

Effects of the Zeolite Framework on the Adsorptions and Hydrogen-Exchange Reactions of Unsaturated Aliphatic, Aromatic and Heterocyclic compounds in ZSM-5 Zeolite: A Combination of Perturbation Theory (MP2) and a Newly Developed Density Functional Theory (M06-2X) in ONIOM Scheme

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SUPPORTING INFORMATION

Table S1. Structure parameters for H-ZSM-5 zeolite from the 5T quantum cluster and ONIOM(5T:34T) models optimized with various methods. Bond lengths are in picometers and bond angles are in degrees.

Parameters	MP2	(MP2:M06-2X)	(MP2:B3LYP)	(MP2:HF)	(MP2:UFF)
Si1-O1	170.0	166.3	166.4	166.3	168.0
O1-Al	185.7	183.3	183.4	183.5	181.4
O-Al _{avg}	173.9	172.2	172.2	172.2	170.6
Al-O2	170.6	169.0	169.0	168.9	168.0
O2-Si2	162.7	159.3	159.3	159.4	160.8
Al...Hz	235.2	236.4	235.9	235.7	228.5
O1-Hz	96.7	97.0	96.9	97.0	96.8
∠ Al-O1-Si1	130.9	130.3	130.4	130.8	131.9
∠ Al-O2-Si2	131.8	132.7	132.5	133.0	133.8
∠ O1-Al-O2	90.0	90.1	89.8	90.3	89.5

Table S2. Structure parameters for ethene/H-ZSM-5 complex from the 5T quantum cluster and ONIOM(5T:34T) models optimized with various methods. Bond lengths are in picometers and bond angles are in degrees.

Parameters	MP2	(MP2:M06-2X)	(MP2:B3LYP)	(MP2:HF)	(MP2:UFF)
Si1-O1	169.4	165.5	165.8	165.7	167.4
O1-Al	184.6	182.0	182.2	182.3	180.2
O-Al _{avg}	173.8	172.1	172.0	172.0	170.4
Al-O2	170.7	169.0	168.9	168.8	167.9
O2-Si2	162.3	158.8	158.7	158.8	160.3
Al...Hz	238.6	240.7	238.9	238.9	233.0
O1-Hz	98.1	98.8	98.9	98.9	98.0
Hz...C1	218.8	216.3	217.1	217.7	226.1
Hz...C2	218.1	220.5	220.3	220.5	225.9
O1...C1	312.8	312.7	311.8	312.1	322.9
O1...C2	313.7	315.0	316.6	316.6	317.0
C1-C2	134.2	134.3	134.3	134.3	134.2
∠ Al-O1-Si1	130.1	129.4	129.1	129.5	131.4
∠ Al-O2-Si2	132.7	133.8	134.2	134.7	134.8
∠ O1-Al-O2	91.3	91.1	91.0	91.5	90.4
∠ O1-Hz-C1	160.0	164.6	159.9	159.8	169.2
∠ O1-Hz-C2	164.2	159.5	164.1	163.6	154.2

Table S3. Structure parameters for benzene/H-ZSM-5 complex from the 5T quantum cluster and ONIOM(5T:34T) models optimized with various methods. Bond lengths are in picometers and bond angles are in degrees.

Parameters	MP2	(MP2:M06-2X)	(MP2:B3LYP)	(MP2:HF)	(MP2:UFF)
Si1-O1	170.1	166.2	166.2	166.1	168.1
O1-Al	184.9	182.5	182.6	182.7	180.6
O-Al _{avg}	173.8	172.1	172.0	172.0	170.5
Al-O2	170.4	168.8	168.6	168.5	167.7
O2-Si2	162.0	158.6	158.4	158.5	160.1
Al...Hz	234.5	234.2	234.4	234.6	228.2
O1-Hz	97.8	98.4	98.4	98.4	97.8
Hz...CB1	222.9	227.7	228.2	229.3	233.6
Hz...CB2	242.5	246.5	257.4	257.0	250.9
O1...CB1	318.5	323.2	322.3	322.9	327.9
O1...CB2	315.2	318.2	350.4	350.8	321.3
CB1-CB2	140.1	140.2	140.0	139.9	140.1
CB1-H1	108.2	108.4	108.2	108.1	108.3
H1...O2	285.2	298.6	282.4	276.0	300.5
∠ Al-O1-Si1	129.2	128.7	128.8	129.3	130.8
∠ Al-O2-Si2	133.7	134.9	135.0	135.5	136.1
∠ O1-Al-O2	91.6	91.2	90.8	91.3	90.9
∠ O1-Hz-CB1	165.2	163.4	159.9	158.6	161.8
∠ O2-H1-CB1	99.7	98.5	97.5	99.0	100.6

Table S4. Structure parameters for ethylbenzene/H-ZSM-5 complex from the 5T quantum cluster and ONIOM(5T:34T) models optimized with various methods. Bond lengths are in picometers and bond angles are in degrees.

Parameters	MP2	(MP2:M06-2X)	(MP2:B3LYP)	(MP2:HF)	(MP2:UFF)
Si1-O1	170.2	166.2	166.3	166.1	168.2
O1-Al	184.9	182.5	182.5	182.6	180.5
O-Al _{avg}	173.9	172.1	172.1	172.0	170.4
Al-O2	170.5	168.7	168.9	168.5	167.7
O2-Si2	162.0	158.4	158.4	158.5	160.0
Al...Hz	234.6	234.8	234.7	234.9	228.6
O1-Hz	97.9	98.3	98.2	98.2	97.7
Hz...CB1	224.8	240.6	258.9	261.2	254.3
Hz...CB2	236.8	256.2	247.4	244.6	260.3
O1...CB1	312.5	329.6	342.9	344.2	340.4
O1...CB2	334.3	352.7	344.0	341.4	354.7
CB1-CB2	140.5	140.6	140.5	140.5	140.4
CB1-H1	108.2	108.4	108.2	108.0	108.2
H1...O2	256.2	268.9	270.8	267.1	278.3
∠ Al-O1-Si1	129.1	128.4	128.7	129.3	130.9
∠ Al-O2-Si2	133.9	135.0	134.8	135.5	135.5
∠ O1-Al-O2	91.5	91.1	90.8	91.4	90.6
∠ O1-Hz-CB1	148.4	150.3	143.5	142.3	146.9
∠ O2-H1-CB1	111.4	100.5	99.8	100.6	100.2

Table S5. Structure parameters for pyridine/H-ZSM-5 complex from the 5T quantum cluster and ONIOM(5T:34T) models optimized with various methods. Bond lengths are in picometers and bond angles are in degrees.

Parameters	MP2	(MP2:M06-2X)	(MP2:B3LYP)	(MP2:HF)	(MP2:UFF)
Si1-O1	164.0	158.9	159.0	158.9	162.3
O1-Al	176.8	173.4	173.5	173.4	172.7
O-Al _{avg}	173.0	171.2	168.5	171.1	169.8
Al-O2	172.1	171.5	171.1	171.1	169.2
O2-Si2	161.1	157.9	157.9	157.9	159.1
Al...Hz	252.5	270.2	260.6	261.4	247.9
O1-Hz	144.5	172.6	169.2	168.9	148.8
Hz-N	110.2	104.8	104.9	105.1	109.4
O1...N	253.7	274.7	270.8	270.8	257.4
∠ Al-O1-Si1	128.0	127.3	128.0	128.7	130.0
∠ Al-O2-Si2	135.9	135.3	136.1	136.6	139.5
∠ O1-Al-O2	94.2	94.2	94.3	94.8	94.4
∠ O1-Hz-N	169.9	163.4	161.6	161.9	171.2

Table S6. Structure parameters for H/H exchange reaction of benzene on H-ZSM-5 active site from the 5T quantum cluster and 5T:34T models optimized with MP2 and ONIOM(MP2:M06-2X) methods, respectively. Bond lengths are in picometers and bond angles are in degrees.

Parameters	MP2			(MP2:M06-2X)		
	AD	TS	PR	AD	TS	PR
Si1-O1	170.1	165.5	162.8	166.2	159.8	158.7
O1-Al	184.9	176.4	170.2	182.5	173.3	168.5
O-Al _{avg}	173.8	173.2	173.5	172.1	171.4	171.9
Al-O2	170.4	177.2	185.4	168.8	174.8	183.5
O2-Si2	162.0	165.1	169.0	158.6	160.7	166.5
Al...Hz	234.5	252.4	390.1	234.2	253.8	362.7
O1-Hz	97.8	135.8	277.3	98.4	151.4	255.6
Hz...CB1	222.9	126.1	108.2	227.7	118.2	108.4
Hz...CB2	242.5	225.7	215.2	246.5	221.0	215.3
O1...CB1	318.5	261.7	324.6	323.2	269.0	324.9
O1...CB2	315.2	346.3	332.5	318.2	354.6	329.6
CB1-CB2	140.1	140.6	140.2	140.2	140.8	140.2
CB1-H1	108.2	127.3	215.0	108.4	122.4	234.0
H1...O2	285.2	134.5	98.1	298.6	144.6	98.3
O2...CB1	321.7	261.8	312.2	332.4	265.2	328.4
∠ Al-O1-Si1	129.2	127.7	125.4	128.7	130.1	127.6
∠ Al-O2-Si2	133.7	133.8	135.6	134.9	134.1	133.1
∠ O1-Al-O2	91.6	91.0	91.9	91.2	91.6	91.6
∠ O1-Hz-CB1	165.2	175.3	106.2	163.4	172.3	120.8
∠ O2-H1-CB1	99.7	177.2	170.7	98.5	166.9	160.7

Table S7. Structure parameters for H/H exchange reaction of ethylbenzene on H-ZSM-5 active site from the 5T quantum cluster and 5T:34T models optimized with MP2 and ONIOM(MP2:M06-2X) methods, respectively. Bond lengths are in picometers and bond angles are in degrees.

Parameters	MP2			(MP2:M06-2X)		
	AD	TS	PR	AD	TS	PR
Si1-O1	170.2	165.3	162.9	166.2	159.7	158.5
O1-Al	184.9	176.3	170.3	182.5	173.4	168.4
O-Al _{avg}	173.9	173.1	173.6	172.1	171.3	171.8
Al-O2	170.5	176.9	185.4	168.7	174.1	183.2
O2-Si2	162.0	164.8	169.1	158.4	160.0	166.1
Al...Hz	234.6	255.1	325.4	234.8	260.7	412.4
O1-Hz	97.9	138.2	272.3	98.3	153.6	294.7
Hz...CB1	224.8	124.9	108.3	240.6	117.2	108.3
Hz...CB2	236.8	225.9	213.7	256.2	220.1	215.2
O1...CB1	312.5	262.8	330.5	329.6	268.5	311.5
O1...CB2	334.3	350.2	363.1	352.7	366.8	337.4
CB1-CB2	140.5	141.1	140.7	140.6	141.2	140.6
CB1-H1	108.2	125.7	213.7	108.4	119.5	296.4
H1...O2	256.2	137.2	98.2	268.9	148.1	99.0
O2...CB1	312.4	262.8	303.5	307.7	266.3	376.3
∠ Al-O1-Si1	129.1	127.5	125.5	128.4	129.3	126.3
∠ Al-O2-Si2	133.9	134.1	135.1	135.0	136.2	133.7
∠ O1-Al-O2	91.5	91.3	92.2	91.1	92.6	92.9
∠ O1-Hz-CB1	148.4	174.7	113.3	150.3	164.9	88.6
∠ O2-H1-CB1	111.4	176.3	151.1	100.5	168.6	138.5

Table S8. The contribution analysis on adsorption energies of ethene, benzene, ethylbenzene and pyridine molecule on 5T models calculated with MP2 full quantum calculation and 5T:34T model with different ONIOM approaches. Energies are in kcal/mol. (High level means contribution from high level of theory: $\Delta E(\text{model, high})$ and Low level means contribution from low level of theory: $\Delta E(\text{real, low}) - \Delta E(\text{model, low})$)

Model	Method	Ethene	Benzene	Ethylbenzene	Pyridine
5T	MP2^a	-8.7	-12.1	-13.9	-24.9
5T:34T	ONIOM(MP2:M06-2X)^b	-13.3	-18.4	-23.3	-43.7
	High level	-8.8	-11.7	-12.8	-23.6
	Low level	-4.5	-6.7	-10.5	-20.1
5T:34T	ONIOM(MP2:B3LYP)^c	-10.5	-12.9	-13.3	-39.1
	High level	-9.1	-11.0	-12.0	-24.2
	Low level	-1.4	-1.9	-1.3	-14.9
5T:34T	ONIOM(MP2:HF)^d	-10.4	-11.8	-11.6	-38.7
	High level	-9.0	-10.7	-11.8	-23.9
	Low level	-1.4	-1.1	0.2	-14.8
5T:34T	ONIOM(MP2:UFF)^e	-16.6	-26.0	-35.3	-38.6
	High level	-8.5	-10.9	-11.8	-26.3
	Low level	-8.1	-15.1	-23.5	-12.3
Expt	H-ZSM-5	-	-	-	-47.6
	FAU	-9	-15.3	-19.6	-43.1

^a MP2/6-311+G(2df,2p)//M06-2X/6-31G(d,p)

^b ONIOM(MP2/6-311+G(2df,2p):M06-2X/6-31G(d,p)//MP2/6-31G(d,p):M06-2X/6-31G(d,p))

^c ONIOM(MP2/6-311+G(2df,2p):B3LYP/6-31G(d,p)//MP2/6-31G(d,p):B3LYP/6-31G(d,p))

^d ONIOM(MP2/6-311+G(2df,2p):HF/6-31G(d,p)//MP2/6-31G(d,p):HF/6-31G(d,p))

^e ONIOM(MP2/6-311+G(2df,2p):UFF//MP2/6-31G(d,p):UFF)

Table S9. Comparison of model size and computational approach on adsorption energies of ethene, benzene, ethylbenzene and pyridine molecule on H-ZSM-5 zeolite; ONIOM(MP2:M06-2X) method on 5T:34T and 5T:128T models, embedded ONIOM(MP2:M06-2X) method on 5T:34T model and M06-2X quantum calculation on 34T model. Energies are in kcal/mol.

Model	Method	Ethene	Benzene	Ethylbenzene	Pyridine
5T:34T	ONIOM(MP2:M06-2X) ^a	-13.2	-17.7	-22.2	-43.2
5T:34T	ONIOM(MP2:M06-2X) ^b	-13.3	-18.4	-23.3	-43.7
5T:128T	ONIOM(MP2:M06-2X) ^b	-13.6	-19.0	-23.6	-47.0
5T:34T	Embedded ONIOM(MP2:M06-2X) ^b	-14.0	-19.8	-24.7	-48.4
34T	M06-2X ^c	-14.0	-18.2	-22.8	-41.5
Expt	H-ZSM-5	-	-	-	-47.6
	FAU	-9	-15.3	-19.6	-43.1

^a ONIOM(MP2/6-31G(d,p):M06-2X/6-31G(d,p))

^b ONIOM(MP2/6-311+G(2df,2p):M06-2X/6-31G(d,p)//MP2/6-31G(d,p):M06-2X/6-31G(d,p))

^c M06-2X/6-31G(d,p)//ONIOM(MP2/6-31G(d,p):M06-2X/6-31G(d,p))

Table S10. Reaction energies for H/H exchange reaction of benzene and ethylbenzene on various models of H-ZSM-5 zeolite calculated with different methodologies. Apparent activation energies are presented in **bold type** while intrinsic activation energies are in parenthesis. Energies are in kcal/mol.

Model	Method	Benzene			Ethyl Benzene		
		AD	TS	PR	AD	TS	PR
5T	MP2 ^a	-12.1	22.7 (34.8)	-8.6	-13.9	19.8 (33.7)	-10.4
5T:34T	ONIOM(MP2:M06-2X) ^b	-18.4	12.6 (31.0)	-14.3	-23.3	4.6 (27.9)	-20.6
5T:128T	ONIOM(MP2:M06-2X) ^b	-19.0	12.6 (31.6)	-13.7	-23.6	4.9 (28.5)	-20.6
5T:34T	Embedded ONIOM(MP2:M06-2X) ^b	-19.8	10.4 (30.2)	-14.1	-24.7	1.9 (26.6)	-21.9
34T	M06-2X ^c	-18.2	13.5 (31.7)	-14.2	-22.8	4.9 (27.7)	-20.0
Expt	H-ZSM-5		11.0			6.9	

^a MP2/6-311+G(2df,2p)//M06-2X/6-31G(d,p)

^b ONIOM(MP2/6-311+G(2df,2p):M06-2X/6-31G(d,p)//MP2/6-31G(d,p):M06-2X/6-31G(d,p))

^c M06-2X/6-31G(d,p)//ONIOM(MP2/6-31G(d,p):M06-2X/6-31G(d,p))

Table S11. Adsorption energies (kcal/mol) of ethane, benzene, ethylbenzene and pyridine molecules on 5T model of H-ZSM-5 zeolite, BSSE corrected.

	ΔE	$\Delta E + \text{BSSE}$
Ethene		
MP2/6-311+G(2df,2p)//MP2/6-31G(d,p)	-8.7	-7.1
MP2/6-31G(d,p)	-8.8	-4.7
M06-2X/6-311+G(2df,2p)//MP2/6-31G(d,p)	-8.2	-7.7
M06-2X/6-31G(d,p)//MP2/6-31G(d,p)	-9.7	-7.6
B3LYP/6-311+G(2df,2p)//MP2/6-31G(d,p)	-4.1	-3.6
B3LYP/6-31G(d,p)//MP2/6-31G(d,p)	-6.5	-4.2
Benzene		
MP2/6-311+G(2df,2p)//MP2/6-31G(d,p)	-12.1	-9.1
MP2/6-31G(d,p)	-11.4	-5.4
M06-2X/6-311+G(2df,2p)//MP2/6-31G(d,p)	-10.7	-9.7
M06-2X/6-31G(d,p)//MP2/6-31G(d,p)	-9.7	-9.3
B3LYP/6-311+G(2df,2p)//MP2/6-31G(d,p)	-2.2	-1.2
B3LYP/6-31G(d,p)//MP2/6-31G(d,p)	-4.6	-1.4
Ethylbenzene		
MP2/6-311+G(2df,2p)//MP2/6-31G(d,p)	-13.9	-10.2
MP2/6-31G(d,p)	-13.0	-5.5
M06-2X/6-311+G(2df,2p)//MP2/6-31G(d,p)	-12.1	-10.2
M06-2X/6-31G(d,p)//MP2/6-31G(d,p)	-13.7	-10.2
B3LYP/6-311+G(2df,2p)//MP2/6-31G(d,p)	-1.7	-0.6
B3LYP/6-31G(d,p)//MP2/6-31G(d,p)	-4.6	-0.5
Pyridine		
MP2/6-311+G(2df,2p)//MP2/6-31G(d,p)	-24.9	-20.5
MP2/6-31G(d,p)	-24.3	-15.4
M06-2X/6-311+G(2df,2p)//MP2/6-31G(d,p)	-21.6	-20.3
M06-2X/6-31G(d,p)//MP2/6-31G(d,p)	-23.1	-19.7
B3LYP/6-311+G(2df,2p)//MP2/6-31G(d,p)	-17.5	-16.2
B3LYP/6-31G(d,p)//MP2/6-31G(d,p)	-20.4	-16.4

Table S12. Comparison of CPU time for different zeolite models at different levels of theory.

Model	Method	Time (mins)
5T	HF/6-31G(d,p)//MP2/6-31G(d,p)	3
5T	B3LYP/6-31G(d,p)//MP2/6-31G(d,p)	3
5T	M06-2X/6-31G(d,p)//MP2/6-31G(d,p)	7
5T	MP2/6-31G(d,p)	5
5T	B3LYP/6-311+G(2df,2p)//MP2/6-31G(2df,2p)	68
5T	M06-2X/6-311+G(2df,2p)//MP2/6-31G(d,p)	79
5T	MP2/6-311+G(2df,2p)//MP2/6-31G(d,p)	153
34T	HF/6-31G(d,p)//MP2/6-31G(d,p):M06-2X/6-31G(d,p)	182
34T	B3LYP/6-31G(d,p)//MP2/6-31G(d,p):M06-2X/6-31G(d,p)	238
34T	M06-2X/6-31G(d,p)//MP2/6-31G(d,p):M06-2X/6-31G(d,p)	297
5T:34T	MP2/6-31G(d,p):HF/6-31G(d,p)	190
5T:34T	MP2/6-31G(d,p):B3LYP/6-31G(d,p)	246
5T:34T	MP2/6-31G(d,p):M06-2X/6-31G(d,p)	305
5T:34T	MP2/6-311+G(2df,2p):HF/6-31G(d,p)//MP2/6-31G(d,p):HF/6-31G(d,p)	338
5T:34T	MP2/6-311+G(2df,2p):B3LYP/6-31G(d,p)//MP2/6-31G(d,p):B3LYP/6-31G(d,p)	394
5T:34T	MP2/6-311+G(2df,2p):M06-2X/6-31G(d,p)//MP2/6-31G(d,p):M06-2X/6-31G(d,p)	597

The full set of coordinates for the 34T cluster model of H-ZSM-5.

Si	13.8720	19.3474	15.9164	O	13.9754	16.8067	19.6891	H	19.8306	13.0198	10.6375
Si	12.4252	16.4545	19.6758	O	13.9754	13.0418	19.6891	H	19.8306	16.8287	10.6375
Si	12.4252	13.3940	19.6758	O	10.0911	19.0533	17.2935	H	11.8718	13.1764	21.0202
Si	11.5651	18.7747	17.8794	O	10.0911	10.7952	17.2935	H	11.8718	16.6721	21.0202
Si	11.5651	11.0738	17.8794	O	9.9309	12.9901	9.4725	H	8.1075	18.7312	18.8336
Si	14.4337	11.1687	12.9655	O	8.3932	14.9242	8.6454	H	8.1075	11.1173	18.8336
Si	13.8720	10.5011	15.9164	O	7.7105	18.8225	16.3768	H	8.4812	9.0287	17.6988
Si	8.5838	19.3573	17.5918	O	7.7105	11.0260	16.3768	H	5.2205	11.0553	16.7006
Si	8.5838	10.4912	17.5918	O	7.4922	16.7928	10.2086	H	6.1378	10.0479	14.6897
Si	8.4623	16.4664	9.0043	O	7.4922	13.0557	10.2086	H	4.0824	13.0681	13.7707
Si	8.4623	13.3821	9.0043	O	6.2348	17.3161	14.9408	H	6.1049	11.0708	10.8867
Si	6.2787	18.7257	15.6825	O	6.2348	12.5324	14.9408	H	4.9912	13.0800	10.1956
Si	6.2787	11.1228	15.6825	O	6.1768	16.8107	12.4087	H	4.9912	16.7685	10.1956
Si	6.1624	17.3089	10.9007	O	6.1768	13.0378	12.4087	H	6.1049	18.7777	10.8867
Si	6.1624	12.5396	10.9007	O	5.7723	14.9242	14.1579	H	4.0824	16.7804	13.7707
Si	5.5169	16.4607	13.7991	O	18.4042	14.9243	11.4291	H	6.1378	19.8006	14.6897
Si	5.5169	13.3878	13.7991	O	18.0819	18.6832	14.5286	H	5.2205	18.7932	16.7006
Si	18.5948	19.3573	15.8657	O	18.0819	11.1653	14.5286	H	8.4812	20.8198	17.6988
Si	18.5948	10.4912	15.8657	O	18.0598	17.2843	12.3646	H	11.8218	19.8522	18.8459
Si	18.4733	16.4664	11.0702	O	18.0598	12.5642	12.3646	H	16.1488	19.8006	18.7678
Si	18.4733	13.3821	11.0702	O	17.7215	18.8225	17.0807	H	18.4922	20.8198	15.7587
Si	17.5763	18.6458	13.0257	O	17.7215	11.0260	17.0807	H	8.0790	12.6240	7.8046
Si	17.5763	11.2027	13.0257	O	17.5032	13.0557	9.8659	H	8.0790	17.2245	7.8046
Si	16.2897	18.7257	17.7750	O	16.2458	17.3161	18.5167	H	18.4922	9.0287	15.7587
Si	16.2897	11.1228	17.7750	O	16.2458	12.5324	18.5167	H	13.9182	9.0322	15.8825
Si	16.1734	12.5396	9.1738	O	15.7833	14.9243	19.2996	H	16.1488	10.0479	18.7678
Si	15.5279	16.4607	19.6584	O	13.9173	12.5185	12.2990	H	11.8218	9.9963	18.8459
Si	15.5279	13.3878	19.6584	O	13.8472	18.7309	14.4389	H	18.1482	19.7785	12.2835
Si	11.4213	12.5437	9.1272	O	9.9309	16.8584	9.4725	H	16.1159	11.0708	9.1878
Si	13.7490	13.3506	10.9739	O	17.5032	16.7928	9.8659	H	16.1867	13.0007	7.7781
Si	14.4043	18.6631	12.9562	O	16.0036	18.7210	12.9962	H	11.5407	11.0800	9.0633
Si	16.1633	17.3012	9.1062	O	14.9124	13.1214	9.9329	H	11.8041	13.1179	7.8293
Si	11.4385	17.2809	9.1385	O	12.3516	13.0896	10.2969	H	13.9299	10.0149	12.2066
O	13.8472	11.1176	14.4389	O	13.9560	17.2109	12.4806	H	18.1482	10.0700	12.2835
O	12.5618	11.0121	16.6511	O	13.9112	14.8487	11.6767	H	13.9389	19.8046	12.2237
O	11.6908	12.4886	18.5970	O	12.1496	16.5617	10.3850	H	16.1145	18.7481	9.1878
O	12.5618	18.8364	16.6511	O	14.8538	16.5826	9.6967	H	11.5384	18.7297	9.0689
O	12.1834	14.9243	19.2568	H	13.9182	20.8163	15.8825	H	16.1848	16.8441	7.7737
O	11.6908	17.3599	18.5970	H	16.1425	16.7867	20.9534	H	11.7985	16.7368	7.8546
O	16.0036	11.1275	12.9962	H	16.1425	13.0618	20.9534	H	13.8811	14.8800	12.6454
O	15.1466	18.7986	16.6752	H	20.0094	19.0720	16.1457	Al	13.7283	16.5235	10.9536
O	15.1466	11.0499	16.6752	H	20.0094	10.7765	16.1457				