Supporting Information

Quantum chemical modeling of benzene ethylation over H-ZSM-5 approaching chemical accuracy: A hybrid MP2:DFT study

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S.1 Location of the acidic site in the MFI framework

The orthorhombic structure of ZSM-5 has 12 unique T-atom positions into which Al can be substituted. Several experimental and computational studies indicate that there is little energetic preference for Al in different sites.[1-5] In the present study we consider the T12 site for Al substitution in accordance with previous theoretical works.[6-8] In contrast to the siting of the Al atom, the position of the acidic proton is likely determined by thermodynamics because proton jumps between oxygen atoms bonded to the same aluminium are facile, in particular when adsorbates are present.[9-11] In the present work we computed the total energies of the Al12-O24(H)-Si12, Al12-O20(H)-Si3, and Al12-O11(H)-Si11 sites for both sets of unit cell parameters (crystallographic position numbers according to Olson et al.[12]). The results are summarized in Table S.1. The order of stability depends on the unit cell parameters used, although the differences between Al12-O11(H)-Si11 and Al12-O20(H)-Si3 are rather small. Because the latter site is more easily accessible for reactants due to its location at the intersection between straight and sinusoidal channels we use Al12-O20(H)-Si3 as reference site in this work. In the recent work of Svelle et al.[8] the Al12-O20(H)-Si3 site was reported to be more stable than the Al12-O24(H)-Si12 by 12.4 kJ/mol compared to 7.7 kJ/mol calculated in the present work. These deviations are a consequence of some differences in the set-up of the VASP calculations (PREC-tag, EDIFFG-tag, LREAL-tag) as confirmed by reproducing the electronic energy of the H-ZSM-5 unit cell using the input set-up of Svelle et al.[8]

Table S.1. Relative stabilities (in kJ/mol) of different bridging hydroxyl groups for Al-substitution at T12 position and two different sets of unit cell parameters. The results of Svelle et al.[8] are given for comparison.

Bridging hydroxyl group	UC1	UC2	UC2 [8]
Al12-O20(H)-Si3	0.0	0.0	0.0
Al12-O24(H)-Si12	6.3	7.7	12.4
Al12-O11(H)-Si11	-0.6	0.2	5.5

S.2 Extrapolation to the complete basis set limit

For the counterpoise-corrected Hartree-Fock (HF) energy contribution to the MP2 adsorption energy, $\Delta E_{\mathrm{HF}}^{\mathrm{cp}}(\mathrm{X})$, an exponential extrapolation scheme[13,14] is employed,

$$\Delta E_{\mathrm{HF}}^{\mathrm{cp}}(\mathrm{X}) = \Delta E_{\mathrm{HF}}^{\mathrm{CBS}} + b\exp(-c\mathrm{X}), \tag{S.1}$$

while an inverse power law[15] is applied for the extrapolation of the counterpoise-corrected correlation energy contribution to the MP2 adsorption energy, $\Delta E_{\mathrm{corr}}^{\mathrm{cp}}(\mathrm{X})$,

$$\Delta E_{\mathrm{corr}}^{\mathrm{cp}}(\mathrm{X}) = \Delta E_{\mathrm{corr}}^{\mathrm{CBS}} + b\mathrm{X}^{-3}. \tag{S.2}$$

Following the recommendations in ref. 14 the parameter *c* in eq. S.1 is set to 1.5. The corresponding CBS limits, $\Delta E_{\mathrm{HF}}^{\mathrm{CBS}}$ and $\Delta E_{\mathrm{corr}}^{\mathrm{CBS}}$, along with the parameter *b* were calculated directly from two data points.

Figure S.1 shows the complete basis set limit correction for ethene, benzene, and ethylbenzene adsorption as well as for benzene adsorption next to the surface ethoxide as function of the cluster size for up to 18 T-atoms. The CBS-limit correction increases with the cluster size, although not always monotonically. Beyond the 14T cluster there are only weak changes of the CBS-limit correction for ethene and benzene which makes it reasonable to take the values from the 18T clusters as estimates for the periodic limit. For ethylbenzene and benzene adsorbed next to ethoxide, the CBS-limit corrections increase up to 16 T-atoms and level off for 18 T-atoms. Here we also took the numbers from the 18T clusters as estimates for the periodic limit. For the co-adsorption of ethene and benzene the CBS-limit correction was computed only for the T16 cluster because of the high computational costs associated with a 3-body counter poise correction. For the formation of ethoxide and for ethene adsorption in all-silica MFI, we computed the CBS-limit correction only for the T18 cluster.

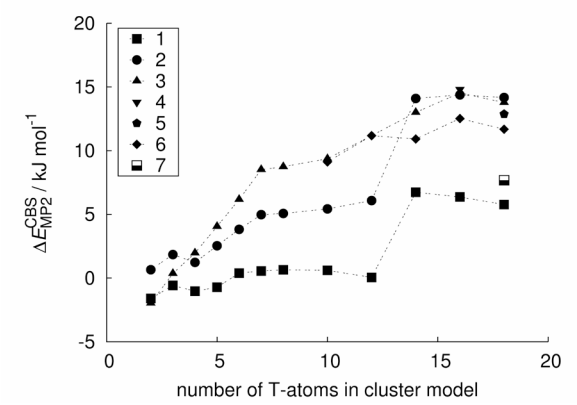

Figure S.1. CBS-limit corrections for the formation of structures **1** to **7**. For structures **4, 5** and **7** the CBS-limit correction was calculated for one cluster size only (16T and 18T, respectively).

S.3 BSSE calculations on transition structures and intermediates

Basis set superposition errors (BSSE) were calculated with the counterpoise procedure[16] (CP). As noted in the main text, CP-corrected CBS-limit corrections for intrinsic energy barriers have been obtained from the CP-corrected CBS-limits for the apparent energy barriers and those of the corresponding adsorbate complexes. Depending on the reaction channel, two-body or three-body CP calculations were performed. The closed-shell subsystems used in these calculations are listed in Table S.2. The fragments used for the ethoxy intermediate resemble the corresponding carbenium ion and the negatively charged zeolite framework.

Table S.2: Subsystems used for calculating BSSE-corrected CBS-limit corrections for apparent activation energies.

	1s		**2s(1)**		**2s(2)**	
Subsystem	forward	reverse	forward	reverse	forward	reverse
zeolite cluster (charge: -1)	+	+	+	+	-	+
protonated ethene (charge: +1)	+	-	+	+	-	-
benzene (charge: 0)	+	-	-	-	+	-
benzene + protonated ethene (charge: +1)	-	+	-	-	-	+
zeolite cluster + protonated ethene (charge: 0)	-	-	-	-	+	-

S.4 Cluster size dependence of the MP2/CBS-DFT+D energy

From Tables 1 and 3 in the main manuscript it becomes evident that higher order correlation effects evaluated as difference between CCSD(T) and MP2 adsorption energies and energy barriers might contribute significantly to the *final estimates*. Unfortunately CCSD(T) calculations are only feasible on small cluster models of the active site. Therefore it becomes necessary to estimate the cluster size dependence of the correlation energy not captured by MP2. Fig. S.2 shows the difference between MP2/CBS and DFT+D adsorption energies for steps **1**, **2**, **3**, and **6**. Assuming that DFT+D describes correctly the dispersion interactions, this difference can be interpreted as that part of the correlation energy not captured by MP2. The important point is that this difference depends only weakly (±2 kJ/mol) on the cluster size. As a result even small clusters can be used to estimate higher order correlation effects.

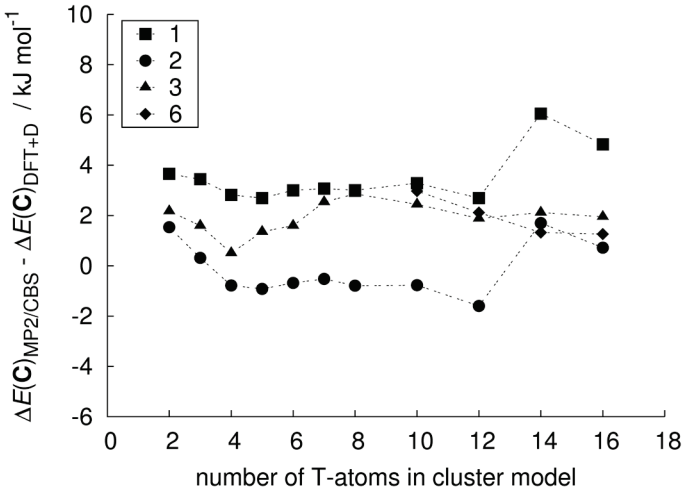

Figure S.2. Differences between MP2/CBS and PBE+D results for adsorption energies.

S.5 Partition functions for reactant and transition states

The partition functions are most easily computed for the case of immobile adsorption because only vibrational contributions are taken into account, which are directly obtained from the dynamical matrix of the stationary point. If the energy of the ground vibrational state is

chosen to be $\sum h\nu/2$, the partition function of the reactant as appearing in eq. 11 of the manuscript is given by

$$Q_{\mathrm{R}}(T) = \prod_{i=1}^{3n-6} \frac{\exp\left[-\Theta_{\mathrm{vib},i}/(2T)\right]}{1-\exp\left[-\Theta_{\mathrm{vib},i}/T\right]}, \tag{S.3}$$

with $\Theta_{\mathrm{vib},i}$ being the vibrational temperatures defined as

$$\Theta_{\mathrm{vib},i} = \frac{\tilde{\nu}_i \cdot c \cdot h}{k_{\mathrm{B}}}, \tag{S.4}$$

where $\tilde{\nu}_i$ is the ith wave number, c is the speed of light, h is Planck's constant and k_{B} is Boltzmann's constant. The partition function of the transitions state is also evaluated with Eq. S.3 but with the product running from $i = 1 \text{ to } 3n-7$ as the vibrational degree of freedom corresponding to the reaction coordinate is missing. The frequency spectrum of physisorbed complexes often displays low wavenumber modes in the range 0 to 100 cm^{-1} which correspond to frustrated rotations and translations of the physisorbed molecules. As these modes make the largest contribution to the partition function it has to be carefully analyzed whether a treatment as vibrations may lead to spurious results and whether the contribution from these modes should be replaced by translational and (hindered) rotational contributions, respectively. In a recent study by De Moor et al.[17] on the adsorption of alkanes and alkenes in H-FAU it was demonstrated how the treatment of low modes influences the enthalpy and entropy of adsorption. Here we are mainly interested in the contributions of physisorbed benzene and ethene to the partition function of the reactant state. Visualization of the vibrations corresponding to harmonic frequencies in the range 0 to 100 cm^{-1} for coadsorbed ethene and benzene in H-ZSM-5 indicate that some frequencies correspond to a rotation of the hydrocarbon relative to the zeolite. For benzene a frequency of 47 cm^{-1} could be associated with a rotation around the C_6-symmetry axis (see Fig. S.3(a)). For ethene, a frequency of 53 cm^{-1} could be associated with a rotation around the $C_2(x)$-symmetry axis (see Fig. S.3(b)). However, both movements were accompanied by significant vibrations of the zeolite lattice

itself. Therefore we have estimated the barriers for a rigid rotation of benzene around its C_6-axis and for ethene around two of its C_2-axes by performing single point energy calculations for discrete points along the rotational pathway. As can be seen from Fig. S.4 a rotation of benzene of 60° is associated with an energy barrier of 6 kJ/mol. For ethene, a rigid rotation of 180° around the $C_2(x)$-axis which is perpendicular to the molecular plane is associated with an energy barrier of around 13 kJ/mol. A frustrated rotation around the $C_2(y)$-axis which goes through the C=C bond is associated with an energy barrier of 46 kJ/mol and can therefore safely be treated as vibration. If the two remaining rotations were treated as harmonic vibrations the corresponding frequencies can be obtained from[18]

$$\nu = \frac{n_r}{2\pi}\left(\frac{V_0}{2I_A}\right)^{1/2}, \tag{S.5}$$

where I_A denotes the moment of inertia and n_r acquires the sense of the degeneration degree during rotation of 2π ($n_r = 2$ for ethene; $n_r = 6$ for benzene). The contributions to the partition function are then given by equation S.3. For the case of free rotation the contribution to the partition function is given by

$$q_{\text{free}} = \frac{1}{n_r}\frac{\left(2\pi k_B T I_A\right)^{1/2}}{h} 2\pi . \tag{S.6}$$

In the case of hindered rotation it can be estimated by using the Tables of Pitzer and Gwinn[19] which tabulate contributions from hindered rotation to the free energy function F_{hind}/T as function of q_{free} and V_0/RT, where V_0 is the rotational barrier. The contribution to the partition function resulting from the hindered rotation can then be obtained from

$$F_{\text{hind}} = -RT \ln q_{\text{hind}} . \tag{S.7}$$

To proceed we compare the contributions of each rotational movement to the reactant partition function for (i) immobile adsorption (Eqs S.3 and S.5), (ii) free rotation (Eq. S.6), and (iii) hindered rotation (Eq. S.7) in order to decide whether the partition function directly calculated from the vibrational spectrum is a reasonable approximation. The results are

summarized in Table S.3. It can be seen that at relevant reaction temperatures the treatment as free rotation leads to a almost twofold increase of the partition function for benzene and an almost threefold increase for ethene, when compared to the assumption of immobile adsorption. However, the treatment as hindered rotations lead to numbers close to the treatment as immobile adsorption leading us to conclude that the calculation of the partition function for the reactant state directly from the frequency spectrum treating all frustrated modes as vibrations is a reasonable approximation in the present study.

Similar investigations were also carried out for ethene adsorbed on the acid site (without benzene coadsorbed) and for benzene adsorbed next to the ethoxide. For ethene adsorbed on the acid site the barrier for rotation around the $C_2(y)$-axis was calculated to 46 kJ/mol while for rotation around the $C_2(x)$-axis a barrier of only 3.5 kJ/mol was determined. While the first barrier is large enough to treat the corresponding movement as normal vibration, the rotation around the $C_2(x)$-axis could also be regarded as free rotation. However, a comparison of the contributions to the reactant partition function for free rotation around the $C_2(x)$-axis and a vibrational contribution from a frequency of 31 cm^{-1} (corresponding to a barrier height of 3.5 kJ/mol according to equation S.5) revealed that the final rate coefficients at reaction temperature are not affected significantly. When assuming free rotation the rate coefficient is smaller by a factor of 1.3 to 1.4 in the temperature range 600 to 700 K. For reasons of simplicity we therefore decided to treat the adsorbate as immobile.

For benzene adsorption next to an ethoxide species we have calculated a barrier of only 2 kJ/mol for rotation around the C_6 axis. This barrier corresponds to a frequency of 24 cm^{-1} according to Eq. S.5. However, in the relevant temperature range from 600 to 700 K the rate coefficient is smaller by a factor of 1.03 to 1.11 when assuming free rotation instead of treating the degree of freedom as vibrational contribution. For reasons of simplicity we have therefore used again the immobile adsorbate assumption. Another argument in favor of the immobile adsorbate assumption is the fact that we also assume immobile transition states

although these structures also display low modes in the range 0 to 100 cm^{-1}. Therefore the contributions from low modes will cancel out to a significant portion in the calculation of the rate coefficients.

Table S.3: Contributions to the reactant partition functions of adsorbed benzene and ethene for different treatments of the rotational motion around the C_6-symmetry axis (C_6H_6) and the C_2(x)-symmetry axis (C_2H_4), respectively.

T [K]	Benzene			Ethene		
	immobile[a]	free rot.[b]	hindered rot.	immobile[a]	free rot.[b]	hindered rot.
298	5.044	13.810	6.368	3.440	14.042	4.252
600	10.167	19.596	12.360	6.944	19.924	8.565
650	11.015	20.396	13.241	7.524	20.738	9.296
700	11.863	21.166	14.086	8.104	21.521	10.034

[a] wavenumbers: 41 cm^{-1} (C_6H_6); 60 cm^{-1} (C_2H_4)

[b] moments of inertia: 2.954×10^{-45} kg m^2 (C_6H_6); 3.393×10^{-46} kg m^2 (C_2H_4)

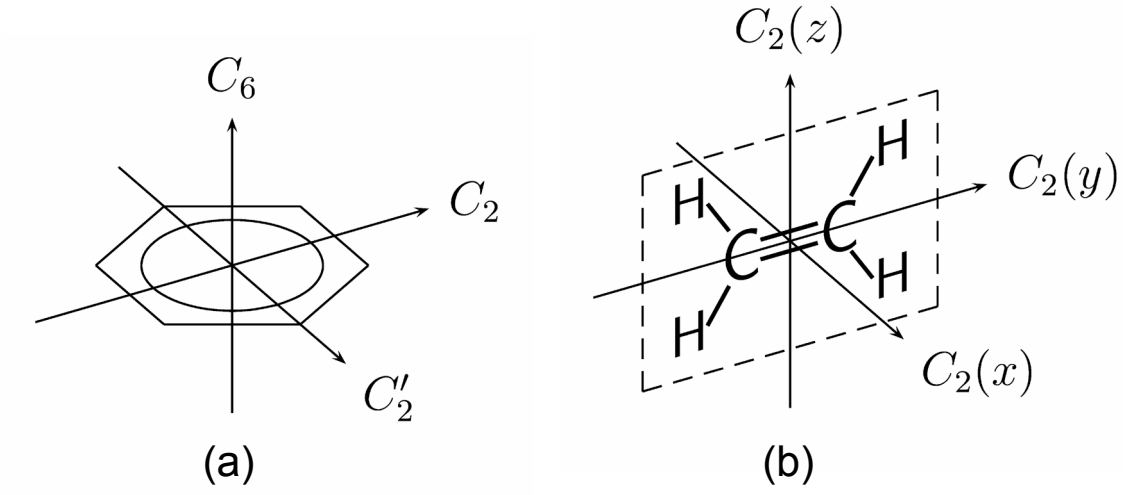

Figure S.3: Definition of symmetry axes for (a) benzene and (b) ethene.

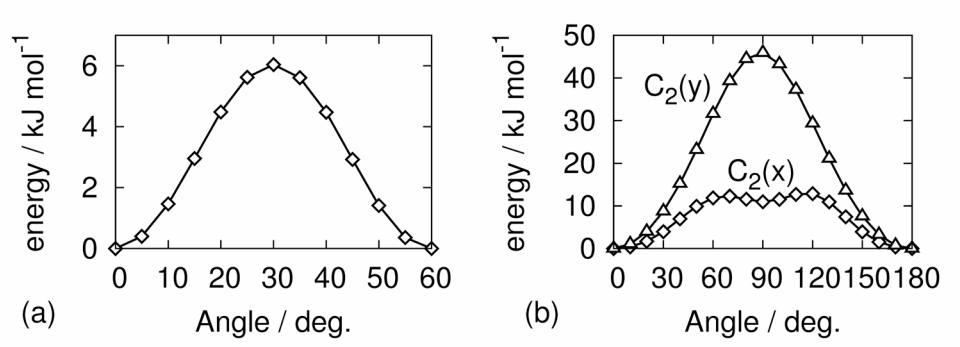

Figure S.4: PBE-barriers for rigid rotations of (a) benzene around the C_6-symmetry axis and (b) ethene around the $C_2(x)$-axis and $C_2(y)$-axis, respectively, for the case of co-adsorbed ethene and benzene

S.6 Influence of unit cell parameters on PBE energies

S.6.1 Adsorption energies

Table S.4 shows adsorption energies obtained for the two different sets of unit cell parameters. It can be seen that the interaction energy with the acid site increases in the order $C_8H_{10} < C_6H_6 < C_2H_4$ for the first set of unit cell parameters while for the second set C_6H_6 and C_8H_{10} show almost the same adsorption energy. The adsorption energy of ethene is hardly influenced by the size of the unit cell, while for benzene and ethylbenzene the changes are 4.3 kJ/mol and -3.4 kJ/mol when going from UC1 to UC2. For ethylbenzene adsorption it was confirmed that the electronic energy obtained with UC1 is reproduced when starting the structure optimization from the stationary point obtained with UC2 after adjusting the cell parameters according to UC1. It can therefore be concluded that the energy differences result exclusively from the change in cell parameters. To estimate the effect of the cell parameters on ZPVE- and finite temperature corrections we have computed these numbers for single molecule adsorption on the acid site using the UC2 cell parameters. The largest effect is obtained for ethene for which the thermal correction is higher by 1.5 kJ/mol for the UC2 cell parameters. For ethene located in pure silica MFI we have also calculated the energy of adsorption in the straight and sinusoidal channels, respectively, in addition to adsorption in

the channel intersections. The electronic adsorption energies are +0.4 kJ/mol and -4.2 kJ/mol, respectively.

Table S.4: DFT (PBE) results for adsorption energies, ΔE, ZPVE-corrected adsorption energies, ΔE_0, and adsorption enthalpies at 298 K, ΔH_{298}. Energies are reported in kJ/mol.

reaction	UC1			UC2		
	ΔE	ΔE_0	ΔH_{298}	ΔE	ΔE_0	ΔH_{298}
1	-31.5	-30.1	-29.0	-31.4	-28.8	-27.5
2	-24.0	-24.2	-21.6	-19.6	-19.5	-16.4
3	-16.6	-13.9	-11.5	-20.0	-18.0	-15.5
4	-40.7	-34.3	-30.4	-42.4	--	--
5	-53.5	-43.1	-45.7	-43.8	--	--
6[a]	-2.0	2.1	5.1	-7.0	--	--
7[b]	-4.2	-6.1	-1.4	--	--	--

[a] The ethyl group is bonded to O24

[b] Adsorption in channel intersection

S.6.2 Energy barriers

Table S.5 summarizes intrinsic energy and enthalpy barriers for the one-step and the two-step alkylation. The PBE energy barrier of the one-step alkylation is lower than the energy barriers of the two-step mechanism in contrast to what was found in our recent cluster study.[7] There, the DFT energy barrier of the ethoxide formation was the lowest of all elementary steps. Note that the energy barriers for the one-step mechanism and for the first step of the two-step scheme are hardly influenced by the set of unit cell parameters used in the calculation. Therefore, there is virtually no uncertainty connected with the choice of the unit cell for these elementary reactions. Only for the second barrier of the two-step scheme a difference of 6.1 kJ/mol is observed. To confirm that this difference is entirely attributable to the change in cell parameters we have changed the cell parameters of the UC2 transition state to UC1 and reoptimized the structure. The total energy of the UC1 transition state was reproduced within 0.1 kJ/mol. For the first step of the two-step mechanism we have calculated the zero-point vibrational energy and thermal correction for both, the UC1 and UC2 cell parameters.

However, the influence of the cell size is rather small. The largest difference (1.9 kJ/mol) is obtained for the ZPVE correction. Regarding the influence of the unit cell size on the reverse reactions, only the first barrier of the two-step mechanism is affected. The reverse barrier of this step is lower by 10.2 kJ/mol for the UC2 set of cell parameters which is a consequence of the lower stability of the ethoxide species in this unit cell.

Table S.5: DFT (PBE) results for intrinsic energy barriers, $E^{\ddagger}$, ZPVE-corrected intrinsic energy barriers, $E_0^{\ddagger}$, and intrinsic enthalpy barriers at 653 K, $H_{653}^{\ddagger}$, for the one-step alkylation (1s) and the two-step alkylation (2s(1) and 2s(2)).

reaction	UC1			UC2		
channel	$E^{\ddagger}$	$E^{\ddagger}_0$	$H^{\ddagger}_{653}$	$E^{\ddagger}$	$E^{\ddagger}_0$	$H^{\ddagger}_{653}$
1s	84.3	79.5	71.8	84.3	--	--
2s(1)	91.6	89.3	80.7	91.2	87.0	79.3
2s(2)	95.9	90.9	87.1	89.8	--	--
1s, rev	173.1	158.5	158.1	174.8	--	--
2s(1), rev	113.7	102.3	99.8	103.5	--	--
2s(2), rev	169.9	163.2	161.2	171.9	--	--

S.7 Cluster size dependence of adsorption energies and intrinsic energy barriers

In addition to the calculations discussed in the main text, two further sets of computations were carried out to study (i) the influence of the cluster termination and (ii) the influence of the size of the unit cell from which the clusters were cut out.

For ethene adsorption on the acid site we have studied the influence of an Al-O-$Si(OH)_3$ cluster termination on the high level correction to see whether it gives results that are different from those of an Al-O-H termination. All clusters used for calculating the data presented in the main text which contain more than 10 T-atoms contain one Al-O-H termination. This termination was replaced by Al-O-$Si(OH)_3$. As can be seen from Figs S.5(a) and S.5(b) the MP2 and PBE adsorption energies are essentially shifted but do not deviate

significantly between the two cluster terminations (open and filled squares). Even more importantly, the difference between MP2 and PBE adsorption energies, extrapolated to the periodic limit is the same in both cases (see Fig. S.6).

In addition we have studied the influence of the unit cell parameters on the high level correction for the case of benzene adsorption on the acid site. In section S.6.1 the influence of the unit cell size on the PBE adsorption energies was evaluated for all elementary steps. It was found that energy differences are within ± 5 kJ/mol with the exception of ethoxide formation (9.7 kJ/mol). As can be seen from Figs S.5(a) and S.5(b), the size of the unit cell used for constructing the cluster series affects the MP2 and PBE adsorption energies, as expected. However, the number of interest is the difference between MP2 and PBE energies, extrapolated to the periodic limit (see Fig. S.6). These numbers differ by only 0.3 kJ/mol which means for the case of benzene adsorption that the UC2 set cell parameters results in an adsorption enthalpy which is less negative by 4.9 kJ/mol if the CBS-limit correction is assumed to be independent of the unit cell size.

Figure S.7 shows the intrinsic energy barriers obtained from single point MP2 (S.7(a)) and PBE (S.7(b)) calculations for all forward and reverse reactions steps as function of the cluster size. Similar to the adsorption energies and apparent energy barriers, the intrinsic energy barriers do not show a systematic behaviour with cluster size. The second barrier of the two-step scheme becomes even negative for larger clusters. The PBE barriers calculated for the T30 clusters are significantly different from the periodic limit. The difference between MP2 and PBE intrinsic energy barriers is plotted in Fig. S.8. Contrary to the corresponding plots for adsorption energies and apparent barriers (Figs 5, 6 and 9 in the main text) the curves do not decay monotonically with cluster size. Therefore, an unambiguous extrapolation to the periodic limit is not possible. Consequently we have determined the high level corrections for the intrinsic energy barriers indirectly from the high level corrections for the apparent barriers and the corresponding adsorbate structures.

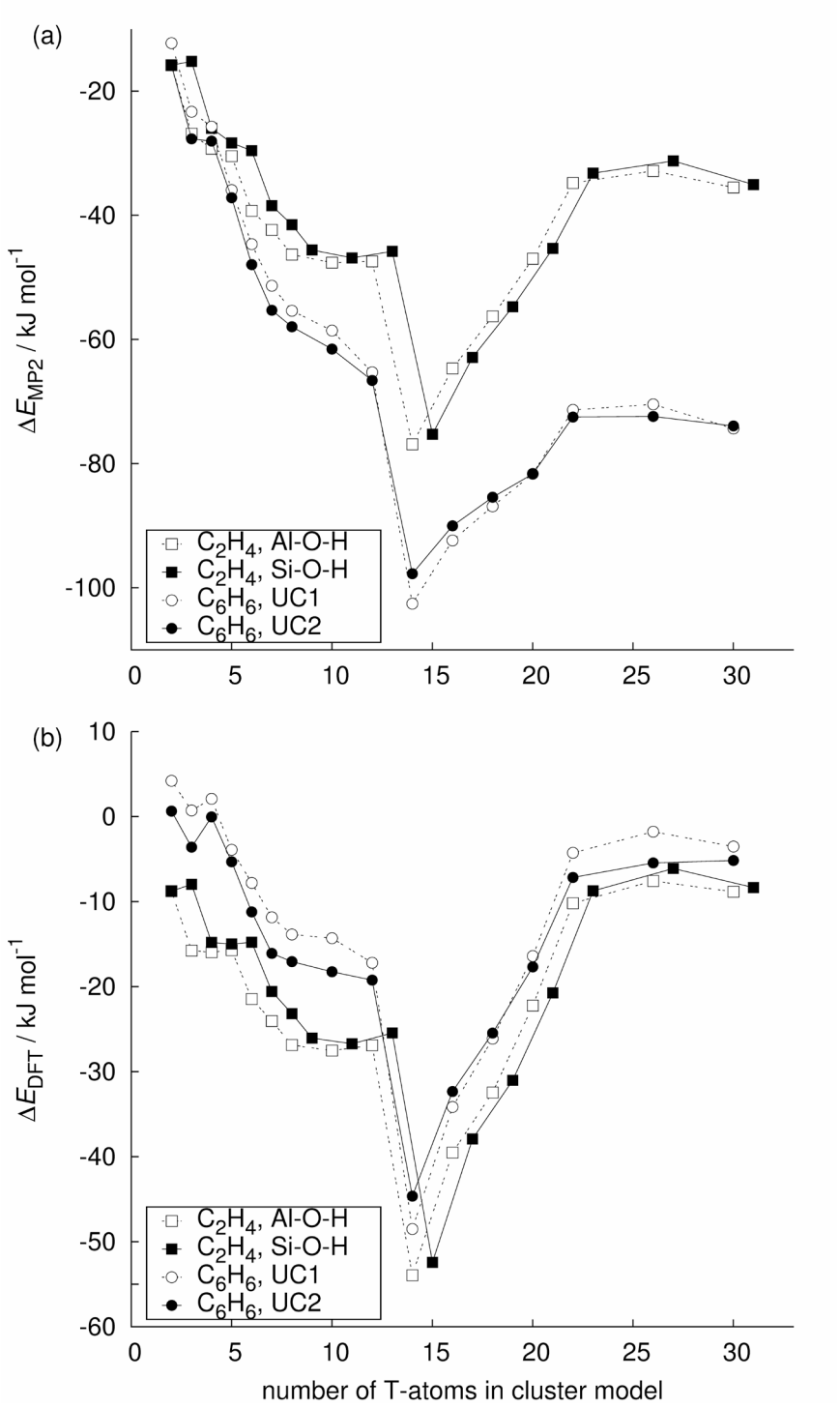

Figure S.5: Adsorption energies of ethene for two different cluster terminations and adsorption energies of benzene for two different sets of unit cell parameters obtained from single-point energy calculations on cluster models of increasing size. (a) MP2/TZVP(P) results. (b) DFT (PBE/QZVP) results.

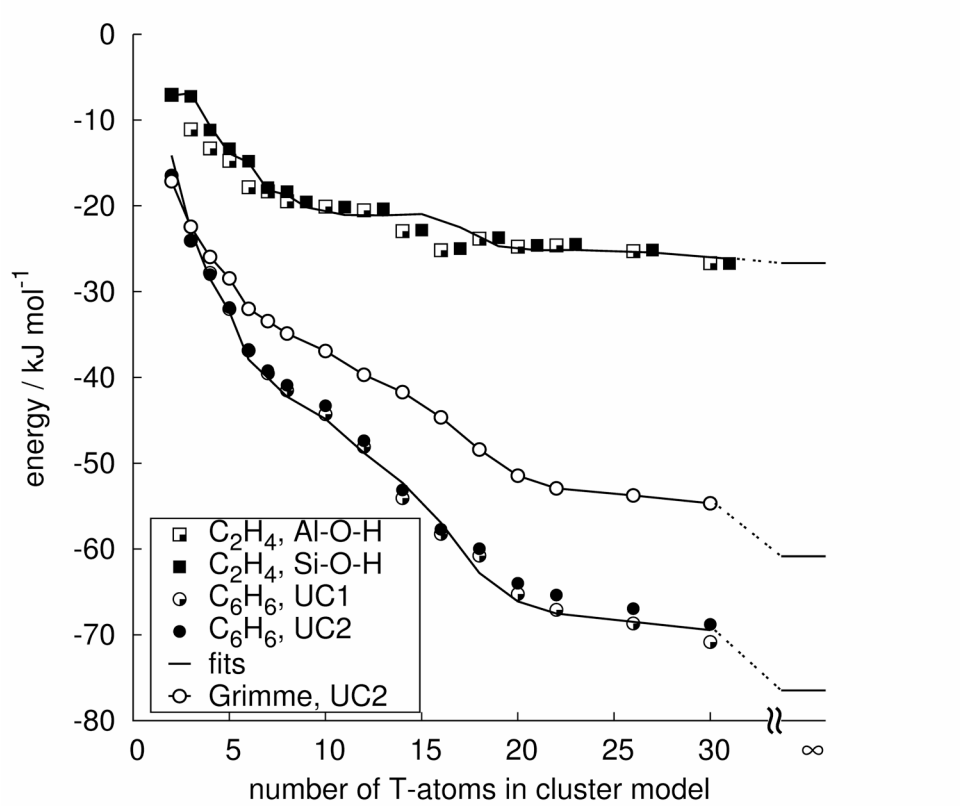

Figure S.6: Differences in adsorption energies between MP2 and PBE (filled and partly filled symbols) and dispersion contributions to the adsorption energies as predicted by the parameter set published by Grimme[20] (open symbols). Extrapolations to the full periodic limit are also included.

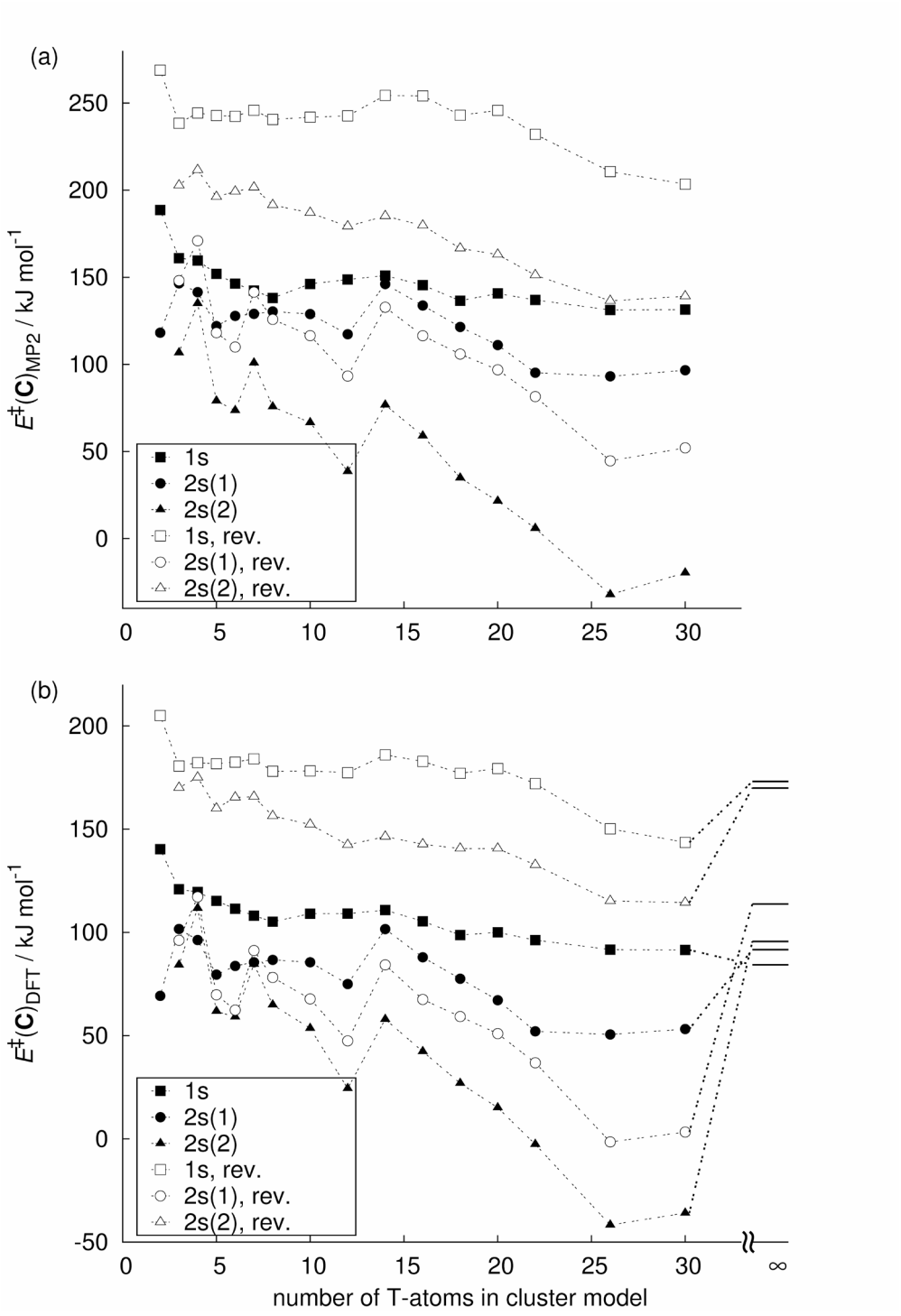

Figure S.7: Intrinsic energy barriers of forward and reverse reaction steps in the one- and two-step alkylation obtained from single-point energy calculations on cluster models of increasing size. (a) MP2/TZVP(P) results. (b) DFT (PBE/QZVP) results. The periodic model limit is given for comparison.

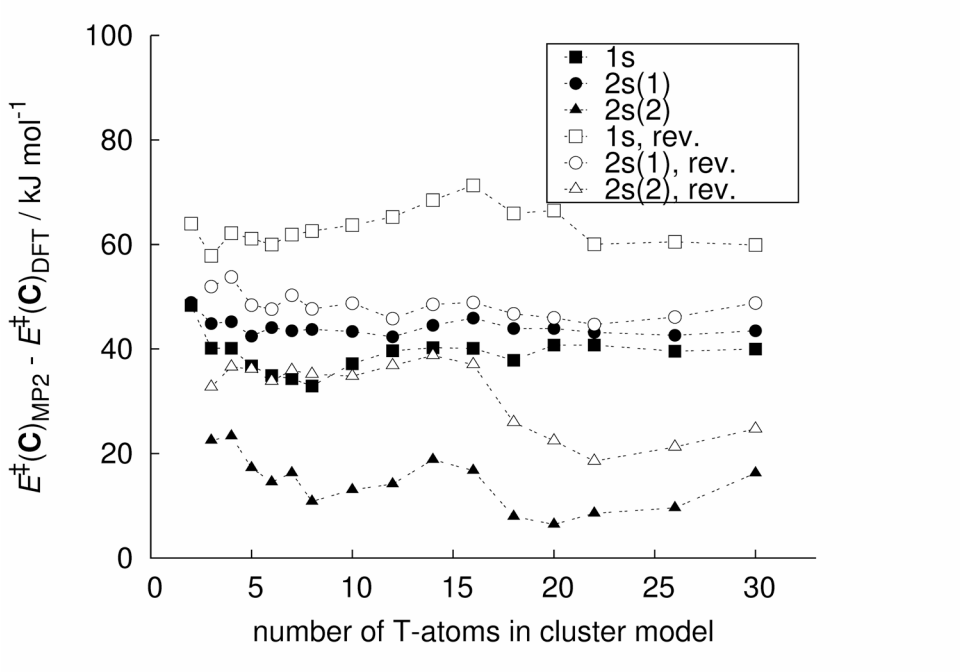

Figure S.8: Differences between MP2 and PBE intrinsic energy barriers for forward and reverse reaction steps.

S.8 Fit parameters

Table S.6: Sets of C_6 parameters (in J nm^6 mol^{-1}) for H, C, Al, Si, and O atoms as well as additive constants, E_{add} (in kJ mol^{-1}) obtained by fitting differences between MP2/TZVP(P) and PBE/QZVP cluster model adsorption energies. Root mean squared errors and the maximum deviation between reference data points and corresponding fitted values are also given (in kJ mol^{-1}).

	C_6							
structure	H	C	Al	Si	O	E_{add}	RMS	max deviation
1	0.8452	7.1538	1.1972	0.9679	0.7975	-31.3671	0.9637	2.5429
2	0.6961	4.2544	1.1108	3.7348	0.7126	-24.8680	1.3311	2.7806
3	0.5322	1.5908	10.7892	9.2059	0.6713	-25.7478	1.2070	-2.2698
4	0.4963	0.8444	11.026	18.9362	0.7117	-9.3222	1.4480	3.7220
5	0.9640	2.3837	1.1514	0.8894	0.7922	-26.6209	1.2595	2.3010
6	0.4857	1.0667	10.6240	18.4515	0.6698	-7.8790	1.5979	3.6477
7	0.7909	5.0718	--	1.1226	0.8271	-5.8854	0.9631	2.2704

Table S.7: Sets of C_6 parameters (in J nm^6 mol^{-1}) for H, C, Al, Si, and O atoms as well as additive constants, E_{add} (in kJ mol^{-1}) obtained by fitting differences between MP2/TZVP(P) and PBE/QZVP cluster model apparent energy barriers. Root mean squared errors and the maximum deviation between reference data points and corresponding fitted values are also given (in kJ mol^{-1}).

	C_6							
structure	H	C	Al	Si	O	E_{add}	RMS	max deviation
1s	0.6299	0.7685	23.7305	13.0105	0.966	-57.6126	0.8992	2.1083
1s, rev	0.6299	0.7685	23.7305	13.0105	0.966	-113.7969	0.8992	2.1083
2s(1)	0.9328	23.6100	7.6409	1.4142	0.9722	-153.1613	0.6268	-1.5038
2s(1), rev	0.9328	23.6100	7.6409	1.4142	0.9722	-153.1613	0.6268	-1.5038
2s(2)	0.5151	1.4267	23.7126	10.4534	0.7634	-48.3866	1.0766	-2.7929
2s(2), rev	0.5151	1.4267	23.7127	10.4534	0.7634	-91.5433	1.0766	-2.7929

S.9 Energies at various levels of theory

This section contains tables (Tables S.8 – S.13) listing the energies of periodic structures and clusters calculated at several levels of theory.

Table S.8: Energies of gas phase molecules.

Method	Energy		
	ethene	benzene	ethylbenzene
Periodic PBE/400 eV (eV)	-31.96453	-76.00720	-109.14188
Scaled disperison (kJ/mol)	-3.152	-13.995	-30.579
DFT/def2-QZVP (Hartree)	-78.507460	-232.036470	-310.586608
MP2/TZVP(P) (Hartree)	-78.388424	-231.715018	-310.153135
MP2/cc-pVTZ (Hartree)	-78.398853	-231.728815	-310.177989
MP2/cc-pVQZ (Hartree)	-78.424772	-231.801948	-310.276883
CCSD(T)/def2-TZVP (Hartree)	-78.429292	-231.793789	-310.267168

Table S.9: Energies of periodic structures.

	UC1		UC2	
	Periodic PBE/400 eV (eV)	Scaled dispersion (kJ/mol)	Periodic PBE/400 eV (eV)	Scaled dispersion (kJ/mol)
Unloaded UC, all-Si	-2280.099070	-2123.933		
Unloaded UC, Al12-O20(H)-Si3	-2281.761284	-2135.608	-2282.475275	-2080.514
Unloaded UC, Al12-O24(H)-Si12	-2281.695671		-2282.395918	
Unloaded UC, Al12-O11(H)-Si11	-2281.767946		-2282.473311	
Adsorbed ethene, all-Si, intersection	-2312.106891	-2145.888		
Adsorbed ethene, all-Si, straight ch.	-2312.059563	-2157.501		
Adsorbed ethene, all-Si, sinusoidal ch.	-2312.107465	-2155.785		
Adsorbed ethene, H on O20	-2314.052070	-2167.911	-2314.765749	
Adsorbed benzene, H on O20	-2358.016802	-2212.577	-2358.685950	-2155.356
Adsorbed ethylbenzene, H on O20	-2391.075443	-2266.956	-2391.824365	
Coadsorbed ethene + benzene, H on O20	-2390.154365	-2250.417	-2390.886406	
Ethoxide, C bonded to O24	-2314.280760	-2172.501	-2314.893505	
Benzene adsorbed next to ethoxide	-2390.308567	-2260.117	-2390.972921	
Transition structure 1s	-2389.281015	-2264.824	-2390.012188	
Transition structure 2s(1)	-2313.102295	-2175.456	-2313.820667	
Transition structure 2s(2)	-2389.314698	-2282.850	-2390.042636	

Table S.10: Zero-point vibrational energies and finite temperature corrections from periodic PBE/400 eV.

	UC1		UC2	
	ZPVE (kJ/mol)	Finite temp. correction (kJ/mol)[a]	ZPVE (kJ/mol)	Finite temp. correction (kJ/mol)[a]
Gas phase ethene	130.262	10.533		
Gas phase benzene	256.923	14.323		
Gas phase ethylbenzene	400.619	22.126		
Unloaded UC, all-Si	2818.328	684.821		
Unloaded UC, Al12-O20(H)-Si3	2841.855	688.318	2830.529	693.150
Adsorbed ethene, all-Si, intersection	2946.626	700.079		
Adsorbed ethene, H on O20	2973.531	699.874	2963.486	704.931
		2648.430		*2656.067*
Adsorbed benzene, H on O20	3098.518	705.225	3087.543	710.574
Adsorbed ethylbenzene, H on O20	3245.245	712.761	3233.177	717.770
		2709.640		
Coadsorbed ethene + benzene, H on O20	3235.323	717.116		
		2716.917		
Ethoxide, C bonded to O24	2982.602	696.203		
		2642.282		
Benzene adsorbed next to ethoxide	3243.563	713.553		
		2711.512		
Transition structure 1s	3230.568	*2709.241*		
Transition structure 2s(1)	2971.161	*2639.814*	2959.294	*2648.394*
Transition structure 2s(2)	3238.523	*2707.712*		

[a] Finite temperature correction to 298 K and 653 K, respectively. The latter are in *italic*

Table S.11: Energies of clusters cut out from the periodic structure (UC1)

		Energies					
Cluster	Method	all-Si Si12-O20-Si3	acid site Al12-O20(H)-Si3	ethene adsorbed on H20	benzene adsorbed on H20	ethylbenzene adsorbed on H20	ethene+benzene adsorbed on H20
2T	MP2/TZVP(P) (Hartree)	-1107.685590	-1061.287304	-1139.681755	-1293.006994	-1371.438751	-1371.408166
	MP2/cc-pVTZ (Hartree)		-1061.634533	-1140.040703	-1293.369179	-1371.813094	
	MP2/cc-pVQZ (Hartree)		-1061.829817	-1140.262404	-1293.637884	-1372.107725	
	DFT/def2-QZVP (Hartree)	-1109.032383	-1062.573566	-1141.084367	-1294.608436	-1373.150404	-1373.125772
	Scaled dispersion (kJ/mol)	-20.686	-26.904	-42.361	-58.244	-82.830	-68.922
3T	MP2/TZVP(P) (Hartree)	-1623.431916	-1577.028574	-1655.427226	-1808.752476	-1887.185580	-1887.156106
	MP2/cc-pVTZ (Hartree)		-1577.527736	-1655.938181	-1809.266822	-1887.712140	
	MP2/cc-pVQZ (Hartree)		-1577.807690	-1656.244360	-1809.619847	-1888.090830	
	DFT/def2-QZVP (Hartree)	-1625.369829	-1578.908225	-1657.421688	-1810.944418	-1889.486840	-1889.464090
	Scaled dispersion (kJ/mol)	-32.626	-38.967	-57.233	-75.479	-101.920	-87.354
4T	MP2/TZVP(P) (Hartree)	-2139.165927	-2092.765603	-2171.165172	-2324.490417	-2402.927420	-2402.895175
	MP2/cc-pVTZ (Hartree)		-2093.415026	-2171.826744	-2325.155417	-2403.604502	
	MP2/cc-pVQZ (Hartree)		-2093.780037	-2172.217914	-2325.593458	-2404.067834	
	DFT/def2-QZVP (Hartree)	-2141.695696	-2095.236929	-2173.750469	-2327.272602	-2405.817271	-2405.793411
	Scaled dispersion (kJ/mol)	-45.346	-51.587	-71.880	-91.376	-119.945	-102.622
5T	MP2/TZVP(P) (Hartree)	-2654.905234	-2608.507209	-2686.907235	-2840.235910	-2918.673168	-2918.638564
	MP2/cc-pVTZ (Hartree)		-2609.307234	-2687.719281	-2841.051600	-2919.500968	
	MP2/cc-pVQZ (Hartree)		-2609.756609	-2688.194873	-2841.573727	-2920.048288	
	DFT/def2-QZVP (Hartree)	-2658.026325	-2611.569738	-2690.083182	-2843.607695	-2922.151780	-2922.126449
	Scaled dispersion (kJ/mol)	-58.103	-64.219	-85.538	-106.783	-137.753	-118.962
6T	MP2/TZVP(P) (Hartree)	-3170.651739	-3124.253296	-3202.656686	-3355.985325	-3434.424940	-3434.388345
	MP2/cc-pVTZ (Hartree)		-3125.204319	-3203.619973	-3356.952294	-3435.404387	
	MP2/cc-pVQZ (Hartree)		-3125.737410	-3204.178855	-3357.557741	-3436.034670	
	DFT/def2-QZVP (Hartree)	-3174.364067	-3127.907223	-3206.422859	-3359.946665	-3438.492284	-3438.465229
	Scaled dispersion (kJ/mol)	-70.296	-76.474	-100.066	-122.820	-155.129	-135.871
7T	MP2/TZVP(P) (Hartree)	-3686.385522	-3639.986126	-3718.390681	-3871.720705	-3950.161706	-3950.122288
	MP2/cc-pVTZ (Hartree)		-3641.087567	-3719.504448	-3872.837925	-3951.291413	
	MP2/cc-pVQZ (Hartree)		-3641.705827	-3720.148444	-3873.528486	-3952.006634	
	DFT/def2-QZVP (Hartree)	-3690.689692	-3644.232058	-3722.748676	-3876.273037	-3954.818910	-3954.789989
	Scaled dispersion (kJ/mol)	-83.215	-89.421	-113.394	-137.427	-172.301	-151.231
8T	MP2/TZVP(P) (Hartree)	-4202.126155	-4155.728626	-4234.134700	-4387.464737	-4465.904790	-4465.865729
	MP2/cc-pVTZ (Hartree)		-4156.980681	-4235.399209	-4388.732764	-4467.185493	
	MP2/cc-pVQZ (Hartree)		-4157.682778	-4236.126986	-4389.507115	-4467.984354	
	DFT/def2-QZVP (Hartree)	-4207.020876	-4160.564899	-4239.082593	-4392.606651	-4471.150455	-4471.122688
	Scaled dispersion (kJ/mol)	-98.307	-104.455	-129.433	-154.092	-192.375	-168.697
10T	MP2/TZVP(P) (Hartree)	-5157.403387	-5111.005329	-5189.411892	-5342.742658	-5421.183788	-5421.147335
	MP2/cc-pVTZ (Hartree)		-5112.468864	-5190.888008	-5344.222296	-5422.676090	
	MP2/cc-pVQZ (Hartree)		-5113.308798	-5191.753600	-5345.134443	-5423.612827	
	DFT/def2-QZVP (Hartree)	-5163.316245	-5116.859864	-5195.377811	-5348.901780	-5427.445475	-5427.419125
	Scaled dispersion (kJ/mol)	-129.745	-136.012	-161.931	-188.082	-228.766	-206.631
12T	MP2/TZVP(P) (Hartree)	-6188.87941	-6142.480404	-6220.886890	-6374.220289	-6452.662488	-6452.626721
	MP2/cc-pVTZ (Hartree)		-6144.247766	-6222.666883	-6376.003736	-6454.458381	
	MP2/cc-pVQZ (Hartree)		-6145.256817	-6223.701987	-6377.085217	-6455.564336	
	DFT/def2-QZVP (Hartree)	-6195.973084	-6149.517699	-6228.035406	-6381.560721	-6460.104631	-6460.078620
	Scaled dispersion (kJ/mol)	-163.786	-169.554	-195.862	-223.951	-265.976	-243.750
14T	MP2/TZVP(P) (Hartree)	-7144.150864	-7097.753854	-7176.171568	-7329.507941	-7407.939864	-7407.900482
	MP2/cc-pVTZ (Hartree)		-7099.733900	-7178.163208	-7331.503092	-7409.948303	
	MP2/cc-pVQZ (Hartree)		-7100.881147	-7179.335629	-7332.721536	-7411.192106	
	DFT/def2-QZVP (Hartree)	-7152.263574	-7105.810034	-7184.338042	-7337.864981	-7416.399122	-7416.370489
	Scaled dispersion (kJ/mol)	-195.468	-201.114	-226.534	-256.776	-300.600	-277.639
16T	MP2/TZVP(P) (Hartree)	-8175.630086	-8129.233091	-8207.646153	-8360.983299	-8439.421961	-8439.380588
	MP2/cc-pVTZ (Hartree)		-8131.514942	-8209.939132	-8363.279894	-8441.732379	-8441.689792
	MP2/cc-pVQZ (Hartree)		-8132.831193	-8211.280849	-8364.667544	-8443.144949	-8443.102633
	DFT/def2-QZVP (Hartree)	-8184.924481	-8138.470760	-8216.993273	-8370.520239	-8449.060483	-8449.030994
	Scaled dispersion (kJ/mol)	-225.939	-231.819	-258.602	-290.385	-335.443	-310.924
18T	MP2/TZVP(P) (Hartree)	-9130.915972	-9084.520372	-9162.930233	-9316.268484	-9394.709175	-9394.668629
	MP2/cc-pVTZ (Hartree)	-9133.448607	-9087.012748	-9165.435129	-9318.777334	-9397.230624	
	MP2/cc-pVQZ (Hartree)	-9134.904231	-9088.466827	-9166.913974	-9320.301967	-9398.781215	
	DFT/def2-QZVP (Hartree)	-9141.227775	-9094.775249	-9173.295073	-9326.821669	-9405.363678	-9405.333838
	Scaled dispersion (kJ/mol)	-256.070	-261.938	-290.153	-325.294	-369.282	-345.970
20T	MP2/TZVP(P) (Hartree)	-10086.188301	-10039.791509	-10118.197830	-10271.537627	-10349.984009	-10349.94397
	DFT/def2-QZVP (Hartree)	-10097.517503	-10051.063897	-10129.579826	-10283.106619	-10361.653531	-10361.62330
	Scaled dispersion (kJ/mol)	-290.280	-296.302	-325.708	-363.164	-407.581	-385.883
22T	MP2/TZVP(P) (Hartree)	-11041.460459	-10995.063606	-11073.465280	-11226.805804	-11305.25630	-11305.220070
	DFT/def2-QZVP (Hartree)	-11053.807003	-11007.353345	-11085.864685	-11239.391441	-11317.94233	-11317.913448
	Scaled dispersion (kJ/mol)	-324.674	-330.659	-360.688	-399.333	-443.558	-425.807
26T	MP2/TZVP(P) (Hartree)	-12875.824580	-12829.427788	-12907.828725	-13061.169641	-13139.61646	-13139.586209
	DFT/def2-QZVP (Hartree)	-12890.042889	-12843.589351	-12922.099696	-13075.626497	-13154.17218	-13154.149905
	Scaled dispersion (kJ/mol)	-392.752	-398.624	-429.017	-468.104	-516.725	-497.058
30T	MP2/TZVP(P) (Hartree)	-14786.383114	-14739.988996	-14818.390948	-14971.732337	-15050.17836	-15050.150933
	DFT/def2-QZVP (Hartree)	-14802.635305	-14756.183680	-14834.694505	-14988.221493	-15066.76579	-15066.745943
	Scaled dispersion (kJ/mol)	-461.058	-467.082	-498.311	-537.708	-587.012	-568.531

Table S.12: Energies of clusters cut out from the periodic structure (UC1).

		Energies					
		ethoxide	benzene adsorbed	ethene	transition state	transition state	transition state
Cluster	Method		next to ethoxide	in all-Si MFI	1-step	2-step(1)	2-step(2)
2T	MP2/TZVP(P) (Hartree)			-1186.073828	-1371.336318	-1139.636742	-1371.368201
	DFT/def2-QZVP (Hartree)			-1187.538856	-1373.072340	-1141.057983	-1373.093918
	Scaled dispersion (kJ/mol)			-26.738	-82.207		-87.892
3T	MP2/TZVP(P) (Hartree)	-1655.427835	-1887.149001	-1701.818856	-1887.094776	-1655.371422	-1887.108346
	DFT/def2-QZVP (Hartree)	-1657.419597	-1889.454154	-1703.874627	-1889.418058	-1657.382970	-1889.422070
	Scaled dispersion (kJ/mol)	-64.272	-96.643	-40.124	-103.011	-66.917	-110.243
4T	MP2/TZVP(P) (Hartree)	-2171.176392	-2402.898247	-2217.553430	-2402.834360	-2171.111278	-2402.846818
	DFT/def2-QZVP (Hartree)	-2173.758424	-2405.793154	-2220.200825	-2405.747886	-2173.713796	-2405.750606
	Scaled dispersion (kJ/mol)	-77.838	-111.543	-53.565	-119.153	-80.646	-126.752
5T	MP2/TZVP(P) (Hartree)	-2686.905782	-2918.628548	-2733.294779	-2918.580672	-2686.860773	-2918.598451
	DFT/def2-QZVP (Hartree)	-2690.079466	-2922.114363	-2736.532826	-2922.082562	-2690.052890	-2922.090835
	Scaled dispersion (kJ/mol)	-92.665	-128.905	-67.308	-136.457	-94.44943126	-143.359
6T	MP2/TZVP(P) (Hartree)	-3202.649892	-3434.377081	-3249.042643	-3434.332601	-3202.607991	-3434.349056
	DFT/def2-QZVP (Hartree)	-3206.414721	-3438.451785	-3252.871384	-3438.422789	-3206.390959	-3438.429296
	Scaled dispersion (kJ/mol)	-106.119	-146.451	-80.778	-154.629	-107.674	-163.172
7T	MP2/TZVP(P) (Hartree)	-3718.395414	-3950.123353	-3764.777199	-3950.068053	-3718.341539	-3950.084916
	DFT/def2-QZVP (Hartree)	-3722.750825	-3954.788043	-3769.197502	-3954.748822	-3722.716100	-3954.755803
	Scaled dispersion (kJ/mol)	-119.799	-161.539	-94.470	-169.952	-121.415	-178.413
8T	MP2/TZVP(P) (Hartree)	-4234.132963	-4465.860681	-4280.518887	-4465.813137	-4234.085025	-4465.831841
	DFT/def2-QZVP (Hartree)	-4239.079353	-4471.115622	-4285.529480	-4471.082633	-4239.049575	-4471.090906
	Scaled dispersion (kJ/mol)	-135.544	-179.076	-110.109	-187.363	-136.834	-197.049
10T	MP2/TZVP(P) (Hartree)	-5189.407186	-5421.137922	-5235.797633	-5421.091652	-5189.362805	-5421.112552
	MP2/cc-pVTZ (Hartree)	-5190.883281	-5422.631255				
	MP2/cc-pVQZ (Hartree)	-5191.749789	-5423.567827				
	DFT/def2-QZVP (Hartree)	-5195.371050	-5427.407886	-5241.825573	-5427.377600	-5195.345239	-5427.387490
	Scaled dispersion (kJ/mol)	-169.081	-217.236	-143.277	-223.534	-169.047	-233.891
12T	MP2/TZVP(P) (Hartree)	-6220.877743	-6452.608903	-6267.275050	-6452.570070	-6220.842211	-6452.594219
	MP2/cc-pVTZ (Hartree)	-6222.657891	-6454.405526				
	MP2/cc-pVQZ (Hartree)	-6223.693770	-6455.511660				
	DFT/def2-QZVP (Hartree)	-6228.024937	-6460.059690	-6274.483463	-6460.037068	-6228.006855	-6460.050394
	Scaled dispersion (kJ/mol)	-202.269	-254.093	-177.341	-260.156	-203.461	-270.887
14T	MP2/TZVP(P) (Hartree)	-7176.166506	-7407.898558	-7222.555298	-7407.842961	-7176.115916	-7407.869336
	MP2/cc-pVTZ (Hartree)	-7178.158018	-7409.906566				
	MP2/cc-pVQZ (Hartree)	-7179.330699	-7411.149584				
	DFT/def2-QZVP (Hartree)	-7184.331458	-7416.365414	-7230.782105	-7416.328296	-7184.299354	-7416.343361
	Scaled dispersion (kJ/mol)	-232.170	-287.889	-208.240	-293.657	-235.613	-304.997
16T	MP2/TZVP(P) (Hartree)	-8207.639525	-8439.375989	-8254.029818	-8439.325175	-8207.595178	-8439.353502
	MP2/cc-pVTZ (Hartree)	-8209.932399	-8441.685312		-8441.633102		-8441.661241
	MP2/cc-pVQZ (Hartree)	-8211.274369	-8443.097527		-8443.047707		-8443.074365
	DFT/def2-QZVP (Hartree)	-8216.985503	-8449.022236	-8263.437332	-8448.990857	-8216.959786	-8449.006123
	Scaled dispersion (kJ/mol)	-263.903	-322.248	-240.064	-326.822	-266.608	-340.629
18T	MP2/TZVP(P) (Hartree)	-9162.924313	-9394.659008	-9209.314355	-9394.616614	-9162.883968	-9394.645725
	MP2/cc-pVTZ (Hartree)	-9165.429114	-9397.181092	-9211.858868		-9165.387768	
	MP2/cc-pVQZ (Hartree)	-9166.908189	-9398.730434	-9213.338043		-9166.869203	
	DFT/def2-QZVP (Hartree)	-9173.288082	-9405.320374	-9219.739142	-9405.296236	-9173.265533	-9405.310120
	Scaled dispersion (kJ/mol)	-294.951	-359.883	-272.395	-363.304	-296.916	-382.482
20T	MP2/TZVP(P) (Hartree)	-10118.192433	-10349.930116	-10164.582617	-10349.890369	-10118.15552	-10349.921908
	DFT/def2-QZVP (Hartree)	-10129.573653	-10361.605732	-10176.024202	-10361.585219	-10129.55424	-10361.599976
	Scaled dispersion (kJ/mol)	-329.666	-399.649	-308.300	-402.292	-331.868	-423.073
22T	MP2/TZVP(P) (Hartree)	-11073.460064	-11305.200969	-11119.850642	-11305.167898	-11073.429003	-11305.198702
	DFT/def2-QZVP (Hartree)	-11085.858894	-11317.890799	-11132.308984	-11317.876802	-11085.844856	-11317.891795
	Scaled dispersion (kJ/mol)	-364.539	-439.957	-344.530	-442.803	-366.427	-462.090
26T	MP2/TZVP(P) (Hartree)	-12907.810243	-13139.552250	-12954.214680	-13139.53623	-12907.793242	-13139.564470
	DFT/def2-QZVP (Hartree)	-12922.079885	-13154.112405	-12968.544540	-13154.11499	-12922.080448	-13154.128286
	Scaled dispersion (kJ/mol)	-436.020	-512.440	-413.052	-513.856	-435.988	-532.364
30T	MP2/TZVP(P) (Hartree)	-14818.373972	-15050.117891	-14864.774579	-15050.100845	-14818.354123	-15050.125380
	DFT/def2-QZVP (Hartree)	-14834.675504	-15066.708530	-14881.137872	-15066.711081	-14834.674241	-15066.722212
	Scaled dispersion (kJ/mol)	-506.469	-584.931	-482.224	-584.340	-505.204	-601.789

Table S.13: CCSD(T) energies for 3T clusters cut out from the periodic structure (UC1).

	CCSD(T)/ def2-TZVP (Hartree)
Unloaded UC, all-Si	-1172.767934
Unloaded UC, Al12-O20(H)-Si3	-1126.300666
Adsorbed ethene, all-Si, intersection	-1251.196404
Adsorbed ethene, H on O20	-1204.740310
Adsorbed benzene, H on O20	-1358.105209
Adsorbed ethylbenzene, H on O20	-1436.583084
Coadsorbed ethene + benzene, H on O20	-1436.544131
Ethoxide, C bonded to O24	-1204.757089
Benzene adsorbed next to ethoxide	-1436.558731
Transition structure 1s	-1436.474423
Transition structure 2s(1)	-1204.686074
Transition structure 2s(2)	-1436.493590

S.10 Complete reference 55

(55) MOLPRO – a package of ab initio programs (version 2006.1). Werner, H.-J.; Knowles, P. J.; Lindh, R.; Manby, F. R.; Schütz, M.; Celani, P.; Korona, T.; Rauhut, G.; Amos, R. D.; Bernhardsson, A.; Berning, A.; Cooper, D. L.; Deegan, M. J. O.; Dobbyn, A. J.; Eckert, F.; Hampel, C.; Hetzer, G.; Lloyd, A. W.; McNicholas, S. J.; Meyer, W.; Mura, M. E.; Nicklass, A.; Palmieri, P.; Pitzer, R.; Schumann, U.; Stoll, H.; Stone, A. J.; Tarroni, R.; Thorsteinsson, T.; Cardiff, UK, 2006.

S.11 Complete reference 82

(82) Sherwood, P.; de Vries, A. H.; Guest, M. F.; Schreckenbach, G.; Catlow, C. R. A.; French, S. A.; Sokol, A. A.; Bromley, S. T.; Thiel, W.; Turner, A. J.; Billeter, S.; Terstegen, F.; Thiel, S.; Kendrick, J.; Rogers, S. C.; Casci, J.; Watson, M.; King, F.; Karlsen, E.; Sjøvoll, M.; Fahmi, A.; Schäfer, A.; Lennartz, C. *J. Mol. Struct. (Theochem)* **2003**, *632*, 1-28.

S.12 Coordinates of stationary points

This section lists the Cartesian coordinates of all UC1 structures optimized with periodic DFT (PBE/400 eV). The cell parameters of the orthorhombic MFI unit cell are a = 20.022 Å, b = 19.899 Å, c = 13.383 Å.

S.12.1 All silica unit cell

Si	8.532	1.150	1.924
Si	1.565	18.836	8.616
Si	11.576	11.100	11.456
Si	18.542	8.886	4.765
Si	11.576	18.842	11.469
Si	18.543	1.145	4.778
Si	8.532	8.892	1.912
Si	1.565	11.094	8.604
Si	6.100	0.592	3.841
Si	3.996	19.395	10.533
Si	14.007	10.541	9.540
Si	16.112	9.445	2.848
Si	14.008	19.394	9.549
Si	16.111	0.592	2.858
Si	6.100	9.445	3.832
Si	3.996	10.542	10.523
Si	5.686	1.339	6.796
Si	4.411	18.648	0.104
Si	14.422	11.288	6.585
Si	15.697	8.699	13.277
Si	14.423	18.640	6.598
Si	15.696	1.346	13.290
Si	5.685	8.691	6.783
Si	4.412	11.296	0.092
Si	2.483	1.374	6.807
Si	7.613	18.612	0.116
Si	17.624	11.324	6.574
Si	12.495	8.663	13.265
Si	17.626	18.605	6.586
Si	12.493	1.381	13.278
Si	2.482	8.655	6.795
Si	7.615	11.331	0.103
Si	1.436	0.628	3.988
Si	8.661	19.358	10.680
Si	18.672	10.578	9.393
Si	11.447	9.408	2.702
Si	18.673	19.359	9.403
Si	11.446	0.627	2.712
Si	1.435	9.410	3.978
Si	8.662	10.577	10.670
Si	3.600	1.112	1.966
Si	6.496	18.875	8.657
Si	16.507	11.062	11.416
Si	13.612	8.925	4.724
Si	16.507	18.881	11.428
Si	13.611	1.105	4.737
Si	3.601	8.932	1.954
Si	6.496	11.055	8.644
Si	8.464	16.508	2.200
Si	1.632	3.478	8.891
Si	11.644	6.559	11.181

Si	18.476	13.427	4.490
Si	11.643	3.477	11.191
Si	18.476	16.509	4.499
Si	8.465	13.427	2.191
Si	1.632	6.559	8.883
Si	6.079	17.351	4.066
Si	4.017	2.636	10.758
Si	14.028	7.401	9.315
Si	16.091	12.585	2.624
Si	14.029	2.634	9.323
Si	16.089	17.353	2.632
Si	6.078	12.583	4.058
Si	4.018	7.403	10.749
Si	5.398	16.519	7.001
Si	4.698	3.468	0.310
Si	14.709	6.569	6.380
Si	15.409	13.418	13.071
Si	14.708	3.466	6.389
Si	15.410	16.521	13.080
Si	5.399	13.416	6.993
Si	4.698	6.571	0.301
Si	2.298	16.492	6.854
Si	7.798	3.494	0.162
Si	17.809	6.543	6.528
Si	12.309	13.444	13.219
Si	17.808	3.491	6.537
Si	12.310	16.495	13.228
Si	2.300	13.441	6.844
Si	7.797	6.546	0.153
Si	1.325	17.388	4.006
Si	8.771	2.599	10.697
Si	18.783	7.438	9.375
Si	11.336	12.548	2.684
Si	18.782	2.600	9.384
Si	11.336	17.386	2.692
Si	1.325	12.549	3.997
Si	8.772	7.437	10.689
Si	3.634	16.546	2.236
Si	6.462	3.440	8.927
Si	16.474	6.597	11.145
Si	16.473	3.440	11.154
Si	13.645	16.546	4.462
Si	3.635	13.390	2.227
Si	6.462	6.597	8.919
Si	13.645	13.390	4.454
O	7.236	1.242	2.890
O	2.860	18.745	9.582
O	12.871	11.192	10.490
O	17.247	8.795	3.799
O	12.871	18.749	10.502
O	17.248	1.238	3.811
O	7.236	8.800	2.878
O	2.860	11.187	9.570
O	6.062	1.438	5.224
O	4.035	18.549	11.915
O	14.046	11.387	8.157
O	16.073	8.599	1.465
O	14.048	18.542	8.170
O	16.071	1.444	1.479
O	6.061	8.592	5.211
O	4.037	11.394	11.903
O	4.082	1.169	7.007
O	6.015	18.817	0.317
O	16.026	11.119	6.373
O	14.093	8.869	13.065
O	16.028	18.807	6.385
O	14.091	1.177	13.077
O	4.080	8.859	6.995
O	6.017	11.127	0.304
O	2.099	1.436	5.235

O	7.997	18.550	11.927
O	18.008	11.386	8.146
O	12.110	8.601	1.454
O	18.009	18.547	8.159
O	12.110	1.439	1.468
O	2.098	8.597	5.222
O	7.999	11.389	11.913
O	2.104	1.121	2.594
O	7.993	18.866	9.286
O	18.004	11.070	10.787
O	12.115	8.916	4.095
O	18.004	18.875	10.799
O	12.115	1.111	4.108
O	2.104	8.925	2.582
O	7.993	11.060	9.273
O	4.649	0.678	3.127
O	5.448	19.309	9.818
O	15.459	10.627	10.254
O	14.660	9.359	3.562
O	15.458	19.311	10.266
O	14.660	0.675	3.574
O	4.649	9.362	3.116
O	5.447	10.625	9.807
O	7.195	16.566	3.200
O	2.902	3.420	9.891
O	12.913	6.617	10.181
O	17.206	13.369	3.490
O	12.914	3.412	10.194
O	17.204	16.574	3.503
O	7.194	13.362	3.187
O	2.903	6.624	9.879
O	6.097	16.718	5.553
O	3.999	3.269	12.245
O	14.010	6.769	7.827
O	16.108	13.218	1.136
O	14.012	3.275	7.840
O	16.106	16.711	1.148
O	6.095	13.225	5.542
O	4.001	6.763	12.234
O	3.845	17.006	6.919
O	6.252	2.981	0.228
O	16.263	7.056	6.462
O	13.856	12.930	13.153
O	16.262	2.977	6.471
O	13.857	17.009	13.163
O	3.846	12.927	6.910
O	6.251	7.059	0.218
O	1.773	16.549	5.322
O	8.322	3.437	12.013
O	18.334	6.600	8.060
O	11.785	13.386	1.368
O	18.329	3.442	8.071
O	11.788	16.545	1.379
O	1.778	13.391	5.310
O	8.319	6.595	12.002
O	2.091	16.792	2.698
O	8.006	3.194	9.389
O	18.017	6.843	10.683
O	12.102	13.144	3.991
O	18.017	3.189	10.694
O	12.102	16.796	4.002
O	2.091	13.139	2.687
O	8.006	6.848	9.379
O	4.611	17.151	3.393
O	5.486	2.836	10.085
O	15.497	7.201	9.987
O	14.622	12.785	3.297
O	15.497	2.829	9.999
O	14.621	17.157	3.307
O	4.610	12.779	3.383

O	5.487	7.207	10.075
O	6.446	18.931	4.138
O	3.650	1.056	10.830
O	13.661	8.981	9.243
O	16.458	11.005	2.551
O	13.664	1.054	9.242
O	16.455	18.933	2.551
O	6.444	11.003	4.140
O	3.652	8.983	10.830
O	1.720	18.945	4.220
O	8.376	1.042	10.912
O	18.388	8.995	9.161
O	11.731	10.991	2.470
O	18.391	1.042	9.163
O	11.727	18.944	2.471
O	1.716	10.992	4.218
O	8.381	8.994	10.910
O	8.706	2.551	1.119
O	1.391	17.435	7.811
O	11.402	12.501	12.262
O	18.716	7.486	5.570
O	11.401	17.443	12.278
O	18.717	2.543	5.587
O	8.706	7.494	1.103
O	1.390	12.492	7.794
O	8.386	19.845	0.840
O	1.711	0.141	7.531
O	11.722	9.896	12.541
O	18.397	10.091	5.850
O	11.721	0.149	12.551
O	18.397	19.837	5.859
O	8.387	10.099	0.830
O	1.711	9.888	7.522
O	8.092	17.213	0.784
O	2.005	2.772	7.476
O	12.016	7.264	12.597
O	18.103	12.722	5.905
O	12.012	2.779	12.611
O	18.108	17.206	5.920
O	8.096	12.729	0.770
O	2.001	7.257	7.462
O	3.919	2.606	1.433
O	6.177	17.381	8.124
O	16.189	12.556	11.948
O	13.931	7.431	5.256
O	16.192	17.388	11.964
O	13.926	2.599	5.272
O	3.916	7.438	1.419
O	6.182	12.549	8.110
O	3.666	0.049	0.737
O	6.431	0.039	7.428
O	16.442	9.999	12.644
O	13.677	9.988	5.952
O	16.440	0.047	12.656
O	13.679	0.041	5.964
O	3.668	9.996	0.726
O	6.429	9.991	7.417
O	3.904	17.281	0.815
O	6.191	2.706	7.506
O	16.203	7.331	12.566
O	13.915	12.655	5.875
O	16.201	2.714	12.579
O	13.916	17.273	5.888
O	3.906	12.663	0.802
O	6.191	7.323	7.494
O	19.865	0.913	3.872
O	10.253	19.074	10.563
O	0.242	10.862	9.509
O	9.854	9.124	2.818
O	0.242	19.071	9.521

O	9.854	0.915	2.830
O	19.865	9.122	3.860
O	10.254	10.864	10.551
O	19.741	17.247	3.784
O	10.377	2.740	10.476
O	0.366	7.297	9.597
O	9.731	12.689	2.906
O	0.365	2.743	9.606
O	9.731	17.244	2.915
O	19.743	12.692	3.775
O	10.377	7.294	10.467
O	8.841	14.969	1.884
O	1.256	5.018	8.575
O	11.267	5.019	11.498
O	18.853	14.967	4.806
O	3.920	14.969	2.028
O	6.177	5.018	8.720
O	16.188	5.019	11.353
O	13.931	14.967	4.661
O	5.489	14.966	7.447
O	4.607	5.021	0.755
O	14.618	5.016	5.935
O	15.500	14.971	12.626
O	2.182	14.965	7.386
O	7.915	5.022	0.694
O	17.926	5.015	5.995
O	12.193	14.971	12.687

S.12.2 Unit cell with Al12-O20(H)-Si3

Si	8.555	1.135	1.963
Si	1.597	18.826	8.644
Si	11.599	11.050	11.575
Si	18.585	8.866	4.865
Si	11.598	18.816	11.503
Si	18.580	1.155	4.825
Si	8.552	8.874	1.981
Si	1.593	11.090	8.653
Si	6.117	0.578	3.872
Si	4.030	19.376	10.566
Si	14.052	10.466	9.703
Si	16.186	9.402	2.938
Si	14.044	19.421	9.611
Si	16.161	0.592	2.904
Si	6.115	9.438	3.876
Si	4.021	10.531	10.570
Si	5.714	1.340	6.828
Si	4.438	18.624	0.133
Si	14.487	11.252	6.761
Si	15.735	8.660	0.003
Si	14.455	18.733	6.641
Si	15.731	1.276	13.334
Si	5.705	8.700	6.852
Si	4.411	11.247	0.140
Si	2.513	1.370	6.839
Si	7.639	18.598	0.147
Si	17.681	11.335	6.663
Si	12.537	8.611	13.359
Si	17.656	18.611	6.613
Si	12.536	1.327	13.315
Si	2.507	8.642	6.870
Si	7.600	11.294	0.162
Si	1.467	0.615	4.021
Si	8.686	19.353	10.711

Si	18.713	10.565	9.485
Si	11.465	9.387	2.748
Si	18.698	19.326	9.435
Si	11.468	0.629	2.736
Si	1.477	9.387	4.052
Si	8.700	10.545	10.741
Si	3.620	1.090	1.984
Si	6.527	18.869	8.683
Si	16.558	11.014	11.542
Si	13.644	8.980	4.791
Si	16.544	18.837	11.476
Si	13.653	1.155	4.752
Si	3.606	8.905	2.003
Si	6.537	11.056	8.722
Si	8.486	16.490	2.214
Si	1.643	3.454	8.918
Si	11.674	6.514	11.275
Si	18.522	13.413	4.560
Si	11.685	3.454	11.215
Si	18.494	16.495	4.525
Si	8.422	13.413	2.210
Si	1.658	6.535	8.943
Si	6.104	17.335	4.094
Si	4.046	2.618	10.779
Si	14.067	7.346	9.422
Si	16.146	12.496	2.719
Si	14.045	2.667	9.326
Si	16.113	17.361	2.681
Si	6.095	12.579	4.118
Si	4.053	7.387	10.786
Si	5.436	16.507	7.026
Si	4.716	3.454	0.331
Si	14.747	6.593	6.471
Si	15.434	13.375	13.179
Si	14.724	3.493	6.378
Si	15.435	16.492	13.123
Si	5.444	13.400	7.071
Si	4.712	6.555	0.344
Si	2.334	16.480	6.879
Si	7.817	3.482	0.201
Si	17.844	6.543	6.633
Si	12.323	13.417	13.321
Si	17.823	3.491	6.580
Si	12.329	16.461	13.248
Si	2.350	13.428	6.903
Si	7.810	6.529	0.203
Si	1.346	17.370	4.034
Si	8.798	2.592	10.739
Si	18.820	7.422	9.474
Si	11.289	12.504	2.742
Si	18.792	2.566	9.423
Si	11.356	17.391	2.705
Si	1.385	12.526	4.058
Si	8.806	7.405	10.750
Si	3.659	16.526	2.269
Si	6.499	3.435	8.953
Si	16.521	6.569	11.252
Si	16.491	3.416	11.189
Si	13.661	16.604	4.519
Si	3.664	13.369	2.281
Si	6.506	6.590	8.963
Al	13.606	13.426	4.443
O	7.259	1.225	2.928
O	2.890	18.737	9.614
O	12.916	11.139	10.627
O	17.293	8.714	3.902
O	12.898	18.755	10.539
O	17.283	1.255	3.863
O	7.259	8.762	2.951
O	2.902	11.181	9.598

O	6.066	1.430	5.251
O	4.068	18.520	11.943
O	14.112	11.339	8.322
O	16.091	8.528	1.575
O	14.101	18.601	8.216
O	16.131	1.429	1.513
O	6.048	8.618	5.273
O	4.013	11.370	11.958
O	4.111	1.189	7.067
O	6.041	18.809	0.349
O	16.064	11.156	6.476
O	14.133	8.848	13.147
O	16.063	18.842	6.413
O	14.129	1.052	13.158
O	4.102	8.844	7.102
O	6.009	10.996	0.313
O	2.155	1.415	5.260
O	8.019	18.547	11.956
O	18.035	11.374	8.241
O	12.163	8.531	1.549
O	18.037	18.520	8.186
O	12.121	1.456	1.494
O	2.156	8.580	5.290
O	8.033	11.350	11.984
O	2.127	1.098	2.620
O	8.023	18.863	9.313
O	18.043	11.042	10.885
O	12.156	8.967	4.160
O	18.033	18.824	10.828
O	12.154	1.093	4.133
O	2.119	8.878	2.654
O	8.038	11.033	9.342
O	4.672	0.664	3.144
O	5.479	19.292	9.848
O	15.509	10.531	10.392
O	14.734	9.366	3.663
O	15.488	19.323	10.340
O	14.701	0.680	3.604
O	4.672	9.351	3.144
O	5.489	10.635	9.891
O	7.216	16.567	3.213
O	2.918	3.379	9.908
O	12.945	6.565	10.275
O	17.277	13.317	3.546
O	12.915	3.463	10.164
O	17.225	16.542	3.525
O	7.183	13.400	3.254
O	2.946	6.591	9.918
O	6.136	16.690	5.577
O	4.028	3.271	12.258
O	14.064	6.722	7.934
O	16.140	13.148	1.230
O	14.015	3.246	7.815
O	16.116	16.746	1.185
O	6.127	13.172	5.621
O	4.023	6.762	12.276
O	3.881	16.992	6.937
O	6.270	2.969	0.256
O	16.302	7.077	6.550
O	13.873	12.912	13.253
O	16.274	2.996	6.468
O	13.877	16.965	13.167
O	3.890	12.906	7.019
O	6.265	7.042	0.269
O	1.801	16.531	5.349
O	8.347	3.432	12.052
O	18.340	6.573	8.176
O	11.792	13.394	1.464
O	18.316	3.412	8.121
O	11.813	16.545	1.397

O	1.876	13.371	5.355
O	8.329	6.560	12.050
O	2.116	16.781	2.726
O	8.039	3.193	9.430
O	18.060	6.848	10.794
O	11.972	13.028	4.094
O	18.034	3.146	10.741
O	12.120	16.838	4.024
O	2.116	13.109	2.724
O	8.051	6.827	9.428
O	4.632	17.131	3.430
O	5.509	2.824	10.096
O	15.534	7.163	10.096
O	14.721	12.591	3.443
O	15.513	2.910	9.986
O	14.646	17.208	3.356
O	4.615	12.781	3.469
O	5.526	7.190	10.122
O	6.457	18.919	4.181
O	3.693	1.036	10.877
O	13.691	8.929	9.340
O	16.612	10.931	2.609
O	13.695	1.082	9.331
O	16.526	18.934	2.623
O	6.475	10.999	4.146
O	3.678	8.967	10.845
O	1.732	18.929	4.253
O	8.397	1.036	10.946
O	18.437	8.983	9.243
O	11.694	10.955	2.423
O	18.403	1.008	9.205
O	11.731	18.951	2.461
O	1.778	10.968	4.274
O	8.418	8.962	10.972
O	8.723	2.532	1.150
O	1.429	17.427	7.835
O	11.423	12.447	12.377
O	18.781	7.496	5.715
O	11.428	17.396	12.274
O	18.749	2.556	5.634
O	8.717	7.495	1.135
O	1.414	12.484	7.835
O	8.415	19.821	0.886
O	1.744	0.135	7.564
O	11.735	9.829	12.638
O	18.408	10.094	5.922
O	11.732	0.101	12.613
O	18.445	19.846	5.907
O	8.412	10.117	0.938
O	1.716	9.874	7.579
O	8.113	17.189	0.794
O	2.004	2.767	7.491
O	12.070	7.212	12.687
O	18.146	12.734	5.997
O	12.131	2.720	12.592
O	18.119	17.214	5.933
O	7.959	12.739	0.803
O	2.009	7.244	7.524
O	3.930	2.581	1.440
O	6.215	17.378	8.141
O	16.196	12.507	12.039
O	13.946	7.524	5.420
O	16.212	17.335	11.979
O	13.951	2.681	5.212
O	3.928	7.414	1.465
O	6.241	12.559	8.200
O	3.681	0.020	0.761
O	6.456	0.038	7.459
O	16.508	9.959	12.777
O	13.673	10.119	5.973

O	16.505	19.879	12.726
O	13.760	0.183	6.052
O	3.628	9.972	0.777
O	6.443	10.005	7.484
O	3.939	17.256	0.847
O	6.245	2.705	7.527
O	16.237	7.296	12.671
O	13.928	12.752	6.185
O	16.176	2.636	12.573
O	13.877	17.415	5.913
O	3.973	12.627	0.871
O	6.244	7.336	7.546
O	19.901	0.926	3.918
O	10.278	19.066	10.597
O	0.280	10.870	9.581
O	9.883	9.052	2.887
O	0.271	19.052	9.547
O	9.878	0.922	2.873
O	19.903	9.112	3.962
O	10.296	10.829	10.636
O	19.764	17.224	3.809
O	10.406	2.717	10.526
O	0.403	7.272	9.680
O	9.664	12.597	2.858
O	0.376	2.715	9.629
O	9.751	17.230	2.922
O	19.800	12.667	3.883
O	10.415	7.260	10.557
O	8.847	14.944	1.905
O	1.268	5.000	8.626
O	11.288	4.977	11.589
O	18.880	14.960	4.863
O	3.938	14.947	2.064
O	6.214	5.014	8.747
O	16.256	4.992	11.465
O	13.955	15.060	4.806
O	5.529	14.959	7.489
O	4.618	5.003	0.788
O	14.647	5.060	5.968
O	15.548	14.926	12.726
O	2.219	14.957	7.426
O	7.932	5.006	0.749
O	17.955	5.027	6.073
O	12.201	14.927	12.736
H	13.864	13.457	6.858

S.12.3 Unit cell with Al12-O24(H)-Si12

Si	8.559	1.151	2.008
Si	1.597	18.800	8.693
Si	11.613	11.107	11.482
Si	18.575	8.848	4.764
Si	11.604	18.856	11.567
Si	18.568	1.102	4.884
Si	8.549	8.909	1.924
Si	1.614	11.058	8.611
Si	6.124	0.572	3.912
Si	4.023	19.372	10.607
Si	14.014	10.456	9.593
Si	16.160	9.491	2.868
Si	14.071	19.420	9.680
Si	16.105	0.563	2.959
Si	6.118	9.433	3.853
Si	4.041	10.538	10.545

Si	5.720	1.303	6.882
Si	4.430	18.652	0.190
Si	14.477	11.170	6.643
Si	15.732	8.809	13.281
Si	14.471	18.702	6.732
Si	15.732	1.359	0.019
Si	5.694	8.645	6.800
Si	4.425	11.297	0.094
Si	2.515	1.352	6.900
Si	7.631	18.617	0.201
Si	17.644	11.241	6.576
Si	12.538	8.696	13.270
Si	17.667	18.574	6.698
Si	12.535	1.366	0.014
Si	2.487	8.602	6.806
Si	7.626	11.334	0.086
Si	1.463	0.614	4.081
Si	8.684	19.354	10.769
Si	18.739	10.615	9.385
Si	11.466	9.381	2.689
Si	18.702	19.349	9.508
Si	11.474	0.604	2.827
Si	1.453	9.383	3.995
Si	8.727	10.547	10.675
Si	3.616	1.113	2.047
Si	6.531	18.838	8.744
Si	16.516	11.089	11.348
Si	13.650	8.899	4.691
Si	16.570	18.891	11.573
Si	13.624	1.131	4.858
Si	3.621	8.936	1.961
Si	6.540	11.016	8.669
Si	8.468	16.474	2.267
Si	1.653	3.466	8.980
Si	11.699	6.514	11.195
Si	18.459	13.405	4.467
Si	11.666	3.460	11.325
Si	18.507	16.473	4.628
Si	8.441	13.396	2.170
Si	1.641	6.552	8.913
Si	6.099	17.324	4.139
Si	4.048	2.618	10.823
Si	14.011	7.330	9.324
Si	16.182	12.640	2.524
Si	14.068	2.664	9.430
Si	16.102	17.303	2.732
Si	6.085	12.567	4.081
Si	4.052	7.398	10.765
Si	5.446	16.493	7.087
Si	4.714	3.458	0.390
Si	14.746	6.591	6.372
Si	15.431	13.387	13.013
Si	14.721	3.483	6.491
Si	15.443	16.494	13.181
Si	5.458	13.389	7.022
Si	4.709	6.561	0.313
Si	2.348	16.460	6.938
Si	7.815	3.498	0.261
Si	17.840	6.532	6.551
Si	12.326	13.440	13.255
Si	17.811	3.469	6.636
Si	12.351	16.490	13.299
Si	2.360	13.410	6.870
Si	7.811	6.544	0.171
Si	1.358	17.367	4.097
Si	8.789	2.590	10.798
Si	18.810	7.475	9.390
Si	11.299	12.510	2.689
Si	18.805	2.592	9.484
Si	11.339	17.353	2.763

Si	1.364	12.521	4.043
Si	8.812	7.402	10.716
Si	3.648	16.527	2.313
Si	6.504	3.422	8.998
Si	16.487	6.622	11.169
Si	16.516	3.470	11.273
Si	13.622	16.623	4.600
Si	3.645	13.365	2.262
Si	6.497	6.578	8.939
Al	13.665	13.239	4.423
O	7.268	1.235	2.980
O	2.888	18.708	9.665
O	12.955	11.178	10.580
O	17.258	8.782	3.826
O	12.900	18.792	10.597
O	17.270	1.140	3.918
O	7.257	8.800	2.895
O	2.933	11.154	9.541
O	6.084	1.395	5.308
O	4.053	18.547	12.002
O	13.989	11.252	8.190
O	16.154	8.689	1.456
O	14.138	18.553	8.304
O	16.077	1.451	1.602
O	6.071	8.568	5.226
O	4.016	11.412	11.912
O	4.114	1.161	7.107
O	6.034	18.834	0.398
O	16.076	10.838	6.575
O	14.125	9.008	13.123
O	16.067	18.779	6.452
O	14.131	1.162	13.170
O	4.088	8.784	7.012
O	6.029	11.090	0.252
O	2.137	1.417	5.325
O	8.021	18.543	12.013
O	18.176	11.439	8.099
O	12.107	8.549	1.442
O	18.000	18.536	8.281
O	12.180	1.399	1.596
O	2.109	8.552	5.232
O	8.054	11.368	11.907
O	2.123	1.110	2.685
O	8.029	18.852	9.372
O	18.024	11.141	10.744
O	12.152	8.878	4.071
O	18.055	18.874	10.918
O	12.125	1.081	4.238
O	2.129	8.926	2.594
O	8.048	10.989	9.268
O	4.673	0.678	3.200
O	5.479	19.268	9.904
O	15.518	10.505	10.205
O	14.684	9.391	3.536
O	15.501	19.314	10.426
O	14.668	0.670	3.703
O	4.673	9.356	3.123
O	5.510	10.634	9.866
O	7.208	16.525	3.278
O	2.927	3.417	9.976
O	12.907	6.449	10.117
O	17.343	13.476	3.304
O	12.930	3.376	10.322
O	17.227	16.604	3.645
O	7.168	13.340	3.167
O	2.931	6.645	9.881
O	6.135	16.727	5.640
O	4.038	3.220	12.322
O	13.994	6.862	7.779
O	16.295	13.054	0.955

O	14.024	3.318	7.949
O	16.113	16.610	1.276
O	6.132	13.232	5.556
O	4.023	6.727	12.237
O	3.891	16.980	7.026
O	6.272	2.978	0.349
O	16.301	7.060	6.493
O	13.877	12.939	13.224
O	16.262	2.955	6.580
O	13.898	17.012	13.258
O	3.905	12.897	6.955
O	6.262	7.044	0.227
O	1.839	16.533	5.402
O	8.321	3.422	12.108
O	18.384	6.628	8.073
O	11.730	13.366	1.368
O	18.340	3.426	8.169
O	11.820	16.541	1.450
O	1.869	13.384	5.325
O	8.329	6.555	12.017
O	2.105	16.785	2.773
O	8.045	3.192	9.481
O	18.021	6.892	10.689
O	12.009	13.112	3.995
O	18.049	3.178	10.801
O	12.103	16.729	4.077
O	2.099	13.087	2.702
O	8.039	6.841	9.397
O	4.625	17.105	3.485
O	5.515	2.827	10.150
O	15.487	7.078	9.964
O	14.732	13.009	3.100
O	15.528	2.900	10.105
O	14.639	17.046	3.427
O	4.603	12.752	3.431
O	5.518	7.200	10.086
O	6.467	18.905	4.174
O	3.676	1.038	10.869
O	13.595	8.895	9.419
O	16.542	11.052	2.667
O	13.761	1.072	9.325
O	16.371	18.897	2.603
O	6.453	10.989	4.184
O	3.709	8.981	10.874
O	1.738	18.928	4.306
O	8.383	1.034	10.996
O	18.427	9.034	9.163
O	11.740	10.959	2.436
O	18.419	1.031	9.265
O	11.749	18.912	2.616
O	1.736	10.960	4.274
O	8.464	8.967	10.951
O	8.732	2.561	1.219
O	1.427	17.395	7.893
O	11.437	12.527	12.248
O	18.743	7.432	5.549
O	11.444	17.446	12.354
O	18.707	2.504	5.689
O	8.715	7.527	1.085
O	1.433	12.445	7.784
O	8.412	19.851	0.917
O	1.749	0.105	7.608
O	11.702	9.909	12.582
O	18.487	10.049	5.860
O	11.749	0.142	12.672
O	18.456	19.792	5.969
O	8.404	10.141	0.871
O	1.727	9.835	7.544
O	8.099	17.218	0.872
O	2.021	2.743	7.571

O	12.176	7.299	12.530
O	17.887	12.636	5.780
O	12.039	2.767	12.749
O	18.146	17.162	6.059
O	8.037	12.768	0.724
O	1.986	7.206	7.465
O	3.922	2.611	1.518
O	6.232	17.337	8.221
O	16.070	12.593	11.752
O	14.016	7.393	5.174
O	16.266	17.405	12.130
O	13.917	2.632	5.372
O	3.927	7.445	1.415
O	6.257	12.510	8.116
O	3.678	0.053	0.816
O	6.449	19.889	7.506
O	16.484	10.105	12.644
O	13.691	9.915	5.955
O	16.515	0.073	12.786
O	13.732	0.109	6.124
O	3.677	10.005	0.739
O	6.417	9.945	7.453
O	3.934	17.284	0.906
O	6.256	2.661	7.587
O	16.185	7.442	12.532
O	14.151	12.567	5.931
O	16.224	2.730	12.690
O	13.876	17.363	6.008
O	3.955	12.664	0.831
O	6.222	7.279	7.502
O	19.892	0.901	3.974
O	10.282	19.090	10.664
O	0.314	10.853	9.559
O	9.874	9.099	2.832
O	0.269	19.043	9.589
O	9.885	0.904	2.908
O	19.890	9.079	3.845
O	10.313	10.864	10.542
O	19.771	17.205	3.910
O	10.400	2.722	10.612
O	0.390	7.311	9.631
O	9.673	12.584	2.842
O	0.388	2.732	9.700
O	9.742	17.200	2.989
O	19.781	12.670	3.871
O	10.412	7.228	10.500
O	8.850	14.945	1.922
O	1.265	5.000	8.656
O	11.305	5.005	11.635
O	18.838	14.920	4.921
O	3.914	14.950	2.083
O	6.215	4.994	8.765
O	16.278	5.051	11.502
O	13.902	15.011	5.049
O	5.545	14.933	7.500
O	4.609	5.019	0.796
O	14.664	5.018	6.004
O	15.516	14.969	12.658
O	2.231	14.924	7.442
O	7.938	5.035	0.762
O	17.934	4.983	6.073
O	12.235	14.979	12.737
H	14.177	14.910	5.984

S.12.4 Unit cell with Al12-O11(H)-Si11

Si	8.559	1.151	2.008
Si	1.597	18.800	8.693
Si	11.613	11.107	11.482
Si	18.575	8.848	4.764
Si	11.604	18.856	11.567
Si	18.568	1.102	4.884
Si	8.549	8.909	1.924
Si	1.614	11.058	8.611
Si	6.124	0.572	3.912
Si	4.023	19.372	10.607
Si	14.014	10.456	9.593
Si	16.160	9.491	2.868
Si	14.071	19.420	9.680
Si	16.105	0.563	2.959
Si	6.118	9.433	3.853
Si	4.041	10.538	10.545
Si	5.720	1.303	6.882
Si	4.430	18.652	0.190
Si	14.477	11.170	6.643
Si	15.732	8.809	13.281
Si	14.471	18.702	6.732
Si	15.732	1.359	0.019
Si	5.694	8.645	6.800
Si	4.425	11.297	0.094
Si	2.515	1.352	6.900
Si	7.631	18.617	0.201
Si	17.644	11.241	6.576
Si	12.538	8.696	13.270
Si	17.667	18.574	6.698
Si	12.535	1.366	0.014
Si	2.487	8.602	6.806
Si	7.626	11.334	0.086
Si	1.463	0.614	4.081
Si	8.684	19.354	10.769
Si	18.739	10.615	9.385
Si	11.466	9.381	2.689
Si	18.702	19.349	9.508
Si	11.474	0.604	2.827
Si	1.453	9.383	3.995
Si	8.727	10.547	10.675
Si	3.616	1.113	2.047
Si	6.531	18.838	8.744
Si	16.516	11.089	11.348
Si	13.650	8.899	4.691
Si	16.570	18.891	11.573
Si	13.624	1.131	4.858
Si	3.621	8.936	1.961
Si	6.540	11.016	8.669
Si	8.468	16.474	2.267
Si	1.653	3.466	8.980
Si	11.699	6.514	11.195
Si	18.459	13.405	4.467
Si	11.666	3.460	11.325
Si	18.507	16.473	4.628
Si	8.441	13.396	2.170
Si	1.641	6.552	8.913
Si	6.099	17.324	4.139
Si	4.048	2.618	10.823
Si	14.011	7.330	9.324
Si	16.182	12.640	2.524
Si	14.068	2.664	9.430
Si	16.102	17.303	2.732
Si	6.085	12.567	4.081
Si	4.052	7.398	10.765
Si	5.446	16.493	7.087

Si	4.714	3.458	0.390
Si	14.746	6.591	6.372
Si	15.431	13.387	13.013
Si	14.721	3.483	6.491
Si	15.443	16.494	13.181
Si	5.458	13.389	7.022
Si	4.709	6.561	0.313
Si	2.348	16.460	6.938
Si	7.815	3.498	0.261
Si	17.840	6.532	6.551
Si	12.326	13.440	13.255
Si	17.811	3.469	6.636
Si	12.351	16.490	13.299
Si	2.360	13.410	6.870
Si	7.811	6.544	0.171
Si	1.358	17.367	4.097
Si	8.789	2.590	10.798
Si	18.810	7.475	9.390
Si	11.299	12.510	2.689
Si	18.805	2.592	9.484
Si	11.339	17.353	2.763
Si	1.364	12.521	4.043
Si	8.812	7.402	10.716
Si	3.648	16.527	2.313
Si	6.504	3.422	8.998
Si	16.487	6.622	11.169
Si	16.516	3.470	11.273
Si	13.622	16.623	4.600
Si	3.645	13.365	2.262
Si	6.497	6.578	8.939
Al	13.665	13.239	4.423
O	7.268	1.235	2.980
O	2.888	18.708	9.665
O	12.955	11.178	10.580
O	17.258	8.782	3.826
O	12.900	18.792	10.597
O	17.270	1.140	3.918
O	7.257	8.800	2.895
O	2.933	11.154	9.541
O	6.084	1.395	5.308
O	4.053	18.547	12.002
O	13.989	11.252	8.190
O	16.154	8.689	1.456
O	14.138	18.553	8.304
O	16.077	1.451	1.602
O	6.071	8.568	5.226
O	4.016	11.412	11.912
O	4.114	1.161	7.107
O	6.034	18.834	0.398
O	16.076	10.838	6.575
O	14.125	9.008	13.123
O	16.067	18.779	6.452
O	14.131	1.162	13.170
O	4.088	8.784	7.012
O	6.029	11.090	0.252
O	2.137	1.417	5.325
O	8.021	18.543	12.013
O	18.176	11.439	8.099
O	12.107	8.549	1.442
O	18.000	18.536	8.281
O	12.180	1.399	1.596
O	2.109	8.552	5.232
O	8.054	11.368	11.907
O	2.123	1.110	2.685
O	8.029	18.852	9.372
O	18.024	11.141	10.744
O	12.152	8.878	4.071
O	18.055	18.874	10.918
O	12.125	1.081	4.238
O	2.129	8.926	2.594

O	8.048	10.989	9.268
O	4.673	0.678	3.200
O	5.479	19.268	9.904
O	15.518	10.505	10.205
O	14.684	9.391	3.536
O	15.501	19.314	10.426
O	14.668	0.670	3.703
O	4.673	9.356	3.123
O	5.510	10.634	9.866
O	7.208	16.525	3.278
O	2.927	3.417	9.976
O	12.907	6.449	10.117
O	17.343	13.476	3.304
O	12.930	3.376	10.322
O	17.227	16.604	3.645
O	7.168	13.340	3.167
O	2.931	6.645	9.881
O	6.135	16.727	5.640
O	4.038	3.220	12.322
O	13.994	6.862	7.779
O	16.295	13.054	0.955
O	14.024	3.318	7.949
O	16.113	16.610	1.276
O	6.132	13.232	5.556
O	4.023	6.727	12.237
O	3.891	16.980	7.026
O	6.272	2.978	0.349
O	16.301	7.060	6.493
O	13.877	12.939	13.224
O	16.262	2.955	6.580
O	13.898	17.012	13.258
O	3.905	12.897	6.955
O	6.262	7.044	0.227
O	1.839	16.533	5.402
O	8.321	3.422	12.108
O	18.384	6.628	8.073
O	11.730	13.366	1.368
O	18.340	3.426	8.169
O	11.820	16.541	1.450
O	1.869	13.384	5.325
O	8.329	6.555	12.017
O	2.105	16.785	2.773
O	8.045	3.192	9.481
O	18.021	6.892	10.689
O	12.009	13.112	3.995
O	18.049	3.178	10.801
O	12.103	16.729	4.077
O	2.099	13.087	2.702
O	8.039	6.841	9.397
O	4.625	17.105	3.485
O	5.515	2.827	10.150
O	15.487	7.078	9.964
O	14.732	13.009	3.100
O	15.528	2.900	10.105
O	14.639	17.046	3.427
O	4.603	12.752	3.431
O	5.518	7.200	10.086
O	6.467	18.905	4.174
O	3.676	1.038	10.869
O	13.595	8.895	9.419
O	16.542	11.052	2.667
O	13.761	1.072	9.325
O	16.371	18.897	2.603
O	6.453	10.989	4.184
O	3.709	8.981	10.874
O	1.738	18.928	4.306
O	8.383	1.034	10.996
O	18.427	9.034	9.163
O	11.740	10.959	2.436
O	18.419	1.031	9.265

O	11.749	18.912	2.616
O	1.736	10.960	4.274
O	8.464	8.967	10.951
O	8.732	2.561	1.219
O	1.427	17.395	7.893
O	11.437	12.527	12.248
O	18.743	7.432	5.549
O	11.444	17.446	12.354
O	18.707	2.504	5.689
O	8.715	7.527	1.085
O	1.433	12.445	7.784
O	8.412	19.851	0.917
O	1.749	0.105	7.608
O	11.702	9.909	12.582
O	18.487	10.049	5.860
O	11.749	0.142	12.672
O	18.456	19.792	5.969
O	8.404	10.141	0.871
O	1.727	9.835	7.544
O	8.099	17.218	0.872
O	2.021	2.743	7.571
O	12.176	7.299	12.530
O	17.887	12.636	5.780
O	12.039	2.767	12.749
O	18.146	17.162	6.059
O	8.037	12.768	0.724
O	1.986	7.206	7.465
O	3.922	2.611	1.518
O	6.232	17.337	8.221
O	16.070	12.593	11.752
O	14.016	7.393	5.174
O	16.266	17.405	12.130
O	13.917	2.632	5.372
O	3.927	7.445	1.415
O	6.257	12.510	8.116
O	3.678	0.053	0.816
O	6.449	19.889	7.506
O	16.484	10.105	12.644
O	13.691	9.915	5.955
O	16.515	0.073	12.786
O	13.732	0.109	6.124
O	3.677	10.005	0.739
O	6.417	9.945	7.453
O	3.934	17.284	0.906
O	6.256	2.661	7.587
O	16.185	7.442	12.532
O	14.151	12.567	5.931
O	16.224	2.730	12.690
O	13.876	17.363	6.008
O	3.955	12.664	0.831
O	6.222	7.279	7.502
O	19.892	0.901	3.974
O	10.282	19.090	10.664
O	0.314	10.853	9.559
O	9.874	9.099	2.832
O	0.269	19.043	9.589
O	9.885	0.904	2.908
O	19.890	9.079	3.845
O	10.313	10.864	10.542
O	19.771	17.205	3.910
O	10.400	2.722	10.612
O	0.390	7.311	9.631
O	9.673	12.584	2.842
O	0.388	2.732	9.700
O	9.742	17.200	2.989
O	19.781	12.670	3.871
O	10.412	7.228	10.500
O	8.850	14.945	1.922
O	1.265	5.000	8.656
O	11.305	5.005	11.635

O	18.838	14.920	4.921
O	3.914	14.950	2.083
O	6.215	4.994	8.765
O	16.278	5.051	11.502
O	13.902	15.011	5.049
O	5.545	14.933	7.500
O	4.609	5.019	0.796
O	14.664	5.018	6.004
O	15.516	14.969	12.658
O	2.231	14.924	7.442
O	7.938	5.035	0.762
O	17.934	4.983	6.073
O	12.235	14.979	12.737
H	14.177	14.910	5.984

S.12.5 Adsorbed ethene in all silica unit cell (intersection)

Si	8.594	1.121	1.978
Si	1.616	18.809	8.670
Si	11.653	11.051	11.529
Si	18.580	8.879	4.835
Si	11.652	18.826	11.527
Si	18.579	1.101	4.834
Si	8.597	8.859	1.980
Si	1.617	11.071	8.672
Si	6.139	0.625	3.815
Si	4.076	19.305	10.506
Si	14.080	10.498	9.617
Si	16.155	9.432	2.918
Si	14.077	19.380	9.610
Si	16.153	0.547	2.921
Si	6.137	9.357	3.815
Si	4.075	10.575	10.509
Si	5.797	1.093	6.880
Si	4.415	18.835	0.188
Si	14.478	11.257	6.664
Si	15.756	8.667	13.352
Si	14.475	18.619	6.660
Si	15.753	1.305	13.351
Si	5.798	8.888	6.881
Si	4.416	11.043	0.191
Si	2.584	1.382	6.899
Si	7.628	18.545	0.208
Si	17.673	11.325	6.635
Si	12.562	8.601	13.323
Si	17.670	18.553	6.631
Si	12.558	1.375	13.323
Si	2.584	8.598	6.901
Si	7.629	11.331	0.209
Si	1.470	0.716	4.072
Si	8.742	19.211	10.762
Si	18.713	10.546	9.438
Si	11.522	9.381	2.742
Si	18.713	19.330	9.433
Si	11.520	0.597	2.744
Si	1.471	9.263	4.074
Si	8.742	10.667	10.764
Si	3.671	1.389	2.148
Si	6.542	18.539	8.838
Si	16.577	11.015	11.491
Si	13.662	8.915	4.793
Si	16.572	18.861	11.482
Si	13.657	1.065	4.795
Si	3.670	8.589	2.149

Si	6.542	11.341	8.840
Si	8.481	16.489	2.375
Si	1.733	3.438	9.068
Si	11.639	6.535	11.251
Si	18.597	13.391	4.563
Si	11.637	3.441	11.252
Si	18.593	16.485	4.559
Si	8.481	13.387	2.377
Si	1.733	6.541	9.070
Si	5.977	17.382	3.904
Si	4.237	2.548	10.599
Si	14.032	7.357	9.374
Si	16.199	12.569	2.687
Si	14.033	2.619	9.375
Si	16.201	17.305	2.682
Si	5.977	12.498	3.908
Si	4.237	7.432	10.600
Si	5.459	16.499	6.866
Si	4.754	3.430	0.177
Si	14.742	6.540	6.430
Si	15.490	13.390	13.128
Si	14.741	3.441	6.433
Si	15.489	16.489	13.121
Si	5.459	13.380	6.868
Si	4.754	6.548	0.178
Si	2.316	16.442	6.900
Si	7.898	3.487	0.207
Si	17.847	6.510	6.576
Si	12.386	13.418	13.270
Si	17.846	3.469	6.576
Si	12.385	16.459	13.267
Si	2.317	13.437	6.902
Si	7.897	6.491	0.209
Si	1.468	17.467	4.041
Si	8.743	2.460	10.729
Si	18.815	7.413	9.407
Si	11.419	12.512	2.714
Si	18.816	2.563	9.404
Si	11.419	17.363	2.715
Si	1.470	12.410	4.042
Si	8.743	7.519	10.732
Si	3.561	16.486	2.027
Si	6.648	3.446	8.719
Si	16.510	6.564	11.217
Si	16.513	3.405	11.217
Si	13.721	16.515	4.526
Si	3.564	13.395	2.030
Si	6.650	6.536	8.719
Si	13.718	13.356	4.531
O	7.342	1.320	2.984
O	2.870	18.613	9.676
O	12.962	11.153	10.584
O	17.272	8.780	3.888
O	12.962	18.728	10.582
O	17.271	1.204	3.887
O	7.343	8.664	2.986
O	2.869	11.268	9.678
O	6.393	0.857	5.393
O	3.822	19.074	12.084
O	14.123	11.357	8.241
O	16.109	8.565	1.547
O	14.116	18.515	8.237
O	16.106	1.404	1.546
O	6.391	9.126	5.394
O	3.821	10.808	12.086
O	4.176	1.096	6.838
O	6.035	18.821	0.147
O	16.079	11.096	6.427
O	14.155	8.838	13.117
O	16.077	18.790	6.430

O	14.152	1.143	13.114
O	4.178	8.878	6.840
O	6.036	11.046	0.148
O	1.992	1.505	5.395
O	8.219	18.425	12.086
O	18.044	11.381	8.212
O	12.189	8.542	1.516
O	18.046	18.493	8.207
O	12.189	1.432	1.517
O	1.993	8.474	5.397
O	8.219	11.454	12.087
O	2.163	1.346	2.746
O	8.050	18.576	9.437
O	18.068	11.009	10.853
O	12.169	8.923	4.158
O	18.065	18.870	10.848
O	12.166	1.060	4.158
O	2.163	8.630	2.748
O	8.050	11.302	9.438
O	4.724	1.303	3.392
O	5.488	18.623	10.080
O	15.533	10.563	10.331
O	14.703	9.374	3.634
O	15.532	19.319	10.321
O	14.701	0.609	3.637
O	4.725	8.674	3.391
O	5.488	11.256	10.083
O	7.342	16.592	3.530
O	2.868	3.333	10.227
O	12.855	6.600	10.184
O	17.377	13.321	3.502
O	12.858	3.373	10.191
O	17.379	16.547	3.491
O	7.345	13.284	3.534
O	2.868	6.646	10.227
O	5.751	17.327	5.503
O	4.462	2.601	12.198
O	14.045	6.739	7.880
O	16.178	13.205	1.201
O	14.049	3.249	7.886
O	16.184	16.687	1.188
O	5.752	12.550	5.507
O	4.465	7.377	12.198
O	3.889	16.662	7.256
O	6.325	3.272	0.565
O	16.299	7.014	6.516
O	13.934	12.912	13.205
O	16.298	2.965	6.515
O	13.933	16.965	13.203
O	3.889	13.218	7.259
O	6.324	6.706	0.569
O	2.083	16.658	5.308
O	8.128	3.267	11.997
O	18.366	6.548	8.111
O	11.873	13.385	1.424
O	18.364	3.433	8.111
O	11.869	16.496	1.420
O	2.085	13.219	5.310
O	8.125	6.714	12.000
O	2.116	16.874	2.674
O	8.093	3.056	9.363
O	18.036	6.843	10.718
O	12.195	13.073	4.029
O	18.039	3.128	10.717
O	12.197	16.797	4.026
O	2.120	13.004	2.675
O	8.095	6.923	9.366
O	4.720	16.690	3.151
O	5.491	3.247	9.847
O	15.474	7.120	10.087

O	14.759	12.793	3.410
O	15.476	2.847	10.090
O	14.760	17.070	3.399
O	4.722	13.198	3.157
O	5.491	6.737	9.844
O	6.106	18.936	3.446
O	4.113	0.994	10.137
O	13.711	8.948	9.304
O	16.525	10.980	2.597
O	13.708	1.030	9.292
O	16.524	18.895	2.611
O	6.100	10.944	3.446
O	4.110	8.987	10.141
O	1.857	19.037	4.203
O	8.352	0.890	10.887
O	18.424	8.969	9.166
O	11.809	10.957	2.463
O	18.426	1.007	9.157
O	11.808	18.919	2.471
O	1.860	10.840	4.203
O	8.353	9.090	10.888
O	8.795	2.459	1.079
O	1.419	17.470	7.771
O	11.477	12.441	12.351
O	18.753	7.483	5.649
O	11.477	17.434	12.344
O	18.753	2.495	5.651
O	8.794	7.519	1.082
O	1.418	12.411	7.775
O	8.369	19.766	0.975
O	1.837	0.165	7.668
O	11.769	9.819	12.590
O	18.462	10.104	5.903
O	11.767	0.156	12.591
O	18.461	19.772	5.898
O	8.375	10.112	0.975
O	1.841	9.818	7.667
O	7.942	17.157	0.991
O	2.277	2.770	7.685
O	12.113	7.185	12.665
O	18.130	12.740	5.980
O	12.104	2.791	12.668
O	18.118	17.138	5.971
O	7.937	12.719	0.994
O	2.273	7.210	7.687
O	3.851	2.801	1.367
O	6.365	17.127	8.054
O	16.266	12.514	12.013
O	13.976	7.412	5.305
O	16.258	17.359	11.995
O	13.971	2.565	5.314
O	3.849	7.178	1.366
O	6.365	12.754	8.058
O	3.904	0.139	1.143
O	6.313	19.791	7.835
O	16.511	9.968	12.733
O	13.731	9.952	6.043
O	16.501	0.001	12.731
O	13.722	0.021	6.041
O	3.900	9.840	1.144
O	6.311	10.091	7.835
O	3.850	17.411	0.727
O	6.352	2.519	7.421
O	16.268	7.304	12.640
O	13.955	12.620	5.958
O	16.274	2.666	12.641
O	13.963	17.254	5.950
O	3.860	12.468	0.732
O	6.359	7.463	7.421
O	19.888	0.887	3.902

O	10.346	19.042	10.592
O	0.281	10.832	9.552
O	9.933	9.093	2.860
O	0.280	19.043	9.552
O	9.930	0.883	2.859
O	19.889	9.094	3.904
O	10.346	10.837	10.594
O	19.876	17.293	3.965
O	10.356	2.635	10.652
O	0.397	7.283	9.629
O	9.815	12.639	2.932
O	0.398	2.693	9.624
O	9.815	17.235	2.935
O	19.878	12.585	3.965
O	10.357	7.344	10.658
O	8.821	14.937	2.068
O	1.396	4.989	8.760
O	11.230	4.989	11.514
O	19.002	14.939	4.826
O	3.541	14.940	1.537
O	6.669	4.991	8.226
O	16.273	4.985	11.452
O	13.959	14.935	4.762
O	5.854	14.939	6.663
O	4.356	4.989	13.356
O	14.638	4.990	5.978
O	15.593	14.938	12.669
O	1.858	14.940	7.302
O	8.360	4.989	0.605
O	17.978	4.989	6.022
O	12.255	14.938	12.715
H	9.879	16.221	8.348
H	11.716	16.201	8.058
H	11.690	13.720	8.050
H	9.854	13.736	8.340
C	10.791	15.636	8.200
C	10.777	14.302	8.196

S.12.6 Adsorbed ethene in all silica unit cell (straight channel)

Si	8.612	1.118	2.016
Si	1.632	18.810	8.706
Si	11.670	11.057	11.533
Si	18.600	8.872	4.859
Si	11.668	18.830	11.557
Si	18.596	1.094	4.868
Si	8.609	8.855	2.030
Si	1.632	11.071	8.704
Si	6.157	0.626	3.853
Si	4.087	19.305	10.544
Si	14.094	10.492	9.628
Si	16.188	9.429	2.931
Si	14.095	19.377	9.638
Si	16.169	0.545	2.955
Si	6.152	9.359	3.864
Si	4.076	10.580	10.556
Si	5.811	1.096	6.917
Si	4.432	18.835	0.225
Si	14.503	11.240	6.668
Si	15.775	8.677	13.372
Si	14.493	18.604	6.692
Si	15.770	1.309	0.004
Si	5.812	8.891	6.928
Si	4.436	11.039	0.230
Si	2.598	1.386	6.935

Si	7.645	18.544	0.243
Si	17.698	11.322	6.651
Si	12.579	8.612	13.335
Si	17.688	18.543	6.664
Si	12.575	1.374	13.361
Si	2.597	8.592	6.934
Si	7.646	11.321	0.246
Si	1.487	0.716	4.108
Si	8.755	19.216	10.797
Si	18.725	10.545	9.458
Si	11.535	9.374	2.761
Si	18.726	19.329	9.466
Si	11.537	0.592	2.781
Si	1.486	9.260	4.105
Si	8.757	10.666	10.798
Si	3.689	1.390	2.186
Si	6.553	18.539	8.876
Si	16.587	11.018	11.504
Si	13.696	8.899	4.789
Si	16.587	18.864	11.517
Si	13.675	1.056	4.834
Si	3.694	8.587	2.191
Si	6.536	11.349	8.893
Si	8.495	16.484	2.408
Si	1.746	3.439	9.106
Si	11.665	6.531	11.264
Si	18.615	13.390	4.579
Si	11.654	3.438	11.290
Si	18.612	16.483	4.590
Si	8.493	13.381	2.414
Si	1.741	6.542	9.109
Si	5.994	17.382	3.943
Si	4.250	2.547	10.637
Si	14.039	7.349	9.377
Si	16.223	12.567	2.702
Si	14.051	2.614	9.408
Si	16.216	17.305	2.714
Si	5.995	12.498	3.953
Si	4.247	7.437	10.638
Si	5.473	16.499	6.903
Si	4.771	3.429	0.214
Si	14.767	6.536	6.439
Si	15.504	13.390	13.148
Si	14.762	3.436	6.471
Si	15.505	16.489	13.154
Si	5.469	13.380	6.908
Si	4.773	6.548	0.214
Si	2.328	16.443	6.932
Si	7.914	3.485	0.246
Si	17.872	6.503	6.602
Si	12.399	13.418	13.289
Si	17.866	3.462	6.612
Si	12.400	16.460	13.296
Si	2.322	13.438	6.932
Si	7.919	6.490	0.254
Si	1.483	17.468	4.073
Si	8.758	2.464	10.766
Si	18.828	7.414	9.436
Si	11.432	12.506	2.734
Si	18.832	2.561	9.441
Si	11.433	17.356	2.748
Si	1.483	12.407	4.068
Si	8.766	7.517	10.771
Si	3.578	16.487	2.065
Si	6.662	3.448	8.757
Si	16.512	6.562	11.229
Si	16.527	3.404	11.251
Si	13.739	16.506	4.555
Si	3.590	13.396	2.071
Si	6.665	6.538	8.761

Si	13.741	13.347	4.542
O	7.360	1.321	3.022
O	2.882	18.610	9.714
O	12.975	11.165	10.583
O	17.289	8.776	3.917
O	12.975	18.732	10.610
O	17.288	1.199	3.921
O	7.359	8.661	3.039
O	2.875	11.274	9.721
O	6.410	0.859	5.431
O	3.835	19.074	12.122
O	14.146	11.335	8.245
O	16.162	8.564	1.558
O	14.142	18.504	8.271
O	16.121	1.407	1.581
O	6.408	9.142	5.443
O	3.816	10.806	12.135
O	4.191	1.107	6.872
O	6.052	18.823	0.181
O	16.106	11.094	6.435
O	14.173	8.871	13.170
O	16.094	18.772	6.455
O	14.168	1.146	13.148
O	4.192	8.850	6.868
O	6.056	11.034	0.162
O	2.004	1.505	5.432
O	8.237	18.428	12.122
O	18.063	11.380	8.229
O	12.167	8.539	1.516
O	18.059	18.491	8.241
O	12.207	1.425	1.555
O	2.000	8.473	5.431
O	8.261	11.446	12.135
O	2.181	1.347	2.783
O	8.062	18.582	9.473
O	18.078	11.019	10.867
O	12.206	8.896	4.155
O	18.079	18.871	10.881
O	12.183	1.054	4.196
O	2.184	8.628	2.783
O	8.042	11.311	9.492
O	4.742	1.303	3.429
O	5.501	18.625	10.119
O	15.544	10.555	10.347
O	14.725	9.371	3.624
O	15.545	19.320	10.357
O	14.718	0.607	3.672
O	4.741	8.672	3.440
O	5.488	11.268	10.142
O	7.356	16.589	3.563
O	2.883	3.336	10.262
O	12.863	6.577	10.176
O	17.390	13.328	3.522
O	12.876	3.360	10.232
O	17.392	16.551	3.528
O	7.366	13.281	3.580
O	2.882	6.647	10.261
O	5.773	17.327	5.542
O	4.475	2.600	12.236
O	14.047	6.758	7.873
O	16.207	13.195	1.212
O	14.069	3.261	7.925
O	16.200	16.680	1.223
O	5.776	12.546	5.552
O	4.474	7.378	12.237
O	3.902	16.662	7.287
O	6.341	3.267	0.602
O	16.324	7.006	6.548
O	13.947	12.915	13.238
O	16.317	2.957	6.555

O	13.948	16.965	13.238
O	3.895	13.219	7.282
O	6.345	6.709	0.599
O	2.095	16.658	5.340
O	8.145	3.272	12.036
O	18.398	6.545	8.135
O	11.868	13.376	1.436
O	18.384	3.433	8.148
O	11.880	16.494	1.448
O	2.082	13.220	5.341
O	8.164	6.716	12.049
O	2.131	16.874	2.706
O	8.109	3.064	9.401
O	18.040	6.842	10.740
O	12.215	13.078	4.041
O	18.054	3.127	10.754
O	12.213	16.782	4.056
O	2.144	12.999	2.707
O	8.110	6.906	9.416
O	4.732	16.694	3.194
O	5.507	3.242	9.886
O	15.483	7.100	10.085
O	14.777	12.789	3.414
O	15.494	2.835	10.127
O	14.774	17.072	3.430
O	4.741	13.204	3.207
O	5.504	6.747	9.884
O	6.127	18.937	3.485
O	4.122	0.994	10.175
O	13.713	8.940	9.340
O	16.560	10.980	2.620
O	13.729	1.026	9.308
O	16.537	18.895	2.637
O	6.114	10.945	3.483
O	4.115	8.993	10.183
O	1.876	19.037	4.237
O	8.365	0.894	10.924
O	18.432	8.968	9.191
O	11.824	10.952	2.488
O	18.439	1.007	9.190
O	11.823	18.913	2.510
O	1.873	10.838	4.236
O	8.376	9.087	10.924
O	8.812	2.454	1.114
O	1.433	17.473	7.804
O	11.497	12.448	12.354
O	18.774	7.474	5.670
O	11.494	17.434	12.370
O	18.771	2.485	5.690
O	8.811	7.511	1.139
O	1.428	12.412	7.809
O	8.386	19.761	1.016
O	1.857	0.167	7.706
O	11.788	9.824	12.590
O	18.490	10.097	5.928
O	11.785	0.155	12.626
O	18.477	19.762	5.929
O	8.384	10.104	1.022
O	1.871	9.823	7.698
O	7.957	17.153	1.024
O	2.288	2.774	7.721
O	12.166	7.192	12.663
O	18.156	12.735	5.995
O	12.115	2.790	12.710
O	18.143	17.127	6.009
O	7.941	12.710	1.037
O	2.273	7.209	7.723
O	3.868	2.802	1.405
O	6.374	17.127	8.095
O	16.266	12.517	12.020

O	14.025	7.395	5.289
O	16.274	17.363	12.033
O	13.987	2.554	5.359
O	3.875	7.176	1.409
O	6.361	12.761	8.110
O	3.922	0.140	1.180
O	6.320	19.789	7.871
O	16.532	9.974	12.749
O	13.775	9.928	6.044
O	16.519	0.006	12.765
O	13.740	0.006	6.073
O	3.929	9.840	1.191
O	6.284	10.100	7.893
O	3.871	17.411	0.765
O	6.372	2.519	7.460
O	16.255	7.312	12.643
O	13.974	12.600	5.962
O	16.289	2.671	12.679
O	13.977	17.241	5.982
O	3.898	12.469	0.777
O	6.389	7.472	7.465
O	19.904	0.883	3.935
O	10.360	19.047	10.625
O	0.293	10.823	9.577
O	9.945	9.098	2.911
O	0.294	19.044	9.584
O	9.948	0.880	2.896
O	19.906	9.088	3.924
O	10.359	10.845	10.602
O	19.890	17.297	3.995
O	10.372	2.636	10.690
O	0.408	7.287	9.673
O	9.829	12.633	2.967
O	0.414	2.688	9.663
O	9.830	17.226	2.970
O	19.892	12.583	3.972
O	10.380	7.344	10.682
O	8.832	14.931	2.101
O	1.403	4.990	8.804
O	11.253	4.988	11.547
O	19.024	14.936	4.845
O	3.564	14.940	1.577
O	6.674	4.993	8.265
O	16.280	4.983	11.478
O	13.984	14.926	4.783
O	5.865	14.939	6.699
O	4.377	4.989	0.010
O	14.664	4.981	6.003
O	15.605	14.940	12.696
O	1.867	14.942	7.334
O	8.375	4.985	0.651
O	17.999	4.981	6.052
O	12.270	14.941	12.739
H	9.612	10.811	5.926
H	10.393	11.014	7.599
H	10.528	8.544	7.832
H	9.743	8.345	6.159
C	10.035	10.341	6.817
C	10.102	9.016	6.943

S.12.7 Adsorbed ethene in all silica unit cell (sinusoidal channel)

Si	8.594	1.119	1.983
Si	1.617	18.807	8.676
Si	11.652	11.052	11.531
Si	18.576	8.878	4.837
Si	11.651	18.824	11.531
Si	18.575	1.099	4.837
Si	8.595	8.859	1.984
Si	1.618	11.069	8.677
Si	6.137	0.624	3.821
Si	4.074	19.304	10.513
Si	14.078	10.498	9.622
Si	16.152	9.432	2.918
Si	14.075	19.378	9.617
Si	16.150	0.544	2.922
Si	6.136	9.355	3.820
Si	4.073	10.574	10.515
Si	5.795	1.094	6.885
Si	4.413	18.834	0.194
Si	14.478	11.253	6.667
Si	15.756	8.671	13.353
Si	14.475	18.620	6.666
Si	15.753	1.302	13.353
Si	5.796	8.884	6.885
Si	4.415	11.041	0.196
Si	2.582	1.382	6.903
Si	7.627	18.545	0.210
Si	17.674	11.326	6.638
Si	12.562	8.606	13.327
Si	17.671	18.550	6.636
Si	12.559	1.370	13.329
Si	2.582	8.595	6.904
Si	7.627	11.329	0.210
Si	1.466	0.717	4.076
Si	8.741	19.212	10.766
Si	18.715	10.545	9.442
Si	11.520	9.381	2.747
Si	18.715	19.329	9.439
Si	11.519	0.595	2.750
Si	1.467	9.260	4.076
Si	8.741	10.665	10.767
Si	3.670	1.389	2.154
Si	6.539	18.539	8.845
Si	16.577	11.017	11.491
Si	13.662	8.910	4.792
Si	16.572	18.858	11.484
Si	13.658	1.066	4.797
Si	3.669	8.588	2.154
Si	6.538	11.337	8.846
Si	8.477	16.488	2.379
Si	1.731	3.437	9.074
Si	11.641	6.533	11.257
Si	18.595	13.390	4.565
Si	11.639	3.442	11.260
Si	18.593	16.484	4.562
Si	8.477	13.386	2.379
Si	1.730	6.539	9.075
Si	5.975	17.380	3.912
Si	4.235	2.547	10.605
Si	14.028	7.356	9.378
Si	16.195	12.572	2.690
Si	14.029	2.619	9.380
Si	16.197	17.302	2.686
Si	5.975	12.497	3.914
Si	4.235	7.431	10.604
Si	5.456	16.497	6.873

Si	4.754	3.429	0.183
Si	14.739	6.540	6.434
Si	15.488	13.389	13.132
Si	14.739	3.438	6.439
Si	15.488	16.488	13.127
Si	5.456	13.379	6.875
Si	4.754	6.547	0.182
Si	2.311	16.441	6.904
Si	7.898	3.486	0.214
Si	17.845	6.509	6.581
Si	12.385	13.417	13.274
Si	17.844	3.467	6.582
Si	12.384	16.458	13.272
Si	2.311	13.436	6.905
Si	7.897	6.490	0.215
Si	1.464	17.468	4.043
Si	8.745	2.461	10.736
Si	18.814	7.411	9.413
Si	11.416	12.513	2.719
Si	18.815	2.563	9.411
Si	11.415	17.360	2.720
Si	1.466	12.408	4.043
Si	8.745	7.516	10.738
Si	3.560	16.485	2.033
Si	6.648	3.444	8.726
Si	16.506	6.563	11.218
Si	16.509	3.406	11.220
Si	13.718	16.513	4.531
Si	3.563	13.393	2.035
Si	6.650	6.535	8.725
Si	13.715	13.355	4.534
O	7.341	1.317	2.989
O	2.871	18.609	9.680
O	12.963	11.159	10.589
O	17.268	8.782	3.891
O	12.963	18.721	10.589
O	17.267	1.199	3.890
O	7.342	8.664	2.989
O	2.871	11.270	9.681
O	6.393	0.857	5.399
O	3.817	19.073	12.090
O	14.115	11.345	8.241
O	16.114	8.567	1.546
O	14.109	18.524	8.240
O	16.109	1.402	1.546
O	6.391	9.124	5.398
O	3.817	10.807	12.092
O	4.175	1.104	6.839
O	6.033	18.824	0.150
O	16.080	11.097	6.431
O	14.155	8.849	13.123
O	16.077	18.785	6.435
O	14.152	1.133	13.120
O	4.176	8.868	6.840
O	6.035	11.044	0.150
O	1.987	1.504	5.400
O	8.219	18.424	12.089
O	18.053	11.377	8.212
O	12.186	8.545	1.519
O	18.055	18.495	8.209
O	12.187	1.427	1.522
O	1.987	8.473	5.401
O	8.219	11.453	12.089
O	2.162	1.347	2.751
O	8.047	18.581	9.440
O	18.069	11.014	10.854
O	12.167	8.920	4.161
O	18.066	18.864	10.851
O	12.164	1.060	4.164
O	2.162	8.628	2.752

O	8.047	11.293	9.440
O	4.723	1.303	3.398
O	5.488	18.625	10.090
O	15.532	10.562	10.333
O	14.698	9.371	3.629
O	15.531	19.317	10.326
O	14.696	0.609	3.634
O	4.723	8.674	3.396
O	5.488	11.251	10.092
O	7.340	16.591	3.534
O	2.868	3.335	10.230
O	12.855	6.591	10.188
O	17.372	13.322	3.507
O	12.859	3.379	10.197
O	17.373	16.547	3.499
O	7.342	13.284	3.538
O	2.869	6.642	10.229
O	5.751	17.325	5.511
O	4.460	2.600	12.203
O	14.036	6.748	7.879
O	16.178	13.210	1.204
O	14.040	3.239	7.887
O	16.183	16.678	1.194
O	5.753	12.550	5.513
O	4.462	7.375	12.203
O	3.885	16.658	7.258
O	6.325	3.268	0.569
O	16.296	7.012	6.524
O	13.932	12.911	13.211
O	16.296	2.964	6.525
O	13.932	16.964	13.210
O	3.885	13.219	7.259
O	6.324	6.708	0.571
O	2.076	16.659	5.312
O	8.130	3.269	12.004
O	18.369	6.548	8.114
O	11.868	13.384	1.426
O	18.367	3.431	8.116
O	11.866	16.494	1.424
O	2.077	13.216	5.313
O	8.128	6.709	12.006
O	2.115	16.874	2.678
O	8.094	3.055	9.370
O	18.034	6.839	10.722
O	12.190	13.082	4.032
O	18.036	3.131	10.723
O	12.192	16.787	4.031
O	2.118	13.002	2.678
O	8.095	6.922	9.371
O	4.717	16.687	3.161
O	5.491	3.243	9.853
O	15.474	7.114	10.083
O	14.753	12.800	3.407
O	15.476	2.850	10.088
O	14.754	17.063	3.399
O	4.719	13.196	3.165
O	5.492	6.739	9.850
O	6.103	18.935	3.453
O	4.108	0.993	10.143
O	13.704	8.946	9.323
O	16.518	10.983	2.600
O	13.702	1.030	9.311
O	16.517	18.892	2.612
O	6.099	10.943	3.452
O	4.105	8.986	10.146
O	1.853	19.038	4.205
O	8.356	0.891	10.896
O	18.423	8.968	9.175
O	11.809	10.958	2.474
O	18.425	1.008	9.168

O	11.808	18.916	2.481
O	1.855	10.838	4.205
O	8.357	9.087	10.898
O	8.795	2.458	1.086
O	1.415	17.468	7.779
O	11.475	12.445	12.350
O	18.748	7.483	5.651
O	11.475	17.429	12.346
O	18.748	2.493	5.654
O	8.794	7.518	1.087
O	1.415	12.410	7.780
O	8.369	19.765	0.979
O	1.841	0.161	7.671
O	11.767	9.823	12.595
O	18.461	10.106	5.901
O	11.765	0.152	12.597
O	18.460	19.768	5.898
O	8.374	10.111	0.978
O	1.845	9.819	7.670
O	7.939	17.157	0.995
O	2.271	2.768	7.690
O	12.118	7.189	12.668
O	18.131	12.741	5.983
O	12.108	2.786	12.673
O	18.122	17.134	5.977
O	7.934	12.717	0.997
O	2.267	7.209	7.691
O	3.851	2.800	1.373
O	6.357	17.127	8.064
O	16.266	12.514	12.019
O	13.979	7.407	5.301
O	16.260	17.358	12.005
O	13.974	2.567	5.312
O	3.850	7.177	1.371
O	6.357	12.751	8.067
O	3.903	0.138	1.150
O	6.305	19.789	7.840
O	16.514	9.969	12.733
O	13.736	9.946	6.043
O	16.505	0.000	12.732
O	13.728	0.024	6.042
O	3.899	9.840	1.150
O	6.302	10.089	7.840
O	3.853	17.410	0.734
O	6.355	2.518	7.427
O	16.260	7.306	12.638
O	13.952	12.612	5.956
O	16.267	2.664	12.642
O	13.959	17.259	5.951
O	3.861	12.468	0.738
O	6.361	7.461	7.426
O	19.884	0.888	3.904
O	10.345	19.038	10.595
O	0.284	10.828	9.558
O	9.931	9.096	2.864
O	0.283	19.046	9.559
O	9.929	0.879	2.864
O	19.885	9.090	3.904
O	10.345	10.839	10.596
O	19.872	17.292	3.963
O	10.358	2.637	10.659
O	0.396	7.282	9.637
O	9.811	12.640	2.936
O	0.397	2.692	9.634
O	9.811	17.232	2.940
O	19.874	12.584	3.962
O	10.359	7.340	10.662
O	8.817	14.937	2.070
O	1.392	4.988	8.765
O	11.232	4.988	11.529

O	19.001	14.938	4.828
O	3.541	14.939	1.543
O	6.669	4.989	8.235
O	16.268	4.984	11.459
O	13.956	14.934	4.780
O	5.853	14.938	6.672
O	4.358	4.988	13.362
O	14.635	4.988	5.988
O	15.588	14.938	12.669
O	1.851	14.938	7.304
O	8.358	4.988	0.615
O	17.976	4.988	6.027
O	12.256	14.937	12.717
H	14.910	14.925	7.751
H	14.669	14.952	9.592
H	17.123	14.960	9.924
H	17.379	14.933	8.083
C	15.361	14.940	8.746
C	16.683	14.945	8.925

S.12.8 Adsorbed ethene, proton on O20

Si	8.576	1.138	1.983
Si	1.608	18.815	8.658
Si	11.613	11.032	11.597
Si	18.553	8.900	4.885
Si	11.628	18.828	11.500
Si	18.565	1.152	4.832
Si	8.580	8.878	2.004
Si	1.591	11.092	8.664
Si	6.114	0.632	3.809
Si	4.049	19.310	10.509
Si	14.066	10.452	9.734
Si	16.179	9.403	2.939
Si	14.063	19.426	9.612
Si	16.174	0.590	2.904
Si	6.101	9.378	3.815
Si	4.047	10.591	10.506
Si	5.780	1.114	6.874
Si	4.403	18.854	0.186
Si	14.463	11.280	6.782
Si	15.736	8.649	0.015
Si	14.469	18.725	6.639
Si	15.741	1.262	13.338
Si	5.775	8.903	6.896
Si	4.375	11.031	0.190
Si	2.563	1.408	6.895
Si	7.611	18.576	0.198
Si	17.650	11.406	6.661
Si	12.553	8.592	13.366
Si	17.666	18.581	6.601
Si	12.554	1.345	13.309
Si	2.561	8.602	6.932
Si	7.566	11.314	0.226
Si	1.444	0.743	4.063
Si	8.721	19.239	10.750
Si	18.686	10.575	9.461
Si	11.504	9.401	2.747
Si	18.701	19.323	9.409
Si	11.491	0.630	2.720
Si	1.464	9.269	4.108
Si	8.712	10.661	10.791
Si	3.649	1.402	2.143
Si	6.511	18.558	8.841
Si	16.581	10.995	11.574

Si	13.661	8.983	4.809
Si	16.561	18.844	11.468
Si	13.674	1.135	4.740
Si	3.614	8.599	2.145
Si	6.531	11.353	8.850
Si	8.447	16.492	2.337
Si	1.701	3.448	9.071
Si	11.618	6.520	11.299
Si	18.623	13.406	4.572
Si	11.643	3.445	11.227
Si	18.568	16.505	4.514
Si	8.397	13.392	2.338
Si	1.707	6.550	9.101
Si	5.964	17.390	3.900
Si	4.215	2.553	10.590
Si	14.008	7.326	9.421
Si	16.209	12.491	2.758
Si	13.996	2.673	9.319
Si	16.185	17.372	2.671
Si	5.952	12.522	3.927
Si	4.220	7.447	10.609
Si	5.448	16.514	6.858
Si	4.735	3.444	0.167
Si	14.724	6.586	6.463
Si	15.466	13.378	13.203
Si	14.719	3.484	6.375
Si	15.473	16.491	13.110
Si	5.458	13.400	6.890
Si	4.725	6.559	0.187
Si	2.291	16.456	6.864
Si	7.882	3.508	0.208
Si	17.828	6.547	6.636
Si	12.353	13.423	13.305
Si	17.826	3.506	6.582
Si	12.359	16.456	13.229
Si	2.332	13.453	6.897
Si	7.859	6.505	0.231
Si	1.432	17.491	4.005
Si	8.734	2.485	10.730
Si	18.796	7.439	9.454
Si	11.342	12.512	2.719
Si	18.791	2.554	9.398
Si	11.389	17.397	2.670
Si	1.509	12.410	4.053
Si	8.715	7.509	10.756
Si	3.554	16.498	2.027
Si	6.638	3.457	8.714
Si	16.498	6.560	11.257
Si	16.476	3.403	11.184
Si	13.706	16.617	4.500
Si	3.564	13.405	2.030
Si	6.634	6.548	8.725
Al	13.651	13.421	4.495
O	7.312	1.333	2.975
O	2.856	18.606	9.669
O	12.934	11.132	10.660
O	17.274	8.712	3.913
O	12.940	18.745	10.555
O	17.252	1.278	3.894
O	7.322	8.686	3.006
O	2.848	11.281	9.664
O	6.369	0.860	5.387
O	3.789	19.075	12.086
O	14.127	11.319	8.355
O	16.069	8.505	1.591
O	14.115	18.602	8.217
O	16.146	1.430	1.515
O	6.329	9.136	5.395
O	3.778	10.840	12.079
O	4.161	1.159	6.833

O	6.023	18.890	0.129
O	16.033	11.295	6.448
O	14.140	8.871	13.141
O	16.075	18.824	6.406
O	14.140	1.026	13.169
O	4.154	8.893	6.901
O	5.994	10.925	0.148
O	1.971	1.518	5.391
O	8.209	18.456	12.079
O	17.983	11.404	8.246
O	12.195	8.518	1.562
O	18.045	18.491	8.175
O	12.131	1.478	1.486
O	1.998	8.470	5.419
O	8.174	11.442	12.109
O	2.141	1.376	2.740
O	8.023	18.606	9.427
O	18.051	11.017	10.888
O	12.171	9.012	4.179
O	18.047	18.851	10.816
O	12.174	1.070	4.126
O	2.117	8.612	2.774
O	8.037	11.302	9.459
O	4.698	1.310	3.388
O	5.471	18.642	10.094
O	15.515	10.519	10.438
O	14.733	9.402	3.674
O	15.512	19.347	10.332
O	14.703	0.638	3.585
O	4.694	8.704	3.363
O	5.466	11.265	10.082
O	7.323	16.599	3.506
O	2.848	3.343	10.217
O	12.824	6.573	10.218
O	17.434	13.263	3.497
O	12.815	3.452	10.108
O	17.332	16.550	3.469
O	7.314	13.318	3.551
O	2.851	6.651	10.251
O	5.773	17.341	5.503
O	4.446	2.616	12.187
O	14.022	6.740	7.916
O	16.103	13.180	1.289
O	13.986	3.222	7.797
O	16.149	16.773	1.169
O	5.729	12.563	5.528
O	4.464	7.395	12.205
O	3.868	16.672	7.203
O	6.306	3.293	0.550
O	16.281	7.061	6.560
O	13.901	12.924	13.216
O	16.275	3.014	6.493
O	13.909	16.944	13.146
O	3.894	13.252	7.309
O	6.289	6.708	0.605
O	2.032	16.676	5.277
O	8.127	3.298	11.999
O	18.321	6.554	8.180
O	11.848	13.420	1.456
O	18.331	3.442	8.120
O	11.852	16.526	1.381
O	2.169	13.221	5.298
O	8.069	6.716	12.017
O	2.103	16.907	2.644
O	8.085	3.091	9.368
O	18.019	6.899	10.778
O	12.024	13.033	4.071
O	18.004	3.090	10.717
O	12.170	16.875	3.991
O	2.119	12.986	2.660

O	8.082	6.916	9.381
O	4.692	16.692	3.176
O	5.473	3.236	9.829
O	15.456	7.086	10.118
O	14.845	12.586	3.591
O	15.446	2.957	10.002
O	14.732	17.230	3.379
O	4.699	13.225	3.181
O	5.470	6.757	9.843
O	6.083	18.944	3.435
O	4.074	0.998	10.139
O	13.685	8.920	9.380
O	16.626	10.917	2.574
O	13.684	1.081	9.340
O	16.594	18.946	2.621
O	6.074	10.969	3.457
O	4.081	9.001	10.151
O	1.817	19.061	4.183
O	8.333	0.917	10.881
O	18.418	8.995	9.183
O	11.745	10.963	2.389
O	18.410	1.000	9.131
O	11.746	18.957	2.403
O	1.893	10.837	4.219
O	8.332	9.083	10.901
O	8.771	2.471	1.075
O	1.407	17.484	7.749
O	11.438	12.428	12.402
O	18.757	7.539	5.752
O	11.455	17.415	12.284
O	18.744	2.543	5.656
O	8.756	7.549	1.082
O	1.414	12.421	7.744
O	8.372	19.771	0.988
O	1.843	0.178	7.668
O	11.721	9.791	12.642
O	18.349	10.148	5.913
O	11.734	0.137	12.589
O	18.455	19.814	5.888
O	8.375	10.154	1.023
O	1.789	9.818	7.680
O	7.891	17.171	0.965
O	2.232	2.794	7.677
O	12.121	7.173	12.701
O	18.170	12.800	6.021
O	12.194	2.756	12.591
O	18.113	17.173	5.927
O	7.762	12.737	0.984
O	2.246	7.216	7.717
O	3.839	2.810	1.358
O	6.326	17.144	8.066
O	16.255	12.486	12.101
O	13.948	7.497	5.377
O	16.235	17.333	11.953
O	13.985	2.663	5.188
O	3.803	7.189	1.361
O	6.374	12.771	8.072
O	3.867	0.145	1.143
O	6.266	19.804	7.834
O	16.544	9.931	12.801
O	13.723	10.055	6.045
O	16.517	19.864	12.735
O	13.780	0.179	6.051
O	3.785	9.856	1.135
O	6.308	10.111	7.834
O	3.885	17.415	0.730
O	6.370	2.529	7.411
O	16.212	7.280	12.678
O	13.791	12.730	6.236
O	16.169	2.618	12.566

O	13.880	17.410	5.915
O	3.901	12.484	0.737
O	6.357	7.484	7.429
O	19.866	0.938	3.890
O	10.324	19.061	10.566
O	0.249	10.893	9.547
O	9.924	9.065	2.885
O	0.270	19.047	9.536
O	9.906	0.929	2.880
O	19.874	9.142	3.981
O	10.321	10.837	10.635
O	19.842	17.315	3.900
O	10.350	2.639	10.656
O	0.378	7.301	9.667
O	9.717	12.590	2.818
O	0.371	2.694	9.627
O	9.786	17.231	2.886
O	19.922	12.593	4.027
O	10.331	7.328	10.715
O	8.763	14.937	2.019
O	1.355	5.003	8.789
O	11.215	4.973	11.569
O	19.000	14.967	4.791
O	3.525	14.950	1.539
O	6.641	5.004	8.226
O	16.304	4.978	11.491
O	13.985	15.073	4.759
O	5.858	14.956	6.672
O	4.326	5.002	13.350
O	14.623	5.050	5.973
O	15.607	14.922	12.732
O	1.840	14.952	7.270
O	8.340	5.007	0.626
O	17.964	5.037	6.055
O	12.211	14.926	12.699
H	11.117	14.670	6.556
H	12.390	15.611	7.535
H	12.335	13.852	9.292
H	11.060	12.913	8.317
H	13.178	13.195	6.884
C	11.750	14.729	7.446
C	11.723	13.779	8.390

S.12.9 Adsorbed benzene, proton on O20

Si	8.590	1.142	1.974
Si	1.630	18.823	8.651
Si	11.622	11.026	11.600
Si	18.563	8.920	4.895
Si	11.646	18.831	11.480
Si	18.584	1.171	4.813
Si	8.593	8.884	2.005
Si	1.598	11.100	8.665
Si	6.131	0.637	3.805
Si	4.063	19.314	10.507
Si	14.087	10.461	9.740
Si	16.184	9.409	2.944
Si	14.074	19.440	9.589
Si	16.199	0.593	2.887
Si	6.112	9.383	3.815
Si	4.054	10.595	10.508
Si	5.794	1.124	6.867
Si	4.425	18.858	0.179
Si	14.476	11.309	6.788

Si	15.755	8.630	0.027
Si	14.495	18.761	6.615
Si	15.756	1.243	13.318
Si	5.784	8.907	6.897
Si	4.383	11.033	0.193
Si	2.578	1.420	6.884
Si	7.631	18.580	0.186
Si	17.659	11.430	6.670
Si	12.572	8.588	13.377
Si	17.691	18.603	6.579
Si	12.572	1.345	13.288
Si	2.572	8.610	6.936
Si	7.572	11.317	0.231
Si	1.458	0.751	4.051
Si	8.741	19.247	10.738
Si	18.691	10.582	9.468
Si	11.520	9.410	2.750
Si	18.725	19.323	9.389
Si	11.503	0.643	2.697
Si	1.476	9.278	4.114
Si	8.713	10.657	10.801
Si	3.670	1.406	2.138
Si	6.522	18.568	8.838
Si	16.602	10.991	11.602
Si	13.667	9.001	4.824
Si	16.570	18.835	11.433
Si	13.696	1.156	4.710
Si	3.620	8.603	2.146
Si	6.541	11.354	8.853
Si	8.466	16.498	2.326
Si	1.713	3.455	9.060
Si	11.624	6.529	11.308
Si	18.642	13.413	4.580
Si	11.667	3.455	11.207
Si	18.575	16.511	4.486
Si	8.411	13.396	2.337
Si	1.715	6.557	9.104
Si	5.985	17.394	3.896
Si	4.226	2.557	10.583
Si	14.028	7.331	9.433
Si	16.204	12.496	2.788
Si	14.006	2.687	9.292
Si	16.210	17.374	2.637
Si	5.970	12.529	3.930
Si	4.227	7.451	10.611
Si	5.463	16.520	6.856
Si	4.747	3.450	0.160
Si	14.733	6.596	6.472
Si	15.475	13.383	13.225
Si	14.735	3.496	6.348
Si	15.490	16.494	13.080
Si	5.472	13.405	6.895
Si	4.733	6.564	0.189
Si	2.303	16.464	6.854
Si	7.898	3.514	0.200
Si	17.837	6.563	6.639
Si	12.363	13.425	13.291
Si	17.842	3.520	6.566
Si	12.373	16.457	13.210
Si	2.347	13.461	6.901
Si	7.865	6.509	0.237
Si	1.443	17.498	3.994
Si	8.756	2.494	10.724
Si	18.802	7.446	9.460
Si	11.360	12.519	2.709
Si	18.806	2.552	9.379
Si	11.409	17.410	2.649
Si	1.530	12.417	4.057
Si	8.715	7.510	10.766
Si	3.576	16.504	2.024

Si	6.654	3.461	8.712
Si	16.516	6.552	11.272
Si	16.487	3.396	11.163
Si	13.733	16.633	4.472
Si	3.582	13.412	2.030
Si	6.642	6.552	8.726
Al	13.651	13.441	4.516
O	7.325	1.337	2.966
O	2.879	18.605	9.659
O	12.930	11.126	10.646
O	17.288	8.734	3.919
O	12.959	18.747	10.535
O	17.268	1.292	3.880
O	7.337	8.694	3.009
O	2.853	11.285	9.669
O	6.391	0.865	5.383
O	3.800	19.079	12.083
O	14.161	11.332	8.365
O	16.079	8.496	1.606
O	14.113	18.625	8.188
O	16.180	1.419	1.489
O	6.337	9.139	5.395
O	3.788	10.845	12.081
O	4.177	1.179	6.816
O	6.044	18.895	0.111
O	16.043	11.345	6.443
O	14.160	8.852	13.144
O	16.103	18.884	6.416
O	14.154	1.003	13.172
O	4.164	8.900	6.906
O	6.002	10.918	0.155
O	1.980	1.525	5.382
O	8.235	18.462	12.068
O	17.979	11.413	8.259
O	12.220	8.521	1.575
O	18.092	18.486	8.147
O	12.129	1.496	1.458
O	2.010	8.475	5.423
O	8.177	11.448	12.114
O	2.161	1.377	2.730
O	8.037	18.623	9.414
O	18.065	11.019	10.899
O	12.178	9.035	4.190
O	18.059	18.846	10.789
O	12.195	1.084	4.098
O	2.125	8.615	2.780
O	8.045	11.294	9.465
O	4.714	1.315	3.388
O	5.490	18.652	10.098
O	15.521	10.544	10.470
O	14.742	9.397	3.685
O	15.530	19.357	10.296
O	14.722	0.646	3.557
O	4.706	8.710	3.358
O	5.471	11.270	10.081
O	7.347	16.608	3.501
O	2.863	3.350	10.202
O	12.828	6.602	10.227
O	17.451	13.247	3.512
O	12.827	3.478	10.073
O	17.353	16.535	3.424
O	7.337	13.320	3.561
O	2.857	6.656	10.257
O	5.802	17.341	5.501
O	4.448	2.623	12.181
O	14.048	6.723	7.936
O	16.062	13.218	1.336
O	13.994	3.214	7.763
O	16.186	16.813	1.121
O	5.742	12.572	5.530

O	4.478	7.400	12.207
O	3.881	16.680	7.186
O	6.321	3.294	0.533
O	16.289	7.076	6.557
O	13.911	12.924	13.193
O	16.291	3.030	6.473
O	13.925	16.940	13.127
O	3.909	13.261	7.318
O	6.295	6.713	0.616
O	2.037	16.679	5.267
O	8.154	3.311	11.992
O	18.322	6.561	8.186
O	11.867	13.426	1.446
O	18.348	3.444	8.103
O	11.865	16.535	1.362
O	2.194	13.226	5.302
O	8.066	6.711	12.021
O	2.125	16.919	2.637
O	8.103	3.098	9.363
O	18.032	6.902	10.787
O	12.039	13.038	4.059
O	18.015	3.081	10.698
O	12.197	16.906	3.970
O	2.140	12.994	2.664
O	8.088	6.920	9.386
O	4.712	16.695	3.175
O	5.491	3.234	9.828
O	15.467	7.087	10.145
O	14.862	12.577	3.656
O	15.458	2.978	9.970
O	14.751	17.219	3.327
O	4.722	13.236	3.178
O	5.474	6.759	9.841
O	6.099	18.948	3.432
O	4.082	1.002	10.135
O	13.727	8.928	9.367
O	16.610	10.925	2.559
O	13.689	1.096	9.336
O	16.627	18.948	2.626
O	6.086	10.975	3.461
O	4.088	9.005	10.153
O	1.823	19.067	4.179
O	8.356	0.926	10.879
O	18.423	9.002	9.190
O	11.758	10.968	2.379
O	18.428	0.998	9.108
O	11.756	18.972	2.371
O	1.914	10.844	4.222
O	8.322	9.081	10.917
O	8.785	2.474	1.065
O	1.423	17.496	7.738
O	11.444	12.425	12.399
O	18.767	7.561	5.764
O	11.473	17.419	12.263
O	18.761	2.565	5.633
O	8.764	7.555	1.082
O	1.428	12.430	7.747
O	8.389	19.774	0.981
O	1.868	0.188	7.664
O	11.749	9.794	12.652
O	18.351	10.167	5.923
O	11.747	0.143	12.565
O	18.489	19.833	5.871
O	8.388	10.161	1.026
O	1.798	9.827	7.681
O	7.907	17.175	0.954
O	2.242	2.807	7.663
O	12.123	7.173	12.716
O	18.204	12.819	6.039
O	12.241	2.757	12.557

O	18.099	17.195	5.883
O	7.759	12.741	0.991
O	2.258	7.224	7.723
O	3.859	2.815	1.356
O	6.334	17.151	8.067
O	16.299	12.473	12.165
O	13.940	7.520	5.410
O	16.232	17.320	11.897
O	14.010	2.686	5.147
O	3.806	7.194	1.360
O	6.391	12.772	8.073
O	3.896	0.150	1.138
O	6.266	19.809	7.828
O	16.571	9.902	12.806
O	13.739	10.083	6.051
O	16.524	19.840	12.712
O	13.799	0.213	6.031
O	3.784	9.862	1.136
O	6.320	10.115	7.834
O	3.912	17.419	0.728
O	6.390	2.534	7.407
O	16.234	7.255	12.703
O	13.777	12.757	6.264
O	16.171	2.594	12.532
O	13.937	17.449	5.868
O	3.916	12.489	0.738
O	6.367	7.488	7.430
O	19.882	0.957	3.867
O	10.342	19.065	10.544
O	0.253	10.901	9.544
O	9.940	9.068	2.883
O	0.295	19.058	9.533
O	9.919	0.937	2.873
O	19.886	9.163	3.993
O	10.324	10.812	10.651
O	19.854	17.319	3.879
O	10.372	2.646	10.644
O	0.385	7.309	9.666
O	9.734	12.594	2.804
O	0.385	2.694	9.614
O	9.807	17.237	2.873
O	19.944	12.603	4.035
O	10.331	7.333	10.730
O	8.774	14.941	2.014
O	1.362	5.011	8.787
O	11.233	4.977	11.565
O	19.011	14.978	4.784
O	3.542	14.957	1.537
O	6.651	5.009	8.226
O	16.328	4.967	11.492
O	14.003	15.092	4.745
O	5.876	14.961	6.676
O	4.338	5.007	13.349
O	14.634	5.066	5.962
O	15.627	14.919	12.730
O	1.855	14.961	7.269
O	8.348	5.012	0.632
O	17.979	5.056	6.051
O	12.220	14.927	12.685
H	13.138	13.166	6.915
H	12.725	16.149	8.534
H	10.959	16.980	6.998
H	9.259	15.410	6.082
H	11.059	12.169	8.278
H	12.759	13.745	9.208
H	9.323	13.002	6.703
C	11.982	15.458	8.135
C	10.988	15.924	7.272
C	10.034	15.041	6.758
C	10.069	13.690	7.104

C	11.055	13.218	7.977
C	12.015	14.102	8.492

S.12.10 Adsorbed ethylbenzene, proton on O20

Si	8.615	1.164	1.992
Si	1.665	18.833	8.658
Si	11.606	11.074	11.495
Si	18.562	8.890	4.777
Si	11.648	18.855	11.524
Si	18.633	1.165	4.868
Si	8.580	8.905	1.948
Si	1.648	11.096	8.599
Si	6.174	0.586	3.892
Si	4.093	19.397	10.567
Si	14.132	10.463	9.721
Si	16.262	9.369	2.707
Si	14.083	19.419	9.619
Si	16.218	0.596	2.974
Si	6.138	9.445	3.838
Si	4.045	10.538	10.552
Si	5.787	1.334	6.851
Si	4.509	18.682	0.149
Si	14.473	11.174	6.669
Si	15.762	8.678	13.199
Si	14.509	18.719	6.656
Si	15.775	1.220	13.373
Si	5.712	8.689	6.813
Si	4.435	11.272	0.100
Si	2.589	1.387	6.867
Si	7.709	18.646	0.158
Si	17.678	11.378	6.620
Si	12.592	8.680	13.279
Si	17.712	18.578	6.607
Si	12.575	1.361	13.354
Si	2.507	8.617	6.832
Si	7.610	11.306	0.117
Si	1.520	0.642	4.050
Si	8.750	19.376	10.709
Si	18.778	10.628	9.454
Si	11.497	9.373	2.657
Si	18.767	19.303	9.408
Si	11.517	0.627	2.780
Si	1.502	9.421	4.036
Si	8.713	10.537	10.712
Si	3.677	1.123	2.019
Si	6.590	18.863	8.694
Si	16.648	11.155	11.481
Si	13.771	8.887	4.543
Si	16.586	18.827	11.450
Si	13.697	1.171	4.805
Si	3.611	8.939	1.970
Si	6.543	11.041	8.706
Si	8.543	16.495	2.208
Si	1.705	3.469	8.937
Si	11.744	6.540	11.163
Si	18.613	13.391	4.485
Si	11.744	3.488	11.277
Si	18.540	16.475	4.483
Si	8.476	13.414	2.158
Si	1.658	6.550	8.939
Si	6.171	17.341	4.102
Si	4.095	2.645	10.800
Si	14.126	7.294	9.343

Si	16.132	12.465	2.784
Si	14.110	2.651	9.402
Si	16.174	17.365	2.680
Si	6.178	12.590	4.107
Si	4.082	7.401	10.755
Si	5.500	16.508	7.027
Si	4.765	3.473	0.366
Si	14.780	6.667	6.377
Si	15.441	13.412	13.232
Si	14.757	3.511	6.463
Si	15.486	16.530	13.104
Si	5.495	13.399	7.060
Si	4.743	6.577	0.317
Si	2.396	16.493	6.866
Si	7.869	3.507	0.240
Si	17.893	6.577	6.572
Si	12.363	13.438	13.184
Si	17.866	3.512	6.633
Si	12.375	16.492	13.252
Si	2.404	13.446	6.864
Si	7.840	6.550	0.189
Si	1.391	17.393	4.035
Si	8.860	2.622	10.763
Si	18.840	7.474	9.457
Si	11.380	12.493	2.625
Si	18.866	2.523	9.412
Si	11.423	17.377	2.729
Si	1.481	12.539	4.019
Si	8.823	7.412	10.745
Si	3.719	16.564	2.274
Si	6.556	3.459	8.976
Si	16.515	6.441	11.131
Si	16.601	3.321	11.241
Si	13.739	16.564	4.520
Si	3.759	13.406	2.243
Si	6.540	6.607	8.929
Al	13.634	13.377	4.530
O	7.307	1.237	2.941
O	2.960	18.730	9.624
O	12.910	11.134	10.533
O	17.336	8.722	3.735
O	12.960	18.755	10.578
O	17.338	1.302	3.906
O	7.285	8.771	2.913
O	2.968	11.176	9.529
O	6.138	1.435	5.274
O	4.134	18.570	11.961
O	13.986	10.944	8.181
O	16.333	8.516	1.325
O	14.112	18.589	8.226
O	16.181	1.364	1.548
O	6.063	8.623	5.234
O	4.000	11.400	11.926
O	4.184	1.178	7.087
O	6.112	18.862	0.361
O	16.051	11.422	6.540
O	14.176	9.046	13.219
O	16.119	18.857	6.472
O	14.165	1.077	13.184
O	4.107	8.777	7.060
O	6.026	10.956	0.224
O	2.222	1.428	5.290
O	8.090	18.587	11.968
O	18.135	11.382	8.168
O	12.093	8.484	1.425
O	18.137	18.453	8.170
O	12.172	1.448	1.537
O	2.148	8.558	5.255
O	8.077	11.382	11.947
O	2.181	1.120	2.647

O	8.086	18.855	9.323
O	18.123	11.227	10.810
O	12.231	8.931	4.040
O	18.079	18.863	10.812
O	12.202	1.102	4.173
O	2.128	8.899	2.632
O	8.054	10.983	9.297
O	4.722	0.672	3.179
O	5.545	19.305	9.856
O	15.547	10.999	10.286
O	14.759	9.229	3.309
O	15.545	19.338	10.312
O	14.755	0.721	3.659
O	4.694	9.365	3.105
O	5.529	10.625	9.903
O	7.276	16.567	3.214
O	2.963	3.430	9.954
O	12.883	6.501	10.007
O	17.382	13.248	3.461
O	13.009	3.450	10.271
O	17.291	16.487	3.455
O	7.321	13.392	3.296
O	2.967	6.623	9.885
O	6.223	16.701	5.588
O	4.075	3.244	12.301
O	14.019	7.143	7.735
O	15.826	13.271	1.406
O	14.068	3.256	7.905
O	16.182	16.886	1.136
O	6.203	13.159	5.621
O	4.079	6.744	12.231
O	3.948	16.994	6.915
O	6.322	2.995	0.297
O	16.348	7.093	6.492
O	13.901	12.924	13.001
O	16.313	3.032	6.518
O	13.923	16.989	13.148
O	3.942	12.918	6.977
O	6.296	7.066	0.263
O	1.851	16.546	5.342
O	8.405	3.427	12.096
O	18.418	6.696	8.099
O	11.905	13.359	1.345
O	18.350	3.454	8.182
O	11.888	16.544	1.413
O	1.942	13.409	5.311
O	8.341	6.545	12.029
O	2.175	16.819	2.726
O	8.096	3.255	9.470
O	18.041	6.843	10.727
O	12.042	13.050	3.966
O	18.129	3.001	10.780
O	12.193	16.825	4.042
O	2.221	13.105	2.685
O	8.079	6.852	9.409
O	4.692	17.133	3.454
O	5.561	2.875	10.128
O	15.551	6.683	9.833
O	14.857	12.441	3.753
O	15.590	2.851	10.049
O	14.706	17.166	3.337
O	4.723	12.844	3.431
O	5.547	7.222	10.068
O	6.523	18.924	4.185
O	3.743	1.061	10.840
O	14.041	8.851	9.806
O	16.599	10.934	2.425
O	13.719	1.078	9.355
O	16.600	18.933	2.767
O	6.511	11.001	4.116

O	3.701	8.978	10.854
O	1.766	18.952	4.272
O	8.457	1.061	10.917
O	18.450	9.042	9.319
O	11.776	10.935	2.334
O	18.490	0.977	9.095
O	11.771	18.947	2.505
O	1.882	10.985	4.272
O	8.427	8.964	10.996
O	8.779	2.578	1.208
O	1.504	17.448	7.824
O	11.422	12.506	12.238
O	18.793	7.494	5.579
O	11.456	17.455	12.324
O	18.792	2.537	5.726
O	8.758	7.534	1.090
O	1.467	12.489	7.780
O	8.489	19.872	0.889
O	1.804	0.168	7.605
O	11.748	9.891	12.597
O	18.222	10.050	5.866
O	11.769	0.161	12.610
O	18.505	19.808	5.895
O	8.434	10.151	0.910
O	1.747	9.877	7.526
O	8.181	17.240	0.812
O	2.118	2.801	7.513
O	12.309	7.299	12.480
O	18.273	12.707	5.923
O	12.149	2.774	12.679
O	18.118	17.183	5.886
O	7.907	12.757	0.781
O	1.976	7.239	7.502
O	3.992	2.625	1.504
O	6.264	17.371	8.161
O	16.421	12.525	12.300
O	14.086	7.408	5.119
O	16.248	17.307	11.900
O	13.977	2.691	5.302
O	3.932	7.460	1.400
O	6.263	12.554	8.205
O	3.753	0.081	0.773
O	6.529	0.021	7.461
O	16.574	9.874	12.468
O	13.962	9.972	5.742
O	16.502	19.802	12.751
O	13.801	0.166	6.079
O	3.619	10.035	0.769
O	6.406	10.014	7.452
O	4.011	17.318	0.869
O	6.321	2.687	7.568
O	15.998	7.288	12.408
O	13.662	12.591	6.228
O	16.283	2.559	12.627
O	13.976	17.397	5.903
O	4.082	12.676	0.831
O	6.295	7.341	7.502
O	19.959	0.978	3.956
O	10.344	19.095	10.592
O	0.353	10.881	9.547
O	9.908	9.096	2.859
O	0.337	19.030	9.565
O	9.928	0.931	2.913
O	19.915	9.241	3.962
O	10.306	10.812	10.566
O	19.812	17.238	3.803
O	10.470	2.759	10.566
O	0.419	7.300	9.692
O	9.752	12.587	2.708
O	0.451	2.676	9.609

O	9.819	17.190	2.943
O	19.903	12.670	3.804
O	10.432	7.283	10.551
O	8.878	14.952	1.850
O	1.276	5.004	8.658
O	11.365	5.029	11.602
O	18.950	14.942	4.796
O	3.994	14.990	2.030
O	6.254	5.029	8.723
O	16.439	4.892	11.562
O	14.031	15.022	4.788
O	5.589	14.958	7.477
O	4.653	5.032	0.787
O	14.642	5.082	6.111
O	15.609	14.954	12.771
O	2.276	14.968	7.409
O	7.974	5.039	0.764
O	18.020	5.034	6.092
O	12.223	14.978	12.687
H	9.528	15.853	5.901
H	11.312	16.745	7.370
H	12.935	12.890	6.856
H	12.041	12.783	8.885
H	10.280	11.880	7.391
H	9.005	13.417	5.892
H	12.864	16.473	9.088
H	12.629	15.099	10.169
H	15.037	15.361	9.533
H	14.623	15.163	7.813
H	14.418	13.809	8.953
C	14.321	14.899	8.837
C	12.893	15.376	9.135
C	10.089	15.170	6.544
C	11.099	15.674	7.368
C	11.837	14.829	8.207
C	11.533	13.452	8.187
C	10.517	12.945	7.364
C	9.795	13.806	6.536

S.12.11 Coadsorbed ethene and benzene, proton on O20

Si	8.561	1.119	1.930
Si	1.621	18.838	8.612
Si	11.625	11.021	11.569
Si	18.608	8.884	4.870
Si	11.611	18.813	11.447
Si	18.601	1.177	4.767
Si	8.572	8.860	1.992
Si	1.607	11.092	8.661
Si	6.127	0.580	3.852
Si	4.048	19.377	10.549
Si	14.074	10.447	9.680
Si	16.204	9.395	2.940
Si	14.040	19.440	9.540
Si	16.209	0.601	2.834
Si	6.143	9.436	3.887
Si	4.029	10.525	10.579
Si	5.720	1.370	6.793
Si	4.459	18.594	0.102
Si	14.508	11.301	6.746
Si	15.759	8.631	0.014
Si	14.471	18.782	6.567
Si	15.740	1.234	13.266
Si	5.723	8.714	6.864
Si	4.435	11.232	0.151

Si	2.516	1.387	6.799
Si	7.662	18.572	0.114
Si	17.698	11.348	6.663
Si	12.558	8.587	13.369
Si	17.672	18.637	6.552
Si	12.552	1.312	13.255
Si	2.525	8.644	6.879
Si	7.626	11.287	0.180
Si	1.480	0.615	3.982
Si	8.696	19.367	10.686
Si	18.726	10.560	9.483
Si	11.484	9.383	2.753
Si	18.723	19.317	9.374
Si	11.473	0.656	2.667
Si	1.497	9.383	4.060
Si	8.715	10.528	10.764
Si	3.641	1.070	1.949
Si	6.535	18.895	8.650
Si	16.569	10.987	11.545
Si	13.659	9.012	4.801
Si	16.541	18.812	11.377
Si	13.691	1.186	4.646
Si	3.634	8.894	2.023
Si	6.550	11.058	8.743
Si	8.519	16.494	2.192
Si	1.644	3.447	8.894
Si	11.690	6.509	11.279
Si	18.542	13.413	4.560
Si	11.712	3.457	11.143
Si	18.495	16.493	4.462
Si	8.453	13.412	2.235
Si	1.679	6.530	8.954
Si	6.126	17.342	4.074
Si	4.055	2.613	10.760
Si	14.095	7.332	9.423
Si	16.163	12.485	2.718
Si	14.038	2.694	9.234
Si	16.165	17.376	2.592
Si	6.127	12.577	4.135
Si	4.060	7.381	10.804
Si	5.463	16.508	7.005
Si	4.729	3.450	0.303
Si	14.771	6.600	6.475
Si	15.454	13.366	13.174
Si	14.749	3.511	6.291
Si	15.454	16.487	13.046
Si	5.473	13.402	7.094
Si	4.731	6.549	0.361
Si	2.355	16.481	6.861
Si	7.829	3.477	0.174
Si	17.872	6.552	6.631
Si	12.336	13.406	13.305
Si	17.851	3.506	6.532
Si	12.340	16.451	13.191
Si	2.377	13.430	6.917
Si	7.829	6.515	0.215
Si	1.364	17.369	4.018
Si	8.810	2.598	10.722
Si	18.839	7.419	9.471
Si	11.326	12.502	2.741
Si	18.795	2.553	9.375
Si	11.385	17.422	2.642
Si	1.416	12.520	4.073
Si	8.820	7.397	10.769
Si	3.680	16.520	2.250
Si	6.506	3.439	8.934
Si	16.547	6.560	11.257
Si	16.477	3.410	11.121
Si	13.718	16.633	4.428
Si	3.693	13.360	2.292

Si	6.515	6.595	8.980
Al	13.652	13.435	4.467
O	7.264	1.215	2.892
O	2.911	18.754	9.583
O	12.931	11.106	10.609
O	17.311	8.725	3.916
O	12.911	18.769	10.484
O	17.299	1.290	3.811
O	7.277	8.749	2.959
O	2.913	11.183	9.610
O	6.080	1.455	5.217
O	4.089	18.497	11.911
O	14.144	11.330	8.313
O	16.120	8.505	1.585
O	14.050	18.646	8.127
O	16.206	1.411	1.426
O	6.082	8.622	5.288
O	4.025	11.356	11.972
O	4.116	1.226	7.025
O	6.063	18.763	0.318
O	16.088	11.150	6.472
O	14.156	8.806	13.159
O	16.083	18.926	6.417
O	14.137	0.974	13.171
O	4.119	8.865	7.096
O	6.035	10.989	0.313
O	2.156	1.427	5.220
O	8.042	18.534	11.921
O	18.051	11.381	8.245
O	12.178	8.520	1.558
O	18.104	18.504	8.109
O	12.078	1.498	1.411
O	2.160	8.569	5.303
O	8.071	11.355	12.004
O	2.146	1.075	2.577
O	8.032	18.912	9.279
O	18.054	11.021	10.886
O	12.172	8.969	4.166
O	18.038	18.796	10.748
O	12.186	1.134	4.043
O	2.145	8.871	2.666
O	8.049	11.012	9.366
O	4.684	0.653	3.122
O	5.494	19.307	9.824
O	15.521	10.506	10.395
O	14.751	9.351	3.660
O	15.501	19.316	10.233
O	14.729	0.688	3.498
O	4.694	9.350	3.166
O	5.499	10.626	9.904
O	7.248	16.599	3.185
O	2.922	3.348	9.876
O	12.963	6.578	10.286
O	17.312	13.293	3.533
O	12.893	3.509	10.036
O	17.263	16.513	3.414
O	7.220	13.409	3.287
O	2.958	6.568	9.945
O	6.151	16.674	5.547
O	4.039	3.295	12.227
O	14.110	6.660	7.954
O	16.145	13.151	1.232
O	14.008	3.213	7.703
O	16.167	16.813	1.077
O	6.150	13.148	5.646
O	4.030	6.777	12.302
O	3.905	16.985	6.913
O	6.282	2.963	0.216
O	16.328	7.078	6.549
O	13.889	12.915	13.238

O	16.300	3.025	6.409
O	13.891	16.938	13.111
O	3.916	12.916	7.050
O	6.285	7.031	0.278
O	1.818	16.528	5.332
O	8.363	3.455	12.026
O	18.361	6.560	8.177
O	11.805	13.387	1.449
O	18.336	3.406	8.074
O	11.818	16.563	1.336
O	1.916	13.365	5.365
O	8.352	6.543	12.065
O	2.139	16.784	2.711
O	8.045	3.180	9.407
O	18.083	6.847	10.793
O	12.022	13.027	4.084
O	18.020	3.119	10.689
O	12.171	16.888	3.956
O	2.146	13.099	2.737
O	8.061	6.829	9.444
O	4.660	17.142	3.395
O	5.515	2.813	10.068
O	15.555	7.171	10.116
O	14.751	12.576	3.461
O	15.503	2.976	9.888
O	14.690	17.233	3.253
O	4.651	12.786	3.480
O	5.537	7.182	10.146
O	6.467	18.927	4.190
O	3.714	1.031	10.893
O	13.720	8.912	9.296
O	16.623	10.919	2.586
O	13.697	1.109	9.302
O	16.604	18.943	2.595
O	6.511	10.998	4.141
O	3.678	8.959	10.842
O	1.739	18.931	4.241
O	8.415	1.044	10.961
O	18.457	8.978	9.227
O	11.712	10.949	2.417
O	18.409	0.996	9.143
O	11.750	18.981	2.380
O	1.805	10.961	4.287
O	8.423	8.950	11.010
O	8.732	2.508	1.105
O	1.452	17.437	7.809
O	11.445	12.423	12.364
O	18.809	7.523	5.733
O	11.450	17.383	12.202
O	18.775	2.573	5.582
O	8.736	7.478	1.150
O	1.434	12.487	7.844
O	8.426	19.797	0.862
O	1.766	0.142	7.526
O	11.770	9.809	12.639
O	18.446	10.123	5.916
O	11.730	0.091	12.565
O	18.474	19.858	5.840
O	8.434	10.102	0.947
O	1.730	9.873	7.588
O	8.155	17.165	0.755
O	1.992	2.777	7.454
O	12.076	7.189	12.702
O	18.157	12.755	6.007
O	12.234	2.696	12.476
O	18.055	17.232	5.842
O	7.983	12.726	0.835
O	2.052	7.244	7.544
O	3.946	2.560	1.400
O	6.234	17.404	8.105

O	16.212	12.482	12.044
O	13.956	7.578	5.482
O	16.190	17.305	11.856
O	14.013	2.712	5.090
O	3.961	7.399	1.499
O	6.259	12.567	8.235
O	3.715	-0.003	0.732
O	6.454	0.065	7.428
O	16.522	9.932	12.779
O	13.675	10.194	5.936
O	16.502	19.839	12.639
O	13.780	0.220	5.952
O	3.662	9.951	0.788
O	6.458	10.021	7.492
O	3.949	17.230	0.815
O	6.252	2.732	7.496
O	16.270	7.267	12.687
O	13.996	12.816	6.206
O	16.121	2.591	12.471
O	13.958	17.448	5.820
O	3.999	12.610	0.886
O	6.251	7.352	7.570
O	19.918	0.940	3.856
O	10.286	19.067	10.548
O	0.292	10.871	9.585
O	9.902	9.045	2.897
O	0.297	19.068	9.517
O	9.882	0.918	2.846
O	19.923	9.117	3.956
O	10.313	10.796	10.641
O	19.784	17.222	3.784
O	10.415	2.717	10.494
O	0.423	7.274	9.680
O	9.701	12.607	2.883
O	0.377	2.705	9.601
O	9.784	17.247	2.891
O	19.831	12.667	3.905
O	10.429	7.259	10.567
O	8.877	14.942	1.916
O	1.279	4.999	8.627
O	11.310	4.965	11.571
O	18.883	14.969	4.842
O	3.959	14.938	2.065
O	6.227	5.021	8.752
O	16.281	4.980	11.451
O	14.007	15.092	4.703
O	5.563	14.968	7.489
O	4.635	4.991	0.786
O	14.662	5.086	5.915
O	15.583	14.911	12.702
O	2.232	14.963	7.424
O	7.944	4.989	0.755
O	17.997	5.047	6.045
O	12.195	14.910	12.705
H	10.081	12.454	7.989
H	9.838	13.710	10.128
H	10.044	17.433	7.972
H	10.300	16.181	5.830
H	9.821	16.188	10.118
H	13.084	15.601	7.932
H	13.189	14.250	9.201
H	15.658	14.141	8.882
H	15.546	15.481	7.597
H	14.059	13.543	6.905
H	10.326	13.693	5.840
C	15.032	14.828	8.305
C	13.705	14.890	8.482
C	10.208	14.240	6.777
C	10.081	13.545	7.983
C	9.941	14.248	9.183

C	9.930	15.645	9.178
C	10.058	16.342	7.972
C	10.196	15.639	6.772

S.12.12 Ethoxide, C bonded to O24

Si	8.553	1.140	1.960
Si	1.645	18.818	8.642
Si	11.663	11.092	11.479
Si	18.585	8.908	4.805
Si	11.637	18.866	11.508
Si	18.557	1.120	4.834
Si	8.558	8.890	1.944
Si	1.654	11.085	8.624
Si	6.093	0.637	3.782
Si	4.084	19.320	10.483
Si	14.110	10.544	9.674
Si	16.093	9.426	2.979
Si	14.128	19.376	9.714
Si	16.068	0.644	2.991
Si	6.112	9.383	3.778
Si	4.094	10.598	10.465
Si	5.780	1.129	6.849
Si	4.406	18.851	0.165
Si	14.465	11.018	6.621
Si	15.814	8.926	13.303
Si	14.441	18.964	6.627
Si	15.791	1.155	13.313
Si	5.784	8.897	6.841
Si	4.402	11.062	0.139
Si	2.565	1.417	6.875
Si	7.613	18.572	0.177
Si	17.649	11.339	6.589
Si	12.602	8.626	13.273
Si	17.647	18.536	6.603
Si	12.580	1.427	13.301
Si	2.572	8.591	6.857
Si	7.606	11.356	0.155
Si	1.444	0.726	4.052
Si	8.723	19.273	10.741
Si	18.769	10.712	9.393
Si	11.471	9.299	2.702
Si	18.748	19.234	9.416
Si	11.467	0.757	2.735
Si	1.466	9.285	4.037
Si	8.750	10.655	10.732
Si	3.626	1.395	2.114
Si	6.546	18.583	8.811
Si	16.568	11.350	11.316
Si	13.659	8.614	4.633
Si	16.581	18.601	11.385
Si	13.655	1.495	4.662
Si	3.648	8.624	2.106
Si	6.560	11.337	8.806
Si	8.500	16.509	2.288
Si	1.662	3.453	9.024
Si	11.707	6.572	11.124
Si	18.520	13.364	4.418
Si	11.681	3.462	11.148
Si	18.522	16.505	4.440
Si	8.478	13.395	2.282
Si	1.680	6.570	9.007
Si	6.011	17.387	3.872
Si	4.183	2.571	10.561
Si	14.213	7.434	9.600

Si	16.023	12.578	2.842
Si	14.208	2.617	9.600
Si	15.962	17.376	2.932
Si	5.999	12.532	3.871
Si	4.193	7.448	10.558
Si	5.493	16.518	6.844
Si	4.713	3.449	0.150
Si	14.732	6.609	6.632
Si	15.479	13.392	13.270
Si	14.713	3.497	6.638
Si	15.465	16.511	13.312
Si	5.504	13.401	6.850
Si	4.721	6.570	0.141
Si	2.340	16.452	6.866
Si	7.857	3.517	0.197
Si	17.881	6.527	6.564
Si	12.314	13.461	13.254
Si	17.858	3.517	6.585
Si	12.340	16.469	13.225
Si	2.363	13.453	6.861
Si	7.878	6.510	0.175
Si	1.461	17.468	4.018
Si	8.721	2.518	10.727
Si	18.762	7.562	9.410
Si	11.423	12.449	2.732
Si	18.733	2.485	9.432
Si	11.456	17.502	2.681
Si	1.492	12.431	4.032
Si	8.755	7.510	10.708
Si	3.584	16.492	2.014
Si	6.619	3.473	8.697
Si	16.659	6.580	11.444
Si	16.632	3.498	11.458
Si	13.532	16.624	4.788
Si	3.566	13.404	2.007
Si	6.629	6.558	8.700
Al	13.611	13.367	4.728
O	7.274	1.342	2.929
O	2.914	18.605	9.623
O	12.938	11.299	10.504
O	17.288	8.772	3.855
O	12.910	18.688	10.525
O	17.270	1.272	3.869
O	7.282	8.671	2.916
O	2.938	11.307	9.583
O	6.358	0.886	5.355
O	3.815	19.064	12.055
O	13.848	10.714	8.098
O	16.400	9.155	1.412
O	13.884	19.146	8.132
O	16.368	0.904	1.425
O	6.376	9.125	5.351
O	3.799	10.855	12.032
O	4.161	1.160	6.825
O	6.028	18.894	0.132
O	16.093	10.920	6.685
O	14.193	8.909	13.336
O	16.048	18.808	6.614
O	14.170	1.126	13.339
O	4.165	8.874	6.806
O	6.021	11.035	0.083
O	1.984	1.515	5.366
O	8.194	18.471	12.050
O	18.251	11.529	8.087
O	12.005	8.498	1.389
O	18.184	18.419	8.126
O	12.016	1.557	1.433
O	1.990	8.483	5.350
O	8.212	11.460	12.037
O	2.118	1.347	2.712

O	8.060	18.652	9.394
O	18.085	11.309	10.740
O	12.150	8.674	4.039
O	18.082	18.643	10.774
O	12.143	1.348	4.091
O	2.139	8.665	2.695
O	8.073	11.259	9.384
O	4.668	1.296	3.365
O	5.517	18.672	10.072
O	15.545	11.204	10.055
O	14.700	8.688	3.377
O	15.523	18.665	10.142
O	14.679	1.385	3.397
O	4.680	8.738	3.363
O	5.531	11.247	10.068
O	7.404	16.645	3.482
O	2.794	3.326	10.187
O	12.833	6.648	9.951
O	17.500	13.198	3.169
O	12.797	3.329	9.972
O	17.391	16.701	3.281
O	7.362	13.315	3.466
O	2.815	6.683	10.167
O	5.814	17.323	5.474
O	4.415	2.643	12.159
O	14.438	7.433	7.998
O	15.848	12.570	1.225
O	14.405	2.660	7.995
O	15.671	17.260	1.354
O	5.805	12.600	5.475
O	4.393	7.379	12.159
O	3.916	16.681	7.203
O	6.283	3.283	0.537
O	16.303	6.757	6.244
O	13.894	13.238	12.939
O	16.280	3.298	6.250
O	13.911	16.693	12.862
O	3.933	13.244	7.235
O	6.299	6.737	0.487
O	2.092	16.660	5.276
O	8.099	3.331	11.985
O	18.152	6.739	8.151
O	12.016	13.258	1.443
O	18.111	3.307	8.176
O	12.120	16.706	1.437
O	2.165	13.253	5.263
O	8.153	6.677	11.966
O	2.142	16.903	2.655
O	8.061	3.100	9.362
O	18.086	6.994	10.775
O	12.042	13.058	4.077
O	18.050	3.037	10.800
O	12.120	16.916	4.056
O	2.118	13.006	2.644
O	8.077	6.933	9.347
O	4.758	16.669	3.132
O	5.432	3.269	9.794
O	15.470	6.719	10.338
O	14.874	13.436	3.561
O	15.440	3.359	10.351
O	14.785	16.607	3.777
O	4.726	13.215	3.135
O	5.458	6.751	9.816
O	6.084	18.947	3.421
O	4.083	1.009	10.123
O	14.097	8.972	10.114
O	15.993	11.013	3.323
O	14.174	1.061	10.077
O	15.943	18.951	3.338
O	6.114	10.973	3.425

O	4.098	9.007	10.110
O	1.815	19.045	4.191
O	8.332	0.947	10.891
O	18.395	9.134	9.227
O	11.829	10.876	2.544
O	18.373	0.910	9.242
O	11.835	19.076	2.568
O	1.869	10.857	4.192
O	8.368	9.078	10.892
O	8.754	2.465	1.042
O	1.443	17.488	7.730
O	11.435	12.447	12.346
O	18.769	7.543	5.673
O	11.434	17.504	12.369
O	18.739	2.468	5.720
O	8.761	7.564	1.025
O	1.455	12.405	7.695
O	8.386	19.754	0.981
O	1.839	0.193	7.656
O	11.861	9.846	12.497
O	18.478	10.158	5.836
O	11.823	0.206	12.540
O	18.402	19.756	5.845
O	8.363	10.169	0.962
O	1.830	9.797	7.652
O	7.900	17.152	0.916
O	2.229	2.814	7.636
O	12.293	7.230	12.492
O	17.870	12.735	5.776
O	12.266	2.820	12.527
O	17.970	17.140	5.838
O	7.861	12.778	0.903
O	2.259	7.185	7.615
O	3.811	2.807	1.336
O	6.376	17.163	8.042
O	16.341	12.787	12.036
O	13.830	7.201	5.425
O	16.414	17.209	12.199
O	13.801	2.923	5.419
O	3.845	7.203	1.347
O	6.400	12.761	8.040
O	3.855	0.148	1.104
O	6.285	19.814	7.792
O	16.334	10.134	12.360
O	13.916	9.848	5.639
O	16.345	19.867	12.365
O	13.981	0.316	5.726
O	3.876	9.857	1.080
O	6.287	10.114	7.781
O	3.886	17.417	0.715
O	6.365	2.541	7.393
O	16.372	7.507	12.742
O	13.984	12.464	6.139
O	16.321	2.588	12.769
O	13.743	17.614	6.040
O	3.870	12.488	0.704
O	6.355	7.485	7.399
O	19.863	0.914	3.901
O	10.329	19.105	10.584
O	0.350	10.891	9.563
O	9.869	9.096	2.866
O	0.327	19.038	9.557
O	9.865	0.942	2.891
O	19.888	9.109	3.864
O	10.351	10.838	10.562
O	19.873	17.264	3.944
O	10.336	2.683	10.665
O	0.352	7.370	9.498
O	9.793	12.573	2.743
O	0.322	2.674	9.519

O	9.852	17.297	2.750
O	19.907	12.613	4.028
O	10.369	7.347	10.618
O	8.856	14.954	2.019
O	1.308	5.011	8.761
O	11.336	5.019	11.421
O	18.829	14.938	4.686
O	3.538	14.951	1.518
O	6.641	5.014	8.201
O	16.731	5.038	11.948
O	13.384	15.089	5.488
O	5.907	14.962	6.673
O	4.318	5.009	13.348
O	14.341	5.052	6.871
O	15.875	14.957	0.065
O	1.890	14.949	7.277
O	8.315	5.012	0.628
O	18.317	5.013	6.164
O	11.878	14.971	12.826
H	13.733	15.961	8.128
H	13.864	14.173	8.034
H	12.441	14.932	8.789
H	11.851	14.108	6.514
H	11.752	15.884	6.565
C	13.179	15.027	7.976
C	12.432	15.027	6.669

S.12.13 Benzene adsorbed next to ethoxide

Si	8.581	1.172	1.992
Si	1.657	18.859	8.643
Si	11.643	11.131	11.440
Si	18.569	8.951	4.785
Si	11.620	18.914	11.451
Si	18.537	1.189	4.805
Si	8.571	8.944	1.964
Si	1.664	11.129	8.626
Si	6.108	0.671	3.805
Si	4.054	19.356	10.525
Si	14.099	10.583	9.646
Si	16.091	9.455	2.939
Si	14.120	19.430	9.666
Si	16.094	0.733	2.928
Si	6.120	9.429	3.795
Si	4.071	10.647	10.497
Si	5.781	1.190	6.863
Si	4.419	18.899	0.190
Si	14.461	11.044	6.590
Si	15.804	8.983	13.272
Si	14.438	19.024	6.575
Si	15.783	1.191	13.260
Si	5.776	8.920	6.850
Si	4.403	11.101	0.158
Si	2.565	1.493	6.890
Si	7.617	18.645	0.173
Si	17.653	11.409	6.561
Si	12.599	8.710	13.276
Si	17.637	18.557	6.556
Si	12.581	1.418	13.304
Si	2.562	8.604	6.866
Si	7.600	11.377	0.144
Si	1.440	0.776	4.075
Si	8.705	19.355	10.739
Si	18.770	10.762	9.365
Si	11.480	9.391	2.722

Si	18.744	19.282	9.374
Si	11.491	0.739	2.768
Si	1.455	9.322	4.047
Si	8.732	10.657	10.728
Si	3.635	1.434	2.142
Si	6.498	18.636	8.843
Si	16.563	11.401	11.288
Si	13.682	8.627	4.599
Si	16.574	18.639	11.338
Si	13.707	1.570	4.617
Si	3.651	8.666	2.126
Si	6.520	11.365	8.829
Si	8.490	16.550	2.263
Si	1.651	3.499	9.066
Si	11.722	6.609	11.170
Si	18.518	13.408	4.370
Si	11.696	3.502	11.199
Si	18.537	16.554	4.378
Si	8.463	13.440	2.250
Si	1.663	6.612	9.040
Si	6.032	17.423	3.901
Si	4.182	2.608	10.583
Si	14.189	7.478	9.573
Si	16.005	12.611	2.814
Si	14.186	2.665	9.566
Si	15.974	17.460	2.886
Si	6.013	12.577	3.893
Si	4.188	7.495	10.576
Si	5.500	16.564	6.867
Si	4.734	3.483	0.177
Si	14.717	6.659	6.618
Si	15.462	13.438	13.240
Si	14.705	3.537	6.622
Si	15.451	16.565	13.276
Si	5.511	13.438	6.870
Si	4.737	6.615	0.164
Si	2.336	16.497	6.853
Si	7.873	3.559	0.258
Si	17.874	6.584	6.570
Si	12.301	13.504	13.194
Si	17.862	3.562	6.593
Si	12.327	16.516	13.156
Si	2.359	13.491	6.851
Si	7.889	6.552	0.224
Si	1.464	17.523	4.005
Si	8.728	2.595	10.773
Si	18.766	7.618	9.413
Si	11.421	12.547	2.710
Si	18.744	2.527	9.438
Si	11.462	17.479	2.667
Si	1.482	12.464	4.022
Si	8.762	7.515	10.747
Si	3.619	16.535	2.044
Si	6.633	3.516	8.720
Si	16.632	6.631	11.400
Si	16.603	3.548	11.401
Si	13.541	16.664	4.760
Si	3.584	13.443	2.037
Si	6.637	6.597	8.721
Al	13.594	13.446	4.713
O	7.303	1.366	2.962
O	2.897	18.626	9.657
O	12.915	11.334	10.461
O	17.279	8.802	3.828
O	12.886	18.751	10.459
O	17.280	1.390	3.808
O	7.296	8.723	2.937
O	2.931	11.368	9.604
O	6.370	0.915	5.380
O	3.783	19.098	12.096

O	13.845	10.744	8.068
O	16.416	9.184	1.375
O	13.883	19.217	8.080
O	16.402	0.984	1.362
O	6.381	9.171	5.369
O	3.766	10.911	12.062
O	4.169	1.320	6.810
O	6.038	18.999	0.120
O	16.088	11.037	6.683
O	14.184	9.025	13.329
O	16.022	18.709	6.586
O	14.166	1.091	13.324
O	4.163	8.811	6.789
O	6.020	11.032	0.070
O	1.956	1.573	5.392
O	8.205	18.536	12.049
O	18.275	11.582	8.052
O	12.004	8.610	1.394
O	18.195	18.476	8.073
O	12.026	1.504	1.440
O	1.956	8.517	5.367
O	8.210	11.480	12.027
O	2.130	1.400	2.745
O	8.020	18.758	9.396
O	18.076	11.370	10.700
O	12.161	8.734	4.042
O	18.070	18.667	10.717
O	12.181	1.367	4.101
O	2.144	8.697	2.717
O	8.040	11.229	9.376
O	4.690	1.342	3.383
O	5.497	18.722	10.126
O	15.528	11.252	10.037
O	14.696	8.708	3.323
O	15.504	18.702	10.103
O	14.691	1.457	3.321
O	4.691	8.781	3.377
O	5.519	11.280	10.114
O	7.414	16.681	3.475
O	2.805	3.386	10.209
O	12.835	6.677	9.985
O	17.486	13.225	3.135
O	12.799	3.376	10.012
O	17.395	16.764	3.234
O	7.361	13.365	3.446
O	2.819	6.718	10.179
O	5.884	17.362	5.508
O	4.438	2.692	12.176
O	14.337	7.483	7.963
O	15.819	12.616	1.198
O	14.297	2.699	7.952
O	15.662	17.325	1.311
O	5.870	12.648	5.501
O	4.401	7.407	12.174
O	3.912	16.751	7.161
O	6.299	3.294	0.579
O	16.296	6.858	6.292
O	13.882	13.273	12.886
O	16.282	3.292	6.312
O	13.901	16.754	12.813
O	3.929	13.257	7.197
O	6.311	6.809	0.517
O	2.051	16.689	5.267
O	8.124	3.397	12.045
O	18.195	6.772	8.150
O	11.995	13.296	1.379
O	18.178	3.376	8.175
O	12.091	16.767	1.359
O	2.124	13.305	5.256
O	8.174	6.687	12.014

O	2.173	16.982	2.647
O	8.074	3.201	9.416
O	18.073	7.061	10.774
O	12.030	13.244	4.015
O	18.039	3.074	10.795
O	12.130	16.767	3.979
O	2.127	13.029	2.638
O	8.086	6.925	9.391
O	4.763	16.698	3.195
O	5.435	3.272	9.795
O	15.483	6.770	10.253
O	14.865	13.467	3.546
O	15.456	3.415	10.246
O	14.795	16.728	3.749
O	4.715	13.254	3.193
O	5.458	6.823	9.821
O	6.088	18.982	3.440
O	4.036	1.045	10.162
O	14.086	9.014	10.097
O	15.981	11.041	3.283
O	14.182	1.110	10.049
O	15.997	19.039	3.278
O	6.121	11.020	3.442
O	4.063	9.056	10.146
O	1.816	19.096	4.221
O	8.322	1.027	10.919
O	18.387	9.184	9.199
O	11.847	10.970	2.607
O	18.363	0.959	9.216
O	11.865	19.053	2.668
O	1.862	10.893	4.206
O	8.365	9.082	10.923
O	8.784	2.515	1.100
O	1.448	17.535	7.725
O	11.413	12.502	12.280
O	18.756	7.596	5.667
O	11.418	17.530	12.277
O	18.737	2.521	5.711
O	8.784	7.606	1.063
O	1.456	12.443	7.692
O	8.407	19.810	0.984
O	1.903	0.234	7.670
O	11.840	9.903	12.478
O	18.447	10.213	5.799
O	11.808	0.226	12.514
O	18.310	19.818	5.792
O	8.368	10.204	0.960
O	1.876	9.839	7.665
O	7.878	17.219	0.910
O	2.193	2.874	7.663
O	12.308	7.295	12.523
O	17.884	12.805	5.749
O	12.279	2.834	12.568
O	18.019	17.175	5.794
O	7.838	12.805	0.884
O	2.215	7.208	7.629
O	3.818	2.838	1.349
O	6.337	17.206	8.097
O	16.337	12.836	12.013
O	13.842	7.197	5.365
O	16.405	17.250	12.158
O	13.837	3.013	5.348
O	3.849	7.248	1.361
O	6.369	12.800	8.087
O	3.848	0.173	1.147
O	6.186	19.845	7.814
O	16.353	10.178	12.328
O	13.999	9.819	5.634
O	16.363	0.016	12.312
O	14.125	0.439	5.702

O	3.866	9.906	1.106
O	6.192	10.165	7.793
O	3.971	17.444	0.747
O	6.440	2.564	7.420
O	16.300	7.547	12.695
O	13.908	12.445	6.069
O	16.235	2.642	12.698
O	13.627	17.766	5.932
O	3.923	12.539	0.735
O	6.412	7.541	7.422
O	19.860	0.953	3.903
O	10.306	19.180	10.542
O	0.351	10.922	9.550
O	9.877	9.185	2.884
O	0.322	19.099	9.528
O	9.890	0.936	2.920
O	19.879	9.150	3.853
O	10.330	10.856	10.528
O	19.880	17.321	3.875
O	10.344	2.742	10.708
O	0.355	7.437	9.542
O	9.788	12.637	2.715
O	0.332	2.693	9.578
O	9.853	17.312	2.730
O	19.896	12.638	3.981
O	10.376	7.363	10.654
O	8.825	14.998	1.962
O	1.268	5.054	8.820
O	11.371	5.059	11.499
O	18.841	14.984	4.604
O	3.556	14.993	1.557
O	6.610	5.055	8.215
O	16.696	5.087	11.896
O	13.577	15.160	5.540
O	5.892	15.004	6.711
O	4.358	5.048	0.001
O	14.371	5.096	6.868
O	15.845	15.007	0.038
O	1.910	14.992	7.282
O	8.302	5.057	0.707
O	18.264	5.066	6.144
O	11.876	15.015	12.761
H	9.849	17.481	7.751
H	9.529	16.185	5.645
H	9.670	13.699	5.681
H	10.105	12.509	7.826
H	10.416	13.810	9.928
H	10.291	16.285	9.889
H	12.709	15.981	7.278
H	12.794	14.204	7.221
H	15.294	14.294	7.508
H	14.455	15.091	8.858
H	15.230	16.078	7.600
C	9.914	16.392	7.761
C	9.732	15.663	6.582
C	13.353	15.127	7.044
C	10.055	13.598	7.805
C	10.232	14.327	8.985
C	10.162	15.722	8.963
C	14.667	15.152	7.779
C	9.803	14.267	6.603

S.12.14 Transition structure 1s

Si	8.553	1.156	1.933
Si	1.603	18.868	8.622
Si	11.625	11.061	11.560
Si	18.594	8.903	4.840
Si	11.607	18.828	11.443
Si	18.585	1.201	4.768
Si	8.570	8.899	1.995
Si	1.607	11.127	8.670
Si	6.122	0.613	3.855
Si	4.022	19.411	10.571
Si	14.044	10.471	9.636
Si	16.191	9.453	2.923
Si	14.039	19.455	9.547
Si	16.190	0.628	2.828
Si	6.141	9.472	3.904
Si	4.034	10.566	10.580
Si	5.702	1.395	6.801
Si	4.447	18.627	0.117
Si	14.480	11.312	6.703
Si	15.732	8.721	13.365
Si	14.464	18.794	6.562
Si	15.735	1.300	13.270
Si	5.720	8.736	6.867
Si	4.439	11.273	0.155
Si	2.496	1.414	6.805
Si	7.652	18.604	0.126
Si	17.667	11.339	6.637
Si	12.536	8.633	13.353
Si	17.668	18.664	6.564
Si	12.544	1.341	13.254
Si	2.518	8.680	6.878
Si	7.639	11.323	0.169
Si	1.460	0.644	3.986
Si	8.691	19.389	10.697
Si	18.732	10.604	9.453
Si	11.481	9.424	2.752
Si	18.706	19.362	9.396
Si	11.464	0.677	2.677
Si	1.480	9.410	4.056
Si	8.720	10.576	10.740
Si	3.630	1.108	1.962
Si	6.508	18.930	8.676
Si	16.530	11.034	11.467
Si	13.665	9.003	4.785
Si	16.538	18.854	11.406
Si	13.682	1.202	4.651
Si	3.643	8.932	2.035
Si	6.547	11.097	8.732
Si	8.502	16.517	2.210
Si	1.638	3.484	8.905
Si	11.692	6.536	11.259
Si	18.491	13.441	4.527
Si	11.691	3.485	11.150
Si	18.487	16.517	4.490
Si	8.466	13.433	2.238
Si	1.672	6.569	8.961
Si	6.115	17.372	4.087
Si	4.044	2.645	10.773
Si	14.054	7.363	9.377
Si	16.177	12.549	2.623
Si	14.030	2.711	9.252
Si	16.145	17.407	2.611
Si	6.115	12.609	4.132
Si	4.053	7.419	10.815
Si	5.438	16.548	7.020

Si	4.721	3.488	0.314
Si	14.761	6.616	6.437
Si	15.451	13.389	13.106
Si	14.754	3.510	6.312
Si	15.439	16.512	13.072
Si	5.457	13.444	7.077
Si	4.731	6.589	0.370
Si	2.337	16.513	6.870
Si	7.820	3.511	0.175
Si	17.855	6.578	6.615
Si	12.336	13.434	13.319
Si	17.845	3.525	6.537
Si	12.331	16.480	13.205
Si	2.360	13.461	6.913
Si	7.832	6.555	0.220
Si	1.349	17.396	4.022
Si	8.794	2.623	10.721
Si	18.830	7.462	9.448
Si	11.338	12.548	2.765
Si	18.791	2.603	9.394
Si	11.366	17.439	2.659
Si	1.381	12.550	4.076
Si	8.824	7.436	10.760
Si	3.671	16.544	2.266
Si	6.488	3.463	8.942
Si	16.510	6.625	11.216
Si	16.465	3.475	11.130
Si	13.707	16.642	4.432
Si	3.672	13.384	2.301
Si	6.505	6.619	8.993
Al	13.713	13.425	4.478
O	7.256	1.253	2.895
O	2.893	18.789	9.595
O	12.940	11.144	10.615
O	17.295	8.756	3.888
O	12.896	18.760	10.462
O	17.279	1.301	3.817
O	7.271	8.804	2.959
O	2.920	11.226	9.612
O	6.083	1.473	5.230
O	4.059	18.526	11.930
O	14.076	11.358	8.281
O	16.109	8.586	1.549
O	14.063	18.657	8.132
O	16.183	1.465	1.436
O	6.092	8.637	5.295
O	4.031	11.392	11.975
O	4.097	1.243	7.015
O	6.053	18.806	0.312
O	16.077	11.038	6.533
O	14.126	8.894	13.151
O	16.074	18.916	6.389
O	14.134	1.037	13.154
O	4.115	8.894	7.086
O	6.043	11.060	0.319
O	2.125	1.458	5.229
O	8.046	18.553	11.935
O	18.110	11.434	8.197
O	12.142	8.560	1.536
O	18.065	18.565	8.132
O	12.076	1.502	1.414
O	2.142	8.604	5.305
O	8.070	11.388	11.989
O	2.134	1.113	2.588
O	8.011	18.919	9.297
O	18.029	11.069	10.842
O	12.173	8.977	4.150
O	18.031	18.827	10.771
O	12.175	1.162	4.052
O	2.150	8.914	2.665

O	8.050	11.077	9.350
O	4.673	0.696	3.136
O	5.475	19.341	9.854
O	15.512	10.491	10.320
O	14.737	9.418	3.641
O	15.491	19.325	10.252
O	14.712	0.699	3.499
O	4.690	9.393	3.186
O	5.504	10.675	9.904
O	7.235	16.610	3.211
O	2.920	3.383	9.884
O	12.953	6.567	10.249
O	17.307	13.387	3.441
O	12.880	3.517	10.053
O	17.235	16.576	3.469
O	7.204	13.416	3.255
O	2.946	6.609	9.958
O	6.150	16.733	5.575
O	4.032	3.333	12.237
O	14.048	6.732	7.889
O	16.252	13.119	1.095
O	13.999	3.216	7.718
O	16.145	16.783	1.119
O	6.144	13.227	5.627
O	4.017	6.825	12.318
O	3.885	17.029	6.922
O	6.273	2.998	0.231
O	16.312	7.103	6.557
O	13.889	12.948	13.268
O	16.301	3.010	6.441
O	13.879	16.983	13.137
O	3.905	12.952	7.025
O	6.285	7.065	0.273
O	1.804	16.563	5.341
O	8.341	3.479	12.022
O	18.374	6.596	8.152
O	11.773	13.422	1.446
O	18.352	3.433	8.072
O	11.788	16.593	1.341
O	1.880	13.397	5.368
O	8.365	6.604	12.074
O	2.130	16.812	2.719
O	8.028	3.194	9.403
O	18.051	6.901	10.763
O	12.047	13.093	4.088
O	18.009	3.198	10.691
O	12.153	16.890	3.967
O	2.125	13.129	2.746
O	8.052	6.846	9.453
O	4.646	17.159	3.421
O	5.506	2.830	10.080
O	15.527	7.193	10.045
O	14.729	12.715	3.268
O	15.491	3.001	9.909
O	14.668	17.297	3.276
O	4.635	12.802	3.482
O	5.530	7.205	10.162
O	6.464	18.956	4.175
O	3.692	1.065	10.915
O	13.645	8.934	9.304
O	16.635	10.976	2.601
O	13.694	1.122	9.318
O	16.581	18.975	2.549
O	6.498	11.031	4.189
O	3.686	9.000	10.839
O	1.722	18.960	4.241
O	8.407	1.065	10.963
O	18.462	9.022	9.193
O	11.718	10.993	2.436
O	18.397	1.044	9.190

O	11.734	18.999	2.408
O	1.771	10.991	4.292
O	8.436	8.996	10.969
O	8.727	2.541	1.104
O	1.435	17.463	7.826
O	11.454	12.465	12.355
O	18.784	7.532	5.693
O	11.444	17.398	12.197
O	18.766	2.601	5.573
O	8.731	7.504	1.175
O	1.430	12.523	7.854
O	8.418	19.830	0.869
O	1.749	0.167	7.532
O	11.722	9.839	12.621
O	18.466	10.141	5.887
O	11.747	0.107	12.554
O	18.458	19.891	5.852
O	8.427	10.119	0.924
O	1.736	9.912	7.594
O	8.130	17.199	0.780
O	1.981	2.802	7.470
O	12.094	7.227	12.672
O	18.038	12.754	5.934
O	12.189	2.724	12.493
O	18.094	17.258	5.884
O	8.034	12.753	0.822
O	2.048	7.282	7.552
O	3.935	2.596	1.408
O	6.210	17.434	8.134
O	16.121	12.542	11.893
O	13.982	7.517	5.350
O	16.190	17.357	11.910
O	14.017	2.720	5.105
O	3.975	7.434	1.520
O	6.252	12.601	8.207
O	3.705	0.028	0.751
O	6.434	0.095	7.452
O	16.481	10.030	12.746
O	13.686	10.081	6.001
O	16.503	0.010	12.642
O	13.769	0.231	5.955
O	3.687	9.979	0.791
O	6.455	10.044	7.497
O	3.955	17.260	0.837
O	6.223	2.761	7.503
O	16.226	7.363	12.628
O	14.056	12.753	6.098
O	16.127	2.663	12.490
O	13.914	17.457	5.841
O	3.976	12.641	0.891
O	6.238	7.376	7.584
O	19.897	0.958	3.851
O	10.279	19.087	10.547
O	0.300	10.900	9.601
O	9.894	9.102	2.901
O	0.278	19.102	9.525
O	9.874	0.952	2.850
O	19.914	9.118	3.926
O	10.316	10.865	10.617
O	19.771	17.236	3.789
O	10.397	2.747	10.493
O	0.410	7.304	9.684
O	9.708	12.647	2.916
O	0.373	2.748	9.625
O	9.765	17.271	2.913
O	19.800	12.697	3.902
O	10.430	7.288	10.550
O	8.868	14.971	1.924
O	1.282	5.035	8.630
O	11.297	4.997	11.571

O	18.854	14.987	4.858
O	3.947	14.963	2.079
O	6.210	5.045	8.766
O	16.249	5.045	11.444
O	14.019	15.114	4.706
O	5.544	15.006	7.497
O	4.631	5.029	0.793
O	14.686	5.079	5.936
O	15.548	14.950	12.668
O	2.228	14.995	7.427
O	7.945	5.023	0.746
O	17.964	5.064	6.043
O	12.206	14.941	12.707
H	9.145	17.012	7.237
H	10.670	15.678	5.775
H	11.630	13.542	6.622
H	11.121	12.764	8.933
H	9.597	14.101	10.391
H	8.613	16.218	9.526
H	12.739	16.193	7.722
H	12.567	15.206	9.284
H	14.789	14.189	8.871
H	14.993	15.349	7.429
H	14.095	13.904	7.228
C	14.318	14.739	8.049
C	13.105	15.384	8.352
C	9.590	16.086	7.605
C	10.441	15.346	6.790
C	11.022	14.162	7.282
C	10.701	13.705	8.576
C	9.841	14.448	9.385
C	9.292	15.637	8.900

S.12.15 Transition structure 2s(1)

Si	8.547	1.140	1.913
Si	1.626	18.862	8.627
Si	11.633	11.071	11.591
Si	18.591	8.922	4.861
Si	11.619	18.810	11.493
Si	18.592	1.145	4.777
Si	8.564	8.885	1.986
Si	1.607	11.114	8.670
Si	6.124	0.599	3.846
Si	4.063	19.392	10.553
Si	14.055	10.463	9.715
Si	16.145	9.502	2.948
Si	14.032	19.414	9.572
Si	16.124	0.524	2.884
Si	6.141	9.459	3.895
Si	4.035	10.551	10.577
Si	5.718	1.379	6.792
Si	4.453	18.607	0.111
Si	14.488	11.222	6.748
Si	15.753	8.696	0.017
Si	14.493	18.856	6.604
Si	15.759	1.253	13.295
Si	5.719	8.738	6.867
Si	4.431	11.251	0.156
Si	2.514	1.399	6.798
Si	7.658	18.572	0.121
Si	17.670	11.319	6.678
Si	12.554	8.618	13.360
Si	17.680	18.671	6.602
Si	12.555	1.344	13.285

Si	2.517	8.669	6.881
Si	7.627	11.315	0.173
Si	1.470	0.619	3.987
Si	8.705	19.368	10.703
Si	18.731	10.589	9.484
Si	11.479	9.390	2.757
Si	18.738	19.327	9.412
Si	11.459	0.686	2.697
Si	1.479	9.405	4.067
Si	8.736	10.578	10.758
Si	3.631	1.090	1.957
Si	6.559	18.913	8.658
Si	16.561	11.014	11.523
Si	13.641	8.955	4.807
Si	16.545	18.813	11.390
Si	13.632	1.233	4.705
Si	3.631	8.915	2.039
Si	6.561	11.086	8.745
Si	8.512	16.501	2.205
Si	1.646	3.465	8.890
Si	11.685	6.514	11.269
Si	18.522	13.434	4.585
Si	11.676	3.471	11.181
Si	18.494	16.493	4.518
Si	8.456	13.420	2.244
Si	1.671	6.550	8.963
Si	6.111	17.358	4.067
Si	4.053	2.634	10.765
Si	14.044	7.351	9.428
Si	16.156	12.652	2.670
Si	14.037	2.671	9.322
Si	16.119	17.222	2.624
Si	6.118	12.599	4.135
Si	4.052	7.400	10.812
Si	5.470	16.534	7.014
Si	4.708	3.472	0.311
Si	14.753	6.622	6.460
Si	15.443	13.389	13.135
Si	14.735	3.497	6.365
Si	15.435	16.484	13.049
Si	5.477	13.427	7.098
Si	4.717	6.575	0.373
Si	2.367	16.502	6.891
Si	7.808	3.498	0.160
Si	17.845	6.567	6.604
Si	12.345	13.419	13.365
Si	17.822	3.497	6.514
Si	12.347	16.471	13.250
Si	2.383	13.453	6.937
Si	7.819	6.540	0.211
Si	1.373	17.378	4.049
Si	8.788	2.601	10.715
Si	18.825	7.443	9.453
Si	11.318	12.504	2.778
Si	18.792	2.567	9.373
Si	11.364	17.457	2.681
Si	1.415	12.542	4.102
Si	8.822	7.438	10.766
Si	3.658	16.532	2.252
Si	6.498	3.455	8.929
Si	16.519	6.586	11.256
Si	16.503	3.433	11.185
Si	13.651	16.595	4.518
Si	3.675	13.374	2.297
Si	6.513	6.617	8.987
Al	13.626	13.397	4.581
O	7.249	1.236	2.874
O	2.930	18.772	9.581
O	12.958	11.191	10.660
O	17.278	8.870	3.920

O	12.914	18.723	10.518
O	17.272	1.130	3.845
O	7.266	8.781	2.951
O	2.923	11.211	9.607
O	6.100	1.461	5.220
O	4.093	18.516	11.918
O	14.106	11.287	8.324
O	16.108	8.599	1.594
O	14.015	18.636	8.142
O	16.188	1.322	1.473
O	6.099	8.642	5.296
O	4.018	11.369	11.977
O	4.114	1.206	6.999
O	6.059	18.752	0.336
O	16.084	11.003	6.525
O	14.148	8.870	13.169
O	16.101	19.045	6.507
O	14.149	1.080	13.149
O	4.113	8.898	7.075
O	6.034	11.028	0.312
O	2.131	1.445	5.224
O	8.032	18.534	11.927
O	18.076	11.420	8.247
O	12.156	8.532	1.545
O	18.132	18.499	8.148
O	12.118	1.507	1.456
O	2.130	8.581	5.311
O	8.070	11.391	11.998
O	2.133	1.080	2.580
O	8.058	18.913	9.285
O	18.055	11.050	10.887
O	12.149	8.960	4.173
O	18.050	18.800	10.783
O	12.128	1.155	4.100
O	2.139	8.903	2.674
O	8.066	11.057	9.359
O	4.671	0.685	3.137
O	5.514	19.308	9.835
O	15.528	10.484	10.385
O	14.692	9.423	3.665
O	15.509	19.276	10.224
O	14.660	0.740	3.549
O	4.685	9.373	3.189
O	5.511	10.671	9.913
O	7.233	16.600	3.188
O	2.915	3.362	9.884
O	12.934	6.506	10.239
O	17.360	13.384	3.477
O	12.885	3.489	10.107
O	17.312	16.480	3.415
O	7.213	13.427	3.285
O	2.942	6.585	9.964
O	6.137	16.701	5.546
O	4.024	3.310	12.234
O	14.044	6.824	7.902
O	16.235	13.229	1.149
O	14.032	3.186	7.791
O	16.171	16.722	1.089
O	6.142	13.184	5.642
O	4.011	6.821	12.320
O	3.914	17.016	6.961
O	6.262	2.986	0.231
O	16.306	7.106	6.554
O	13.893	12.910	13.307
O	16.279	2.979	6.417
O	13.889	16.993	13.159
O	3.924	12.941	7.080
O	6.273	7.048	0.284
O	1.860	16.541	5.352
O	8.314	3.471	12.002

O	18.375	6.600	8.137
O	11.797	13.411	1.501
O	18.335	3.380	8.047
O	11.833	16.582	1.400
O	1.943	13.392	5.380
O	8.337	6.590	12.060
O	2.120	16.790	2.726
O	8.035	3.158	9.384
O	18.047	6.863	10.761
O	11.992	13.017	4.135
O	18.029	3.173	10.677
O	12.140	16.964	4.022
O	2.132	13.116	2.754
O	8.056	6.875	9.443
O	4.645	17.156	3.392
O	5.511	2.847	10.076
O	15.511	7.134	10.096
O	14.745	12.976	3.347
O	15.488	2.940	10.006
O	14.685	16.802	3.281
O	4.643	12.803	3.480
O	5.529	7.177	10.162
O	6.463	18.941	4.168
O	3.732	1.047	10.891
O	13.625	8.920	9.460
O	16.480	11.049	2.613
O	13.684	1.086	9.370
O	16.343	18.829	2.679
O	6.504	11.021	4.156
O	3.689	8.983	10.821
O	1.752	18.941	4.255
O	8.411	1.044	10.973
O	18.458	9.006	9.227
O	11.720	10.959	2.435
O	18.403	1.003	9.190
O	11.733	19.010	2.413
O	1.799	10.980	4.310
O	8.453	8.998	10.999
O	8.719	2.520	1.075
O	1.450	17.462	7.822
O	11.442	12.454	12.418
O	18.757	7.510	5.651
O	11.439	17.389	12.263
O	18.726	2.584	5.522
O	8.725	7.496	1.154
O	1.432	12.511	7.854
O	8.421	19.802	0.863
O	1.756	0.167	7.542
O	11.747	9.829	12.632
O	18.500	10.118	5.962
O	11.773	0.093	12.601
O	18.528	19.872	5.908
O	8.427	10.120	0.933
O	1.730	9.899	7.594
O	8.161	17.170	0.765
O	2.017	2.798	7.454
O	12.115	7.215	12.669
O	18.048	12.730	5.974
O	12.148	2.719	12.537
O	17.979	17.267	5.852
O	7.990	12.750	0.836
O	2.056	7.271	7.561
O	3.924	2.583	1.409
O	6.274	17.422	8.099
O	16.164	12.512	11.979
O	13.972	7.453	5.316
O	16.196	17.315	11.888
O	13.940	2.754	5.162
O	3.959	7.417	1.524
O	6.287	12.596	8.225

O	3.724	0.018	0.740
O	6.470	0.093	7.447
O	16.523	9.993	12.787
O	13.699	9.969	6.077
O	16.481	19.854	12.635
O	13.753	0.277	6.018
O	3.675	9.962	0.796
O	6.456	10.041	7.504
O	3.919	17.249	0.819
O	6.214	2.756	7.492
O	16.254	7.334	12.671
O	14.002	12.638	6.133
O	16.235	2.619	12.564
O	14.043	17.550	5.771
O	3.976	12.622	0.892
O	6.228	7.374	7.582
O	19.903	0.920	3.854
O	10.298	19.076	10.592
O	0.300	10.888	9.602
O	9.891	9.071	2.892
O	0.314	19.093	9.552
O	9.867	0.957	2.834
O	19.907	9.143	3.941
O	10.330	10.872	10.640
O	19.789	17.232	3.864
O	10.393	2.733	10.502
O	0.406	7.280	9.684
O	9.688	12.600	2.900
O	0.376	2.718	9.584
O	9.766	17.268	2.916
O	19.831	12.695	3.963
O	10.428	7.278	10.567
O	8.892	14.952	1.943
O	1.283	5.017	8.623
O	11.273	4.983	11.594
O	18.877	14.979	4.942
O	3.942	14.952	2.063
O	6.249	5.040	8.749
O	16.281	5.003	11.503
O	13.625	15.090	5.117
O	5.584	14.993	7.494
O	4.612	5.014	0.788
O	14.676	5.070	6.028
O	15.496	14.928	12.625
O	2.244	14.986	7.453
O	7.941	5.008	0.736
O	17.942	5.045	6.048
O	12.229	14.929	12.767
H	12.584	16.190	7.018
H	11.361	15.208	6.019
H	11.452	13.425	7.713
H	13.094	13.465	7.086
H	12.772	14.348	8.635
C	12.290	14.135	7.674
C	12.114	15.229	6.809

S.12.16 Transition structure 2s(2)

Si	8.937	1.325	1.829
Si	2.022	19.091	8.544
Si	12.046	11.225	11.586
Si	18.979	9.148	4.829
Si	12.034	18.992	11.366
Si	19.008	1.397	4.661
Si	8.964	9.062	1.987

Si	2.009	11.342	8.687
Si	6.518	0.808	3.785
Si	4.456	19.596	10.483
Si	14.446	10.677	9.619
Si	16.535	9.703	2.915
Si	14.428	19.643	9.443
Si	16.573	0.755	2.753
Si	6.553	9.664	3.897
Si	4.426	10.750	10.578
Si	6.108	1.622	6.713
Si	4.859	18.771	0.023
Si	14.901	11.504	6.710
Si	16.129	8.876	13.365
Si	14.927	19.114	6.461
Si	16.163	1.436	13.173
Si	6.122	8.989	6.876
Si	4.829	11.417	0.168
Si	2.903	1.621	6.699
Si	8.070	18.744	0.034
Si	18.076	11.539	6.672
Si	12.926	8.769	13.363
Si	18.098	18.927	6.484
Si	12.964	1.538	13.144
Si	2.921	8.919	6.879
Si	8.030	11.504	0.190
Si	1.866	0.821	3.887
Si	9.110	19.557	10.610
Si	19.157	10.788	9.464
Si	11.873	9.592	2.753
Si	19.143	19.543	9.309
Si	11.855	0.918	2.551
Si	1.864	9.606	4.053
Si	9.132	10.801	10.764
Si	4.043	1.271	1.866
Si	6.939	19.142	8.573
Si	16.929	11.196	11.447
Si	14.042	9.199	4.810
Si	16.932	19.005	11.253
Si	14.065	1.462	4.532
Si	4.044	9.083	2.066
Si	6.949	11.323	8.775
Si	8.934	16.717	2.141
Si	2.039	3.672	8.795
Si	12.066	6.729	11.243
Si	18.885	13.644	4.552
Si	12.091	3.684	11.032
Si	18.863	16.700	4.417
Si	8.863	13.631	2.267
Si	2.087	6.754	8.948
Si	6.504	17.572	3.994
Si	4.445	2.831	10.687
Si	14.451	7.570	9.379
Si	16.561	12.850	2.585
Si	14.419	2.901	9.173
Si	16.555	17.470	2.486
Si	6.523	12.810	4.136
Si	4.430	7.598	10.816
Si	5.830	16.745	6.923
Si	5.100	3.672	0.218
Si	15.145	6.818	6.433
Si	15.876	13.585	13.072
Si	15.150	3.705	6.218
Si	15.856	16.689	12.939
Si	5.838	13.633	7.098
Si	5.116	6.775	0.373
Si	2.731	16.717	6.813
Si	8.201	3.689	0.068
Si	18.240	6.787	6.573
Si	12.767	13.609	13.349
Si	18.237	3.726	6.408

Si	12.759	16.660	13.163
Si	2.742	13.669	6.933
Si	8.218	6.735	0.191
Si	1.748	17.574	3.965
Si	9.195	2.796	10.627
Si	19.229	7.644	9.413
Si	11.737	12.710	2.761
Si	19.181	2.783	9.277
Si	11.783	17.697	2.577
Si	1.782	12.746	4.087
Si	9.210	7.663	10.745
Si	4.054	16.727	2.176
Si	6.889	3.667	8.863
Si	16.916	6.804	11.214
Si	16.871	3.656	11.059
Si	14.106	16.855	4.368
Si	4.070	13.574	2.295
Si	6.890	6.830	8.989
Al	14.096	13.619	4.504
O	7.648	1.414	2.801
O	3.330	18.995	9.492
O	13.361	11.319	10.644
O	17.669	9.070	3.886
O	13.316	18.912	10.371
O	17.679	1.402	3.738
O	7.661	8.965	2.948
O	3.343	11.447	9.601
O	6.499	1.695	5.142
O	4.488	18.692	11.830
O	14.432	11.582	8.278
O	16.495	8.805	1.557
O	14.409	18.908	7.991
O	16.654	1.535	1.332
O	6.548	8.884	5.318
O	4.391	11.532	11.997
O	4.505	1.443	6.912
O	6.468	18.888	0.238
O	16.501	11.174	6.624
O	14.519	8.989	13.142
O	16.531	19.354	6.431
O	14.553	1.223	13.100
O	4.516	9.189	7.032
O	6.437	11.215	0.303
O	2.533	1.646	5.122
O	8.450	18.717	11.839
O	18.571	11.649	8.216
O	12.549	8.714	1.554
O	18.583	18.728	8.018
O	12.452	1.750	1.287
O	2.497	8.804	5.320
O	8.494	11.608	12.023
O	2.543	1.251	2.478
O	8.440	19.101	9.200
O	18.442	11.216	10.857
O	12.546	9.200	4.175
O	18.440	18.977	10.655
O	12.559	1.398	3.932
O	2.546	9.075	2.681
O	8.456	11.327	9.382
O	5.072	0.889	3.062
O	5.908	19.522	9.763
O	15.928	10.681	10.274
O	15.088	9.621	3.641
O	15.908	19.495	10.086
O	15.086	0.947	3.377
O	5.082	9.557	3.224
O	5.918	10.874	9.948
O	7.648	16.855	3.112
O	3.313	3.527	9.776
O	13.340	6.791	10.253

O	17.734	13.584	3.436
O	13.252	3.752	9.905
O	17.694	16.664	3.300
O	7.635	13.666	3.330
O	3.329	6.749	9.989
O	6.513	16.868	5.456
O	4.406	3.544	12.140
O	14.455	6.920	7.898
O	16.718	13.395	1.053
O	14.423	3.330	7.617
O	16.633	17.001	0.942
O	6.539	13.340	5.666
O	4.380	7.083	12.347
O	4.281	17.231	6.858
O	6.652	3.185	0.113
O	16.696	7.309	6.536
O	14.323	13.137	13.303
O	16.698	3.203	6.290
O	14.303	17.165	13.080
O	4.286	13.160	7.059
O	6.672	7.241	0.268
O	2.218	16.738	5.277
O	8.727	3.666	11.916
O	18.771	6.789	8.108
O	12.190	13.616	1.472
O	18.739	3.583	7.941
O	12.222	16.798	1.302
O	2.286	13.578	5.385
O	8.743	6.816	12.045
O	2.520	16.991	2.654
O	8.426	3.348	9.302
O	18.446	7.083	10.726
O	12.439	13.210	4.105
O	18.403	3.400	10.567
O	12.580	17.256	3.920
O	2.527	13.341	2.762
O	8.437	7.090	9.431
O	5.049	17.377	3.295
O	5.907	3.031	9.999
O	15.912	7.395	10.074
O	15.121	13.200	3.176
O	15.865	3.211	9.853
O	15.085	17.107	3.088
O	5.050	13.041	3.487
O	5.914	7.351	10.189
O	6.836	19.154	4.152
O	4.134	1.245	10.855
O	14.047	9.139	9.282
O	16.880	11.244	2.572
O	14.065	1.319	9.307
O	16.850	19.065	2.581
O	6.917	11.235	4.103
O	4.060	9.178	10.760
O	2.114	19.140	4.178
O	8.832	1.233	10.885
O	18.889	9.210	9.165
O	12.092	11.158	2.394
O	18.788	1.218	9.111
O	12.133	19.245	2.252
O	2.180	11.185	4.270
O	8.820	9.220	10.970
O	9.098	2.698	0.982
O	1.829	17.692	7.742
O	11.887	12.615	12.410
O	19.151	7.753	5.647
O	11.872	17.568	12.141
O	19.155	2.833	5.409
O	9.118	7.668	1.162
O	1.811	12.749	7.890
O	8.808	0.084	0.784

O	2.158	0.388	7.452
O	12.133	9.987	12.630
O	18.901	10.365	5.904
O	12.179	0.288	12.457
O	18.958	0.218	5.787
O	8.826	10.295	0.931
O	2.127	10.143	7.593
O	8.597	17.348	0.677
O	2.387	3.018	7.346
O	12.442	7.371	12.688
O	18.406	12.956	5.946
O	12.645	2.905	12.342
O	18.342	17.524	5.718
O	8.376	12.928	0.884
O	2.519	7.517	7.583
O	4.325	2.759	1.303
O	6.640	17.661	7.986
O	16.528	12.700	11.884
O	14.348	7.698	5.342
O	16.555	17.506	11.729
O	14.393	2.984	4.977
O	4.388	7.580	1.570
O	6.619	12.827	8.265
O	4.156	0.190	0.660
O	6.864	0.343	7.382
O	16.846	10.187	12.720
O	14.110	10.231	6.055
O	16.880	0.141	12.504
O	14.168	0.513	5.851
O	4.100	10.115	0.811
O	6.869	10.280	7.529
O	4.307	17.418	0.729
O	6.597	3.003	7.410
O	16.667	7.519	12.650
O	14.543	12.887	6.013
O	16.577	2.802	12.407
O	14.559	17.797	5.612
O	4.367	12.781	0.913
O	6.579	7.616	7.606
O	0.289	1.161	3.729
O	10.697	19.233	10.477
O	0.725	11.083	9.642
O	10.287	9.256	2.895
O	0.721	19.335	9.478
O	10.263	1.159	2.744
O	0.273	9.344	3.902
O	10.731	11.052	10.645
O	0.148	17.413	3.754
O	10.796	2.930	10.397
O	0.807	7.466	9.656
O	10.108	12.833	2.926
O	0.764	2.936	9.495
O	10.187	17.494	2.841
O	0.180	12.904	3.936
O	10.815	7.507	10.541
O	9.293	15.157	1.925
O	1.706	5.233	8.549
O	11.669	5.177	11.490
O	19.234	15.198	4.889
O	4.344	15.145	2.016
O	6.641	5.256	8.721
O	16.660	5.217	11.421
O	14.097	15.345	4.913
O	5.950	15.215	7.443
O	5.009	5.201	0.732
O	15.075	5.287	5.925
O	15.938	15.123	12.562
O	2.615	15.215	7.410
O	8.336	5.188	0.671
O	18.353	5.281	5.976

O	12.618	15.107	12.711
H	8.499	16.197	8.574
H	8.727	14.787	6.528
H	10.525	13.062	6.413
H	12.095	12.763	8.325
H	11.860	14.186	10.365
H	10.071	15.893	10.480
H	11.868	14.849	5.684
H	13.154	14.466	6.962
H	13.094	16.844	7.707
H	11.428	16.326	7.945
H	11.808	17.212	6.468
C	9.287	15.446	8.508
C	9.412	14.659	7.368
C	12.435	15.175	6.553
C	11.319	13.529	8.376
C	11.182	14.314	9.523
C	10.175	15.275	9.586
C	12.218	16.469	7.164
C	10.437	13.706	7.291

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