62792	7.79188	–3.15056	H	–10.4457	1.24026	3.34408
Si	2.36963	4.62511	–4.11691	H	–10.4771	1.2791	–1.14923
Si	3.75718	0.92745	–0.39352	H	–9.98847	–4.35501	–3.76792
Si	3.90492	1.03067	2.95393	H	–10.2645	–4.40676	1.24943
Si	8.96966	1.14343	–0.71548	Al	1.62887	3.03514	–1.17427
Si	9.16364	1.06402	2.68017	H	–6.45789	–7.65848	–3.20516
O	6.56212	–6.29078	–0.96731	H	–6.43689	–7.55727	1.27802
O	1.92582	–6.83808	–0.30191	H	–2.17027	–8.0564	–2.51942
Si	6.67733	–6.18669	0.73384	H	2.2817	–8.07893	–2.54636
Si	6.51999	–6.27864	–2.6695	H	2.164	–7.54491	2.19512
Si	1.76038	–6.45154	1.35189	H	–2.04079	–7.47303	2.21422
Si	1.75551	–6.85713	–1.99676	H	6.56559	–7.62455	–3.1733
O	2.5309	–5.51744	–2.70003	H	6.73614	–7.50286	1.30685
O	5.12474	–5.46048	–3.20035	H	8.47584	–3.68515	–5.15314
O	7.82951	–5.3799	–3.28739	H	3.41331	–4.16086	–4.7265
O	2.71968	–5.07767	1.62814	H	–3.28778	–4.06713	–4.68496
O	5.36177	–5.28851	1.32596	H	–8.1877	–3.60696	–5.12598
O	8.07141	–5.28183	1.10741	H	6.26392	3.61906	–5.36928
O	4.00751	–3.10623	–2.43036	H	1.65172	4.23145	–5.29971
O	4.05125	–0.58598	–0.9348	H	–1.66821	3.99267	–5.06742
O	3.76294	0.908	1.24949	H	–6.15873	3.40753	–5.44012
O	4.1148	–0.51717	3.61823	H	–6.35834	5.55587	–4.44617
O	4.31524	–3.22434	2.98638	H	–6.6152	6.3234	1.22504
O	4.21652	–3.0903	0.25491	H	6.33603	5.74992	–4.34173
O	8.50735	–2.80474	–2.71307	H	6.60333	6.48457	1.25434
O	8.54512	–0.43277	–1.19945	H	2.30499	8.84826	–3.85319
O	9.13958	1.095	0.98091	H	2.33143	9.25914	0.73325
O	8.69758	–0.45883	3.28349	H	–2.54501	9.04432	0.83244
O	8.61575	–3.09199	2.71938	H	–2.52102	8.64408	–3.90842
O	8.65978	–2.89348	–0.01192	P	–1.6474	2.91332	–1.15213
O	6.2959	–2.10814	–1.25621	Al	–3.89607	0.86042	–0.38092
O	6.44421	–1.93653	4.05782	H	–2.73464	–0.89474	–1.69981
Si	3.72619	–4.49539	–3.36701	H	–1.25404	0.56249	–3.59342
Si	4.60606	–2.1924	–1.12817	C	–1.32723	–0.52918	–3.64121
Si	4.74206	–2.01869	4.11121	H	–0.42078	–0.93461	–4.10175
Si	4.13361	–4.13567	1.57375	H	–2.19178	–0.80903	–4.24799
Si	8.81964	–4.07966	–3.80397	H	1.17987	–0.92551	1.15576
Si	7.98161	–2.02103	–1.29923	C	0.24879	–0.82605	0.58793
Si	8.13637	–1.94704	3.88374	H	–0.32804	0.01998	0.97996
Si	9.06127	–3.9049	1.29039	H	–0.33673	–1.74241	0.70306
H	–6.62034	3.37723	5.07095	O	0.52871	–0.66714	–0.80501
H	–2.07977	3.71704	5.24983	H	1.1373	0.10628	–0.92961
H	1.99507	3.71132	5.36335	O	–1.50645	–1.09462	–2.34059
H	6.63587	3.40646	5.07991	H	–0.70814	–0.88066	–1.75577
H	–8.7137	–2.4318	5.20038				

Table B19 Coordinates of TS on P–H^4–ZSM–5, in Å

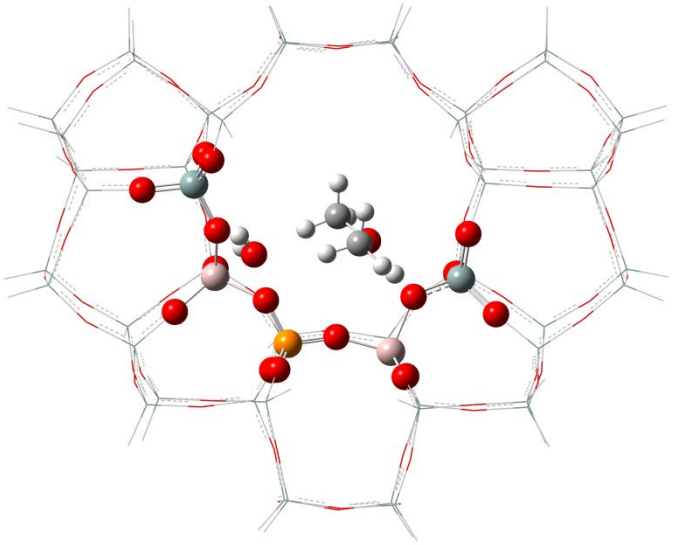


TS

Atoms	X	Y	Z
Si	–1.9223	7.94803	0.16243
Si	–1.91579	7.63258	–3.18429
O	–3.83216	–3.12316	–2.37829
O	–3.74214	–0.80853	–1.14993
O	–3.91064	0.71731	1.3794
O	–4.10109	–0.7317	3.77231
O	–4.16637	–3.39013	3.03429
O	–4.05301	–3.05945	0.28792
O	–8.1538	–2.91239	–2.77289
O	–8.56668	–0.66789	–1.15957
O	–9.27593	0.75628	1.0519
O	–8.65493	–0.81611	3.29242
O	–8.45056	–3.42431	2.64591
O	–8.38499	–3.15203	–0.0716
O	–6.06313	–2.08171	–1.20281
O	–6.37927	–2.25285	4.101
O	–2.22898	–5.43782	–2.76287
O	–4.80888	–5.44418	–3.34261
O	–7.48909	–5.44997	–3.42599
O	–2.44214	–5.06986	1.56441
O	–5.06766	–5.36607	1.20105
O	–7.75234	–5.541	0.97664
Si	–3.43034	–4.44885	–3.4394
Si	–4.48461	–2.37493	–1.09928
Si	–3.94452	0.8097	3.08068
Si	–4.67814	–2.26469	4.21313
Si	–3.8914	–4.20096	1.58666
Si	–8.45845	–4.13143	–3.93297
Si	–7.7972	–2.15387	–1.30118
Si	–9.223	0.82253	–0.648
Si	–9.19662	0.70615	2.75275
Si	–8.06313	–2.30251	3.86854
Si	–8.80758	–4.21837	1.18557
O	–8.04768	1.81998	3.31429
O	–5.31071	1.70934	3.56043
O	–2.63619	1.7355	3.64664
O	–8.09939	1.99175	–1.14453
O	–5.33172	1.73487	–0.93167
O	–2.45103	1.45991	–1.08095
Si	–6.30689	–6.34849	0.57683
Si	–6.16541	–6.34256	–2.83056
Si	–1.4719	–6.44705	1.27
Si	–1.4618	–6.80832	–2.08014
O	–6.53035	3.98668	2.60735
O	–6.42276	3.43232	–2.86031
O	–6.56792	4.05959	–0.16437
O	–2.20955	4.20698	2.68578
O	–2.21227	6.39963	0.82267
O	–2.2121	7.82804	–1.51704
O	–2.26194	6.01708	–3.63495
O	–2.13058	3.49646	–2.54281
O	–2.22123	3.75697	–0.04901
O	–4.42308	4.96595	1.225
O	–4.19383	4.21063	–4.26937
Si	–6.66195	2.71825	3.7387
Si	–6.1272	4.9149	1.23787
Si	–5.90352	4.10804	–4.3351
Si	–6.61328	2.79623	–1.30154
Si	–1.75983	3.16347	3.97179
Si	–2.7396	4.85824	1.2316
Si	–2.5294	4.39382	–4.0083
O	–0.07752	2.9839	3.94208
O	–0.22366	2.6069	–1.1402
O	–0.27754	8.31597	0.33986
O	–0.25436	7.88396	–3.40471
O	–6.1869	–6.35773	–1.12825
O	–1.67913	–6.78151	–0.39143
O	0.19605	–6.21697	1.48685
O	0.21507	–6.77986	–2.33571
O	6.29482	4.37773	2.62096
O	6.04008	3.75823	–2.81105
O	6.1455	4.33777	–0.11912
O	1.93998	4.48643	2.82122
O	1.82429	6.69899	0.98872
O	1.6623	7.98673	–1.50826
O	1.91775	6.30707	–3.81194
O	1.82018	3.78461	–2.77516
O	1.92903	4.08349	0.09024
O	4.10552	5.36961	1.37039
O	3.94339	4.58271	–4.43378
O	7.91053	2.25926	3.28179
O	5.17454	1.99248	3.36641
O	2.52673	1.91457	3.55276
O	7.67997	2.29612	–1.12278
O	4.94397	1.94872	–0.93247
O	2.31344	1.44881	–1.05956
Si	6.45905	3.05754	3.68141

Si	5.79453	5.2754	1.25689	H	–4.23888	–2.65374	5.5217
Si	5.64067	4.495	–4.29854	H	4.26024	–2.32575	5.38603
Si	6.18179	3.08631	–1.26472	H	8.71967	–2.09902	5.16995
Si	1.60793	3.28542	3.97774	H	10.40766	1.57335	3.17151
Si	2.42063	5.13455	1.31659	H	10.52059	–4.09791	1.3627
Si	1.41852	8.12568	0.17666	H	10.1991	1.70293	–1.31609
Si	1.44833	7.80652	–3.19198	H	10.34879	–4.33927	–3.6934
Si	2.25713	4.6581	–4.15817	H	–10.5018	0.98659	3.2886
Si	3.72633	0.95086	–0.45687	H	–10.5262	1.05113	–1.20267
Si	3.83806	1.05251	2.8946	H	–9.84974	–4.52525	–3.92306
Si	8.96721	1.27411	–0.71353	H	–10.1799	–4.63659	1.1425
Si	9.1031	1.20847	2.6854	Al	1.55409	3.01442	–1.23299
O	6.71096	–6.22378	–0.962	H	–6.17125	–7.677	–3.35917
O	2.0476	–6.84519	–0.36784	H	–6.27437	–7.68572	1.09568
Si	6.80324	–6.10353	0.73981	H	–2.04524	–7.99293	–2.65241
Si	6.69091	–6.21096	–2.66423	H	2.41782	–8.08123	–2.61313
Si	1.87753	–6.46165	1.28665	H	2.28266	–7.55492	2.12887
Si	1.90204	–6.85493	–2.06456	H	–1.92768	–7.5373	2.09053
O	2.67848	–5.51577	–2.76227	H	6.77082	–7.55625	–3.16615
O	5.28253	–5.42786	–3.21409	H	6.88548	–7.41517	1.32088
O	7.98615	–5.28381	–3.26876	H	8.62216	–3.58477	–5.13221
O	2.81138	–5.07514	1.56936	H	3.5825	–4.16631	–4.78055
O	5.45712	–5.23665	1.30911	H	–3.11157	–3.96075	–4.74608
O	8.17067	–5.16404	1.12398	H	–8.06523	–3.6758	–5.24761
O	4.10048	–3.08655	–2.47285	H	6.16184	3.69769	–5.38991
O	4.04931	–0.56786	–0.98706	H	1.56485	4.26948	–5.35818
O	3.72995	0.9262	1.19209	H	–1.77585	3.88862	–5.11334
O	4.07429	–0.48635	3.57467	H	–6.27283	3.24549	–5.43606
O	4.35263	–3.19056	2.94929	H	–6.4682	5.42713	–4.51442
O	4.27877	–3.06905	0.20667	H	–6.72532	6.21765	1.28872
O	8.59514	–2.6895	–2.69685	H	6.21648	5.82328	–4.35394
O	8.56803	–0.3102	–1.19586	H	6.43542	6.55966	1.21961
O	9.10977	1.23347	0.98601	H	2.09352	8.88685	–3.88843
O	8.66385	–0.32356	3.28726	H	2.10199	9.27499	0.70234
O	8.64438	–2.95912	2.7352	H	–2.76957	8.93256	0.77427
O	8.71387	–2.76479	0.00258	H	–2.72464	8.52474	–3.96751
O	6.35042	–2.03598	–1.27452	P	–1.72009	2.82847	–1.19329
O	6.43275	–1.85007	4.0458	Al	–3.97193	0.89556	–0.32175
Si	3.87578	–4.48169	–3.41214	H	–2.89351	–0.788	–1.62115
Si	4.6603	–2.15043	–1.1666	H	–0.54234	–1.9654	–1.28152
Si	4.73179	–1.9698	4.0765	C	–0.40543	–1.10673	–1.9051
Si	4.20713	–4.10209	1.53394	H	0.27436	–1.34522	–2.69625
Si	8.95379	–3.96198	–3.775	H	–0.91948	–0.19543	–1.68111
Si	8.03341	–1.90789	–1.29469	H	2.42827	–0.89782	0.67237
Si	8.12606	–1.81944	3.88879	C	1.45283	–0.46017	0.71576
Si	9.12476	–3.76204	1.3123	H	1.50889	0.48792	1.20859
H	–6.79381	3.23324	5.07337	H	0.7958	–1.10644	1.25939
H	–2.16509	3.72093	5.23466	O	0.95238	–0.27863	–0.61146
H	1.93105	3.71811	5.31224	H	1.54066	0.30256	–1.09906
H	6.49629	3.48808	5.05255	O	–1.83531	–1.56893	–3.13096
H	–8.7032	–2.66491	5.10437	H	–2.48466	–2.26473	–3.00526

Table B20 Coordinates of DME/H[1]Z on P–H[1]–ZSM–5, in Å



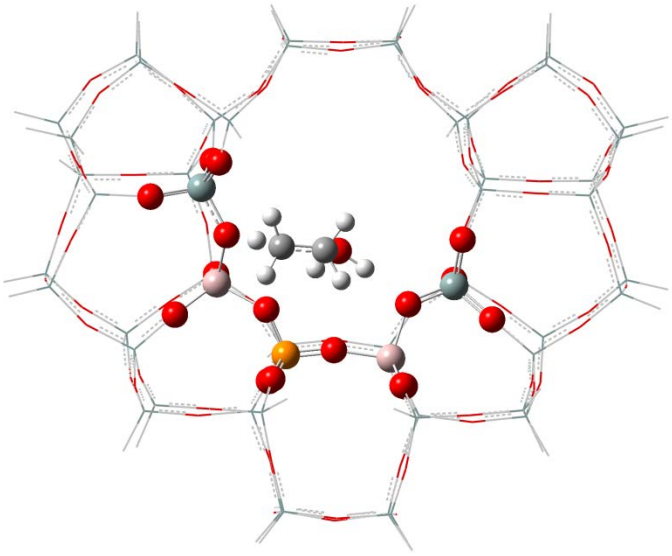
DME/H[1]Z

Atoms	X	Y	Z
Si	–1.58125	8.00798	0.14708
Si	–1.58596	7.62456	–3.19834
O	–4.08629	–3.07626	–2.35267
O	–3.83824	–0.70606	–1.18269
O	–3.79934	0.81278	1.37167
O	–4.05552	–0.56395	3.82194
O	–4.26302	–3.22022	3.0779
O	–4.18661	–2.92845	0.30322
O	–8.43229	–2.7373	–2.59585
O	–8.59867	–0.40373	–1.06829
O	–9.17265	1.1178	1.12445
O	–8.62661	–0.44379	3.40842
O	–8.57744	–3.07713	2.83034
O	–8.57398	–2.85631	0.09967
O	–6.20887	–1.96963	–1.14255
O	–6.4033	–1.97327	4.20173
O	–2.54498	–5.45325	–2.70476
O	–5.15426	–5.46167	–3.16976
O	–7.85227	–5.33255	–3.18657
O	–2.65126	–4.96968	1.60451
O	–5.28631	–5.19852	1.34278
O	–7.99963	–5.25232	1.20433
Si	–3.78302	–4.4592	–3.33616
Si	–4.57909	–2.15019	–1.08224
Si	–3.85228	0.9385	3.05478
Si	–4.70121	–2.07206	4.25835
Si	–4.07238	–4.033	1.60978
Si	–8.80325	–3.99606	–3.68497
Si	–7.92504	–1.94724	–1.1777
Si	–9.11142	1.14362	–0.58032
Si	–9.09954	1.08343	2.82264
Si	–8.092	–1.94473	4.00419
Si	–8.99443	–3.87868	1.38648
O	–7.90422	2.15366	3.37999
O	–5.1557	1.92188	3.55956
O	–2.50916	1.83175	3.6363
O	–7.9199	2.24285	–1.08022
O	–5.13292	1.92271	–0.90192
O	–2.27536	1.53137	–0.97919
Si	–6.59746	–6.13383	0.80493
Si	–6.54728	–6.25844	–2.59957
Si	–1.74465	–6.38213	1.33743
Si	–1.76055	–6.79421	–2.01023
O	–6.30582	4.25333	2.65696
O	–6.22999	3.64766	–2.80457
O	–6.34461	4.2774	–0.12857
O	–2.00771	4.33032	2.72525
O	–1.9017	6.48544	0.84077
O	–1.85194	7.87047	–1.53315
O	–1.96723	6.01703	–3.62369
O	–1.93479	3.54744	–2.48209
O	–2.02116	3.86287	0.00201
O	–4.20041	5.19834	1.25566
O	–3.99242	4.32574	–4.25257
Si	–6.46496	2.9737	3.77599
Si	–5.9115	5.14315	1.2615
Si	–5.70916	4.23895	–4.30659
Si	–6.40056	2.98677	–1.24533
Si	–1.63933	3.24126	3.99875
Si	–2.53391	4.98194	1.26733
Si	–2.32983	4.39952	–3.97478
O	0.05381	3.04525	3.98443
O	–0.05061	2.66405	–1.0589
O	0.08133	8.32246	0.31948
O	0.08981	7.82373	–3.41591
O	–6.53646	–6.26342	–0.89756
O	–1.92315	–6.77036	–0.31512
O	–0.06098	–6.18495	1.54622
O	–0.07585	–6.72937	–2.27905
O	6.53481	4.19312	2.69504
O	6.22047	3.59981	–2.75452
O	6.34875	4.20083	–0.04234
O	2.16521	4.46989	2.89174
O	2.15324	6.66657	1.00513
O	2.01926	7.88941	–1.51632
O	2.238	6.20563	–3.80283
O	2.06485	3.71632	–2.72254
O	2.20361	4.03829	0.17353
O	4.37982	5.2699	1.47018
O	4.17724	4.37927	–4.41885
O	8.03868	2.0006	3.35505
O	5.2984	1.87265	3.43233
O	2.63033	1.91346	3.65085
O	7.7205	2.04014	–1.02349
O	4.97121	1.92398	–0.86551
O	2.37008	1.37731	–0.96931
Si	6.63534	2.87211	3.76301

Si	6.06445	5.13768	1.35546	H	–4.25182	–2.47672	5.5611
Si	5.87302	4.29029	–4.28193	H	4.17729	–2.40239	5.45655
Si	6.31567	2.96708	–1.19604	H	8.63655	–2.40579	5.21447
Si	1.73069	3.31035	4.06291	H	10.50113	1.18834	3.22277
Si	2.68914	5.10607	1.40568	H	10.33982	–4.47061	1.40104
Si	1.7651	8.08749	0.16219	H	10.22749	1.40719	–1.26505
Si	1.78296	7.72441	–3.1991	H	10.12036	–4.64416	–3.70565
Si	2.49929	4.55081	–4.1436	H	–10.39	1.43653	3.35412
Si	3.87501	0.87594	–0.31817	H	–10.3976	1.47551	–1.12732
Si	3.90498	0.99983	3.01844	H	–10.2025	–4.35912	–3.61231
Si	9.0018	0.9912	–0.64439	H	–10.3823	–4.24972	1.39802
Si	9.17544	0.89141	2.75191	Al	1.67209	3.1033	–1.16183
O	6.41738	–6.35476	–0.95108	H	–6.63022	–7.60365	–3.09973
O	1.79761	–6.81337	–0.32734	H	–6.61196	–7.44297	1.39676
Si	6.51887	–6.27914	0.75206	H	–2.28767	–8.01701	–2.55677
Si	6.38295	–6.35131	–2.65349	H	2.13217	–8.03209	–2.58773
Si	1.6037	–6.46339	1.33206	H	2.02277	–7.56345	2.15888
Si	1.60296	–6.81981	–2.01992	H	–2.19123	–7.45641	2.184
O	2.41205	–5.47985	–2.70026	H	6.3962	–7.69605	–3.15917
O	5.01828	–5.484	–3.18622	H	6.53805	–7.59985	1.31483
O	7.71779	–5.48083	–3.25926	H	8.41022	–3.78653	–5.11275
O	2.58117	–5.09796	1.62798	H	3.3512	–4.12313	–4.71604
O	5.22944	–5.33997	1.33792	H	–3.50211	–4.07912	–4.69084
O	7.93303	–5.41248	1.14437	H	–8.46362	–3.60894	–5.03758
O	3.95411	–3.12095	–2.40626	H	6.39624	3.4355	–5.3257
O	4.0734	–0.62189	–0.89042	H	1.78415	4.12676	–5.3139
O	3.7734	0.90449	1.29535	H	–1.56139	3.86917	–5.05825
O	4.08289	–0.56409	3.63583	H	–6.09232	3.35723	–5.38705
O	4.20892	–3.27408	3.01058	H	–6.22937	5.56841	–4.54429
O	4.12885	–3.11157	0.29862	H	–6.48193	6.45992	1.29667
O	8.45458	–2.93325	–2.66594	H	6.47253	5.60451	–4.36557
O	8.54148	–0.57005	–1.13735	H	6.75776	6.39218	1.31985
O	9.15312	0.9365	1.05134	H	2.46916	8.77289	–3.90351
O	8.65358	–0.61708	3.341	H	2.49684	9.21706	0.66421
O	8.51613	–3.24208	2.76894	H	–2.37977	9.04624	0.7336
O	8.60856	–3.04061	0.04333	H	–2.34746	8.54419	–3.99625
O	6.26684	–2.17694	–1.19304	P	–1.57047	2.88494	–1.11887
O	6.36157	–2.03655	4.09205	Al	–3.86153	0.86391	–0.369
Si	3.63627	–4.49854	–3.36195	H	–3.09573	–0.37606	–2.91105
Si	4.57997	–2.26094	–1.08822	H	–0.44121	–0.27655	–3.4341
Si	4.65854	–2.08664	4.14215	C	0.58767	–0.58957	–3.23095
Si	4.00738	–4.18577	1.60012	H	0.72802	–1.62684	–3.56202
Si	8.74272	–4.20695	–3.76914	H	1.2963	0.05617	–3.75323
Si	7.95839	–2.15184	–1.244	H	–0.03951	–2.24345	–1.21218
Si	8.05501	–2.09408	3.93641	C	–0.04649	–1.17085	–0.98272
Si	8.96213	–4.06996	1.34865	H	0.28639	–1.01482	0.045
H	–6.53835	3.49063	5.11583	H	–1.05219	–0.76531	–1.11126
H	–2.01178	3.8007	5.27072	O	0.88931	–0.48944	–1.83122
H	2.07826	3.74334	5.38967	H	1.75979	0.62093	–1.30681
H	6.68318	3.29763	5.13368	O	–2.74276	–0.27191	–3.81934
H	–8.71488	–2.23544	5.26901	H	–3.22821	–0.92755	–4.33393

APPENDIX C

Table C1 Coordinates of TS on P-H[1]-ZSM-5 for Ethylene formation, in Å

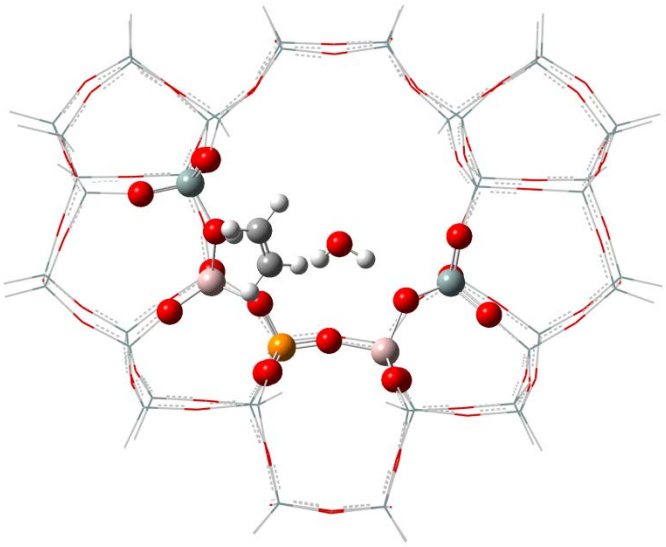


TS

Atoms	X	Y	Z
H	-2.33626	0.23456	-3.7181
C	-1.84221	-0.62308	-3.2613
H	-2.1519	-1.59588	-3.64127
H	0.03114	0.46387	-3.14597
C	-0.47533	-0.48406	-3.01033
H	0.17076	-1.3517	-2.95149
H	-2.6006	-0.71278	-2.15334
H	0.82431	0.31154	-0.90714
O	0.00076	-0.24743	-0.9389
H	-0.72055	0.3436	-0.65935
H	-10.3774	1.12092	-1.21464
Si	-9.08571	0.87422	-0.63944
O	-8.42915	-0.61566	-1.13985
O	-9.17747	0.82068	1.06049
O	-7.94009	2.02915	-1.12032
Si	-7.64129	-2.09849	-1.25864
Si	-9.13375	0.80268	2.76255
Si	-6.43853	2.79846	-1.30437
O	-8.05491	-2.88515	-2.70498
O	-8.25465	-3.0614	-0.00912
O	-5.91666	-2.00946	-1.19198
O	-8.60986	-0.7058	3.35254
O	-7.98373	1.91729	3.3231
H	-10.4457	1.10784	3.26792
O	-5.1518	1.7341	-0.99028
O	-6.30188	3.46301	-2.86181
O	-6.39396	4.08077	-0.18552
Si	-8.46725	-4.12563	-3.8038
Si	-8.7628	-4.09425	1.24177
Si	-4.31116	-2.27468	-1.10502
Si	-8.02186	-2.1928	3.93254
Si	-6.57456	2.79136	3.71547
Al	-3.82453	0.80633	-0.39284
Si	-5.85666	4.25285	-4.29801
Si	-6.07825	4.98801	1.21376
O	-7.56223	-5.48479	-3.28226
H	-9.87799	-4.43977	-3.74359
H	-8.0937	-3.74489	-5.14855
O	-8.43323	-3.30859	2.71408
O	-7.74884	-5.45759	1.09685
H	-10.1477	-4.4636	1.15559
O	-3.78265	-3.19604	-2.34658
O	-3.52777	-0.79221	-1.23697
O	-3.92746	-2.97596	0.30611
O	-6.33668	-2.15861	4.15624
H	-8.6569	-2.54156	5.17527
O	-5.23534	1.7814	3.47948
O	-6.47482	4.06945	2.58955
H	-6.65908	3.30002	5.05677
O	-3.80794	0.69985	1.33076
O	-2.27915	1.58962	-0.95324
O	-4.14403	4.37931	-4.25629
H	-6.22705	3.4654	-5.45338
H	-6.43982	5.57351	-4.37885
O	-4.37922	5.14453	1.28199
H	-6.74338	6.2591	1.20798
Si	-6.25901	-6.40632	-2.68467
Si	-6.30629	-6.2818	0.71907
Si	-3.47959	-4.59753	-3.32557
Si	-3.85292	-4.11113	1.60532
Si	-4.63294	-2.18032	4.23768
Si	-3.87893	0.85311	3.01991
P	-1.67425	3.00781	-1.10815
Si	-2.49088	4.53073	-3.93974
Si	-2.70149	5.01568	1.32321
O	-4.8802	-5.55808	-3.22123
O	-6.24447	-6.41125	-0.98399
H	-6.31263	-7.7454	-3.20051
O	-5.05455	-5.26206	1.24542
H	-6.25612	-7.58416	1.32056
O	-2.30069	-5.60934	-2.6344
H	-3.13176	-4.18041	-4.65285
O	-4.13306	-3.30842	3.06013
O	-2.4447	-5.05305	1.64263
O	-4.05192	-0.65265	3.78342
H	-4.18265	-2.55975	5.54621
O	-2.58023	1.79515	3.59892

O	-2.1271	3.6234	-2.46715	Si	3.67078	-4.52519	-3.34137
O	-2.18344	3.93785	0.02069	Si	4.11269	-4.13574	1.57859
O	-0.16049	2.86303	-1.08074	Si	3.83042	1.03224	2.93506
O	-2.17701	6.14211	-3.55194	Si	5.72554	4.46655	-4.27207
H	-1.70957	3.99884	-5.01418	Si	5.91822	5.22082	1.29605
O	-2.17023	4.32026	2.75619	Si	6.11737	3.01325	-1.23761
O	-2.12548	6.54791	0.93772	Si	4.50409	-2.18383	-1.12928
Si	-1.55748	-6.96852	-1.91344	O	5.09528	-5.45159	-3.19372
Si	-1.5396	-6.48109	1.42061	O	3.90279	-3.11314	-2.42238
Si	-1.72416	3.21226	3.99059	H	3.3243	-4.2	-4.69571
Al	1.63046	3.12433	-1.16262	O	5.35946	-5.26417	1.31158
Si	-1.79046	7.74634	-3.09387	O	4.2956	-3.21841	2.98602
Si	-1.78258	8.07394	0.25517	O	4.15036	-3.08784	0.25788
O	-1.74505	-6.89756	-0.22325	O	5.19943	1.94391	3.36325
O	0.11913	-6.94747	-2.19486	O	4.06352	-0.50881	3.60645
H	-2.14173	-8.17122	-2.44512	O	6.04011	3.68582	-2.78721
O	0.13829	-6.30061	1.62627	H	6.24594	3.67096	-5.36442
H	-2.02149	-7.51812	2.29332	H	6.34294	5.77628	-4.28617
O	-0.03698	3.04509	3.94678	O	6.40513	4.29352	2.64351
H	-2.11732	3.71866	5.27848	O	6.15044	4.2607	-0.09056
O	1.95983	3.82566	-2.71633	H	6.63164	6.46424	1.22987
O	2.09186	4.13558	0.16388	O	7.57927	2.16536	-1.08228
O	2.1814	1.44004	-0.96649	O	6.19145	-2.07071	-1.26898
O	-2.06929	7.9449	-1.4251	Si	6.49718	-6.27133	-2.67961
O	-0.1222	7.94695	-3.32398	Si	6.66522	-6.17701	0.72273
H	-2.57435	8.66417	-3.87227	Si	4.70219	-2.00267	4.10728
O	-0.12415	8.38798	0.41937	Si	6.51527	2.96432	3.70012
H	-2.58964	9.10023	0.85186	Si	8.8873	1.15365	-0.7167
Si	1.80625	-6.95124	-1.94085	Si	7.87908	-1.99962	-1.31385
Si	1.81401	-6.52938	1.40459	O	6.5466	-6.28704	-0.97848
Si	1.6489	3.31184	4.02899	O	7.79518	-5.36322	-3.30723
Si	2.35769	4.70244	-4.11289	H	6.54219	-7.6142	-3.19076
Si	2.55596	5.18149	1.40953	O	8.06255	-5.27341	1.088
Si	3.63632	0.92518	-0.40711	H	6.72019	-7.49156	1.29922
Si	1.57868	7.84937	-3.11815	O	6.40472	-1.91522	4.05395
Si	1.56605	8.16923	0.25094	H	4.23986	-2.34071	5.42429
O	1.98595	-6.92302	-0.24816	O	7.94556	2.132	3.29755
O	2.51442	-5.57579	-2.65195	H	6.55358	3.38203	5.07468
H	2.3798	-8.14827	-2.49664	O	8.45909	-0.41832	-1.20969
O	2.73306	-5.12333	1.65459	O	9.07756	1.0986	0.97694
H	2.25666	-7.60246	2.25366	H	10.10072	1.58992	-1.34979
O	2.04937	4.51554	2.89481	O	8.40016	-2.77646	-2.73288
O	2.5487	1.92618	3.60292	O	8.56443	-2.87269	-0.03189
H	1.96254	3.7202	5.37298	Si	8.75548	-4.04024	-3.82304
O	2.03505	6.34885	-3.75217	Si	9.01857	-3.87154	1.26327
O	4.03271	4.60072	-4.43557	Si	8.09638	-1.94191	3.87825
H	1.62851	4.29938	-5.28593	Si	9.11624	1.07067	2.67655
O	1.96128	6.74259	1.07055	H	10.15238	-4.41264	-3.75875
O	4.24134	5.40561	1.46598	H	8.40584	-3.65519	-5.17341
O	4.81729	1.93162	-0.93137	O	8.57061	-3.07647	2.70112
O	3.89517	-0.5914	-0.96446	H	10.41676	-4.19993	1.2746
O	3.66934	0.90076	1.23223	O	8.66986	-0.45536	3.28554
O	1.80274	8.01359	-1.43459	H	8.696	-2.25505	5.14836
H	2.23771	8.9227	-3.81218	H	10.43562	1.4214	3.13043
H	2.27306	9.31004	0.76378				

Table C2 Coordinates of $C_2H_4/H_2O/H^1Z$ on P-H^1-ZSM-5 for Ethylene formation, in Å

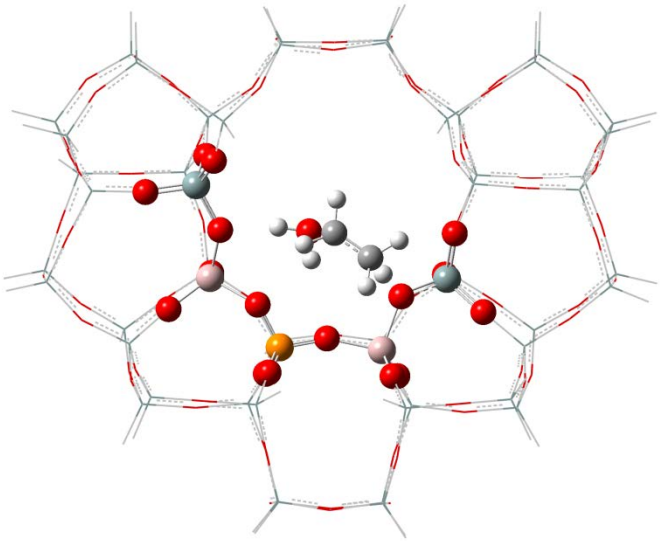


$C_2H_4/H_2O/H^1Z$

Atoms	X	Y	Z
H	-3.25277	-1.19736	-5.19235
C	-2.34016	-1.10722	-4.60715
H	-1.69521	-1.98145	-4.56622
H	-2.63092	0.90947	-4.04733
C	-1.99861	0.02677	-3.98556
H	-1.0795	0.09893	-3.40749
H	1.06245	0.07667	-1.42898
O	0.22268	-0.41564	-1.53972
H	-0.39981	0.10116	-1.01068
H	-10.4354	1.27068	3.31545
Si	-9.13519	0.94075	2.79641
O	-9.19448	0.97778	1.09431
O	-8.64189	-0.58604	3.36739
O	-7.95095	2.01912	3.35395
Si	-9.1311	1.01661	-0.60625
Si	-8.08641	-2.07208	3.98005
Si	-6.52313	2.86839	3.73489
O	-8.55404	-0.51485	-1.08851
O	-7.9462	2.11566	-1.12042
H	-10.4185	1.30643	-1.16934
O	-8.51587	-3.20805	2.78575
O	-6.39992	-2.06776	4.19932
H	-8.72693	-2.3839	5.22929
O	-5.208	1.82572	3.49651
O	-6.40285	4.13549	2.6004
H	-6.58986	3.38097	5.07523
Si	-7.83113	-2.02762	-1.19617
Si	-6.44275	2.88126	-1.30038
Si	-8.88343	-4.01652	1.33605
Si	-4.69869	-2.13047	4.29416
Si	-3.86734	0.87188	3.04916
Si	-5.98986	5.04325	1.22132
O	-8.23132	-2.81785	-2.64024
O	-8.4309	-2.98183	0.06235
O	-6.09601	-1.97808	-1.12699
O	-5.17311	1.79548	-0.9636
O	-6.25806	3.52192	-2.85902
O	-6.37881	4.15153	-0.17221
O	-7.85538	-5.36504	1.16604
H	-10.265	-4.403	1.29161
O	-4.07776	-0.62817	3.81069
O	-4.21737	-3.2745	3.1225
H	-4.2621	-2.50844	5.60669
O	-3.81534	0.71792	1.35277
O	-2.543	1.77706	3.61527
O	-4.28654	5.11417	1.25688
H	-6.60422	6.33911	1.22939
Si	-8.61231	-4.0617	-3.75076
Si	-4.52082	-2.31659	-1.05042
Al	-3.84449	0.90059	-0.35107
Si	-5.7359	4.25941	-4.30243
Si	-6.43055	-6.2127	0.77433
Si	-3.95063	-4.07738	1.6686
Si	-1.65403	3.18206	3.9955
Si	-2.6089	4.95884	1.30208
O	-7.69244	-5.40609	-3.22109
H	-10.0193	-4.39224	-3.70127
H	-8.22786	-3.66534	-5.08721
O	-3.966	-3.18007	-2.29881
O	-3.7052	-0.78925	-1.22123
O	-4.08784	-2.934	0.36815
O	-2.3006	1.53465	-1.01438
O	-4.02647	4.36055	-4.21629
H	-6.09452	3.43935	-5.43866
H	-6.30033	5.58407	-4.43473
O	-5.15946	-5.21675	1.30417
O	-6.37182	-6.31502	-0.92988
H	-6.40007	-7.52025	1.36416
O	-2.52914	-4.99011	1.66065
O	-2.10067	4.2738	2.74834
O	0.02803	2.99472	3.95512
H	-2.05049	3.69848	5.27839
O	-2.0222	6.48541	0.9191
O	-2.11752	3.84643	0.01921
Si	-6.39292	-6.33841	-2.63137
Si	-3.60825	-4.55151	-3.31569
P	-1.607	2.92147	-1.11938
Si	-2.36485	4.52085	-3.92812
Si	-1.59832	-6.40402	1.41972
Si	1.7171	3.26656	4.02941
Si	-1.68846	8.03359	0.27911
O	-5.01298	-5.50467	-3.18521
H	-6.46561	-7.68242	-3.12983
O	-2.4249	-5.55146	-2.62751
H	-3.29419	-4.11227	-4.6416
O	-2.0037	3.58681	-2.47334

O	-0.10528	2.71623	-1.04721	O	4.03314	-0.61258	-0.95133
O	-2.07729	6.1321	-3.51983	H	2.33116	8.91298	-3.78474
H	-1.59858	4.02614	-5.02896	O	5.3429	-5.32132	1.31849
O	-1.82672	-6.80878	-0.22292	O	4.31497	-3.25871	2.99059
O	0.07712	-6.21372	1.61587	O	4.19521	-3.11834	0.2565
H	-2.07673	-7.44326	2.29214	O	6.47297	4.24938	2.66368
O	2.1048	4.4704	2.89286	O	6.27622	4.2323	-0.0759
O	2.61794	1.88295	3.60699	H	6.67194	6.43381	1.2713
H	2.02168	3.67957	5.3743	O	8.01787	2.07579	3.2969
O	-1.98658	7.93843	-1.40054	H	6.65215	3.33276	5.08814
O	-0.03329	8.35323	0.45226	O	6.44339	-1.97576	4.05857
H	-2.50424	9.0352	0.90553	H	4.27409	-2.38081	5.42653
Si	-1.63436	-6.88993	-1.91306	Si	3.67745	-4.54	-3.35176
Al	1.68023	3.05757	-1.16812	Si	5.77841	4.44632	-4.25128
Si	-1.70231	7.74142	-3.06931	Si	6.26168	2.98971	-1.23099
Si	1.75058	-6.48503	1.39124	Si	4.57719	-2.22251	-1.13111
Si	2.61567	5.12092	1.39985	Si	6.64969	-6.2295	0.72322
Si	3.90669	0.99756	2.93662	Si	9.17885	1.00073	2.68075
Si	1.6578	8.13428	0.27711	Si	8.13466	-2.0057	3.87963
O	0.03777	-6.8558	-2.20065	O	5.07495	-5.51026	-3.20047
H	-2.2154	-8.09836	-2.43587	O	3.97765	-3.153	-2.42092
O	1.96853	3.81347	-2.70762	H	3.34684	-4.21613	-4.7093
O	2.1178	4.08353	0.16291	O	6.14537	3.67623	-2.77232
O	2.34433	1.42822	-1.01098	H	6.28148	3.65108	-5.35221
O	-0.03704	7.9592	-3.29746	H	6.38989	5.75914	-4.28377
H	-2.49799	8.64946	-3.84742	O	7.72965	2.14561	-1.09679
O	1.89793	-6.88726	-0.26059	O	6.26864	-2.14815	-1.25947
O	2.71209	-5.11146	1.64675	O	6.52877	-6.33767	-0.97727
H	2.15204	-7.57464	2.24019	O	8.05137	-5.33484	1.09296
O	2.04489	6.69531	1.07668	H	6.70018	-7.54581	1.2973
O	4.30375	5.32457	1.45533	O	9.15982	1.03065	0.98147
O	5.27312	1.89987	3.39363	O	8.71254	-0.52191	3.28466
O	3.77218	0.89249	1.23256	H	10.49787	1.33568	3.14862
O	4.11739	-0.54778	3.60701	O	8.6014	-3.15017	2.70941
O	1.88949	8.00202	-1.41007	H	8.7344	-2.31586	5.15079
H	2.36495	9.26752	0.80623	Si	6.47757	-6.32155	-2.67927
Si	1.72926	-6.90544	-1.95535	Si	8.9924	1.08244	-0.71544
Si	2.40292	4.68598	-4.0937	Si	7.95374	-2.06558	-1.30564
Si	3.76803	0.90899	-0.41131	Si	9.04127	-3.9575	1.27544
Si	1.66444	7.84202	-3.0944	O	7.78175	-5.41993	-3.30386
Si	4.12157	-4.16259	1.57535	H	6.52444	-7.66709	-3.18468
Si	5.98688	5.17294	1.31252	O	8.5333	-0.48335	-1.20191
Si	6.59585	2.91601	3.71355	H	10.22684	1.47834	-1.33493
Si	4.74025	-2.04703	4.10936	O	8.47281	-2.8485	-2.72292
O	2.49274	-5.56496	-2.66593	O	8.63399	-2.94389	-0.02284
H	2.25023	-8.12922	-2.50527	H	10.42963	-4.32526	1.30433
O	2.09666	6.33714	-3.72893	Si	8.77037	-4.11908	-3.82217
O	4.08397	4.58126	-4.38646	H	10.15698	-4.53208	-3.77812
H	1.68809	4.31696	-5.28596	H	8.41675	-3.71879	-5.16713
O	4.98247	1.89381	-0.90551	H	-3.13265	-0.75886	-2.01841

Table C3 Coordinates of TS on P-H^4-ZSM-5 for Ethylene formation, in Å

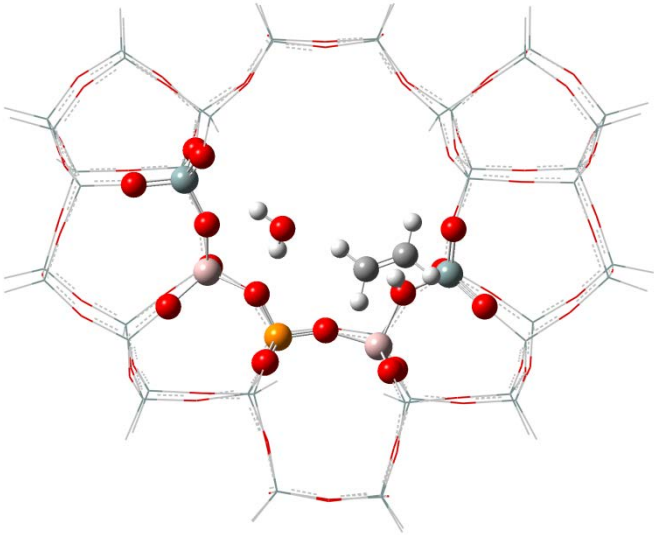


TS

Atoms	X	Y	Z
Si	-1.86044	8.05782	0.25228
Si	-1.8433	7.76169	-3.10142
O	-3.73088	-3.16048	-2.32832
O	-3.56171	-0.82044	-1.06693
O	-3.86332	0.77851	1.35818
O	-4.08657	-0.66647	3.77155
O	-4.14236	-3.36108	3.06603
O	-3.96906	-3.0791	0.31426
O	-8.06619	-2.93982	-2.74967
O	-8.44685	-0.68161	-1.18004
O	-9.23195	0.76675	1.00688
O	-8.64225	-0.76273	3.29481
O	-8.44273	-3.37344	2.66253
O	-8.29244	-3.12462	-0.06072
O	-5.93049	-2.08962	-1.20149
O	-6.36011	-2.19029	4.10878
O	-2.20769	-5.53414	-2.69129
O	-4.78548	-5.52564	-3.25201
O	-7.47585	-5.52124	-3.34729
O	-2.45432	-5.11659	1.65554
O	-5.06107	-5.37467	1.28837
O	-7.75613	-5.52319	1.03781
Si	-3.4136	-4.51616	-3.34556
Si	-4.30514	-2.27459	-1.06847
Si	-3.94472	0.86269	3.04433
Si	-4.65676	-2.2048	4.20871
Si	-3.88053	-4.19064	1.618
Si	-8.42419	-4.18654	-3.85678
Si	-7.64461	-2.16126	-1.29763
Si	-9.13607	0.79543	-0.69521
Si	-9.18155	0.74105	2.70715
Si	-8.04276	-2.24645	3.8734
Si	-8.7749	-4.1634	1.19082
O	-8.05239	1.87409	3.27765
O	-5.30582	1.77092	3.53586
O	-2.65234	1.807	3.65037
O	-8.0312	1.99189	-1.17712
O	-5.24854	1.70358	-0.97449
O	-2.40214	1.60342	-1.00877
Si	-6.30973	-6.34727	0.67367
Si	-6.15191	-6.40016	-2.73076
Si	-1.52205	-6.51041	1.37233
Si	-1.49667	-6.90903	-1.97867
O	-6.53042	4.03968	2.5767
O	-6.34668	3.44609	-2.87075
O	-6.48592	4.05016	-0.20532
O	-2.21884	4.32246	2.75303
O	-2.18978	6.52526	0.92012
O	-2.12545	7.95189	-1.4327
O	-2.19921	6.15684	-3.57039
O	-2.0897	3.64856	-2.47674
O	-2.17478	3.92269	0.01348
O	-4.42843	5.09125	1.24206
O	-4.15465	4.37235	-4.23778
Si	-6.6654	2.76581	3.70567
Si	-6.13289	4.94297	1.1913
Si	-5.86648	4.21011	-4.30588
Si	-6.52377	2.76021	-1.32259
Si	-1.80581	3.23104	4.01316
Si	-2.75165	4.98425	1.30374
Si	-2.50089	4.53771	-3.94559
O	-0.11408	3.05252	3.98093
O	-0.2061	2.71909	-1.06613
O	-0.20009	8.37271	0.42738
O	-0.1715	7.97372	-3.32123
O	-6.18369	-6.43012	-1.02924
O	-1.6874	-6.87731	-0.28727
O	0.15618	-6.29942	1.59293
O	0.18886	-6.89668	-2.23628
O	6.32487	4.33336	2.65042
O	5.99304	3.70859	-2.78576
O	6.10889	4.3051	-0.08595
O	1.97899	4.49095	2.89344
O	1.87209	6.69845	1.05021
O	1.74542	8.01112	-1.41954
O	1.97195	6.34972	-3.7265
O	1.86862	3.80405	-2.72545
O	2.02836	4.07576	0.16752
O	4.15688	5.38867	1.44622
O	3.94948	4.57681	-4.4131
O	7.87149	2.18936	3.32158
O	5.12454	1.97626	3.34311
O	2.47093	1.92364	3.60134
O	7.56259	2.21388	-1.06321
O	4.80682	1.96391	-0.92261

O	2.19215	1.40556	-1.05994	H	6.43829	3.4169	5.08468
Si	6.42843	3.00459	3.70868	H	-8.67952	-2.59609	5.11596
Si	5.83983	5.25799	1.30198	H	-4.21925	-2.56691	5.52791
Si	5.64593	4.46635	-4.27799	H	4.20388	-2.28898	5.4321
Si	6.10477	3.05981	-1.23071	H	8.65669	-2.16744	5.1988
Si	1.56775	3.3059	4.04628	H	10.37847	1.51905	3.19226
Si	2.47421	5.1485	1.40562	H	10.44644	-4.13381	1.37058
Si	1.48667	8.14927	0.26467	H	10.09636	1.68929	-1.2993
Si	1.52337	7.8618	-3.10431	H	10.23701	-4.33658	-3.69802
Si	2.27344	4.70939	-4.10824	H	-10.4963	1.02906	3.21755
Si	3.66225	0.92817	-0.40794	H	-10.4343	1.00818	-1.27108
Si	3.76039	1.05221	2.93113	H	-9.82314	-4.5544	-3.80989
Si	8.88822	1.22884	-0.67487	H	-10.1574	-4.54838	1.12512
Si	9.07119	1.14872	2.72128	Al	1.5471	3.10961	-1.17319
O	6.61674	-6.22594	-0.94753	H	-6.16016	-7.73947	-3.25252
O	2.04257	-6.89132	-0.26696	H	-6.29889	-7.67102	1.23149
Si	6.71342	-6.13067	0.75578	H	-2.06465	-8.10933	-2.5336
Si	6.58177	-6.2171	-2.64886	H	2.45932	-8.09859	-2.52042
Si	1.83075	-6.51841	1.38636	H	2.28574	-7.58816	2.23329
Si	1.86728	-6.91251	-1.96041	H	-1.96413	-7.60088	2.20042
O	2.59244	-5.53133	-2.65354	H	6.63766	-7.55844	-3.16093
O	5.18388	-5.39558	-3.17177	H	6.77896	-7.44647	1.32673
O	7.87945	-5.29876	-3.26302	H	8.49415	-3.58384	-5.12357
O	2.75038	-5.11016	1.65104	H	3.42303	-4.14569	-4.69224
O	5.39214	-5.23212	1.33214	H	-3.07271	-4.09922	-4.67539
O	8.09538	-5.2104	1.13934	H	-8.06358	-3.78736	-5.20035
O	3.96623	-3.06757	-2.4147	H	6.15593	3.654	-5.36224
O	3.93275	-0.57839	-0.96627	H	1.54889	4.30934	-5.28363
O	3.59976	0.93724	1.21786	H	-1.71411	4.02696	-5.02676
O	4.02346	-0.4903	3.57848	H	-6.19458	3.40635	-5.46294
O	4.29394	-3.19876	3.00109	H	-6.45569	5.52574	-4.42734
O	4.18739	-3.06037	0.28482	H	-6.76997	6.22946	1.19733
O	8.46725	-2.71329	-2.68242	H	6.25103	5.78051	-4.31618
O	8.49175	-0.35258	-1.16141	H	6.52583	6.51605	1.2428
O	9.05171	1.18531	1.02045	H	2.20977	8.91845	-3.79624
O	8.63334	-0.38288	3.3198	H	2.20579	9.26958	0.80422
O	8.56804	-3.00721	2.75447	H	-2.66731	9.08112	0.85347
O	8.62156	-2.81101	0.02488	H	-2.62196	8.68368	-3.87935
O	6.25132	-2.02122	-1.21873	P	-1.71707	2.97256	-1.12216
O	6.37524	-1.85521	4.07218	Al	-3.90738	0.78033	-0.38092
Si	3.75103	-4.48691	-3.33749	H	1.0908	0.83153	-3.69247
Si	4.56925	-2.17359	-1.10001	C	1.22096	-0.0338	-3.04135
Si	4.6742	-1.96924	4.11431	H	2.15202	-0.58582	-3.18383
Si	4.12712	-4.12515	1.59743	H	1.62429	0.59985	-1.96874
Si	8.83849	-3.97398	-3.77359	H	-0.88812	-0.5131	-3.22008
Si	7.94169	-1.9451	-1.2626	C	0.08314	-0.83209	-2.85977
Si	8.06949	-1.87114	3.91945	H	-1.70093	-0.87172	-0.99197
Si	9.0481	-3.81001	1.33147	H	0.17592	-1.88996	-2.64412
H	-6.80193	3.29174	5.03677	O	-0.72361	-0.71741	-0.92188
H	-2.18413	3.7759	5.28959	H	-0.66026	0.22246	-0.68093
H	1.91761	3.71556	5.38021				

Table C4 Coordinates of $C_2H_4/H_2O/H^4$Zon P-H^4-ZSM-5 for Ethylene formation, in Å

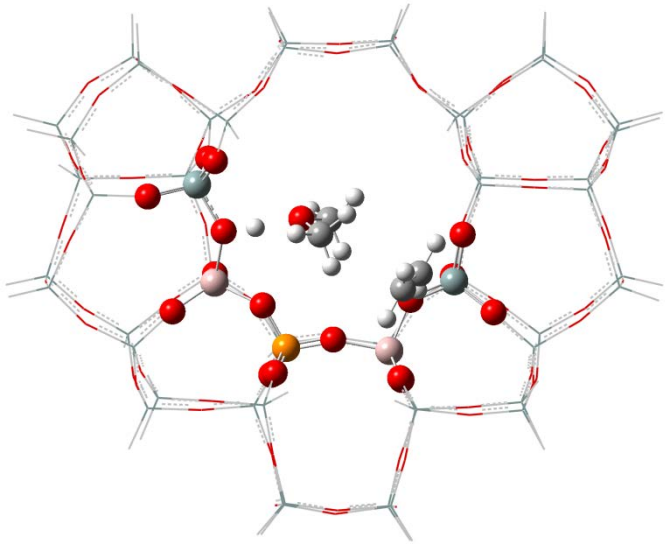


$C_2H_4/H_2O/H^4Z$

Atoms	X	Y	Z
Si	-1.53912	7.98936	0.21027
Si	-1.50492	7.67463	-3.14114
O	-4.05278	-3.04074	-2.33674
O	-3.88042	-0.71819	-1.08413
O	-3.79139	0.88555	1.37491
O	-4.11725	-0.55339	3.79164
O	-4.34922	-3.23448	3.07596
O	-4.29111	-2.97852	0.31206
O	-8.47015	-2.70754	-2.68321
O	-8.60068	-0.36709	-1.16192
O	-9.17723	1.16822	1.02377
O	-8.684	-0.39297	3.32076
O	-8.65477	-3.02556	2.74502
O	-8.64718	-2.81633	0.01175
O	-6.24781	-1.98088	-1.18943
O	-6.48278	-1.93548	4.1418
O	-2.59517	-5.46075	-2.72612
O	-5.18759	-5.38718	-3.18756
O	-7.8858	-5.30512	-3.25271
O	-2.76385	-5.03106	1.62144
O	-5.39926	-5.23045	1.3571
O	-8.10754	-5.21726	1.13249
Si	-3.79305	-4.41192	-3.34874
Si	-4.6191	-2.15293	-1.06338
Si	-3.8825	0.96098	3.05869
Si	-4.78265	-2.05486	4.22586
Si	-4.17253	-4.07664	1.62058
Si	-8.83322	-3.9732	-3.76808
Si	-7.96054	-1.92729	-1.26107
Si	-9.09457	1.18697	-0.68042
Si	-9.13221	1.1361	2.72281
Si	-8.16843	-1.89859	3.9229
Si	-9.08057	-3.82727	1.30304
O	-7.93512	2.19499	3.29953
O	-5.18853	1.94907	3.54969
O	-2.54521	1.8352	3.68351
O	-7.88391	2.27638	-1.1591
O	-5.09433	1.96174	-0.93137
O	-2.25124	1.51305	-1.02735
Si	-6.71375	-6.12427	0.75904
Si	-6.57397	-6.20973	-2.64501
Si	-1.85154	-6.43299	1.32428
Si	-1.8377	-6.81181	-2.02884
O	-6.30822	4.2833	2.6183
O	-6.1694	3.69809	-2.84238
O	-6.31965	4.30879	-0.173
O	-2.00932	4.31075	2.73571
O	-1.85894	6.44375	0.84867
O	-1.78883	7.89662	-1.47663
O	-1.86181	6.0648	-3.58392
O	-1.91648	3.56131	-2.49097
O	-1.99236	3.82766	0.00133
O	-4.17672	5.19145	1.2314
O	-3.93499	4.43081	-4.25444
Si	-6.50075	3.00325	3.73298
Si	-5.88973	5.16336	1.22459
Si	-5.65462	4.36626	-4.3118
Si	-6.36203	3.01881	-1.29246
Si	-1.6661	3.24044	4.03215
Si	-2.51558	4.94698	1.26552
Si	-2.27482	4.46697	-3.96322
O	0.0267	3.03843	4.02769
O	-0.02585	2.64779	-1.10071
O	0.12053	8.30353	0.41389
O	0.17108	7.89555	-3.33716
O	-6.60536	-6.23005	-0.94246
O	-2.01538	-6.79756	-0.33419
O	-0.16815	-6.24126	1.54953
O	-0.14857	-6.78054	-2.28097
O	6.52792	4.10682	2.7526
O	6.30491	3.55819	-2.69357
O	6.40399	4.12639	0.01709
O	2.16319	4.42508	2.91873
O	2.18993	6.6259	1.05731
O	2.08049	7.94668	-1.41023
O	2.34197	6.31163	-3.71589
O	2.09295	3.78352	-2.71842
O	2.21226	4.00314	0.19268
O	4.39887	5.18987	1.49625
O	4.27365	4.46452	-4.31013
O	7.98741	1.88131	3.40285
O	5.24105	1.79631	3.40545
O	2.57772	1.86713	3.64569
O	7.82089	1.97892	-0.97173
O	5.07774	1.83737	-0.84803
O	2.45439	1.403	-1.10152
Si	6.5866	2.7626	3.79555

Si	6.08591	5.06017	1.41035	H	-8.80795	-2.18139	5.18142
Si	5.9681	4.33791	-4.18032	H	-4.35764	-2.44437	5.54176
Si	6.41598	2.90178	-1.14556	H	4.0492	-2.4192	5.43789
Si	1.70631	3.2722	4.08951	H	8.50624	-2.53819	5.26355
Si	2.7061	5.0552	1.4391	H	10.45151	1.06344	3.33275
Si	1.80658	8.08045	0.27158	H	10.23775	-4.59081	1.45514
Si	1.86189	7.81798	-3.09763	H	10.29986	1.23638	-1.16656
Si	2.59142	4.66532	-4.09323	H	10.05729	-4.72307	-3.68109
Si	3.91559	0.84452	-0.34308	H	-10.427	1.50616	3.23199
Si	3.83248	0.95231	2.98209	H	-10.3677	1.54063	-1.24464
Si	9.04705	0.87082	-0.56951	H	-10.2334	-4.33491	-3.70158
Si	9.13723	0.76935	2.82988	H	-10.4744	-4.17614	1.31558
O	6.32252	-6.41525	-0.95573	Al	1.68264	3.13228	-1.17924
O	1.70924	-6.87212	-0.31521	H	-6.629	-7.55435	-3.1519
Si	6.40345	-6.35421	0.74864	H	-6.77806	-7.4413	1.33031
Si	6.29614	-6.40043	-2.65841	H	-2.37555	-8.02701	-2.58276
Si	1.49684	-6.51143	1.33931	H	2.065	-8.07612	-2.57915
Si	1.52633	-6.86864	-2.00949	H	1.92142	-7.59946	2.1795
O	2.35219	-5.52949	-2.67274	H	-2.29812	-7.52366	2.15031
O	4.94507	-5.51082	-3.18658	H	6.30073	-7.74086	-3.17507
O	7.64457	-5.5391	-3.24845	H	6.39824	-7.67792	1.3041
O	2.47771	-5.14328	1.6209	H	8.3605	-3.83193	-5.08376
O	5.12404	-5.39541	1.32341	H	3.26077	-4.16386	-4.70694
O	7.82497	-5.50933	1.16444	H	-3.50771	-4.04356	-4.70467
O	3.88664	-3.148	-2.41261	H	-8.48889	-3.59315	-5.12146
O	4.04844	-0.65634	-0.92037	H	6.47374	3.52775	-5.26708
O	3.70957	0.90367	1.25174	H	1.90599	4.27928	-5.294
O	4.00387	-0.61956	3.57443	H	-1.51176	3.92671	-5.04617
O	4.11413	-3.33357	3.00311	H	-6.04091	3.54503	-5.43758
O	4.05496	-3.15016	0.2991	H	-6.15739	5.71259	-4.48068
O	8.40711	-3.00741	-2.62731	H	-6.43595	6.49062	1.25432
O	8.52045	-0.66425	-1.07559	H	6.58873	5.64464	-4.19497
O	9.15802	0.81387	1.12872	H	6.77663	6.31618	1.39068
O	8.59302	-0.73562	3.40551	H	2.54611	8.88401	-3.77614
O	8.41069	-3.35211	2.80898	H	2.53127	9.18924	0.82644
O	8.5345	-3.13634	0.08806	H	-2.34728	9.0095	0.81454
O	6.21643	-2.23506	-1.16828	H	-2.26794	8.59171	-3.93995
O	6.25945	-2.10534	4.10548	P	-1.54774	2.87485	-1.13951
Si	3.55281	-4.5371	-3.35432	Al	-3.85695	0.87566	-0.36707
Si	4.52824	-2.3134	-1.08629	H	3.38632	0.53984	-4.32603
Si	4.55509	-2.13672	4.12551	C	2.53936	-0.09217	-4.06666
Si	3.90555	-4.23841	1.58893	H	2.75904	-1.13574	-3.85075
Si	8.68399	-4.27247	-3.74453	H	2.2201	0.85863	-1.88754
Si	7.90949	-2.23491	-1.20204	H	1.07879	1.41967	-4.26921
Si	7.95337	-2.20502	3.97837	C	1.28579	0.37777	-4.03666
Si	8.86402	-4.17883	1.38999	H	-2.21849	-1.32626	-2.65685
H	-6.60318	3.52246	5.07013	H	0.43228	-0.24868	-3.78681
H	-2.03815	3.82438	5.29281	O	-1.43419	-0.77739	-2.80706
H	2.08012	3.68758	5.41431	H	-1.58485	-0.04071	-2.19287
H	6.60589	3.15913	5.17544				

Table C5 Coordinates of DME/C_2H_4/H^1Z on P-H^1-ZSM-5 for DME conversion to propylene, in Å

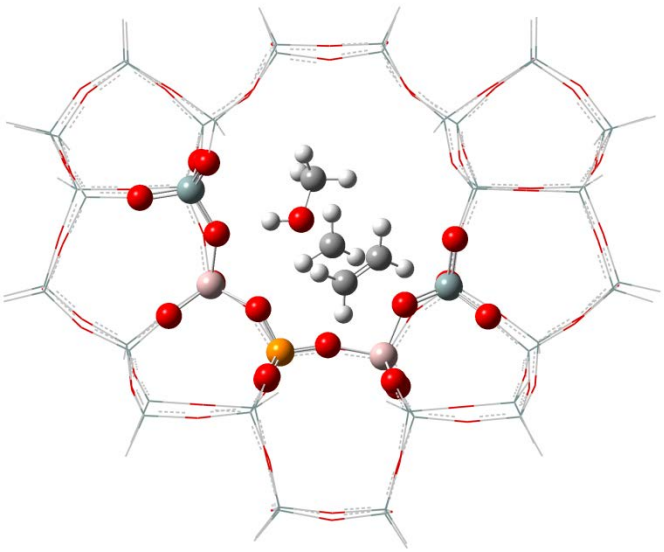


DME/C_2H_4/H^1Z

Atoms	X	Y	Z
Si	1.84587	8.03318	-0.30934
Si	1.84031	7.74519	3.04139
O	3.88888	-3.16448	2.30859
O	3.627	-0.8272	1.08637
O	3.88465	0.72999	-1.38657
O	4.11898	-0.68974	-3.79139
O	4.21921	-3.35991	-3.09277
O	4.0588	-3.0455	-0.35332
O	8.11773	-2.8333	2.71016
O	8.55097	-0.5899	1.11352
O	9.27573	0.85265	-1.0828
O	8.68365	-0.71748	-3.33701
O	8.50422	-3.32704	-2.69889
O	8.35978	-3.05755	0.01556
O	6.02654	-1.98007	1.13471
O	6.41858	-2.17331	-4.14655
O	2.30885	-5.50668	2.67164
O	4.88502	-5.48841	3.25594
O	7.56354	-5.40811	3.33615
O	2.51533	-5.08279	-1.65578
O	5.14196	-5.34076	-1.27521
O	7.83028	-5.46583	-1.05177
Si	3.49913	-4.50162	3.34948
Si	4.45103	-2.32742	1.03887
Si	3.94852	0.84357	-3.08274
Si	4.71729	-2.20917	-4.25217
Si	3.95128	-4.18757	-1.65105
Si	8.47434	-4.05238	3.85413
Si	7.75622	-2.06459	1.24361
Si	9.20472	0.90499	0.61747
Si	9.20701	0.80605	-2.7839
Si	8.10346	-2.20693	-3.91784
Si	8.84805	-4.10946	-1.22844
O	8.04657	1.90813	-3.34615
O	5.30588	1.76044	-3.55568
O	2.63805	1.7599	-3.66653
O	8.06026	2.05226	1.11813
O	5.29085	1.71385	0.93891
O	2.42145	1.56365	1.0051
Si	6.4008	-6.30896	-0.66797
Si	6.26769	-6.34025	2.73844
Si	1.56124	-6.47181	-1.37529
Si	1.54498	-6.86636	1.97214
O	6.50736	4.04882	-2.61527
O	6.36148	3.45901	2.84301
O	6.47836	4.07491	0.15822
O	2.20185	4.26168	-2.7814
O	2.16294	6.48796	-0.9631
O	2.13173	7.92635	1.3718
O	2.20501	6.14183	3.51771
O	2.09171	3.611	2.45243
O	2.16369	3.86076	-0.04214
O	4.3873	5.04441	-1.27439
O	4.13921	4.34183	4.19313
Si	6.64239	2.78519	-3.75172
Si	6.09046	4.95991	-1.23868
Si	5.84641	4.20611	4.28296
Si	6.54926	2.80586	1.2893
Si	1.76972	3.17875	-4.04049
Si	2.70562	4.94075	-1.33005
Si	2.47963	4.5238	3.91078
O	0.08611	2.99462	-4.01487
O	0.19546	2.68458	1.06606
O	0.1944	8.3709	-0.49072
O	0.17411	7.97342	3.25716
O	6.28686	-6.35692	1.036
O	1.75722	-6.82794	0.28249
O	-0.10851	-6.24167	-1.59426
O	-0.13427	-6.83001	2.22672
O	-6.32278	4.31831	-2.74462
O	-6.07965	3.72997	2.68606
O	-6.16289	4.28151	-0.0077
O	-1.96661	4.48587	-2.93204
O	-1.88625	6.71663	-1.12093
O	-1.74355	8.03417	1.35902
O	-1.98334	6.3735	3.67361
O	-1.88952	3.82797	2.67355
O	-1.98103	4.10539	-0.20025
O	-4.15408	5.36032	-1.50197

O	-4.02578	4.66922	4.28885	H	-6.4809	3.40196	-5.17151
O	-7.89758	2.17095	-3.40358	H	8.74409	-2.55751	-5.15688
O	-5.156	1.9471	-3.45184	H	4.28074	-2.58376	-5.56638
O	-2.50304	1.90047	-3.63921	H	-4.18381	-2.34475	-5.47782
O	-7.67016	2.22303	0.99206	H	-8.64392	-2.20389	-5.27967
O	-4.92583	1.91676	0.84139	H	-10.3907	1.46506	-3.29893
O	-2.28657	1.46331	0.984	H	-10.433	-4.19599	-1.45988
Si	-6.45443	2.98718	-3.7955	H	-10.185	1.6067	1.19206
Si	-5.84023	5.22979	-1.38336	H	-10.2601	-4.41001	3.59705
Si	-5.71956	4.54303	4.14421	H	10.51116	1.10498	-3.31222
Si	-6.18773	3.03837	1.14634	H	10.5014	1.14519	1.18247
Si	-1.59989	3.28027	-4.07344	H	9.88123	-4.38748	3.84017
Si	-2.46692	5.14556	-1.43958	H	10.23127	-4.4859	-1.15319
Si	-1.49819	8.15904	-0.32682	Al	-1.58137	3.06712	1.13531
Si	-1.52645	7.87388	3.04438	H	6.31828	-7.67571	3.26307
Si	-2.3361	4.73222	4.03548	H	6.39296	-7.636	-1.2139
Si	-3.69244	0.94063	0.37075	H	2.11436	-8.06423	2.53064
Si	-3.80594	1.0287	-2.97954	H	-2.35784	-8.09951	2.5063
Si	-8.9497	1.18912	0.58922	H	-2.20407	-7.56761	-2.24364
Si	-9.08442	1.1125	-2.80925	H	2.01799	-7.55253	-2.20763
O	-6.60588	-6.27417	0.87379	H	-6.64963	-7.60035	3.08418
O	-1.9689	-6.87214	0.25812	H	-6.749	-7.47262	-1.40901
Si	-6.69268	-6.15967	-0.82852	H	-8.53854	-3.63775	5.0342
Si	-6.58632	-6.25694	2.57586	H	-3.47845	-4.18046	4.66895
Si	-1.78843	-6.48409	-1.39413	H	3.16824	-4.0406	4.66385
Si	-1.8196	-6.88431	1.95469	H	8.06607	-3.62979	5.17547
O	-2.58486	-5.53139	2.64404	H	-6.24117	3.78448	5.26225
O	-5.18663	-5.45156	3.11662	H	-1.66002	4.3439	5.24551
O	-7.89029	-5.34081	3.17805	H	1.71105	4.03138	5.01193
O	-2.71616	-5.08844	-1.66448	H	6.18538	3.38439	5.42408
O	-5.36065	-5.26633	-1.39021	H	6.4332	5.52116	4.41629
O	-8.07319	-5.24253	-1.21997	H	6.70894	6.25425	-1.25353
O	-4.01315	-3.10169	2.37265	H	-6.32057	5.86106	4.13183
O	-3.97573	-0.58558	0.90856	H	-6.51048	6.49862	-1.34412
O	-3.68034	0.90671	-1.27582	H	-2.1859	8.95134	3.73171
O	-4.02541	-0.51506	-3.65298	H	-2.19887	9.29129	-0.86654
O	-4.27424	-3.21894	-3.04226	H	2.67501	9.03112	-0.92398
O	-4.18691	-3.07994	-0.30644	H	2.63386	8.6607	3.81309
O	-8.51351	-2.75573	2.59431	P	1.69673	2.92403	1.10695
O	-8.52779	-0.38694	1.07864	Al	3.93022	0.86333	0.32941
O	-9.09367	1.14011	-1.10975	C	0.58125	-0.80406	2.78638
O	-8.62823	-0.41626	-3.40637	H	0.23913	0.23192	2.71835
O	-8.56646	-3.04692	-2.83835	H	-0.26599	-1.45003	3.03997
O	-8.63186	-2.84641	-0.10682	H	1.35674	-0.8987	3.54854
O	-6.27983	-2.07046	1.16793	H	-0.14082	-0.07353	0.37515
O	-6.3679	-1.90487	-4.14365	C	0.25484	-1.09116	0.42987
Si	-3.78055	-4.5036	3.30403	H	-0.57277	-1.79925	0.54727
Si	-4.58955	-2.17224	1.06793	H	0.82486	-1.33276	-0.46892
Si	-4.66569	-2.00177	-4.16883	O	1.15918	-1.22525	1.54344
Si	-4.11842	-4.12657	-1.62553	H	2.62007	-0.94468	1.29972
Si	-8.86758	-4.02423	3.67911	H	-2.47483	0.94047	3.74963
Si	-7.96625	-1.97433	1.18716	C	-2.53171	0.34389	4.65563
Si	-8.0627	-1.90613	-3.99717	H	-3.07146	-0.59806	4.58206
Si	-9.03972	-3.84987	-1.41314	C	-1.97637	0.73806	5.80443
H	6.74943	3.30476	-5.08697	H	-2.04122	0.13822	6.70974
H	2.17765	3.70362	-5.31623	H	-1.44356	1.68337	5.88397
H	-1.91931	3.69376	-5.41465				

Table C6 Coordinates of TS1 on P-H[1]-ZSM-5 for DME conversion to propylene, in Å

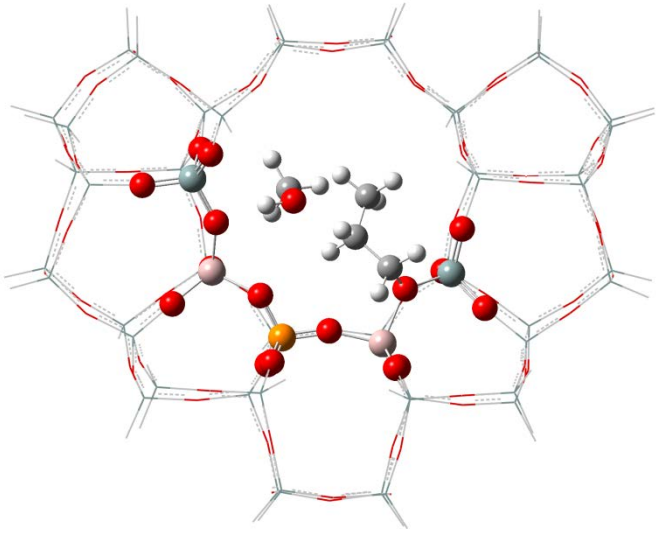


TS1

Atoms	X	Y	Z
Si	-1.65792	8.05608	0.29815
Si	-1.63753	7.82952	-3.05815
O	-3.92571	-3.1041	-2.32144
O	-3.62734	-0.79376	-1.02802
O	-3.77959	0.86338	1.33935
O	-4.08349	-0.59537	3.73426
O	-4.28203	-3.29313	3.07453
O	-4.13933	-3.03031	0.3215
O	-8.23378	-2.75796	-2.70613
O	-8.53238	-0.46883	-1.15166
O	-9.20609	1.02504	1.03788
O	-8.67634	-0.53197	3.3213
O	-8.55803	-3.15142	2.70881
O	-8.44435	-2.91912	-0.01703
O	-6.06886	-1.95137	-1.17984
O	-6.42767	-2.0163	4.12202
O	-2.42759	-5.47112	-2.70808
O	-5.03169	-5.46193	-3.21358
O	-7.71927	-5.35925	-3.29422
O	-2.64184	-5.05478	1.62317
O	-5.27938	-5.3088	1.32593
O	-7.97895	-5.33129	1.08574
Si	-3.65478	-4.46582	-3.34414
Si	-4.45517	-2.19926	-1.05459
Si	-3.87136	0.93721	3.02593
Si	-4.72542	-2.09307	4.20565
Si	-4.07957	-4.14098	1.62936
Si	-8.63419	-4.00068	-3.80304
Si	-7.78616	-1.9762	-1.26372
Si	-9.12033	1.05208	-0.66448
Si	-9.14781	0.99678	2.73812
Si	-8.11418	-2.0263	3.90732
Si	-8.94514	-3.93367	1.24726
O	-7.9606	2.06889	3.30501
O	-5.21104	1.87669	3.51878
O	-2.556	1.82508	3.66153
O	-7.94395	2.17103	-1.15649
O	-5.15846	1.81549	-0.9816
O	-2.31653	1.60026	-1.10778
Si	-6.57647	-6.22462	0.71925
Si	-6.42671	-6.28678	-2.68466
Si	-1.72107	-6.45824	1.34176
Si	-1.70449	-6.84874	-2.01066
O	-6.38623	4.18379	2.59044
O	-6.24686	3.58573	-2.86038
O	-6.35258	4.18413	-0.19282
O	-2.07279	4.31541	2.75028
O	-1.98178	6.4984	0.90835
O	-1.92604	8.00199	-1.3893
O	-2.04147	6.23957	-3.54521
O	-2.01036	3.68942	-2.49852
O	-2.06718	3.88244	0.00341
O	-4.25775	5.15074	1.24091
O	-4.06152	4.52316	-4.22402
Si	-6.53721	2.91053	3.71702
Si	-5.96497	5.06956	1.20001
Si	-5.77653	4.39724	-4.27279
Si	-6.41676	2.89775	-1.31199
Si	-1.67453	3.23182	4.02134
Si	-2.58542	4.97344	1.29296
Si	-2.40248	4.63762	-3.93351
O	0.01257	3.03379	4.00173
O	-0.10186	2.74842	-1.15381
O	-0.00201	8.38052	0.48748
O	0.03726	8.01331	-3.26977
O	-6.45313	-6.31478	-0.98318
O	-1.89197	-6.82056	-0.31847
O	-0.04294	-6.22603	1.54725
O	-0.01985	-6.81187	-2.27083
O	6.45969	4.19711	2.71137
O	6.1886	3.63244	-2.71965
O	6.2921	4.18827	-0.02184
O	2.10976	4.47552	2.91881
O	2.0798	6.7195	1.11557
O	1.94653	8.04662	-1.3553
O	2.19294	6.40343	-3.67614
O	2.00436	3.83524	-2.70716
O	2.11145	4.11292	0.18174
O	4.31105	5.29717	1.4821
O	4.15932	4.60151	-4.32545
O	7.97512	2.00465	3.35852
O	5.23258	1.85251	3.39827
O	2.57775	1.88627	3.60899
O	7.74629	2.08825	-1.02935
O	4.99743	1.85439	-0.88239
O	2.34671	1.47121	-1.04228
Si	6.55452	2.85764	3.75608

Si	5.99307	5.13484	1.36332	H	8.60438	-2.40567	5.21096
Si	5.85276	4.4646	-4.1726	H	10.44909	1.22815	3.25183
Si	6.29028	2.94838	-1.17569	H	10.32147	-4.42354	1.37283
Si	1.6985	3.27989	4.05879	H	10.2385	1.38922	-1.24322
Si	2.61705	5.13528	1.43266	H	10.11733	-4.57973	-3.7028
Si	1.68802	8.167	0.33061	H	-10.4456	1.34362	3.25488
Si	1.7324	7.90518	-3.04128	H	-10.4069	1.3419	-1.23273
Si	2.47891	4.75741	-4.05138	H	-10.0422	-4.32967	-3.74497
Si	3.74013	0.91878	-0.40628	H	-10.3407	-4.27072	1.20246
Si	3.84718	0.98093	2.94108	Al	1.6739	3.10587	-1.15602
Si	8.99407	1.01198	-0.63347	H	-6.48021	-7.62505	-3.20576
Si	9.13253	0.91507	2.76399	H	-6.61977	-7.54557	1.28118
O	6.42719	-6.35686	-0.96807	H	-2.26457	-8.04971	-2.57105
O	1.82614	-6.86747	-0.3025	H	2.22038	-8.06777	-2.5677
Si	6.52128	-6.26997	0.73646	H	2.05005	-7.57267	2.19978
Si	6.39838	-6.32919	-2.66862	H	-2.15901	-7.54827	2.17141
Si	1.62951	-6.49016	1.35189	H	6.40663	-7.66645	-3.19451
Si	1.65961	-6.87221	-1.99658	H	6.53899	-7.59077	1.29977
O	2.41578	-5.49808	-2.67103	H	8.40539	-3.74461	-5.12004
O	5.02285	-5.46255	-3.18368	H	3.30166	-4.13746	-4.6913
O	7.72269	-5.44834	-3.2775	H	-3.34104	-4.0572	-4.6834
O	2.57662	-5.09979	1.61005	H	-8.26841	-3.61993	-5.15051
O	5.22003	-5.33837	1.30747	H	6.36036	3.69793	-5.29197
O	7.92942	-5.3979	1.1316	H	1.78155	4.37894	-5.25324
O	3.87177	-3.08596	-2.4188	H	-1.64397	4.10795	-5.02786
O	3.94948	-0.61173	-0.97741	H	-6.13488	3.63902	-5.45185
O	3.71862	0.87262	1.23201	H	-6.34555	5.72537	-4.34058
O	4.03366	-0.57472	3.59404	H	-6.56148	6.37521	1.20472
O	4.20007	-3.28048	2.99003	H	6.47265	5.7727	-4.15257
O	4.08863	-3.11636	0.2626	H	6.69427	6.38642	1.32745
O	8.41681	-2.89167	-2.6723	H	2.41259	8.97333	-3.72245
O	8.50848	-0.54354	-1.13171	H	2.39596	9.29159	0.87659
O	9.13983	0.94879	1.06334	H	-2.47461	9.05369	0.92933
O	8.63321	-0.60443	3.34945	H	-2.3949	8.77456	-3.83008
O	8.49114	-3.22637	2.76264	P	-1.61354	2.96908	-1.16597
O	8.55541	-3.01689	0.0329	Al	-3.83253	0.85693	-0.40079
O	6.21758	-2.16593	-1.22148	C	0.05311	-0.46303	-2.12291
O	6.3332	-2.03008	4.08332	H	0.80031	-0.06511	-1.44606
Si	3.62696	-4.49993	-3.33981	H	0.04429	-1.4949	-2.43812
Si	4.52938	-2.22	-1.10305	H	-0.8622	0.10646	-2.23306
Si	4.62893	-2.07691	4.11843	H	0.52156	-2.48488	0.31707
Si	4.00338	-4.17902	1.57419	C	-0.56595	-2.49156	0.20351
Si	8.73558	-4.15684	-3.77283	H	-0.86007	-3.30548	-0.47201
Si	7.90915	-2.11556	-1.24835	H	-1.01991	-2.66183	1.18596
Si	8.0267	-2.08084	3.93396	O	-0.94529	-1.21302	-0.30551
Si	8.9388	-4.03781	1.33508	H	-1.91476	-1.16861	-0.48568
H	-6.63869	3.42888	5.05413	H	2.36263	0.24699	-3.10548
H	-2.05776	3.78577	5.29272	C	1.54561	-0.1234	-3.71687
H	2.04822	3.67799	5.39685	H	1.64833	-1.10947	-4.16323
H	6.59098	3.26208	5.13442	C	0.45994	0.65325	-3.96036
H	-8.74649	-2.35109	5.15864	H	-0.34222	0.32353	-4.6149
H	-4.28779	-2.46076	5.52322	H	0.41627	1.66848	-3.5779
H	4.14302	-2.4043	5.42904				

Table C7 Coordinates of C_3H_7-Z/MeOH on P-H[1]-ZSM-5 for DME conversion to propylene, in Å

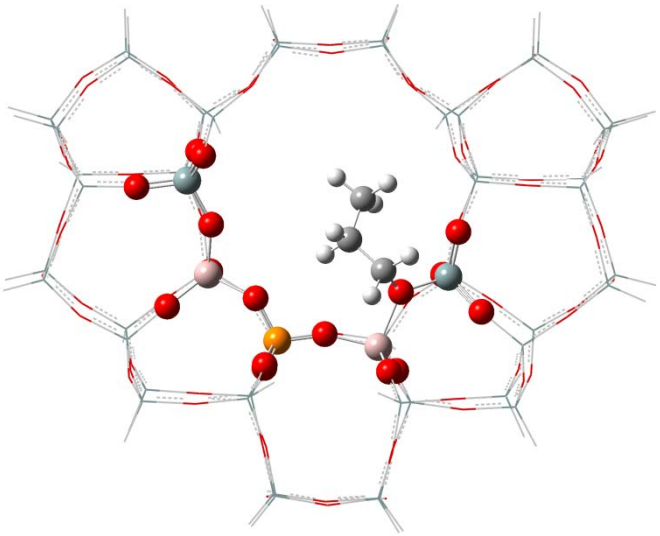


C_3H_7-Z/MeOH

Atoms	X	Y	Z
Si	-1.73599	8.02089	0.22623
Si	-1.69667	7.72985	-3.12853
O	-3.99014	-3.10633	-2.34591
O	-3.77329	-0.79806	-1.0083
O	-3.87408	0.86865	1.33743
O	-4.18122	-0.61866	3.72414
O	-4.31872	-3.31484	3.04537
O	-4.23768	-3.0632	0.29725
O	-8.31527	-2.83567	-2.77901
O	-8.60372	-0.5236	-1.24564
O	-9.26899	0.98786	0.93143
O	-8.75266	-0.57724	3.21724
O	-8.63658	-3.21303	2.62885
O	-8.55406	-2.98205	-0.09479
O	-6.16592	-2.01991	-1.22322
O	-6.52052	-2.06159	4.052
O	-2.38022	-5.41466	-2.80592
O	-4.98042	-5.46208	-3.27466
O	-7.6764	-5.42096	-3.35543
O	-2.64009	-5.05156	1.60438
O	-5.27488	-5.36303	1.31339
O	-7.97568	-5.38028	1.01548
Si	-3.63369	-4.41635	-3.40177
Si	-4.54228	-2.2209	-1.07812
Si	-3.98483	0.91827	3.02047
Si	-4.82039	-2.13073	4.16652
Si	-4.09567	-4.16687	1.59951
Si	-8.63667	-4.10048	-3.8772
Si	-7.87704	-2.04516	-1.33812
Si	-9.16596	1.00919	-0.7713
Si	-9.23094	0.94745	2.63059
Si	-8.20425	-2.07289	3.81501
Si	-8.99341	-4.02076	1.17141
O	-8.06467	2.03393	3.21853
O	-5.31861	1.86453	3.51694
O	-2.66487	1.80788	3.66021
O	-7.98344	2.13227	-1.24245
O	-5.19024	1.84177	-1.00815
O	-2.34254	1.56912	-1.04949
Si	-6.56122	-6.26247	0.66203
Si	-6.35638	-6.30865	-2.74046
Si	-1.65438	-6.39412	1.26056
Si	-1.59711	-6.74707	-2.09826
O	-6.47776	4.15861	2.53848
O	-6.27745	3.5717	-2.91856
O	-6.43776	4.17684	-0.25007
O	-2.16161	4.30416	2.72266
O	-2.06529	6.48311	0.87735
O	-1.98345	7.92891	-1.46169
O	-2.03771	6.12329	-3.59464
O	-2.00438	3.61349	-2.51029
O	-2.09355	3.88081	-0.01847
O	-4.34004	5.12713	1.19551
O	-4.04766	4.41584	-4.27914
Si	-6.6602	2.88749	3.66429
Si	-6.05037	5.04561	1.15133
Si	-5.76248	4.29013	-4.36399
Si	-6.46726	2.88677	-1.37037
Si	-1.79003	3.21893	3.99911
Si	-2.66973	4.95536	1.25879
Si	-2.39131	4.51317	-3.97683
O	-0.09658	3.02074	3.97229
O	-0.11945	2.71329	-1.10734
O	-0.07443	8.32845	0.42317
O	-0.02203	7.9548	-3.33101
O	-6.40823	-6.33701	-1.03795
O	-1.79604	-6.73023	-0.40624
O	0.02389	-6.15262	1.48457
O	0.09198	-6.68317	-2.34767
O	6.39675	4.26667	2.67944
O	6.17099	3.71331	-2.77452
O	6.24793	4.2843	-0.06071
O	2.03816	4.43309	2.88878
O	1.97928	6.61902	1.02538
O	1.88642	7.98509	-1.40942
O	2.14122	6.35261	-3.71596
O	1.99766	3.80143	-2.73272
O	2.1399	3.97977	0.17346
O	4.24916	5.30681	1.45498
O	4.11072	4.57059	-4.37708
O	7.88691	2.09113	3.363

O	5.1369	1.91882	3.26849	H	-8.85082	-2.38069	5.06395
O	2.47907	1.87425	3.55771	H	-4.4096	-2.49222	5.49525
O	7.67002	2.14971	-1.02767	H	4.13337	-2.2998	5.3775
O	4.91573	1.9926	-0.95466	H	8.5911	-2.24921	5.25172
O	2.3354	1.34282	-1.22489	H	10.39763	1.41767	3.27345
Si	6.44193	2.91595	3.71505	H	10.43696	-4.30223	1.50366
Si	5.93653	5.21211	1.33812	H	10.20468	1.63429	-1.2159
Si	5.80878	4.47924	-4.26195	H	10.34563	-4.513	-3.62984
Si	6.25741	3.05896	-1.22324	H	-10.5369	1.28234	3.13572
Si	1.58379	3.25364	4.03442	H	-10.4438	1.31705	-1.35083
Si	2.5671	5.07362	1.40837	H	-10.0311	-4.48795	-3.83999
Si	1.60965	8.09405	0.27376	H	-10.375	-4.4144	1.14174
Si	1.66891	7.86101	-3.09681	Al	1.60797	3.11325	-1.19983
Si	2.43007	4.71597	-4.10741	H	-6.3834	-7.65217	-3.25246
Si	3.83855	0.89851	-0.45996	H	-6.62048	-7.58979	1.20941
Si	3.75805	1.01511	2.86351	H	-2.10537	-7.97548	-2.65184
Si	8.989	1.1568	-0.62018	H	2.28785	-8.0161	-2.62084
Si	9.09788	1.05317	2.77915	H	2.10681	-7.50836	2.12953
O	6.62384	-6.28775	-0.94409	H	-2.05484	-7.52388	2.05835
O	1.92062	-6.79014	-0.36899	H	6.68575	-7.62718	-3.15462
Si	6.67468	-6.19314	0.76006	H	6.71722	-7.50673	1.33774
Si	6.62293	-6.28501	-2.64615	H	8.64935	-3.67704	-5.06666
Si	1.69184	-6.42188	1.28216	H	3.57523	-4.14651	-4.7643
Si	1.76515	-6.79489	-2.06543	H	-3.35487	-3.98842	-4.74169
O	2.62189	-5.47972	-2.73795	H	-8.27359	-3.70527	-5.22146
O	5.24348	-5.45627	-3.20043	H	6.32099	3.67535	-5.35055
O	7.94505	-5.37544	-3.22267	H	1.72605	4.3182	-5.29437
O	2.68034	-5.05979	1.5579	H	-1.6097	3.99743	-5.05937
O	5.34412	-5.28482	1.29889	H	-6.09878	3.47613	-5.51126
O	8.05514	-5.28334	1.17546	H	-6.31362	5.61922	-4.51748
O	4.13449	-3.09886	-2.46514	H	-6.63415	6.35737	1.16627
O	4.17729	-0.58166	-1.00562	H	6.40303	5.79802	-4.28886
O	3.61419	0.94356	1.13637	H	6.60686	6.4787	1.30864
O	4.01646	-0.53463	3.48404	H	2.35844	8.92389	-3.77503
O	4.27035	-3.23857	2.95304	H	2.34071	9.18945	0.84676
O	4.26322	-3.06278	0.24289	H	-2.54014	9.04643	0.82689
O	8.64927	-2.81493	-2.6238	H	-2.46746	8.65148	-3.9145
O	8.62414	-0.42759	-1.11924	P	-1.64281	2.92338	-1.15579
O	9.10369	1.10641	1.07806	Al	-3.89566	0.84593	-0.4106
O	8.63758	-0.47685	3.36161	C	1.12013	-1.6596	-1.2905
O	8.54676	-3.10384	2.81006	H	1.4403	-1.4243	-0.27166
O	8.73516	-2.89653	0.09016	H	1.93489	-2.18745	-1.80575
O	6.41132	-2.097	-1.21386	H	0.26742	-2.33212	-1.19072
O	6.34204	-1.90653	4.06839	H	-0.35444	-1.73072	2.39881
Si	3.84487	-4.49996	-3.40084	C	-1.36783	-1.646	1.99274
Si	4.72759	-2.21909	-1.14255	H	-1.89635	-2.59664	2.18118
Si	4.64009	-2.01029	4.06676	H	-1.89522	-0.83751	2.52309
Si	4.10264	-4.14568	1.53534	O	-1.24088	-1.37483	0.60867
Si	8.9643	-4.09177	-3.71696	H	-2.12156	-1.26161	0.21101
Si	8.10297	-2.03189	-1.2217	H	1.46323	1.33841	-3.0951
Si	8.03931	-1.9544	3.95668	C	1.81477	0.57348	-2.40244
Si	9.05521	-3.92434	1.40665	H	2.67331	0.07569	-2.8544
H	-6.80049	3.41725	4.99381	C	0.70228	-0.39921	-2.04902
H	-2.14824	3.78945	5.2702	H	0.26453	-0.6846	-3.01675
H	1.95269	3.64138	5.36926	H	-0.08648	0.12143	-1.50097
H	6.40012	3.29822	5.09862				

Table C8 Coordinates of C_3H_7-Z on P-H[1]-ZSM-5 for DME conversion to propylene, in Å

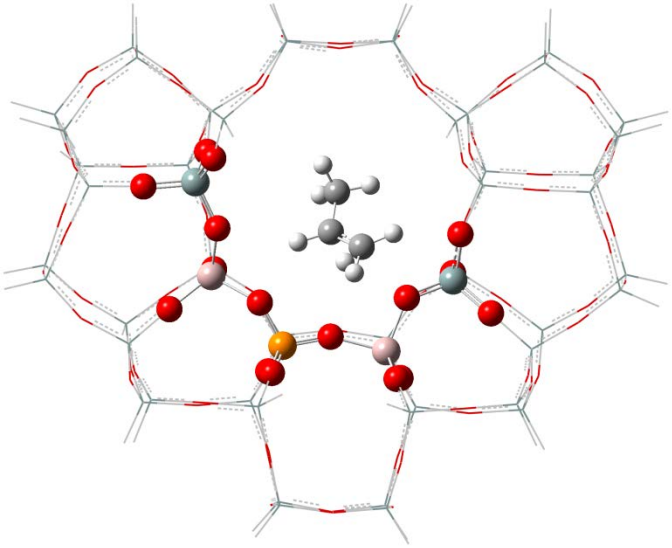


C_3H_7-Z

Atoms	X	Y	Z
Si	-1.76969	7.99895	0.22716
Si	-1.73286	7.70078	-3.12701
O	-4.00222	-3.13861	-2.31896
O	-3.7891	-0.827	-0.98652
O	-3.89131	0.84453	1.35571
O	-4.19303	-0.63831	3.74591
O	-4.32534	-3.33623	3.07306
O	-4.2474	-3.09034	0.32433
O	-8.32832	-2.87821	-2.74861
O	-8.62034	-0.56347	-1.21994
O	-9.28684	0.95123	0.95449
O	-8.76501	-0.60783	3.24317
O	-8.6438	-3.24463	2.66035
O	-8.56431	-3.01933	-0.06386
O	-6.17929	-2.05447	-1.19658
O	-6.5289	-2.08557	4.07905
O	-2.38775	-5.44445	-2.77551
O	-4.98827	-5.49848	-3.24173
O	-7.6844	-5.46335	-3.32007
O	-2.64431	-5.07242	1.63424
O	-5.27868	-5.3902	1.34638
O	-7.97972	-5.41391	1.05103
Si	-3.64392	-4.45013	-3.37233
Si	-4.55509	-2.25165	-1.05257
Si	-4.00061	0.89753	3.03875
Si	-4.82852	-2.1508	4.19213
Si	-4.10179	-4.19089	1.62882
Si	-8.648	-4.14607	-3.84378
Si	-7.89046	-2.08366	-1.30983
Si	-9.18544	0.96912	-0.74837
Si	-9.24713	0.91456	2.6537
Si	-8.21283	-2.10101	3.84365
Si	-9.00023	-4.05625	1.20498
O	-8.08267	2.00481	3.23821
O	-5.33596	1.84197	3.53443
O	-2.68198	1.79136	3.67534
O	-8.00578	2.09373	-1.22304
O	-5.21174	1.80975	-0.99072
O	-2.3635	1.54315	-1.03413
Si	-6.56369	-6.29381	0.69815
Si	-6.36191	-6.34686	-2.70442
Si	-1.65603	-6.41359	1.29239
Si	-1.60111	-6.77364	-2.06571
O	-6.50097	4.13144	2.55212
O	-6.30446	3.53323	-2.90383
O	-6.46359	4.14376	-0.2365
O	-2.18498	4.28669	2.73196
O	-2.09507	6.46187	0.88189
O	-2.01852	7.90281	-1.46033
O	-2.07087	6.09249	-3.58935
O	-2.03111	3.5851	-2.49963
O	-2.11855	3.85759	-0.00831
O	-4.36659	5.10168	1.20508
O	-4.07776	4.37924	-4.2683
Si	-6.67963	2.86236	3.68083
Si	-6.07679	5.01637	1.16266
Si	-5.79238	4.24965	-4.35128
Si	-6.49136	2.85122	-1.354
Si	-1.80987	3.20501	4.01039
Si	-2.69586	4.93364	1.26717
Si	-2.42134	4.48079	-3.96775
O	-0.11602	3.01042	3.98242
O	-0.14294	2.69199	-1.09652
O	-0.10862	8.31052	0.42188
O	-0.05889	7.92891	-3.33153
O	-6.41212	-6.37168	-1.00181
O	-1.79851	-6.75359	-0.37356
O	0.02193	-6.16799	1.51431
O	0.08761	-6.70664	-2.31684
O	6.3734	4.26756	2.68084
O	6.14377	3.70197	-2.7717
O	6.222	4.27897	-0.0592
O	2.01465	4.42503	2.89389
O	1.94933	6.60681	1.02585
O	1.85127	7.96744	-1.41179
O	2.10745	6.33056	-3.71505
O	1.97031	3.78119	-2.7262
O	2.11485	3.96609	0.17946
O	4.22243	5.30042	1.45615
O	4.08018	4.55137	-4.37418
O	7.86888	2.09671	3.36769
O	5.11916	1.91826	3.27611
O	2.46171	1.86859	3.5679

O	7.64779	2.14538	-1.0229	H	1.9332	3.63848	5.37614
O	4.89392	1.98248	-0.94698	H	6.38111	3.30433	5.10209
O	2.31475	1.32657	-1.21341	H	-8.85757	-2.40751	5.09385
Si	6.42246	2.91917	3.71931	H	-4.41572	-2.50854	5.52125
Si	5.9099	5.20911	1.33792	H	4.12669	-2.29796	5.39512
Si	5.77853	4.46392	-4.26044	H	8.58418	-2.23803	5.26507
Si	6.23305	3.05115	-1.2191	H	10.38096	1.42847	3.27724
Si	1.5639	3.24707	4.04249	H	10.43099	-4.29513	1.51972
Si	2.54084	5.06351	1.41162	H	10.18338	1.63502	-1.21238
Si	1.57582	8.07942	0.2714	H	10.33536	-4.51713	-3.61323
Si	1.63246	7.83926	-3.09871	H	-10.5533	1.24772	3.15932
Si	2.39947	4.6937	-4.10326	H	-10.4645	1.27298	-1.32738
Si	3.81956	0.88714	-0.44893	H	-10.0415	-4.53646	-3.80443
Si	3.7419	1.01072	2.87436	H	-10.381	-4.45294	1.17745
Si	8.96929	1.15619	-0.6145	Al	1.58352	3.09547	-1.19148
Si	9.08155	1.06011	2.78494	H	-6.3865	-7.69154	-3.21351
O	6.6199	-6.29412	-0.9202	H	-6.61958	-7.62007	1.24844
O	1.91831	-6.80541	-0.33965	H	-2.10723	-8.00434	-2.61619
Si	6.67211	-6.19574	0.78369	H	2.2861	-8.03542	-2.58919
Si	6.6174	-6.29505	-2.62226	H	2.10836	-7.51785	2.16024
Si	1.69027	-6.43409	1.31092	H	-2.0533	-7.5425	2.09298
Si	1.76127	-6.81414	-2.03592	H	6.68265	-7.63817	-3.12791
O	2.61455	-5.49858	-2.71206	H	6.71803	-7.50799	1.36415
O	5.23566	-5.47048	-3.17704	H	8.63594	-3.68793	-5.05027
O	7.93702	-5.38387	-3.20198	H	3.56313	-4.16768	-4.74217
O	2.67609	-5.06929	1.58282	H	-3.36727	-4.02448	-4.71343
O	5.3401	-5.28913	1.32181	H	-8.28703	-3.75297	-5.18922
O	8.051	-5.28207	1.19584	H	6.29147	3.6588	-5.34778
O	4.12226	-3.11388	-2.44578	H	1.6952	4.29187	-5.28871
O	4.16099	-0.59347	-0.99172	H	-1.63963	3.96441	-5.04991
O	3.59659	0.93514	1.14751	H	-6.12799	3.43246	-5.49648
O	4.00422	-0.53712	3.49798	H	-6.34653	5.57721	-4.50712
O	4.26345	-3.24164	2.97256	H	-6.66338	6.3269	1.17533
O	4.25343	-3.07171	0.26204	H	6.36991	5.78392	-4.29073
O	8.63627	-2.82057	-2.60926	H	6.57747	6.47708	1.3051
O	8.60739	-0.43006	-1.10982	H	2.31906	8.90217	-3.77985
O	9.08567	1.1097	1.08374	H	2.30505	9.17763	0.84137
O	8.62509	-0.46964	3.37112	H	-2.5755	9.02404	0.82635
O	8.53943	-3.09801	2.8253	H	-2.50636	8.61905	-3.91424
O	8.72486	-2.89614	0.10479	P	-1.6668	2.89869	-1.14399
O	6.39809	-2.10443	-1.19878	Al	-3.91447	0.81799	-0.39224
O	6.3333	-1.90275	4.08311	C	1.10589	-1.6786	-1.27142
Si	3.8348	-4.51762	-3.3782	H	1.42651	-1.44043	-0.25339
Si	4.7147	-2.22999	-1.12564	H	1.92132	-2.20581	-1.78631
Si	4.63157	-2.01018	4.08329	H	0.25474	-2.35274	-1.16941
Si	4.09639	-4.15217	1.55697	H	1.44085	1.31625	-3.08279
Si	8.95304	-4.09908	-3.69997	C	1.79469	0.55358	-2.38881
Si	8.08958	-2.03569	-1.20834	H	2.65388	0.05666	-2.8405
Si	8.03056	-1.9472	3.96992	C	0.68463	-0.42075	-2.03226
Si	9.04834	-3.92042	1.42318	H	0.2466	-0.70916	-2.99898
H	-6.81982	3.39467	5.00934	H	-0.10474	0.09937	-1.4846
H	-2.16813	3.77749	5.28059				

Table C9 Coordinates of TS2 on P-H[1]-ZSM-5 for DME conversion to propylene, in Å

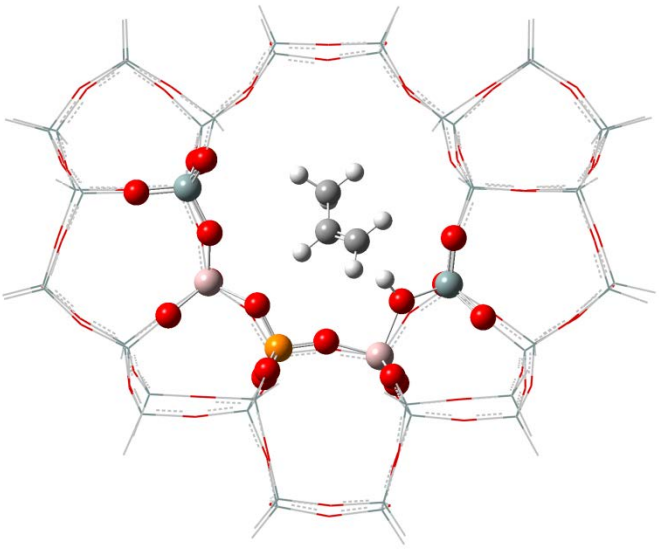


TS2

Atoms	X	Y	Z
Si	-1.76514	8.03971	0.20701
Si	-1.74127	7.75457	-3.14591
O	-3.90098	-3.13841	-2.37686
O	-3.75487	-0.77442	-1.14455
O	-3.8419	0.81114	1.31112
O	-4.07158	-0.63161	3.72464
O	-4.19783	-3.31303	3.02676
O	-4.08429	-3.03057	0.26642
O	-8.27776	-2.8886	-2.72107
O	-8.52994	-0.58397	-1.17234
O	-9.22076	0.89799	1.01871
O	-8.64699	-0.64261	3.30461
O	-8.50666	-3.26777	2.70048
O	-8.4592	-3.03622	-0.02796
O	-6.0912	-2.09662	-1.22031
O	-6.38263	-2.10332	4.10022
O	-2.34939	-5.48082	-2.75289
O	-4.94764	-5.5163	-3.26083
O	-7.64599	-5.4663	-3.31873
O	-2.5353	-5.03752	1.57238
O	-5.16527	-5.33065	1.27966
O	-7.87032	-5.42728	1.07275
Si	-3.58934	-4.49177	-3.39488
Si	-4.45501	-2.2314	-1.11925
Si	-3.91033	0.89658	2.99756
Si	-4.67962	-2.1508	4.17795
Si	-3.98317	-4.13954	1.569
Si	-8.61551	-4.14501	-3.82335
Si	-7.80579	-2.10462	-1.28732
Si	-9.14822	0.92409	-0.68543
Si	-9.15528	0.87268	2.71757
Si	-8.07007	-2.13187	3.88992
Si	-8.88851	-4.06924	1.24671
O	-7.99162	1.9739	3.2816
O	-5.24186	1.83137	3.51692
O	-2.57802	1.79595	3.58756
O	-8.0237	2.09991	-1.17225
O	-5.24732	1.8149	-0.97505
O	-2.40207	1.57925	-1.09219
Si	-6.44589	-6.27893	0.68945
Si	-6.32491	-6.35768	-2.71559
Si	-1.60461	-6.43407	1.29781
Si	-1.59881	-6.83901	-2.05256
O	-6.44328	4.12688	2.59899
O	-6.33645	3.57676	-2.85401
O	-6.46982	4.15575	-0.1828
O	-2.12615	4.30514	2.70209
O	-2.08548	6.49744	0.85849
O	-2.03021	7.94692	-1.47832
O	-2.11481	6.15301	-3.61329
O	-2.01535	3.63627	-2.52197
O	-2.11816	3.88097	-0.02944
O	-4.33974	5.11194	1.21858
O	-4.10298	4.39574	-4.23684
Si	-6.58929	2.83988	3.71078
Si	-6.04938	5.02609	1.2092
Si	-5.82021	4.30141	-4.29749
Si	-6.51915	2.87662	-1.31258
Si	-1.721	3.21244	3.96267
Si	-2.66516	4.96683	1.25451
Si	-2.44069	4.53693	-3.98007
O	-0.03173	3.01189	3.92945
O	-0.16782	2.64339	-1.10896
O	-0.10793	8.36519	0.3889
O	-0.0677	7.95481	-3.35859
O	-6.34095	-6.37688	-1.01313
O	-1.77267	-6.81132	-0.35829
O	0.07333	-6.1911	1.50562
O	0.08769	-6.78512	-2.30827
O	6.4017	4.28075	2.61222
O	6.05791	3.62968	-2.81876
O	6.17655	4.23975	-0.12108
O	2.05109	4.4766	2.8664
O	1.96717	6.70656	1.03806
O	1.84287	7.99159	-1.45033
O	2.06384	6.31454	-3.75134
O	1.91136	3.77519	-2.7423
O	2.04548	4.08591	0.14054
O	4.2252	5.33803	1.41086
O	4.00833	4.51121	-4.43851
O	7.95375	2.13165	3.29665
O	5.21362	1.9311	3.34926
O	2.5493	1.89837	3.57241
O	7.63299	2.14822	-1.09515
O	4.87848	1.89277	-0.93608
O	2.22686	1.41044	-1.00616

Si	6.52098	2.96601	3.68454	H	6.54835	3.39482	5.0553
Si	5.90666	5.19896	1.26117	H	-8.69275	-2.45599	5.14648
Si	5.70346	4.37684	-4.31438	H	-4.2307	-2.52129	5.49106
Si	6.16851	2.98767	-1.26038	H	4.2346	-2.35053	5.41793
Si	1.64855	3.28402	4.01217	H	8.69046	-2.2426	5.16542
Si	2.53593	5.13938	1.37472	H	10.44393	1.4074	3.16549
Si	1.5804	8.14568	0.23165	H	10.42752	-4.26353	1.33713
Si	1.62617	7.83114	-3.13528	H	10.16511	1.6039	-1.32523
Si	2.3349	4.66598	-4.12672	H	10.21177	-4.45123	-3.72246
Si	3.68255	0.91483	-0.41655	H	-10.4573	1.19331	3.24104
Si	3.84701	1.0187	2.92511	H	-10.4471	1.17758	-1.24403
Si	8.95039	1.15644	-0.70414	H	-10.0086	-4.53401	-3.76942
Si	9.12945	1.06654	2.6919	H	-10.2704	-4.46134	1.23402
O	6.55654	-6.2736	-0.97908	Al	1.58905	3.08061	-1.18715
O	1.94739	-6.82575	-0.34454	H	-6.35888	-7.70145	-3.22531
Si	6.65992	-6.18524	0.72381	H	-6.44872	-7.59827	1.2581
Si	6.51943	-6.25865	-2.68049	H	-2.13613	-8.05503	-2.60324
Si	1.74366	-6.4589	1.31042	H	2.32987	-8.03998	-2.6028
Si	1.76613	-6.84255	-2.03823	H	2.1686	-7.54392	2.15319
O	2.52805	-5.47326	-2.71545	H	-2.02858	-7.52297	2.13671
O	5.13858	-5.40529	-3.19838	H	6.54446	-7.59932	-3.19632
O	7.83428	-5.36391	-3.29154	H	6.7079	-7.50255	1.29268
O	2.68984	-5.06942	1.58922	H	8.48542	-3.66111	-5.14965
O	5.34592	-5.27473	1.30157	H	3.4301	-4.10223	-4.73326
O	8.05116	-5.2812	1.1086	H	-3.2834	-4.09482	-4.73884
O	3.95691	-3.06159	-2.42949	H	-8.26665	-3.74438	-5.16959
O	3.90222	-0.6143	-0.98822	H	6.19382	3.5476	-5.39529
O	3.68434	0.87725	1.21733	H	1.6027	4.27894	-5.3022
O	4.06769	-0.52857	3.58323	H	-1.6824	4.01498	-5.0759
O	4.28626	-3.22934	2.97791	H	-6.18415	3.50074	-5.446
O	4.17738	-3.06614	0.25929	H	-6.35571	5.63881	-4.4316
O	8.47521	-2.79176	-2.70776	H	-6.64146	6.33343	1.24149
O	8.54791	-0.42576	-1.1899	H	6.32735	5.68173	-4.37214
O	9.1123	1.10581	0.99159	H	6.59576	6.45553	1.19781
O	8.6643	-0.46069	3.28417	H	2.32093	8.88161	-3.82866
O	8.57971	-3.09088	2.72509	H	2.29402	9.27395	0.76204
O	8.63285	-2.89306	-0.0027	H	-2.58045	9.05078	0.81772
O	6.28059	-2.05673	-1.2373	H	-2.50961	8.68253	-3.92721
O	6.40437	-1.92929	4.04902	P	-1.67897	2.92961	-1.17227
Si	3.73008	-4.46267	-3.37729	Al	-3.93339	0.81728	-0.43166
Si	4.59927	-2.1834	-1.12028	C	0.0077	-1.81741	-0.0283
Si	4.70305	-2.01903	4.10228	H	1.06308	-2.01218	0.18418
Si	4.10801	-4.13921	1.56534	H	-0.44168	-2.71916	-0.45663
Si	8.82157	-4.05863	-3.79991	H	-0.51523	-1.61111	0.90768
Si	7.9737	-2.00821	-1.28796	H	0.56424	0.43186	-2.7004
Si	8.09828	-1.94539	3.88861	C	0.79074	-0.31153	-1.94325
Si	9.03796	-3.90404	1.30127	H	1.79148	-0.73457	-1.9442
H	-6.70621	3.34679	5.05108	C	-0.17964	-0.66862	-0.99832
H	-2.09623	3.75542	5.2407	H	-1.20631	-0.35984	-1.21044
H	1.98441	3.69061	5.35063	H	0.27559	0.3382	-0.57921

Table C10 Coordinates of C_3H_6/H^1Z on P-H^1-ZSM-5 for DME conversion to propylene, in Å

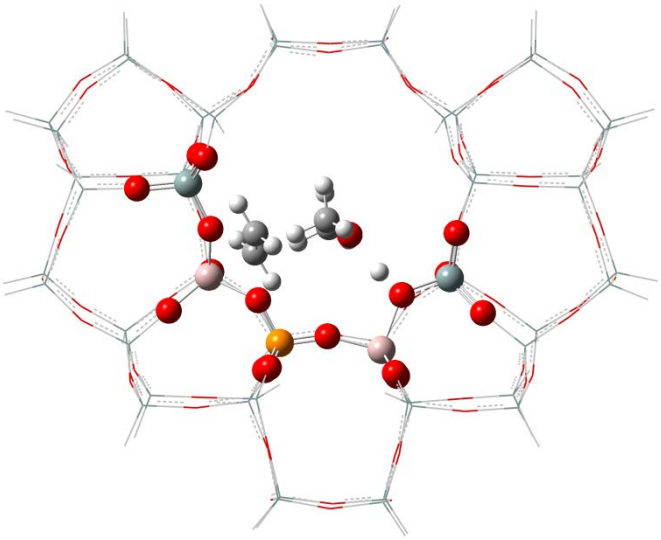


C_3H_6/H^1Z

Atoms	X	Y	Z
Si	-1.58727	8.03822	0.16708
Si	-1.5649	7.71458	-3.1845
O	-4.01553	-3.10295	-2.34895
O	-3.82236	-0.7289	-1.13625
O	-3.78651	0.86977	1.32578
O	-4.07932	-0.5499	3.75832
O	-4.28265	-3.23434	3.0572
O	-4.19549	-2.96925	0.29175
O	-8.40086	-2.75638	-2.68443
O	-8.56146	-0.42375	-1.16142
O	-9.17753	1.09979	1.0239
O	-8.65462	-0.45051	3.32126
O	-8.58697	-3.08307	2.74162
O	-8.56879	-2.86807	0.0102
O	-6.17997	-2.00846	-1.20327
O	-6.42762	-1.96018	4.13171
O	-2.51471	-5.48754	-2.72898
O	-5.10579	-5.4518	-3.22456
O	-7.80658	-5.35036	-3.26676
O	-2.67955	-5.01774	1.61008
O	-5.30851	-5.23423	1.32841
O	-8.01611	-5.26702	1.12274
Si	-3.72289	-4.4571	-3.36742
Si	-4.54469	-2.16882	-1.09961
Si	-3.86923	0.96048	3.00809
Si	-4.72552	-2.05575	4.20488
Si	-4.0941	-4.06896	1.59892
Si	-8.75682	-4.01753	-3.77556
Si	-7.89237	-1.97167	-1.26339
Si	-9.09639	1.1165	-0.68053
Si	-9.12188	1.07275	2.7226
Si	-8.11445	-1.94931	3.91875
Si	-9.00096	-3.88523	1.29627
O	-7.93339	2.14646	3.28964
O	-5.18159	1.93524	3.50896
O	-2.53713	1.8532	3.61958
O	-7.9129	2.23345	-1.16402
O	-5.12241	1.92338	-0.96908
O	-2.28207	1.57414	-1.0545
Si	-6.61083	-6.15258	0.7414
Si	-6.49538	-6.25805	-2.66337
Si	-1.77337	-6.4267	1.33116
Si	-1.77102	-6.84013	-2.01856
O	-6.33705	4.25757	2.5986
O	-6.21972	3.67383	-2.85615
O	-6.34633	4.27068	-0.18934
O	-2.03052	4.34951	2.70043
O	-1.91941	6.50537	0.82955
O	-1.84273	7.93412	-1.51847
O	-1.94281	6.11141	-3.63255
O	-1.94989	3.61605	-2.52228
O	-2.03425	3.89559	-0.03216
O	-4.2239	5.21418	1.21657
O	-3.99846	4.44071	-4.27353
Si	-6.50482	2.9717	3.71053
Si	-5.93599	5.14254	1.20277
Si	-5.71837	4.3682	-4.31756
Si	-6.39414	2.98081	-1.30924
Si	-1.67052	3.26289	3.97932
Si	-2.55845	5.00006	1.24329
Si	-2.33675	4.50578	-3.99583
O	0.02334	3.06294	3.96935
O	-0.06536	2.71342	-1.11655
O	0.07639	8.34174	0.35279
O	0.11324	7.90665	-3.39098
O	-6.51179	-6.26626	-0.9603
O	-1.93974	-6.80937	-0.3234
O	-0.0895	-6.22686	1.54825
O	-0.08205	-6.8106	-2.27408
O	6.51832	4.17214	2.67835
O	6.19983	3.58609	-2.76988
O	6.32006	4.18167	-0.05691
O	2.15182	4.46481	2.88728
O	2.1441	6.67458	1.02129
O	2.02774	7.93686	-1.47779
O	2.25412	6.2775	-3.78005
O	2.06624	3.77211	-2.7433
O	2.19216	4.05589	0.16191
O	4.3689	5.26545	1.46479
O	4.18496	4.44648	-4.4222
O	8.00246	1.96935	3.33531

O	5.25817	1.86374	3.40796	H	-2.03999	3.83135	5.24803
O	2.5917	1.90596	3.63106	H	2.05617	3.72761	5.38272
O	7.69645	2.02453	-1.03704	H	6.65252	3.26993	5.11635
O	4.94852	1.9019	-0.89026	H	-8.74518	-2.24374	5.17908
O	2.33928	1.40734	-1.00412	H	-4.28765	-2.43458	5.51982
Si	6.60503	2.84848	3.74459	H	4.14042	-2.39831	5.43527
Si	6.05202	5.12229	1.34205	H	8.59893	-2.44342	5.18761
Si	5.87802	4.31176	-4.28683	H	10.46985	1.16705	3.20956
Si	6.29366	2.95123	-1.21288	H	10.2925	-4.47691	1.35151
Si	1.70116	3.30633	4.05445	H	10.20176	1.38106	-1.28077
Si	2.67765	5.11085	1.40816	H	10.06317	-4.6265	-3.74584
Si	1.76053	8.11066	0.20163	H	-10.4176	1.4297	3.23899
Si	1.804	7.79374	-3.16398	H	-10.3789	1.43802	-1.24271
Si	2.50866	4.62908	-4.15087	H	-10.1558	-4.38525	-3.71439
Si	3.84497	0.86919	-0.33805	H	-10.3916	-4.2466	1.30414
Si	3.86347	0.99278	2.99568	Al	1.65037	3.16123	-1.19141
Si	8.9749	0.97038	-0.65955	H	-6.56182	-7.60599	-3.16026
Si	9.1463	0.86506	2.73655	H	-6.64871	-7.46856	1.31776
O	6.3644	-6.35363	-0.99182	H	-2.31253	-8.05892	-2.56019
O	1.7877	-6.85369	-0.31428	H	2.15636	-8.06787	-2.57156
Si	6.46929	-6.29008	0.71142	H	2.00807	-7.577	2.1812
Si	6.32583	-6.34416	-2.69428	H	-2.21534	-7.50871	2.17057
Si	1.57623	-6.4924	1.34055	H	6.32937	-7.68603	-3.20701
Si	1.5944	-6.86878	-2.00731	H	6.48272	-7.61322	1.26796
O	2.38048	-5.51214	-2.68472	H	8.34652	-3.77483	-5.14937
O	4.96924	-5.45841	-3.21643	H	3.25665	-4.13018	-4.72299
O	7.66585	-5.47933	-3.29783	H	-3.41979	-4.08352	-4.71823
O	2.5447	-5.11517	1.62168	H	-8.4112	-3.6311	-5.12696
O	5.19096	-5.34098	1.30513	H	6.38135	3.46053	-5.34276
O	7.88871	-5.43138	1.10461	H	1.78976	4.22552	-5.32583
O	3.86935	-3.11611	-2.42107	H	-1.57858	3.9648	-5.08231
O	3.98664	-0.62865	-0.92349	H	-6.10668	3.56218	-5.45386
O	3.72893	0.90577	1.26894	H	-6.23032	5.7138	-4.46381
O	4.04913	-0.57352	3.60061	H	-6.51196	6.45738	1.22611
O	4.17491	-3.28456	2.99132	H	6.50938	5.61207	-4.34606
O	4.07895	-3.11104	0.28597	H	6.7549	6.37099	1.30118
O	8.38455	-2.93237	-2.6988	H	2.50384	8.84354	-3.85239
O	8.49428	-0.58214	-1.15831	H	2.49086	9.23063	0.72625
O	9.12613	0.91234	1.03562	H	-2.38356	9.07142	0.76501
O	8.62643	-0.64435	3.32337	H	-2.31861	8.64482	-3.97688
O	8.47139	-3.26386	2.73659	P	-1.58891	2.9331	-1.16525
O	8.54168	-3.0513	0.01296	Al	-3.85195	0.86273	-0.42074
O	6.20236	-2.1631	-1.21752	C	-0.04851	-2.05162	-1.15447
O	6.3259	-2.04635	4.06881	H	-0.0302	-1.77689	-0.09259
Si	3.5636	-4.50303	-3.37353	H	0.79761	-2.71472	-1.36518
Si	4.51774	-2.26744	-1.10721	H	-0.98206	-2.60504	-1.30636
Si	4.62275	-2.09392	4.11889	H	0.79155	0.33215	-3.59232
Si	3.96391	-4.19593	1.58183	C	0.87812	-0.54973	-2.96224
Si	8.6824	-4.19942	-3.80807	H	1.70955	-1.22239	-3.16958
Si	7.89557	-2.15759	-1.27191	C	-0.04023	-0.82918	-2.02213
Si	8.01867	-2.12079	3.91189	H	-0.86896	-0.1409	-1.86714
Si	8.91196	-4.08523	1.31065	H	1.79717	0.70328	-1.43831
H	-6.60101	3.48521	5.0504				

Table C11 Coordinates of DME/C_2H_4/H^4Z on P-H^4-ZSM-5 for DME conversion to propylene, in Å

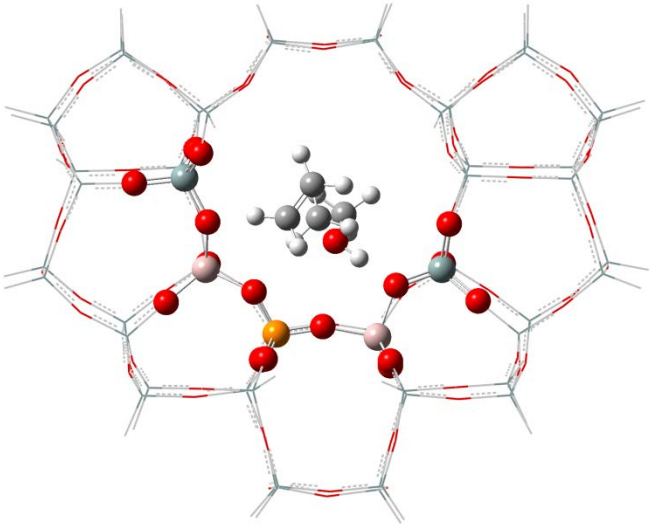


DME/C_2H_4/H^4Z

Atoms	X	Y	Z
Si	1.57061	8.03141	-0.17652
Si	1.55329	7.69364	3.17281
O	4.02966	-3.10109	2.29694
O	3.81735	-0.72404	1.10892
O	3.7499	0.85635	-1.363
O	4.0243	-0.54698	-3.80406
O	4.23538	-3.22319	-3.11588
O	4.16711	-2.95276	-0.35006
O	8.40816	-2.75962	2.57584
O	8.55835	-0.42248	1.05449
O	9.15077	1.10443	-1.13275
O	8.60872	-0.44476	-3.42559
O	8.54385	-3.07928	-2.85091
O	8.54882	-2.86793	-0.1199
O	6.1761	-2.00357	1.1194
O	6.37287	-1.95126	-4.21443
O	2.51256	-5.47919	2.67052
O	5.11485	-5.46659	3.14043
O	7.81528	-5.35376	3.16009
O	2.63046	-4.98832	-1.65767
O	5.26696	-5.22448	-1.39606
O	7.97746	-5.26309	-1.23146
Si	3.73853	-4.46751	3.30195
Si	4.5411	-2.16594	1.04164
Si	3.82475	0.96088	-3.04629
Si	4.67066	-2.04733	-4.26919
Si	4.05495	-4.05548	-1.65554
Si	8.7717	-4.02275	3.66244
Si	7.88998	-1.96994	1.16142
Si	9.08922	1.11933	0.57251
Si	9.07943	1.07918	-2.83085
Si	8.06246	-1.94194	-4.0209
Si	8.96704	-3.88537	-1.41054
O	7.88165	2.14887	-3.38572
O	5.12827	1.938	-3.56136
O	2.47495	1.84293	-3.63269
O	7.9129	2.23727	1.07081
O	5.12518	1.92602	0.90846
O	2.27532	1.56075	1.01969
Si	6.57691	-6.14959	-0.8364
Si	6.50359	-6.26779	2.56861
Si	1.719	-6.39594	-1.38263
Si	1.74824	-6.82403	1.96422
O	6.29632	4.26151	-2.67448
O	6.23426	3.68071	2.78119
O	6.33548	4.27476	0.11091
O	1.97847	4.34114	-2.72307
O	1.89687	6.50016	-0.84771
O	1.83228	7.9196	1.50744
O	1.93857	6.08939	3.6119
O	1.93576	3.59518	2.49145
O	2.02656	3.88329	0.00211
O	4.19378	5.20978	-1.27369
O	4.01026	4.43051	4.20709
Si	6.44816	2.97501	-3.787
Si	5.90563	5.14691	-1.27555
Si	5.73021	4.37384	4.24348
Si	6.39791	2.98869	1.23365
Si	1.6034	3.25105	-3.99433
Si	2.52762	4.99597	-1.27474
Si	2.34251	4.48382	3.9606
O	-0.08772	3.03252	-3.97118
O	0.05417	2.69812	1.07186
O	-0.09208	8.34123	-0.3549
O	-0.12443	7.87754	3.38357
O	6.50161	-6.27211	0.86569
O	1.9034	-6.78744	0.26793
O	0.03533	-6.18455	-1.58473
O	0.06285	-6.78175	2.23447
O	-6.56112	4.19629	-2.65589
O	-6.18931	3.59341	2.79017
O	-6.3176	4.19735	0.07767
O	-2.19464	4.46325	-2.90626
O	-2.15687	6.68058	-1.04022
O	-2.04007	7.9082	1.47623
O	-2.24299	6.21842	3.76471
O	-2.08801	3.7216	2.70629
O	-2.19891	4.05695	-0.18634
O	-4.38842	5.2812	-1.46754
O	-4.16308	4.39658	4.44836
O	-8.07583	2.0073	-3.30721

O	-5.33797	1.88098	-3.42669	H	8.6787	-2.23457	-5.28859
O	-2.6639	1.89678	-3.64248	H	4.21742	-2.42212	-5.57984
O	-7.66469	2.0271	1.05718	H	-4.25642	-2.41552	-5.45959
O	-4.91279	1.93224	0.8944	H	-8.71556	-2.40282	-5.15624
O	-2.317	1.3723	0.89179	H	-10.5372	1.19932	-3.13772
Si	-6.68021	2.88272	-3.73083	H	-10.3619	-4.45964	-1.31026
Si	-6.06995	5.13975	-1.32305	H	-10.178	1.43351	1.34506
Si	-5.85793	4.27356	4.32542	H	-10.0881	-4.63217	3.77244
Si	-6.26664	2.96346	1.23016	H	10.36899	1.43915	-3.3599
Si	-1.76543	3.29153	-4.06649	H	10.37833	1.43712	1.12128
Si	-2.69718	5.11692	-1.42039	H	10.16949	-4.39203	3.58808
Si	-1.77605	8.10581	-0.20084	H	10.35599	-4.25234	-1.4298
Si	-1.81512	7.74471	3.16076	Al	-1.67646	3.11601	1.14982
Si	-2.49368	4.56664	4.13004	H	6.57885	-7.61551	3.06408
Si	-3.85266	0.86645	0.31363	H	6.60307	-7.46152	-1.42206
Si	-3.9533	0.99093	-3.02477	H	2.2889	-8.0467	2.49776
Si	-8.96947	0.99845	0.70419	H	-2.1612	-8.05963	2.54028
Si	-9.20506	0.89853	-2.68811	H	-2.05181	-7.5559	-2.20398
O	-6.41419	-6.35055	0.98145	H	2.15193	-7.47297	-2.23299
O	-1.82017	-6.82808	0.28863	H	-6.36967	-7.69249	3.18875
Si	-6.53546	-6.27676	-0.72033	H	-6.56259	-7.59761	-1.28236
Si	-6.36274	-6.34748	2.68369	H	-8.36204	-3.78644	5.16701
Si	-1.62867	-6.46434	-1.36783	H	-3.29197	-4.13603	4.70956
Si	-1.6166	-6.85053	1.98042	H	3.45269	-4.09122	4.65701
O	-2.40335	-5.50415	2.67417	H	8.43663	-3.63805	5.01685
O	-4.99581	-5.47624	3.20313	H	-6.3581	3.39784	5.3627
O	-7.69385	-5.47979	3.30213	H	-1.74631	4.15852	5.28584
O	-2.6076	-5.09617	-1.65015	H	1.60956	3.92947	5.05744
O	-5.25442	-5.33771	-1.32466	H	6.13447	3.57387	5.37838
O	-7.95395	-5.409	-1.09554	H	6.23179	5.72416	4.38221
O	-3.91556	-3.12469	2.40775	H	6.47802	6.463	-1.30519
O	-4.04643	-0.6242	0.90306	H	-6.48332	5.5744	4.42493
O	-3.80252	0.87541	-1.30438	H	-6.76981	6.38995	-1.27083
O	-4.13739	-0.56761	-3.65267	H	-2.52401	8.78117	3.86032
O	-4.25434	-3.27339	-3.00814	H	-2.50686	9.23311	-0.70893
O	-4.14046	-3.11151	-0.29675	H	2.37018	9.06254	-0.77381
O	-8.42169	-2.92845	2.72182	H	2.3062	8.62231	3.96791
O	-8.51952	-0.56615	1.19405	P	1.57437	2.91842	1.13162
O	-9.15328	0.94369	-0.9884	Al	3.8487	0.86697	0.38314
O	-8.69602	-0.61047	-3.28645	H	-0.44834	-0.86463	2.58096
O	-8.56149	-3.23672	-2.71163	C	0.11386	-1.07666	1.67011
O	-8.60067	-3.03373	0.01421	H	0.20527	-2.1614	1.53954
O	-6.24467	-2.17094	1.22844	H	1.107	-0.62477	1.72119
O	-6.42278	-2.03983	-4.06823	H	0.99354	-0.16583	-0.68013
Si	-3.59999	-4.50633	3.35942	C	0.01783	-0.65828	-0.69117
Si	-4.55937	-2.26189	1.10062	H	0.14201	-1.72142	-0.92962
Si	-4.721	-2.09413	-4.14054	H	-0.6306	-0.18936	-1.43423
Si	-4.03372	-4.18505	-1.59967	O	-0.6367	-0.52163	0.57789
Si	-8.70761	-4.20254	3.82541	H	-1.59523	0.64748	0.80056
Si	-7.93559	-2.14816	1.29607	H	1.88454	0.67143	4.55879
Si	-8.11406	-2.09211	-3.88725	C	2.43697	-0.2622	4.64182
Si	-8.9822	-4.06355	-1.28267	H	2.98208	-0.58353	3.75848
H	6.52248	3.48364	-5.1299	C	2.43754	-0.96673	5.77584
H	1.96382	3.81433	-5.2679	H	1.89024	-0.63899	6.65686
H	-2.10837	3.70984	-5.39891	H	2.98816	-1.90082	5.86495
H	-6.74652	3.31685	-5.09791				

Table C12 Coordinates of TS1 on P-H[4]-ZSM-5 for DME conversion to propylene, in Å

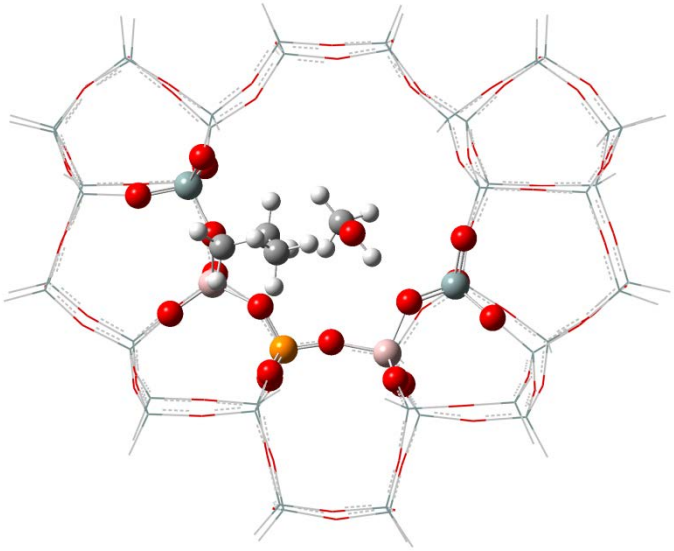


TS1

Atoms	X	Y	Z
C	-0.2425	-0.85684	-1.28118
H	-1.01275	-0.09488	-1.22899
H	-0.42166	-1.77624	-0.74353
H	0.75365	-0.57793	-1.59196
H	-0.25666	-1.33838	1.97197
C	0.61737	-0.71268	1.77403
H	1.50142	-1.34777	1.63632
H	0.77183	-0.05034	2.63474
O	0.32524	0.05679	0.60848
H	1.09745	0.5897	0.29999
H	-0.82538	-3.05724	-2.69571
C	-0.46265	-2.11331	-3.09722
H	0.55177	-2.10265	-3.48679
C	-1.27739	-1.0321	-3.1948
H	-0.92936	-0.11653	-3.66448
H	-2.30979	-1.06059	-2.85325
H	-10.4379	1.40752	-1.14087
Si	-9.14332	1.09674	-0.60148
O	-8.61864	-0.44927	-1.08644
O	-9.18809	1.07557	1.10333
O	-7.97103	2.20926	-1.11699
Si	-7.93866	-1.98951	-1.18613
Si	-9.10661	1.05675	2.80201
Si	-6.46068	2.97	-1.2902
O	-8.45436	-2.80475	-2.58743
O	-8.56417	-2.89345	0.10611
O	-6.22118	-2.00539	-1.17269
O	-8.62451	-0.4658	3.3941
O	-7.91021	2.12941	3.34893
H	-10.3969	1.40675	3.33538
O	-5.19078	1.89688	-0.98153
O	-6.30868	3.65989	-2.83919
O	-6.38987	4.25078	-0.16485
Si	-8.84787	-4.07987	-3.6486
Si	-8.98526	-3.90586	1.40095
Si	-4.59053	-2.16998	-1.11133
Si	-8.06599	-1.95408	3.99736
Si	-6.47268	2.959	3.73459
Al	-3.89758	0.86301	-0.45251
Si	-5.80658	4.39192	-4.28474
Si	-5.94064	5.1245	1.21704
O	-7.87809	-5.40475	-3.1518
H	-10.243	-4.44845	-3.53965
H	-8.53456	-3.71464	-5.01349
O	-8.55804	-3.09953	2.83798
O	-7.99205	-5.28262	1.2267
H	-10.373	-4.27601	1.41533
O	-4.08486	-3.08294	-2.39384
O	-3.84227	-0.73662	-1.19126
O	-4.19406	-2.97252	0.26088
O	-6.37341	-1.96917	4.16271
H	-8.66437	-2.24236	5.27406
O	-5.15966	1.91642	3.49511
O	-6.3367	4.24114	2.61675
H	-6.53766	3.46536	5.07855
O	-3.8014	0.84763	1.28794
O	-2.34134	1.54951	-1.14631
O	-4.08759	4.43195	-4.26464
H	-6.22269	3.61452	-5.43202
H	-6.30967	5.74428	-4.39012
O	-4.23132	5.17054	1.2108
H	-6.51139	6.4412	1.24489
Si	-6.57098	-6.32527	-2.5656
Si	-6.59677	-6.17628	0.83661
Si	-3.86125	-4.47399	-3.38843
Si	-4.07048	-4.05949	1.58246
Si	-4.6705	-2.05291	4.20208
Si	-3.8437	0.95979	2.97414
P	-1.62389	2.91258	-1.22389
Si	-2.41682	4.51376	-4.02785
Si	-2.56107	4.96891	1.20458
O	-5.18564	-5.51561	-3.14424
O	-6.54502	-6.3255	-0.86542
H	-6.63697	-7.67083	-3.06577
O	-5.27483	-5.2397	1.34797
H	-6.60868	-7.47769	1.44418
O	-2.52629	-5.37162	-2.79739
H	-3.64991	-4.10686	-4.75977
O	-4.23839	-3.22464	3.03904
O	-2.62793	-4.96413	1.54145
O	-4.03342	-0.55672	3.72132
H	-4.2015	-2.43561	5.5044
O	-2.50202	1.83769	3.5701
O	-2.00523	3.61104	-2.56988
O	-2.08515	3.84988	-0.07574
O	-0.11442	2.6827	-1.1824
O	-2.0248	6.12105	-3.69048

H	-1.70391	3.9483	-5.13331	Si	3.97384	1.01629	2.99676
O	-2.00812	4.3222	2.65431	Si	5.84473	4.28495	-4.3222
O	-1.95293	6.4789	0.77139	Si	6.00295	5.15276	1.27377
Si	-1.73233	-6.7189	-2.11209	Si	6.25347	2.94044	-1.24272
Si	-1.70695	-6.36195	1.24402	Si	4.59592	-2.2149	-1.11872
Si	-1.6151	3.24145	3.92863	O	5.07213	-5.46274	-3.18718
Al	1.66031	3.02747	-1.16924	O	3.95449	-3.07111	-2.44393
Si	-1.59566	7.71206	-3.23353	H	3.46752	-4.08735	-4.77182
Si	-1.62835	8.01867	0.11627	O	5.27041	-5.32882	1.32832
O	-1.89476	-6.71024	-0.41783	O	4.24216	-3.24552	2.97307
O	-0.05049	-6.60332	-2.37583	O	4.14984	-3.11327	0.24531
H	-2.24213	-7.94073	-2.67571	O	5.33822	1.91434	3.45044
O	-0.02754	-6.12885	1.44286	O	4.13279	-0.54429	3.64731
H	-2.13432	-7.46255	2.06538	O	6.18808	3.57634	-2.80585
O	0.071	3.01416	3.92994	H	6.35722	3.44021	-5.38082
H	-1.99587	3.80504	5.19684	H	6.45548	5.59497	-4.403
O	2.05833	3.68162	-2.728	O	6.51311	4.2404	2.62505
O	2.09622	4.08047	0.13842	O	6.28829	4.19606	-0.10679
O	2.2739	1.38359	-0.82772	H	6.6866	6.41307	1.21559
O	-1.89163	7.92257	-1.56931	O	7.69271	2.05645	-1.07289
O	0.08297	7.8639	-3.43869	O	6.28306	-2.1578	-1.23991
H	-2.33216	8.6569	-4.02585	Si	6.43453	-6.3375	-2.65357
O	0.02802	8.34529	0.30049	Si	6.57389	-6.2549	0.75053
H	-2.44461	9.03317	0.72071	Si	4.71422	-2.07195	4.11695
Si	1.62811	-6.74455	-2.11477	Si	6.66547	2.94507	3.71525
Si	1.64018	-6.42038	1.24387	Si	8.99243	1.03719	-0.69999
Si	1.75192	3.29203	4.01624	Si	7.97447	-2.11621	-1.28215
Si	2.47675	4.5344	-4.13394	O	6.46478	-6.34875	-0.95231
Si	2.62577	5.12449	1.36007	O	7.76917	-5.47485	-3.26611
Si	3.76391	0.89748	-0.34982	H	6.42921	-7.6814	-3.16225
Si	1.77478	7.72053	-3.20491	O	7.9812	-5.37489	1.12964
Si	1.71667	8.11595	0.15431	H	6.60123	-7.57195	1.32203
O	1.81869	-6.74875	-0.42281	O	6.41641	-2.02801	4.05638
O	2.43621	-5.40423	-2.79325	H	4.2402	-2.42396	5.4257
H	2.12573	-7.96543	-2.69108	O	8.06718	2.07041	3.30063
O	2.61424	-5.06255	1.56972	H	6.74736	3.40093	5.0751
H	2.03842	-7.54234	2.05063	O	8.56432	-0.53944	-1.18441
O	2.14671	4.47862	2.8634	O	9.16883	0.98209	0.99474
O	2.65455	1.89701	3.60479	H	10.21181	1.46095	-1.32921
H	2.0783	3.71178	5.3534	O	8.47577	-2.91409	-2.69574
O	2.20143	6.19279	-3.79679	O	8.62346	-3.00833	0.00472
O	4.14956	4.3927	-4.45903	Si	8.79405	-4.198	-3.77522
H	1.74636	4.1253	-5.30399	Si	9.00691	-4.02391	1.31044
O	2.09766	6.70433	1.01022	Si	8.1102	-2.04142	3.89534
O	4.32066	5.28537	1.41024	Si	9.19277	0.95267	2.69434
O	4.93371	1.8876	-0.9095	H	10.17231	-4.62892	-3.68735
O	4.00068	-0.62167	-0.91647	H	8.47609	-3.80478	-5.13073
O	3.82952	0.86386	1.29113	O	8.58137	-3.19371	2.73443
O	1.98338	7.91555	-1.52209	H	10.3855	-4.42414	1.3417
H	2.48097	8.75478	-3.91205	O	8.67897	-0.55753	3.29241
H	2.43018	9.25878	0.65354	H	8.70299	-2.33958	5.17179
Si	3.71631	-4.45531	-3.40714	H	10.52151	1.2451	3.16144
Si	4.05537	-4.16237	1.56536				

Table C13 Coordinates of C_3H_7-Z/MeOH on P-H^4-ZSM-5 for DME conversion to propylene, in Å

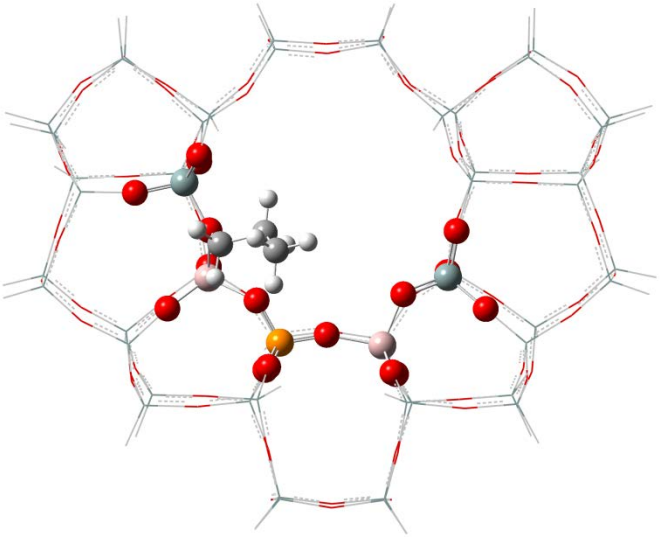


C_3H_7-Z/MeOH

Atoms	X	Y	Z
Si	-1.57766	8.0624	0.2407
Si	-1.6072	7.72001	-3.10375
O	-4.13644	-3.21822	-2.3148
O	-3.80423	-0.72611	-1.39561
O	-3.8059	0.68338	1.34498
O	-4.05415	-0.56675	3.84991
O	-4.2266	-3.16914	3.0998
O	-4.10926	-2.78849	0.32702
O	-8.37473	-2.78271	-2.55829
O	-8.60982	-0.43433	-1.04601
O	-9.17408	1.08489	1.14224
O	-8.61727	-0.45768	3.43134
O	-8.54851	-3.08623	2.87819
O	-8.49287	-2.88818	0.1478
O	-6.18446	-1.92299	-1.14247
O	-6.39244	-1.9793	4.24961
O	-2.56924	-5.56762	-2.64653
O	-5.1905	-5.57172	-3.13018
O	-7.86897	-5.39492	-3.09082
O	-2.5544	-4.85743	1.60326
O	-5.19394	-5.07132	1.29257
O	-7.89464	-5.25383	1.282
Si	-3.79936	-4.60812	-3.3109
Si	-4.60059	-2.24562	-1.10527
Si	-3.83337	0.90341	3.03541
Si	-4.69121	-2.067	4.3165
Si	-3.97122	-3.93635	1.62546
Si	-8.78878	-4.05315	-3.62612
Si	-7.92007	-1.96425	-1.14563
Si	-9.13016	1.11652	-0.55924
Si	-9.09773	1.06706	2.84394
Si	-8.08182	-1.94648	4.05437
Si	-8.92817	-3.90825	1.43961
O	-7.89316	2.13476	3.37779
O	-5.15369	1.88965	3.47283
O	-2.49436	1.80517	3.57255
O	-7.92403	2.18751	-1.08399
O	-5.16142	1.81764	-0.94513
O	-2.30368	1.5708	-0.96671
Si	-6.47645	-6.10461	0.87355
Si	-6.57817	-6.352	-2.5214
Si	-1.65253	-6.29652	1.40293
Si	-1.71536	-6.85735	-1.91695
O	-6.31633	4.22465	2.60475
O	-6.21979	3.55433	-2.83959
O	-6.31321	4.21219	-0.16276
O	-2.02656	4.31422	2.74617
O	-1.927	6.53198	0.91367
O	-1.88273	7.93935	-1.43622
O	-2.00647	6.11312	-3.54202
O	-1.95471	3.57794	-2.46305
O	-2.02378	3.88781	0.02376
O	-4.19531	5.16723	1.24225
O	-3.97796	4.35339	-4.20415
Si	-6.44383	2.95675	3.73738
Si	-5.89901	5.11593	1.21603
Si	-5.69022	4.30023	-4.27585
Si	-6.40919	2.92921	-1.27376
Si	-1.60065	3.19978	3.98003
Si	-2.51742	5.00662	1.29654
Si	-2.3125	4.4986	-3.92387
O	0.08094	3.00238	3.95398
O	-0.06319	2.68062	-1.04921
O	0.08212	8.36449	0.4026
O	0.06012	7.91289	-3.33931
O	-6.4987	-6.29383	-0.82325
O	-1.89128	-6.74519	-0.22656
O	0.0267	-6.13257	1.59257
O	-0.04645	-6.77178	-2.21952
O	6.53895	4.21757	2.67335
O	6.21922	3.64303	-2.76609
O	6.36106	4.2092	-0.06779
O	2.16403	4.4669	2.88775
O	2.1331	6.67964	1.04792
O	1.99431	7.95483	-1.45784
O	2.17373	6.26184	-3.75905
O	2.02267	3.7529	-2.704

O	2.16241	4.0603	0.16222	H	2.07031	3.69677	5.37521
O	4.36998	5.2853	1.45038	H	6.74392	3.31511	5.10028
O	4.14591	4.48629	-4.39643	H	-8.7108	-2.23078	5.31592
O	8.07287	2.03065	3.30124	H	-4.24254	-2.48397	5.61279
O	5.32949	1.88263	3.43598	H	4.28732	-2.40654	5.4399
O	2.67009	1.88339	3.62716	H	8.74886	-2.37051	5.15486
O	7.78484	2.09581	-1.0913	H	10.54163	1.25671	3.15514
O	5.03622	1.89166	-0.88294	H	10.42144	-4.41906	1.32611
O	2.39749	1.39671	-0.96945	H	10.27717	1.41294	-1.32819
Si	6.66542	2.88961	3.72947	H	10.13892	-4.63677	-3.77856
Si	6.05471	5.14269	1.32237	H	-10.3884	1.42021	3.37143
Si	5.84166	4.37009	-4.26416	H	-10.4151	1.44123	-1.10918
Si	6.33117	2.96521	-1.22091	H	-10.1971	-4.36944	-3.53662
Si	1.76991	3.27318	4.03263	H	-10.309	-4.29891	1.41291
Si	2.67962	5.10006	1.38858	Al	1.71774	3.01823	-1.15566
Si	1.76877	8.11327	0.22806	H	-6.70431	-7.70281	-2.98974
Si	1.76058	7.77826	-3.13935	H	-6.40354	-7.38033	1.52619
Si	2.46589	4.60305	-4.10031	H	-2.25529	-8.09816	-2.40729
Si	3.83469	0.89907	-0.37996	H	2.14168	-8.07685	-2.54182
Si	3.95995	0.99053	2.96935	H	2.06809	-7.55241	2.20137
Si	9.03974	1.02289	-0.71082	H	-2.14949	-7.3009	2.30541
Si	9.21879	0.93916	2.68567	H	6.45532	-7.69775	-3.17721
O	6.48592	-6.36773	-0.97082	H	6.66149	-7.5873	1.29749
O	1.82669	-6.83529	-0.29103	H	8.41403	-3.78043	-5.16079
Si	6.61776	-6.26814	0.72937	H	3.35051	-4.1809	-4.71188
Si	6.42818	-6.35123	-2.67276	H	-3.53545	-4.19523	-4.65663
Si	1.69286	-6.44427	1.36434	H	-8.43232	-3.69128	-4.98027
Si	1.64641	-6.84524	-1.98487	H	6.34782	3.5505	-5.34569
O	2.44243	-5.52056	-2.68955	H	1.74977	4.22169	-5.28834
O	5.03604	-5.52262	-3.1946	H	-1.56359	3.97712	-5.02501
O	7.74495	-5.46904	-3.29893	H	-6.07651	3.50102	-5.41835
O	2.68596	-5.09703	1.63931	H	-6.22327	5.63941	-4.39007
O	5.31944	-5.35431	1.33531	H	-6.49823	6.41893	1.21367
O	8.02778	-5.38627	1.09799	H	6.44342	5.686	-4.33214
O	3.99617	-3.14861	-2.41345	H	6.73467	6.40666	1.29043
O	4.11272	-0.62081	-0.91304	H	2.43706	8.83371	-3.84413
O	3.8385	0.88637	1.26422	H	2.49683	9.24133	0.73977
O	4.14842	-0.56135	3.63218	H	-2.37891	9.08619	0.8498
O	4.31073	-3.27459	3.00155	H	-2.39281	8.63171	-3.88802
O	4.21659	-3.13403	0.26707	P	-1.5615	2.91827	-1.10067
O	8.50142	-2.91323	-2.71662	Al	-3.8394	0.88717	-0.35591
O	8.57793	-0.54203	-1.19855	H	-2.36204	-0.80959	-5.34835
O	9.20245	0.96967	0.98648	C	-1.70416	-0.34832	-4.60079
O	8.73337	-0.57846	3.28739	H	-0.67541	-0.63048	-4.83951
O	8.60472	-3.20913	2.71622	H	-1.77867	0.73971	-4.71218
O	8.66322	-3.00547	-0.01546	H	-0.29203	-0.19163	0.60014
O	6.30684	-2.19596	-1.25322	C	0.22209	-1.04459	0.13471
O	6.45761	-2.01853	4.06731	H	-0.4665	-1.8965	0.12033
Si	3.66111	-4.52113	-3.35346	H	1.08832	-1.31205	0.75747
Si	4.61532	-2.24064	-1.11732	O	0.59707	-0.77414	-1.20583
Si	4.75407	-2.07155	4.1232	H	1.22324	-0.02011	-1.20072
Si	4.11499	-4.1766	1.58509	H	-4.21339	-0.92164	-3.44302
Si	8.76237	-4.1908	-3.81743	C	-3.47558	-0.40628	-2.82509
Si	7.99216	-2.1224	-1.30003	H	-3.64106	0.66638	-2.92822
Si	8.14824	-2.05854	3.8845	C	-2.05032	-0.79098	-3.17191
Si	9.0402	-4.02624	1.2864	H	-1.92674	-1.87369	-3.07952
H	-6.47996	3.46686	5.07986	H	-1.3543	-0.34153	-2.45982
H	-2.00548	3.70024	5.26679				

Table C14 Coordinates of C_3H_7-Z on P-H[4]-ZSM-5 for DME conversion to propylene, in Å

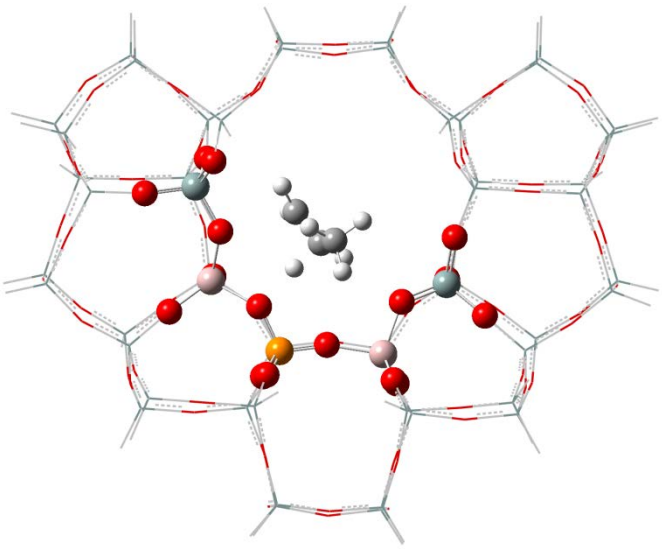


C_3H_7-Z

Atoms	X	Y	Z
Si	-1.56978	8.05207	0.23485
Si	-1.59943	7.70969	-3.1096
O	-4.13227	-3.22771	-2.32065
O	-3.79924	-0.73571	-1.40146
O	-3.80045	0.67378	1.33913
O	-4.0491	-0.57627	3.84407
O	-4.22242	-3.1786	3.09395
O	-4.10495	-2.79799	0.32118
O	-8.37042	-2.7908	-2.56414
O	-8.60473	-0.44235	-1.05186
O	-9.16849	1.07706	1.1364
O	-8.61219	-0.46569	3.42549
O	-8.54429	-3.09426	2.87234
O	-8.4886	-2.89624	0.14196
O	-6.17986	-1.93181	-1.14832
O	-6.38786	-1.98804	4.24376
O	-2.56584	-5.57763	-2.65238
O	-5.18711	-5.58086	-3.13603
O	-7.86552	-5.40318	-3.09667
O	-2.55076	-4.86744	1.59742
O	-5.19038	-5.08045	1.28672
O	-7.89114	-5.26208	1.27615
Si	-3.79565	-4.61772	-3.31675
Si	-4.5961	-2.25496	-1.11112
Si	-3.82785	0.89383	3.02956
Si	-4.68666	-2.0763	4.31065
Si	-3.96729	-3.94589	1.61961
Si	-8.78488	-4.06111	-3.63196
Si	-7.91549	-1.97249	-1.15148
Si	-9.12456	1.10868	-0.56508
Si	-9.09215	1.05921	2.8381
Si	-8.07723	-1.95467	4.04852
Si	-8.92423	-3.91616	1.43376
O	-7.88722	2.1265	3.37194
O	-5.14783	1.8805	3.46699
O	-2.48853	1.79515	3.5667
O	-7.91808	2.17927	-1.08984
O	-5.15559	1.80849	-0.95098
O	-2.29793	1.56071	-0.97256
Si	-6.47323	-6.11332	0.8677
Si	-6.57503	-6.36068	-2.52725
Si	-1.64937	-6.30682	1.39708
Si	-1.71239	-6.86763	-1.9228
O	-6.30971	4.21588	2.5989
O	-6.21339	3.54553	-2.84544
O	-6.3066	4.20342	-0.16861
O	-2.01991	4.30404	2.74032
O	-1.91962	6.52177	0.90782
O	-1.87488	7.92912	-1.44207
O	-1.99923	6.10293	-3.54787
O	-1.9483	3.56773	-2.4689
O	-2.01727	3.87763	0.01792
O	-4.18838	5.15776	1.23641
O	-3.97129	4.34385	-4.20999
Si	-6.43763	2.94802	3.73153
Si	-5.89209	5.10702	1.21018
Si	-5.68358	4.29125	-4.2817
Si	-6.403	2.92047	-1.27961
Si	-1.59437	3.18945	3.97418
Si	-2.51055	4.9966	1.29069
Si	-2.30579	4.48851	-3.92972
O	0.08716	2.9915	3.94813
O	-0.05708	2.6698	-1.05506
O	0.0901	8.35361	0.39675
O	0.06795	7.90202	-3.34515
O	-6.49554	-6.30254	-0.8291
O	-1.88827	-6.75542	-0.23241
O	0.02991	-6.14343	1.58672
O	-0.04345	-6.78262	-2.22537
O	6.54557	4.20457	2.6675
O	6.22565	3.63013	-2.77194
O	6.36768	4.19626	-0.07363
O	2.17073	4.45534	2.8819
O	2.14053	6.66809	1.04207
O	2.00216	7.94332	-1.46369
O	2.18102	6.25027	-3.7649
O	2.02913	3.74138	-2.70985
O	2.16898	4.04873	0.15637
O	4.37695	5.27301	1.44454
O	4.15261	4.47407	-4.40227
O	8.07877	2.01715	3.2954
O	5.33534	1.87002	3.43013
O	2.67594	1.87166	3.62131

O	7.79076	2.0824	-1.09714	H	2.07675	3.68524	5.36936
O	5.04208	1.87915	-0.88878	H	6.75024	3.30204	5.09443
O	2.40318	1.38507	-0.9753	H	-8.7063	-2.23877	5.31008
Si	6.6716	2.87656	3.72362	H	-4.23812	-2.49342	5.60694
Si	6.06163	5.12985	1.31653	H	4.29176	-2.4188	5.43406
Si	5.84833	4.35731	-4.27001	H	8.75331	-2.38424	5.14901
Si	6.33738	2.95228	-1.22676	H	10.54727	1.24239	3.14929
Si	1.77622	3.26175	4.02678	H	10.42521	-4.43334	1.32026
Si	2.68653	5.08832	1.38273	H	10.28286	1.39871	-1.33404
Si	1.77667	8.10183	0.22221	H	10.14262	-4.65095	-3.78441
Si	1.76837	7.76683	-3.1452	H	-10.3827	1.41278	3.36559
Si	2.47264	4.59139	-4.10616	H	-10.4094	1.43381	-1.11503
Si	3.84022	0.88696	-0.38581	H	-10.1933	-4.37693	-3.54247
Si	3.9655	0.97838	2.9635	H	-10.3052	-4.30636	1.40707
Si	9.04531	1.00907	-0.71667	Al	1.72397	3.00681	-1.16151
Si	9.22433	0.92527	2.67982	H	-6.70161	-7.71145	-2.99559
O	6.48905	-6.38071	-0.97667	H	-6.40074	-7.38907	1.52034
O	1.82967	-6.84674	-0.29688	H	-2.25273	-8.10826	-2.41314
Si	6.62093	-6.28116	0.72352	H	2.14425	-8.0884	-2.54767
Si	6.43132	-6.36419	-2.67861	H	2.07083	-7.56394	2.19552
Si	1.69597	-6.45568	1.35849	H	-2.14667	-7.31104	2.29956
Si	1.64939	-6.85663	-1.99072	H	6.45802	-7.71073	-3.18305
O	2.44584	-5.53221	-2.69539	H	6.66422	-7.60035	1.29165
O	5.03945	-5.53513	-3.20045	H	8.41801	-3.79405	-5.16664
O	7.74837	-5.48244	-3.30478	H	3.35437	-4.19285	-4.71772
O	2.68951	-5.10877	1.63346	H	-3.5316	-4.20491	-4.66247
O	5.32291	-5.36691	1.32947	H	-8.4283	-3.69935	-4.98612
O	8.03123	-5.39976	1.09214	H	6.35422	3.53756	-5.35154
O	4.00036	-3.16077	-2.4193	H	1.75639	4.21026	-5.29419
O	4.11774	-0.63301	-0.91889	H	-1.55705	3.96678	-5.03086
O	3.84402	0.87426	1.25837	H	-6.07012	3.49217	-5.4242
O	4.15346	-0.57357	3.62633	H	-6.21618	5.63061	-4.39592
O	4.31488	-3.28686	2.9957	H	-6.49089	6.41022	1.20782
O	4.22079	-3.14627	0.26122	H	6.45052	5.67303	-4.33799
O	8.50569	-2.92687	-2.72247	H	6.74201	6.39359	1.28458
O	8.58298	-0.55571	-1.2044	H	2.44519	8.82205	-3.84997
O	9.208	0.95579	0.98063	H	2.5051	9.22966	0.73392
O	8.73841	-0.59218	3.28154	H	-2.37069	9.07612	0.84396
O	8.6089	-3.22282	2.71037	H	-2.38474	8.62165	-3.89387
O	8.66746	-3.01917	-0.02131	P	-1.5553	2.90793	-1.10652
O	6.31134	-2.20888	-1.25907	Al	-3.83388	0.87758	-0.36176
O	6.46218	-2.03151	4.06146	H	-2.35708	-0.81967	-5.3542
Si	3.66485	-4.53319	-3.3593	C	-1.69905	-0.35861	-4.60664
Si	4.61982	-2.253	-1.12317	H	-0.67039	-0.6411	-4.84536
Si	4.75862	-2.08397	4.11735	H	-1.77319	0.72945	-4.71803
Si	4.11885	-4.1888	1.57924	H	-4.20846	-0.9311	-3.44887
Si	8.76622	-4.20453	-3.82328	C	-3.47049	-0.41599	-2.83094
Si	7.9967	-2.13588	-1.30588	H	-3.63561	0.65673	-2.93407
Si	8.15279	-2.07207	3.87865	C	-2.04535	-0.80116	-3.17776
Si	9.0441	-4.04006	1.28055	H	-1.92212	-1.88391	-3.08537
H	-6.47359	3.45814	5.07401	H	-1.34918	-0.35193	-2.46567
H	-1.99903	3.69005	5.26094				

Table C15 Coordinates of TS2 on P-H^4-ZSM-5 for DME conversion to propylene, in Å

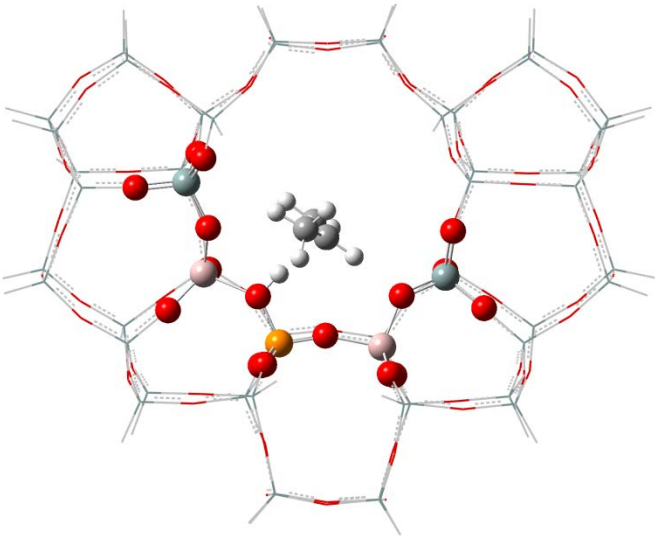


TS2

Atoms	X	Y	Z
Si	-1.79294	8.04902	0.21988
Si	-1.77017	7.77388	-3.13314
O	-3.77182	-3.13885	-2.33533
O	-3.55493	-0.80809	-1.0881
O	-3.76679	0.79066	1.32495
O	-4.03326	-0.64359	3.72265
O	-4.1532	-3.32486	3.04949
O	-3.97263	-3.04054	0.30442
O	-8.11631	-2.88746	-2.70929
O	-8.45779	-0.61398	-1.14318
O	-9.19615	0.84767	1.04615
O	-8.62778	-0.692	3.33114
O	-8.44696	-3.30139	2.70688
O	-8.31065	-3.05924	-0.01658
O	-5.96015	-2.04264	-1.1901
O	-6.33985	-2.12235	4.11489
O	-2.29784	-5.49291	-2.71435
O	-4.9017	-5.50307	-3.21953
O	-7.58751	-5.47833	-3.29534
O	-2.48559	-5.06725	1.59928
O	-5.11979	-5.3367	1.28812
O	-7.81502	-5.46218	1.0831
Si	-3.52877	-4.50621	-3.36805
Si	-4.34345	-2.24681	-1.07624
Si	-3.87399	0.89326	3.01415
Si	-4.63739	-2.15764	4.19725
Si	-3.92778	-4.16723	1.60526
Si	-8.52106	-4.13244	-3.80397
Si	-7.68003	-2.10339	-1.26656
Si	-9.10939	0.88095	-0.65604
Si	-9.14446	0.82152	2.74656
Si	-8.0281	-2.17374	3.91113
Si	-8.81041	-4.08514	1.24002
O	-7.98452	1.92342	3.31391
O	-5.23243	1.80207	3.50208
O	-2.56486	1.80944	3.61421
O	-7.97139	2.0403	-1.14474
O	-5.18503	1.75234	-0.98172
O	-2.32411	1.58643	-1.09316
Si	-6.38723	-6.31094	0.70835
Si	-6.26929	-6.37563	-2.69582
Si	-1.57244	-6.48102	1.32507
Si	-1.56961	-6.87534	-2.02546
O	-6.47439	4.08139	2.597
O	-6.31601	3.49803	-2.85805
O	-6.43363	4.08983	-0.18281
O	-2.15628	4.31245	2.71532
O	-2.12354	6.50546	0.86885
O	-2.06406	7.95248	-1.46427
O	-2.16114	6.17659	-3.60816
O	-2.09662	3.66613	-2.51874
O	-2.19897	3.89128	-0.02116
O	-4.38292	5.1249	1.25793
O	-4.15162	4.42239	-4.25906
Si	-6.58354	2.80254	3.72039
Si	-6.0862	4.98996	1.21137
Si	-5.86433	4.28582	-4.29267
Si	-6.46822	2.81196	-1.31062
Si	-1.71529	3.23787	3.97992
Si	-2.70739	4.9823	1.27745
Si	-2.49044	4.56616	-3.98876
O	-0.02983	3.0509	3.9447
O	-0.16868	2.81389	-1.12228
O	-0.13887	8.37513	0.40586
O	-0.09871	7.97178	-3.34333
O	-6.28226	-6.40604	-0.99413
O	-1.76146	-6.8399	-0.33318
O	0.10192	-6.25374	1.53447
O	0.11236	-6.84772	-2.28063
O	6.38838	4.29071	2.65132
O	6.06827	3.67266	-2.77728
O	6.17242	4.24962	-0.08236
O	2.04634	4.51501	2.8776
O	1.95846	6.74664	1.0605
O	1.80773	8.02899	-1.43629
O	2.05688	6.36303	-3.74929
O	1.95142	3.83274	-2.7293
O	2.05812	4.13653	0.14672
O	4.2297	5.38652	1.44166
O	4.04965	4.60271	-4.41553
O	7.93915	2.13211	3.31555
O	5.19649	1.93692	3.37889
O	2.54153	1.92164	3.58627
O	7.62568	2.16338	-1.07123
O	4.8695	1.90739	-0.91525

O	2.22212	1.45642	-0.98393	H	6.54294	3.38726	5.08483
Si	6.50771	2.96602	3.71131	H	-8.64322	-2.51906	5.16492
Si	5.90959	5.21265	1.29621	H	-4.18479	-2.51813	5.51099
Si	5.74097	4.44834	-4.26285	H	4.20053	-2.35821	5.41256
Si	6.15667	3.00041	-1.22835	H	8.65651	-2.25223	5.1804
Si	1.6566	3.316	4.01874	H	10.42563	1.40283	3.1803
Si	2.54167	5.17947	1.38698	H	10.40776	-4.23494	1.33428
Si	1.55432	8.17488	0.24711	H	10.14694	1.57409	-1.30843
Si	1.59953	7.86579	-3.12236	H	10.20354	-4.43845	-3.69746
Si	2.37061	4.71576	-4.11502	H	-10.4515	1.13314	3.2611
Si	3.6517	0.92733	-0.41445	H	-10.4046	1.12243	-1.22612
Si	3.83188	1.02964	2.93158	H	-9.9253	-4.47221	-3.72786
Si	8.92413	1.14661	-0.68784	H	-10.1997	-4.44344	1.1812
Si	9.1099	1.06325	2.70785	Al	1.628	3.10749	-1.18185
O	6.55187	-6.29142	-0.96348	H	-6.28839	-7.71246	-3.22129
O	1.96358	-6.88083	-0.32031	H	-6.3743	-7.62601	1.284
Si	6.65077	-6.18323	0.73863	H	-2.14461	-8.06952	-2.58498
Si	6.52451	-6.27512	-2.66533	H	2.35055	-8.10233	-2.57351
Si	1.77835	-6.5007	1.33361	H	2.20824	-7.58003	2.18077
Si	1.796	-6.89797	-2.01525	H	-2.02719	-7.56003	2.15992
O	2.53556	-5.52769	-2.70449	H	6.56521	-7.61824	-3.17563
O	5.1345	-5.4448	-3.19497	H	6.69355	-7.49709	1.31731
O	7.83479	-5.37368	-3.27563	H	8.47905	-3.67222	-5.13615
O	2.69287	-5.0931	1.6015	H	3.41488	-4.17049	-4.73546
O	5.33581	-5.2698	1.30915	H	-3.23579	-4.09756	-4.71042
O	8.04348	-5.28119	1.12168	H	-8.17087	-3.749	-5.15425
O	3.94298	-3.09754	-2.43829	H	6.2449	3.6408	-5.35434
O	3.91244	-0.59594	-0.96822	H	1.65432	4.32972	-5.30139
O	3.67669	0.89007	1.22955	H	-1.73082	4.03681	-5.07918
O	4.04032	-0.51711	3.60086	H	-6.23581	3.50276	-5.45064
O	4.26195	-3.21995	2.97118	H	-6.44672	5.60739	-4.37161
O	4.14022	-3.08079	0.24102	H	-6.73058	6.27185	1.21892
O	8.44741	-2.79054	-2.69689	H	6.37305	5.75099	-4.28904
O	8.49881	-0.42833	-1.17704	H	6.61544	6.46086	1.23895
O	9.09404	1.09349	1.00823	H	2.27058	8.93658	-3.80878
O	8.6449	-0.46125	3.30851	H	2.24693	9.31808	0.77403
O	8.55641	-3.08756	2.73609	H	-2.6145	9.05487	0.83152
O	8.58629	-2.888	0.00411	H	-2.54122	8.70552	-3.90784
O	6.23041	-2.07878	-1.24986	P	-1.67367	3.00459	-1.1748
O	6.37641	-1.92897	4.05817	Al	-3.8516	0.81353	-0.40837
Si	3.72559	-4.50126	-3.37433	H	0.96731	-1.26958	-3.02641
Si	4.54202	-2.1785	-1.13642	C	0.0696	-0.64547	-2.97459
Si	4.67426	-2.01286	4.10155	H	0.32511	0.32112	-3.41266
Si	4.09506	-4.13268	1.55901	H	-0.72246	-1.10838	-3.57104
Si	8.81013	-4.05741	-3.78134	H	-1.35732	-1.35105	0.18192
Si	7.91945	-2.00884	-1.28345	C	-1.15367	-1.41808	-0.8829
Si	8.07063	-1.94655	3.90224	H	-1.5808	-2.26696	-1.40843
Si	9.01397	-3.89013	1.30567	C	-0.35362	-0.46662	-1.5257
H	-6.6814	3.30799	5.06211	H	0.38188	0.05881	-0.8933
H	-2.10884	3.77629	5.2543	H	-1.20259	0.34315	-1.41207
H	1.9823	3.72331	5.35996				

Table C16 Coordinates of C_3H_6/H^4Z on P-H^4-ZSM-5 for DME conversion to propylene, in Å



C_3H_6/H^4Z

Atoms	X	Y	Z
Si	-1.69794	7.96238	0.14684
Si	-1.67036	7.63431	-3.199
O	-3.97821	-3.08485	-2.34785
O	-3.83068	-0.72918	-1.1065
O	-3.81507	0.85175	1.38653
O	-4.08593	-0.59422	3.79024
O	-4.25028	-3.26354	3.0485
O	-4.15465	-2.97954	0.30079
O	-8.37288	-2.80778	-2.67997
O	-8.53967	-0.48174	-1.14016
O	-9.16156	1.026	1.04935
O	-8.64733	-0.54715	3.33304
O	-8.55624	-3.17302	2.74571
O	-8.54482	-2.93964	0.0207
O	-6.16512	-2.03296	-1.1845
O	-6.40986	-2.03232	4.14046
O	-2.45801	-5.46585	-2.72104
O	-5.0538	-5.43641	-3.22558
O	-7.74913	-5.38564	-3.27744
O	-2.61362	-5.02574	1.60715
O	-5.25122	-5.25975	1.30626
O	-7.95262	-5.33753	1.11313
Si	-3.66734	-4.44855	-3.36109
Si	-4.53415	-2.19528	-1.0848
Si	-3.87582	0.93088	3.08493
Si	-4.7082	-2.1191	4.22071
Si	-4.03648	-4.10192	1.59551
Si	-8.71497	-4.0652	-3.78433
Si	-7.88201	-2.0348	-1.25015
Si	-9.09009	1.05004	-0.65364
Si	-9.13089	0.97521	2.74971
Si	-8.09751	-2.04342	3.93125
Si	-8.96143	-3.97716	1.29918
O	-7.95241	2.0517	3.33357
O	-5.19877	1.89684	3.56134
O	-2.53042	1.81415	3.65239
O	-7.90488	2.17181	-1.13423
O	-5.11781	1.94084	-0.93683
O	-2.23118	1.48821	-1.00819
Si	-6.5368	-6.20426	0.72369
Si	-6.42624	-6.28288	-2.68192
Si	-1.67863	-6.42201	1.32359
Si	-1.68693	-6.8174	-2.02505
O	-6.41196	4.1863	2.64524
O	-6.24193	3.64339	-2.83452
O	-6.40164	4.24594	-0.14742
O	-2.08227	4.27888	2.72065
O	-2.00616	6.40981	0.79421
O	-1.97279	7.83108	-1.53449
O	-2.01544	6.00642	-3.62196
O	-2.02729	3.53194	-2.50163
O	-2.1545	3.80245	-0.00178
O	-4.30852	5.15568	1.28217
O	-4.04406	4.31419	-4.29722
Si	-6.5463	2.90462	3.76729
Si	-6.02039	5.09985	1.26833
Si	-5.76513	4.2683	-4.33823
Si	-6.42224	2.97763	-1.28299
Si	-1.63791	3.21866	4.00312
Si	-2.64628	4.93939	1.29161
Si	-2.38711	4.41204	-4.01318
O	0.04395	3.03661	3.93523
O	-0.07245	2.73891	-1.07809
O	-0.05177	8.31199	0.33694
O	-0.0078	7.88026	-3.4056
O	-6.44695	-6.29609	-0.97924
O	-1.87353	-6.78931	-0.3316
O	-0.00237	-6.20859	1.53886
O	-0.00494	-6.78065	-2.28737
O	6.4694	4.23846	2.66959
O	6.18692	3.64052	-2.75938
O	6.29979	4.21024	-0.06843
O	2.11445	4.50708	2.86145
O	2.06324	6.72768	1.02659
O	1.89372	7.98033	-1.49236
O	2.15704	6.30971	-3.79936
O	1.99919	3.8094	-2.7471
O	2.13743	4.13001	0.13272
O	4.32784	5.34741	1.43514
O	4.14616	4.52961	-4.40756
O	8.00762	2.06004	3.32089
O	5.26297	1.89681	3.39682
O	2.61536	1.91351	3.57761

O	7.7717	2.11811	-1.06883	H	2.04899	3.72753	5.34462
O	5.01883	1.86871	-0.8976	H	6.63344	3.33291	5.09732
O	2.37694	1.46278	-1.0193	H	-8.72606	-2.34521	5.18986
Si	6.58763	2.90797	3.72514	H	-4.26687	-2.5022	5.53168
Si	6.01167	5.16353	1.31122	H	4.18813	-2.39071	5.42018
Si	5.84104	4.39	-4.25266	H	8.65036	-2.33871	5.19798
Si	6.30489	2.95908	-1.2146	H	10.47643	1.27783	3.21323
Si	1.73314	3.30536	4.00582	H	10.37538	-4.37871	1.37391
Si	2.63973	5.16165	1.3778	H	10.26245	1.42505	-1.27775
Si	1.64758	8.13849	0.19102	H	10.17228	-4.58079	-3.69854
Si	1.69403	7.81169	-3.17846	H	-10.4346	1.317	3.25313
Si	2.46478	4.65609	-4.14323	H	-10.3691	1.37559	-1.21895
Si	3.77843	0.90583	-0.41654	H	-10.1106	-4.44343	-3.72495
Si	3.89726	0.99778	2.933	H	-10.3474	-4.35351	1.30222
Si	9.01881	1.03977	-0.67065	Al	1.75018	3.08592	-1.18993
Si	9.15953	0.96119	2.72765	H	-6.47033	-7.6255	-3.19231
O	6.48852	-6.35152	-0.95083	H	-6.55363	-7.52209	1.29421
O	1.84943	-6.85217	-0.32572	H	-2.24333	-8.02568	-2.57577
Si	6.58385	-6.24841	0.7515	H	2.19699	-8.08724	-2.57396
Si	6.45931	-6.33976	-2.65312	H	2.07975	-7.5663	2.1699
Si	1.66992	-6.47329	1.3287	H	-2.12894	-7.50244	2.16085
Si	1.67707	-6.86412	-2.02059	H	6.49602	-7.68543	-3.15792
O	2.47754	-5.53111	-2.71328	H	6.61965	-7.56428	1.32681
O	5.07988	-5.50297	-3.1949	H	8.45887	-3.76151	-5.11788
O	7.78401	-5.45414	-3.259	H	3.39603	-4.18736	-4.73559
O	2.63353	-5.10061	1.60982	H	-3.36929	-4.04488	-4.70429
O	5.27755	-5.32789	1.32771	H	-8.368	-3.65743	-5.12859
O	7.98745	-5.36288	1.13857	H	6.34632	3.57757	-5.33935
O	3.9752	-3.13802	-2.43575	H	1.75178	4.26405	-5.3289
O	4.02233	-0.6192	-0.95873	H	-1.61311	3.8191	-5.05696
O	3.76992	0.88195	1.2285	H	-6.17101	3.40834	-5.42629
O	4.07429	-0.54684	3.61014	H	-6.26742	5.61015	-4.53002
O	4.24006	-3.25896	2.97918	H	-6.60579	6.40841	1.30123
O	4.15707	-3.11945	0.25058	H	6.4521	5.70227	-4.29741
O	8.47941	-2.8852	-2.67684	H	6.71062	6.41647	1.26836
O	8.54476	-0.51971	-1.15984	H	2.34525	8.89159	-3.86793
O	9.16313	0.99199	1.02801	H	2.31822	9.29981	0.70491
O	8.65758	-0.55093	3.32725	H	-2.54173	8.95456	0.74911
O	8.54597	-3.18008	2.75631	H	-2.47524	8.51134	-4.00108
O	8.61058	-2.9787	0.02664	P	-1.55457	2.98327	-1.14321
O	6.26586	-2.15857	-1.23591	Al	-3.9751	0.81085	-0.32756
O	6.37436	-1.99712	4.07392	H	-0.01777	-1.56248	-4.03817
Si	3.68981	-4.52748	-3.37305	C	-0.69056	-0.91682	-3.4586
Si	4.57339	-2.22999	-1.12961	H	-0.87996	-0.03455	-4.08309
Si	4.67045	-2.06044	4.10829	H	-1.63423	-1.44443	-3.29853
Si	4.05259	-4.16918	1.5656	H	0.11544	-0.62909	-0.06056
Si	8.78847	-4.16213	-3.76693	C	-0.4504	-0.91454	-0.94365
Si	7.9528	-2.09817	-1.26547	H	-1.31988	-1.55233	-0.80592
Si	8.06772	-2.0327	3.91809	C	-0.03381	-0.53221	-2.16423
Si	8.99107	-3.99786	1.32966	H	0.86154	0.08645	-2.22037
H	-6.64836	3.41597	5.10602	H	-1.54865	0.75202	-1.14653
H	-2.01498	3.78444	5.26989				

VITAE

Name:	Miss TREERAT CHOMPOOPUDPONG
Date of Birth:	July 17, 1986
Place of Birth:	Satun, Thailand
Address:	105/310 My Condo Pinklao, Soi Charansanitwong 49, Charansanitwong Road, Bang Bamru, Bangplad, Bangkok 10700, Thailand
Telephone:	081-7434360
E-mail address:	giggle_pink@hotmail.com

Educations:

2009 – 2011	M.Sc. (Petrochemistry and Polymer Science), Chulalongkorn University, Thailand
2005 – 2008	B.Sc. (Chemistry), Chulalongkorn University, Thailand
2002 – 2004	Prachuapwittayalai School, Prachuapkhirikhan, Thailand
1999 – 2001	Uttaraditdarunee School, Uttaradit, Thailand
1998	Uttaradit Kindergarten School, Uttaradit, Thailand
1994 – 1997	Wat Phra Mahathat School, Nakorn Si Thammarat, Thailand
1993	Prachuapkhirikhan Kindergarten School, Prachuapkhirikhan, Thailand

Presentation:

2012	An oniom study on catalytic activity of phosphorus-modified H-ZSM-5 catalyst (Poster Session): Pure and Applied Chemistry International Conference (PACCON2012), January 11-13, 2012 at Chiang Mai, Thailand