Supporting Information

Genesis and Stability of Hydronium Ions in Zeolite Channels

Meng Wang,† Nicholas R. Jaegers,†,‡ Mal-Soon Lee,† Chuan Wan,† Jian Zhi Hu,*,† Hui Shi,† Donghai Mei,† Sarah D. Burton,† Donald M. Camaioni,† Oliver Y. Gutierrez,† Vassiliki-Alexandra Glezakou,† Roger Rousseau,† Yong Wang,†,‡ and Johannes A. Lercher*,†,§

† Institute for Integrated Catalysis, Pacific Northwest National Laboratory Richland, Washington 99354, USA

‡ Voiland School of Chemical Engineering and Bioengineering, Washington State University, Pullman, WA 99163, USA

§ Department of Chemistry and Catalysis Research Center, TU München, Lichtenbergstrasse 4, 85748 Garching, Germany

Content

Analysis of the structure of the aluminum hexahydrate complex

A combination of spectroscopic and theoretical methods was used to better understand the nature of the aluminum hexahydrate complex. As a reference point for comparison, solid $Al(NO_3)_3 \cdot 9H_2O$ was investigated with ^1H NMR since it is comprised of $Al(H_2O)_6^{3+}$ octahedra[1] as the first coordination shell structure while the second coordination shell consists of 3 H_2O and 3 NO_3^- molecules. Two peaks are present (Figure S8) at 9.3 and 4.3 ppm, which relate to protons surrounding the Al in the first and second coordination shells, respectively. This assignment is validated by DFT cluster calculations of the chemical shift (Table S1), where the proton species in the first coordination shell of Al^{3+} is predicted at 9.4 ppm. Analogous cluster calculations show that given sufficient neighboring water molecules, or in water clusters without Al^{3+}, the average shift accurately converges to 4.8-4.9 ppm, in excellent agreement with the experimental value of pure bulk water. The results in Table S1 demonstrate the necessity of a second solvation shell for the aluminum hexahydrate, $Al(H_2O)_6^{3+}$ to present ^1H signals at the observed value (~9.5 ppm) since an isolated aluminum hexahydrate complex, $Al(H_2O)_6^{3+}$, without second shell is predicted to have a ^1H chemical shift of 5.7 ppm (see Table S1). This second solvation shell contains 12 additional water molecules to total 18 H_2O in the water-abundant Al^{3+} complex. The water in the second hydration shell of the $Al(H_2O)_6^{3+} \cdot 12H_2O$ cluster greatly influence the geometries of the first shell water molecules, i.e., the Al-O distances and the H-O-H bond angles. The net result is to deshield the first shell water protons, causing the NMR resonance to be shifted downfield relative to the protons in a bare $Al(H_2O)_6^{3+}$ cluster in vacuum. For details, please see the Figure S9, including Table S2 and Table S3. Note here we refer to the 18 waters, of the $Al(H_2O)_6^{3+} \cdot 12H_2O$ rather than the waters inside the zeolite associated with the BA site. Even though the protons in the first shell of this $Al(H_2O)_6^{3+} \cdot 12H_2O$ cluster have chemical shifts approximately 9.3 ppm, fast exchange with the protons in the second shell would result in an average chemical shift of about 6 ppm. Considering this evidence, we conclude that the 9-ppm peak observed in this study cannot be attributed to $Al(H_2O)_6^{3+} \cdot 12H_2O$. The assignment of 9.2 ppm to hexaquo complexes[2] was based on the report by Akitt, et al. for the aluminum hexahydrate complex in a mixture at 10.2 ppm,[3,4] Akitt et al. purposely created a condition where exchange is slow so that the different protons could be seen.

Analysis of NMR signals of perchloric acid in solution and in zeolite pores

A free hydronium ion in aqueous phase is expected to have a chemical shift in the range of 7 – 12 ppm.[2, 5] To test the assignment of the 9-ppm peak to a hydrated hydronium ion, the ^1H NMR spectra of perchloric acid in a wide range of concentrations in water were investigated (Figure S10). In agreement with previous reports,[6] the chemical shift moved downfield as the ratio of H_2O/H^+ increased. At H_2O/H^+ ratios of 2.4 and 8, the ^1H chemical shifts were between 8.8 and 6.6 ppm, respectively.

To understand the chemical species corresponding to the 9-ppm peak in the zeolite environment, acid solutions were injected into the zeolite with a micro syringe in a glovebox and sealed in the rotor. After the rotor was heated to 140 °C and cooled to room temperature, the ^1H NMR spectra (Figure S11) showed a narrow peak at about 9 ppm with higher intensity compared to the sample which had only adsorbed water (Figures 1 and 6). By introducing more hydronium ions into this mixture, the signal at 9 ppm increased, confirming the attribution of the 9 ppm peak to hydronium ions that do not rapidly exchange protons with water outside their hydration sphere, similar to the depiction in Figure 2b.

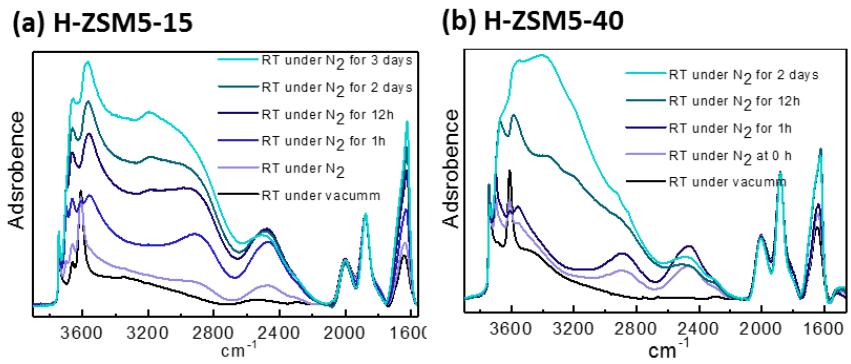

Figure S1. IR spectra of dehydrated H-ZSM5-15 (a) and H-ZSM5-40 (b) zeolites acquired at different time after the zeolite cooled down and exposed to nitrogen (10 ml/min) from 400°C to room temperature.

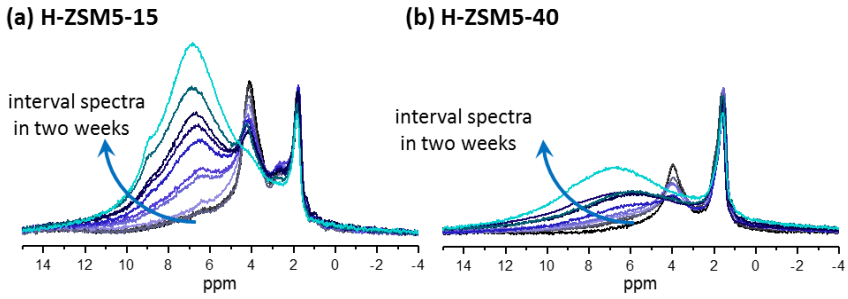

Figure S2. [1]H one-pulse MAS solid-state NMR spectra acquired two weeks after the dehydrated H-ZSM5-15 and H-ZSM5-40 zeolites were loaded into the probe. The recycle delay was 10 s, the number of scans was 16, and the spinning rate was 9.5 kHz.

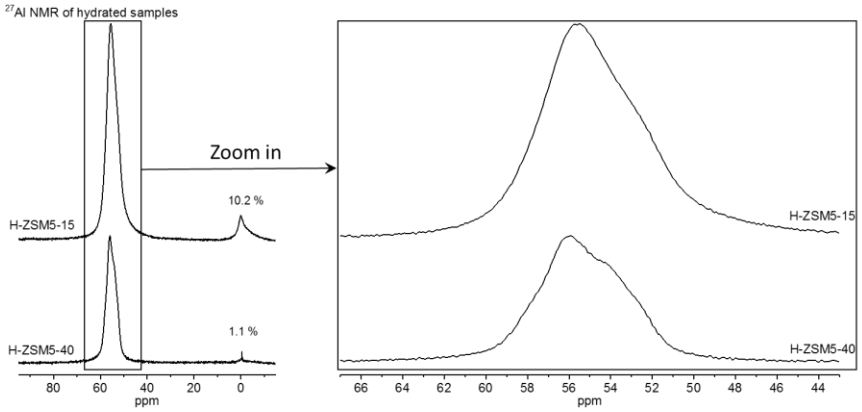

Figure S3. [27]Al MAS Solid state NMR spectra of the full hydrated H-ZSM-5 zeolites. Pulse length of 1.0 μs, corresponding to a pulse angle of 15°, was selected for acquiring each [27]Al MAS NMR spectrum with a recycle time of 1 s and total accumulation of 5000 scans. Magnetic field strength was 19.97 T (850MHz NMR spectrometer) and spinning rate was 20 kHz. The results indicate a greater abundance of extra-framework Al species for the more substituted zeolite that appear more solid in nature. The concentrations are employed in Table 1. There is a slight difference in the relative distribution of the tetrahedral Al species due to the enhanced Al content of H-ZSM5-15.[7]

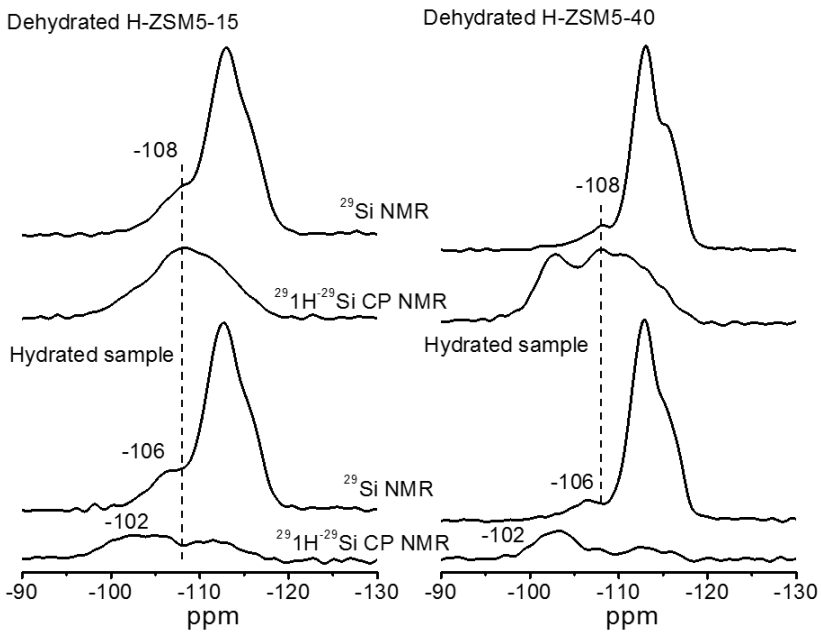

Figure S4. Comparison of ^{29}Si one-pulse and ^{1}H-^{29}Si Cross Polarization (CP) MAS Solid state NMR spectra of dehydrated and full hydrated H-ZSM-5 zeolites. For one-pulse experiments, pulse length was 4.5 us (90°), recycle delay was 200 s, and number of scans was 1000. CP/MAS NMR measurements were performed with a contact time of 3 ms, a recycle delay of 5 s, and a sample spinning rate of 5 kHz.

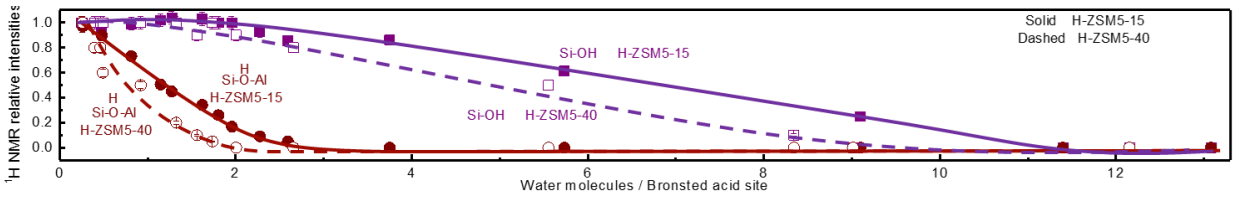

Figure S5. The dependencies of ^{1}H NMR relative intensities of the silanol group (1.7 ppm) and Brønsted acid site (4 ppm) on water loading of dehydrated zeolites.

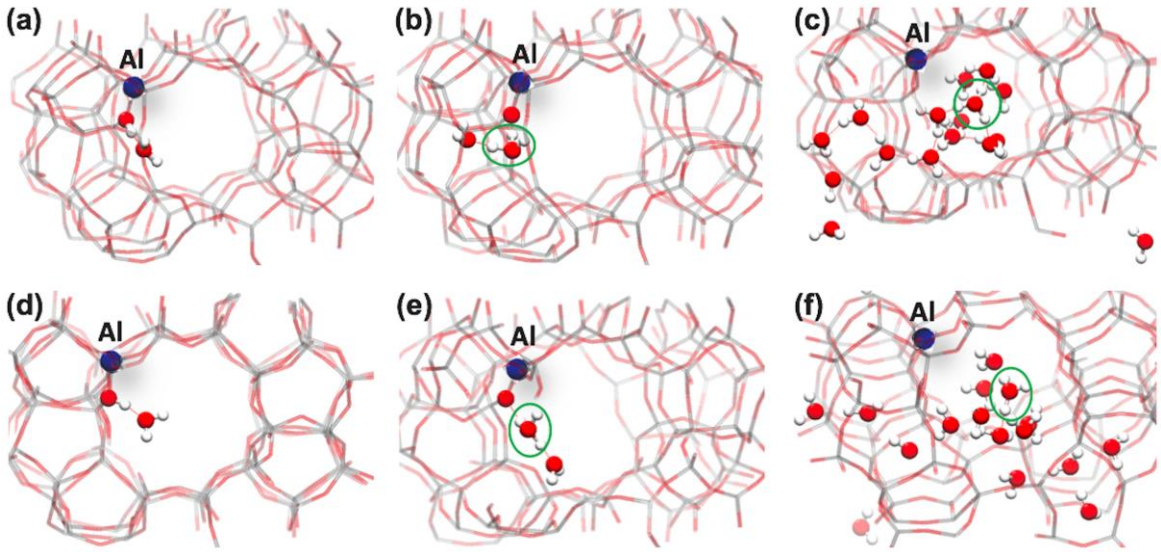

Figure S6. Snapshot of H-ZSM-5 structures with water:BAS ratio of 1 (a,d), 2 (b,e) and 16 (c,f) obtained from AIMD simulations at 300 K (upper panel) and 500 K (lower panel). Green circles show H_3O^+ formation.

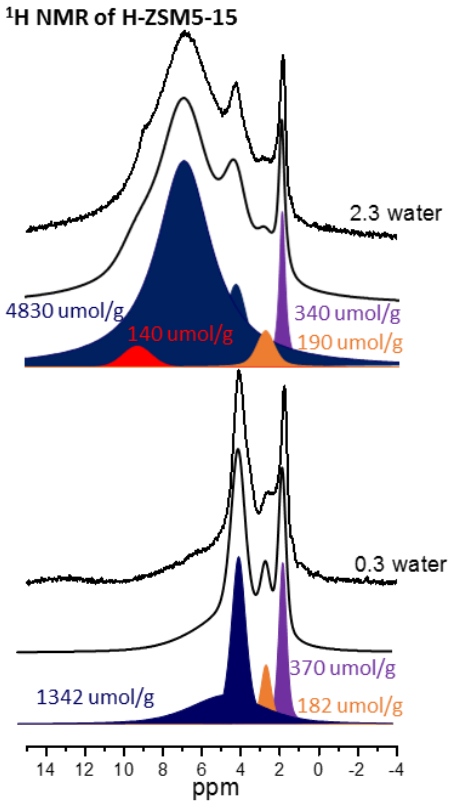

Figure S7. [1]H one-pulse MAS solid-state NMR spectra with simulations and spin-counting results of H-ZSM5-15 zeolite with different water loadings.

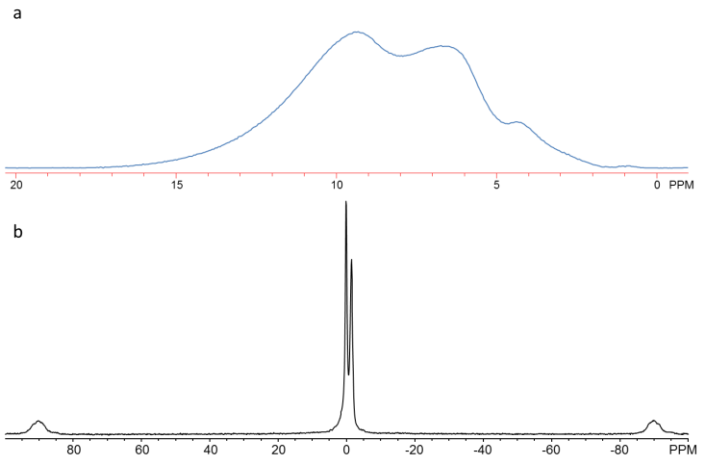

Figure S8. [1]H (a) and [27]Al (b) NMR spectra of $Al(NO_3)_3 \cdot 9H_2O$ at 20 kHz MAS. The proton spectrum shows signals relating to water surrounding Al ions (9.3 ppm), system background as determined by pulse width calibration (6.6 ppm), and water in an outer shell that link octahedral within the same layer and nitrate anions (4.3). Two [27]Al signals are present (0.1 and -1.4 ppm) which relate to the two similar, but distinct, Al octahedral in the crystal structure.

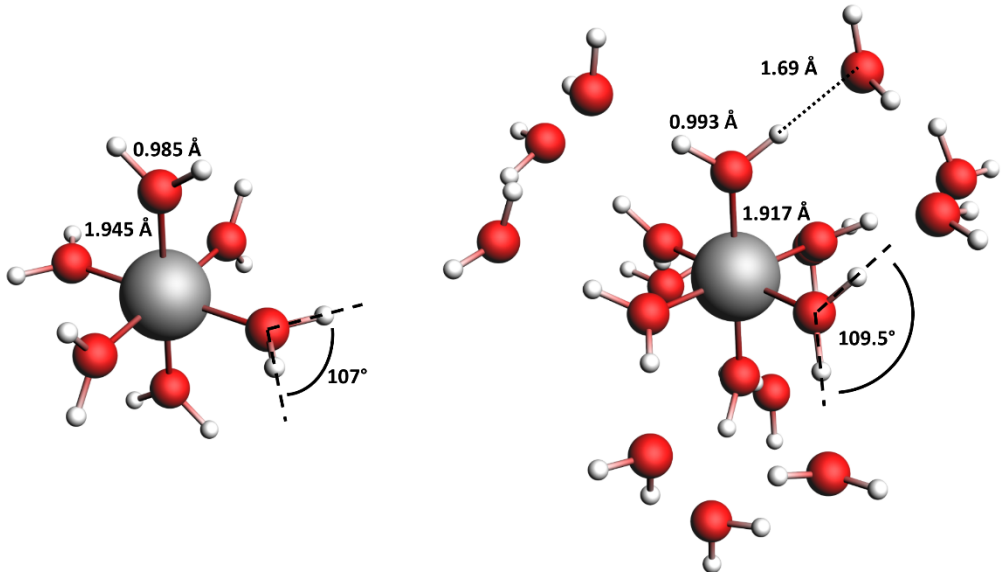

Figure S9. Geometry optimized structures of $Al(H_2O)_6^{3+}$ (one water shell) and $Al(H_2O)_6^{3+}\cdot 12H_2O$ (two water shells). Optimized geometry coordinates are attached in the end of the supporting information.

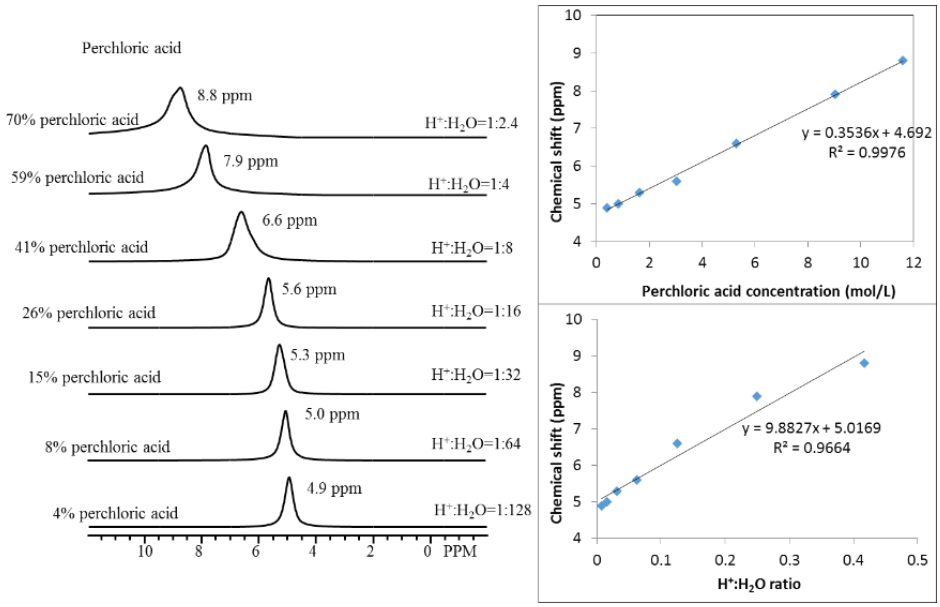

Figure S10. ^1H one-pulse NMR spectra of perchloric acid with different concentrations (left), dependences of ^1H chemical shift on mole fraction of the acid (upper right) or the ratio between H^+ and H_2O (lower right).

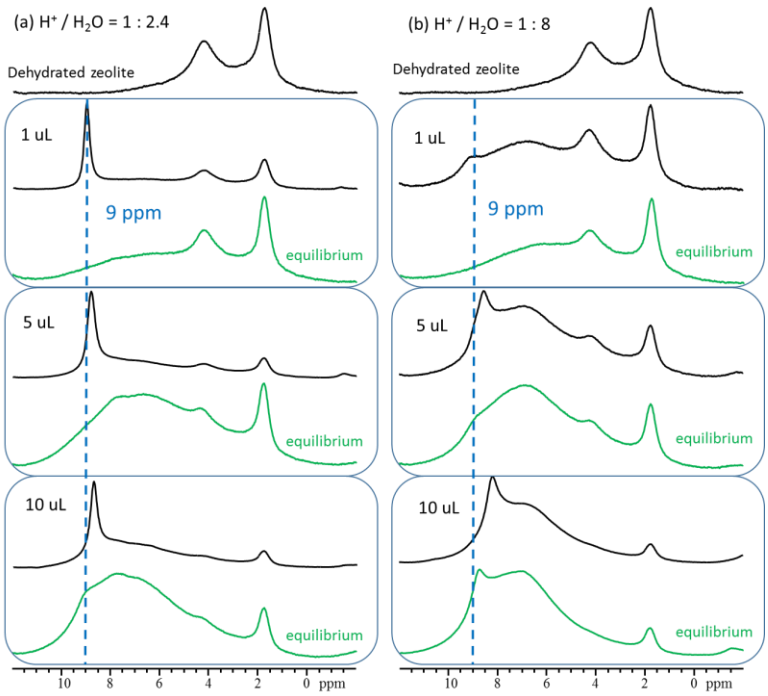

Figure S11. ^{1}H one-pulse NMR spectra of dehydrated H-ZSM5-15 with different amounts of perchloric acid solution in two different concentrations. In each unit, the upper spectrum was acquired as the beginning when rotor was loaded into the probe, the lower spectrum was acquired after the rotor was heated to 140 °C and cooled to room temperature. The mass of the catalyst was 115.1 (a) and 109.8 mg (b), and from top to the bottom, the total amount of added solution was 1, 5 and 10 uL.

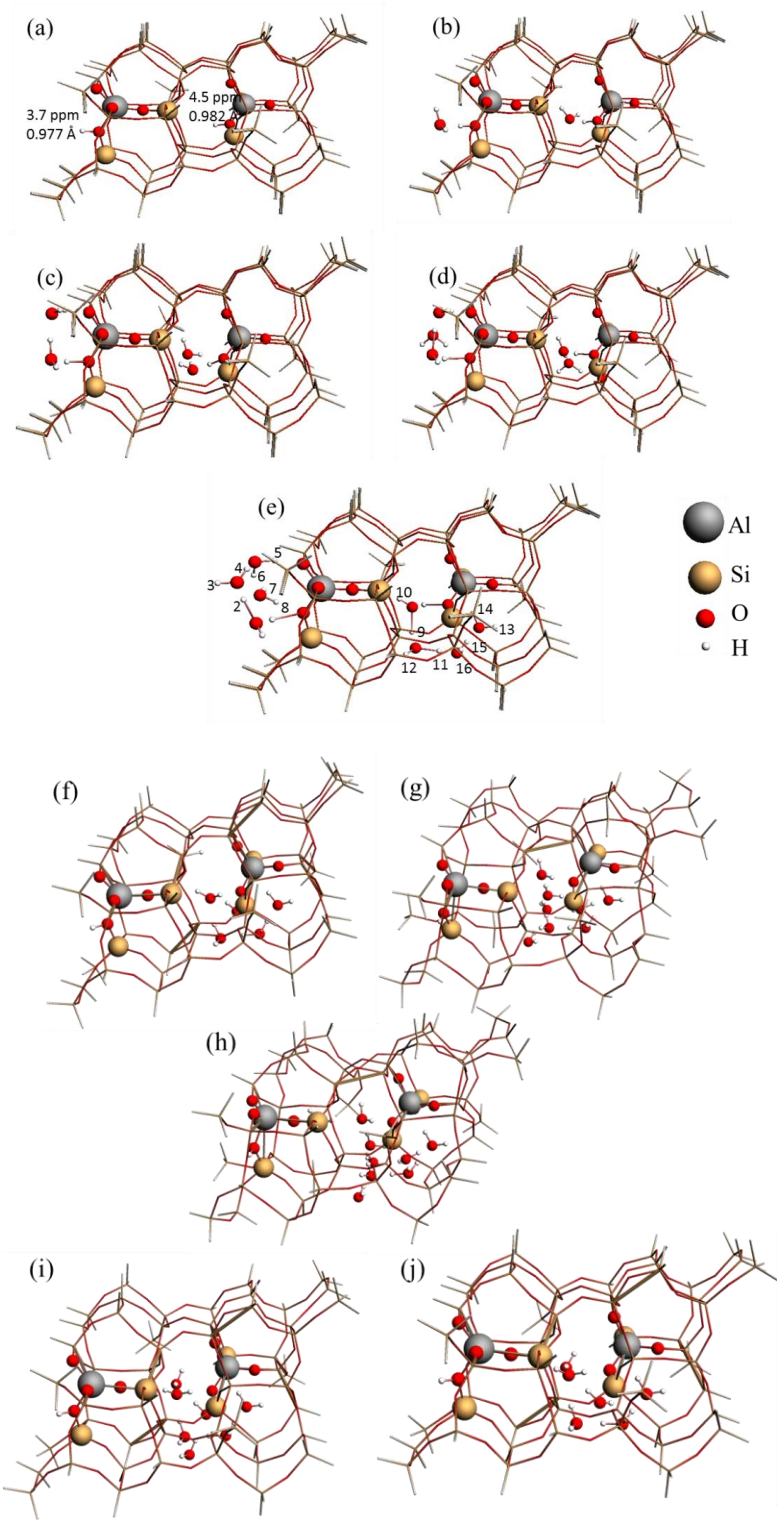

Figure S12. Geometry optimized structures for H_2O molecules bonding with H-ZSM5 clusters. (a) 58T H-ZSM5 cluster, (b) 58T-1H_2O, (c) 58T-2H_2O, (d) 58T-3H_2O, (e) 58T-4H_2O, (f) 58T-5H_2O, (g) 58T-6H_2O, (h) 58T-7H_2O, (i) 58T-8H_2O, (j) 58T-9H_2O. Optimized geometry coordinates are attached in the end of the supporting information.

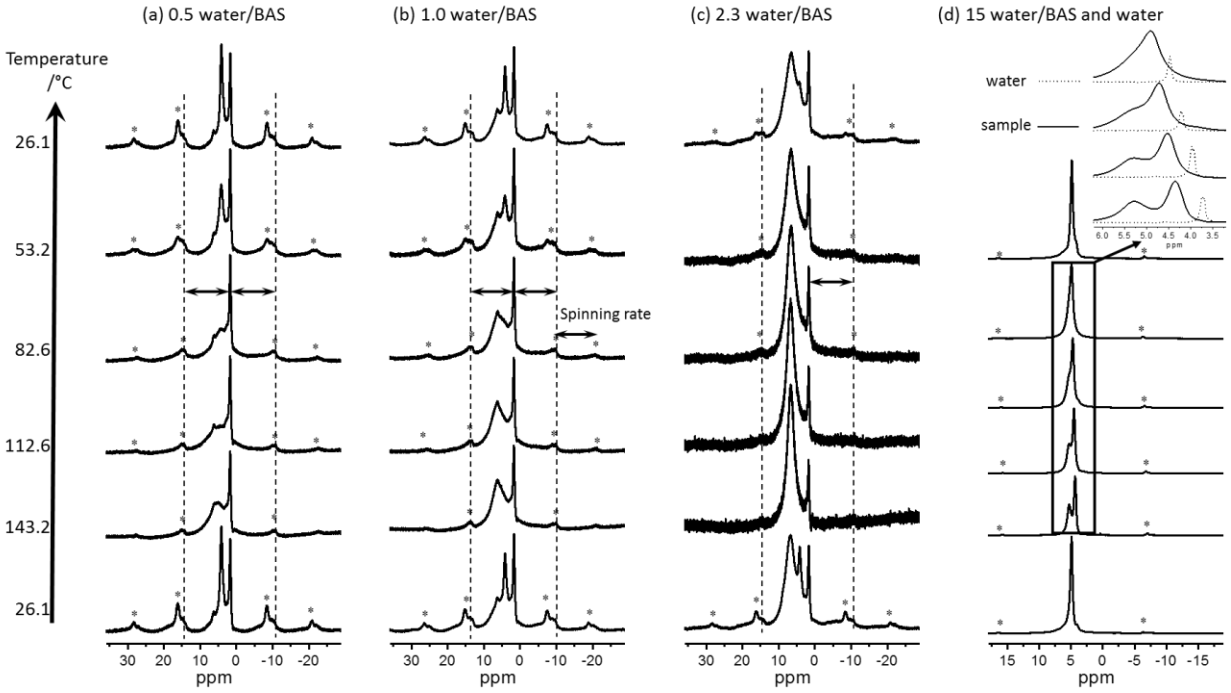

Figure S13. In-situ ^{1}H one-pulse NMR spectra of H-ZSM5-15 at different temperatures with different water loadings. From a to d, 0.5, 1.0, 2.3 and 15 water molecules per acid site were obtained from the samples respectively, and the insert figure in d shows the comparison between the sample and water in a narrow range. The bottom spectrum was the first scan for each sample. The rotor was then heated to the highest temperature and stepwise cooled and monitored. Calibrated temperatures are listed on the left. The spinning rates were from 3400 to 3760 Hz, and ± 10 Hz in each experiment. Asterisks denote spinning sidebands and the dashed lines in a, b and c indicate the positions of sidebands from the terminal silanol groups.

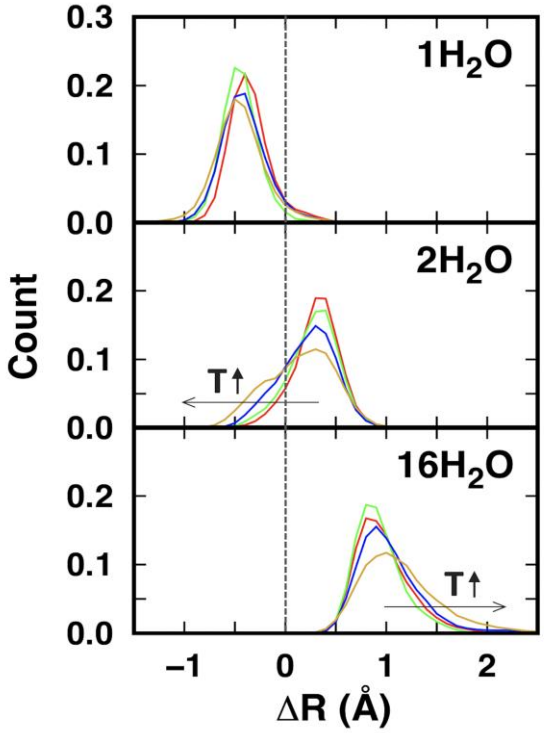

Figure S14. Histogram of bond length differences between R(H-OB) and R(Ow-H) at different temperatures obtained from AIMD simulations. Line color codes: red at 27 °C, green at 77 °C, blue at 127 °C, and gold at 227 °C.

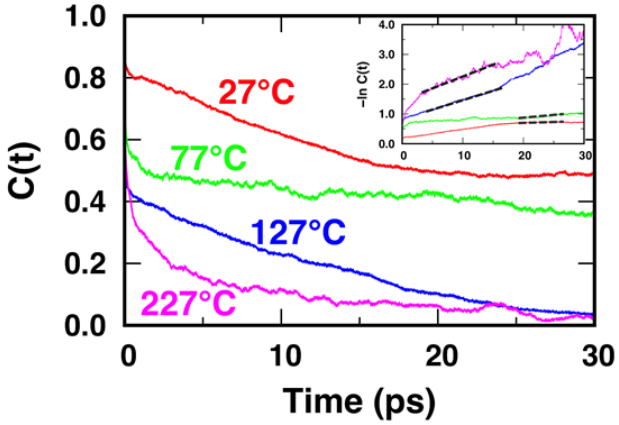

Figure S15. H_3O^+ population decay correlation function $C(t)$ at different temperatures in the 16 water/BAS system. Inset: plot of -ln $\boldsymbol{C(t)}$ vs. time where dotted lines show slopes to estimate hoping rate D. For the fitting of the lines, we took data showing stead change of -ln $C(t)$ which allow us to avoid the ambiguity due to cutoff criteria as well as limited statistics.

Table S1. DFT ^{1}H NMR calculations of selected hydrated clusters

Model	**Δ ppm ^{1}H**
TMS	0
$Al(H_2O)_6^{3+}$	5.65
$Al(H_2O)_6^{3+}\cdot 12H_2O$	1st Shell: 9.5 2nd Shell: 3.6 Avg.: 5.6
$Al(NO_3)_3\cdot 9H_2O$	1st Shell: 9.4 2nd Shell: 3.7 Avg.:7.4
$1H_2O$	0.06
$2H_2O$	0.40
$3H_2O$	0.58
$4H_2O$	4.39
$5H_2O$	4.3
$6H_2O$	4.2
$7H_2O$	4.9
$8H_2O$	4.3
$9H_2O$	5.1
$10H_2O$	5.0
$12H_2O$	4.9
10 Water/Site 2	7.0*

*This average chemical shift value is apparently distorted due to migration of water molecules into positions which would house the framework in an extended, uncut model.

Table S2. DFT ^{1}H NMR calculations of hydrated Al^{3+} clusters in Table S1. Optimized geometry coordinates are attached in the end of the supporting information.

$Al(H_2O)_6^{3+}$	**Δ ppm**	$Al(H_2O)_6^{3+}\cdot 12H_2O$	**Δ ppm**	$Al(NO_3)_3\cdot 9H_2O$	**Δ ppm**
		1st Shell	9.5	1st Shell	9.4
Average	5.5	2nd Shell	3.6	2nd Shell	3.7
		Average	5.6	Average	7.4
H(11):	5.53	H(10):	9.41	H(1):	11.12
H(13):	5.52	H(11):	9.41	H(2):	20.18
H(15):	5.53	H(12):	9.41	H(3):	6.93
H(17):	5.52	H(13):	9.41	H(4):	2.42
H(19):	5.52	H(14):	9.41	H(5):	11.77
H(2):	5.53	H(15):	9.41	H(6):	15.91
H(3):	5.53	H(16):	9.41	H(7):	5.99
H(4):	5.52	H(17):	9.41	H(8):	10.04
H(5):	5.52	H(18):	9.41	H(9):	3.22
H(6):	5.52	H(19):	9.41	H(10):	9.99
H(7):	5.53	H(32):	4.38	H(11):	1.33
H(9):	5.53	H(33):	4.38	H(12):	12.33
		H(34):	4.38	H(13):	4.73
		H(35):	4.38	H(14):	5.16
		H(36):	4.38	H(15):	4.22
		H(37):	4.38	H(16):	1.42
		H(38):	4.38	H(17):	3.59
		H(39):	4.38	H(18):	2.42
		H(40):	4.38		
		H(41):	4.38		
		H(42):	4.38		
		H(43):	4.38		
		H(44):	2.6		
		H(45):	2.6		
		H(46):	2.6		
		H(47):	2.6		
		H(48):	2.6		
		H(49):	2.6		
		H(50):	2.6		
		H(51):	2.6		
		H(52):	2.6		
		H(53):	2.6		
		H(54):	2.6		
		H(55):	2.6		
		H(8):	9.41		
		H(9):	9.41		

Table S3: The Mulliken charges extracted from DFT population analysis.

	$Al(H_2O)_6^{3+}$	$Al(H_2O)_6^{3+}\cdot 12H_2O$
Mulliken Al	2.118	1.860
Mulliken H -1st	0.251	0.237
Mulliken O - 1st	-0.355	-0.395
Mulliken H - 2nd		0.263
Mulliken O - 2nd		-0.470

Table S4. DFT ^{1}H NMR calculations of different water loadings on Site 2 in Table 3.

Water/BAS		**Δ ppm ^{1}H**
0	H(192):	4.5
1	H(192):	14.4
	H(209):	4.3
	H(210):	4.0
2	H(192):	18.6
	H(209):	11.6
	H(210):	5.0
	H(212):	3.0
	H(213):	4.5
3	H(192):	16.1
	H(209):	17.4
	H(210):	6.0
	H(212):	10.8
	H(213):	2.1
	H(218):	1.5
	H(219):	7.6
4	H(192):	6.9
	H(209):	11.6
	H(210):	2.3
	H(212):	17.2
	H(213):	2.3
	H(218):	3.1
	H(219):	11.3
	H(224):	17.9
	H(225):	6.1
5	H(192):	7.4
	H(205):	5.8
	H(207):	10
	H(209):	8.2
	H(210):	2.3
	H(212):	15.4
	H(213):	2
	H(215):	17.7
	H(216):	3.5
	H(218):	0.3
	H(219):	4.4
6	H(192):	7.3
	H(205):	6
	H(207):	9.5
	H(209):	8.4
	H(210):	3.1
	H(212):	15.7
	H(213):	1.8
	H(215):	16.9
	H(216):	5.6
	H(218):	-0.1
	H(219):	4.4
	H(220):	5.9
	H(222):	1
7	H(192):	7.9
	H(205):	2.1
	H(207):	7.6
	H(209):	16
	H(210):	4
	H(212):	12.8
	H(213):	10.5
	H(215):	6.5
	H(216):	0.5
	H(218):	3.8
	H(219):	3.1
	H(220):	4.8
	H(222):	2.7
	H(223):	5.4
	H(225):	6.7
8	H(192):	6.1
	H(205):	9.5
	H(207):	8.9
	H(209):	11.1
	H(210):	11
	H(212):	17.2
	H(213):	4.2
	H(215):	13.5
	H(216):	3.9
	H(218):	1.5
	H(219):	4.4
	H(220):	5.2
	H(222):	0.7
	H(223):	2.5
	H(225):	1.2
	H(226):	4.7
	H(228):	5.9
9	H(192):	6.6
	H(205):	9.4
	H(207):	8.8
	H(209):	11.1
	H(210):	9.8
	H(212):	17.7
	H(213):	4.6
	H(215):	13.1
	H(216):	4
	H(218):	1.6
	H(219):	4.4
	H(220):	4.9
	H(222):	0.7
	H(223):	2.6
	H(225):	0.9
	H(226):	5.4
	H(228):	6.5
	H(229):	1.8
	H(231):	3.4

Table S5. DFT ^{1}H NMR calculations of different water loadings on Site 1 in Table 3.

Water/BAS		**Δ ppm ^{1}H**
0	H(58):	3.7
1	H(58):	13.6
	H(206):	4.9
	H(207):	2.4
2	H(58):	16.7
	H(206):	5.9
	H(207):	16.9
	H(215):	8.2
	H(216):	3.5
3	H(58):	7.5
	H(206):	4.3
	H(207):	17.2
	H(215):	3.5
	H(216):	0.8
	H(221):	14.8
	H(222):	5.0
4	H(58):	5.2
	H(206):	4.1
	H(207):	11.2
	H(215):	2.0
	H(216):	16.9
	H(221):	12.3
	H(222):	12.6
	H(227):	2.1
	H(228):	7.3

Reference

1. Hermansson, K., A Neutron-diffraction Determination Of The Structure Of Deuterated Aluminum Nitrate Nonahydrate, Al(NO3)3.9D2O. *Acta Crystallogr., Sect. C: Struct. Chem.* **1983,** *39* (AUG), 925-930.
2. Hunger, M.; Freude, D.; Pfeifer, H., Magic-angle spinning nuclear magnetic resonance studies of water molecules adsorbed on Bronsted- and Lewis-acid sites in zeolites and amorphous silica-aluminas. *J. Chem. Soc., Faraday Trans.* **1991,** *87* (4), 657-662.
3. Akitt, J. W.; Elders, J. M.; Fontaine, X. L. R., Hydrogen-deuterium isotope effects in the proton NMR spectra of hydrated Al species. *J. Chem. Soc., Chem. Commun.* **1986,** (13), 1047-1049.
4. Batamack, P.; Doremieux-Morin, C.; Fraissard, J.; Freude, D., Broad-line and high-resolution NMR studies concerning the hydroxonium ion in HZSM-5 zeolites. *J. Phys. Chem.* **1991,** *95* (9), 3790-3796.
5. Sauer, J., Acidic sites in heterogeneous catalysis: structure, properties and activity. *J. Mol. Catal.* **1989,** *54* (3), 312-323.
6. Maemets, V.; Koppel, I., 17O and 1H chemical shifts of water in solutions of some ammonium salts: evaluation of the anionic effect on the 17O and 1H chemical shifts of water in aqueous solutions of mineral acids. *J. Chem. Soc., Faraday Trans.* **1996,** *92* (19), 3533-3538.
7. Vjunov, A.; Fulton, J. L.; Huthwelker, T.; Pin, S.; Mei, D.; Schenter, G. K.; Govind, N.; Camaioni, D. M.; Hu, J. Z.; Lercher, J. A., Quantitatively Probing the Al Distribution in Zeolites. *Journal of the American Chemical Society* **2014,** *136* (23), 8296-8306.

Optimized geometries of the structures in Figure S12.

Figure S12a

Atom	X	Y	Z (Angstrom)
1.H	11.724897	18.758996	8.990065
2.O	7.905434	6.718915	2.918203
3.O	8.769086	14.904732	8.621397
4.O	10.256288	7.300206	3.850785
5.O	3.747943	14.866833	8.541266
6.Si	3.608383	1.178364	8.991497
7.Si	8.510158	16.468016	8.942364
8.Si	6.080702	17.246897	10.874931
9.O	3.927836	12.435724	7.779864
10.H	19.669389	12.824277	10.664242
11.O	11.261974	4.979486	4.760475
12.Si	3.641757	16.399351	9.064493
13.O	8.258402	11.367538	5.329838
14.O	3.757783	11.203355	5.502358
15.O	11.853464	16.505999	7.829272
16.Si	7.623219	18.561818	6.886585
17.O	3.679898	6.802193	5.761159
18.O	8.683827	7.382991	8.034960
19.Si	1.562565	3.409045	2.285621
20.Si	3.925210	2.598888	4.229845
21.Si	4.628036	3.352819	7.183220
22.Si	7.642333	3.445997	7.064690
23.Si	8.606398	2.597838	4.229984
24.Si	6.348566	3.452390	2.343302
25.Si	11.617472	10.879672	4.575116
26.Si	14.052075	10.462394	2.554765
27.O	9.852796	17.164946	9.534970
28.O	7.169574	8.791325	9.704741
29.O	13.920543	14.873119	11.460635
30.Si	16.430657	11.072603	4.498444
31.Si	11.569735	6.533465	4.432283
32.Si	13.938170	7.247473	2.431637
33.O	6.246889	4.989009	1.836310
34.H	6.133215	13.066610	12.315747
35.O	15.509939	14.915550	5.851883
36.Si	16.365481	6.500210	4.326441
37.Si	18.492784	8.870413	11.394933
38.Si	16.093857	9.406061	9.366069
39.Si	15.645651	8.731120	6.480304
40.Si	12.429454	8.587330	6.604200
41.Si	11.354801	9.421519	9.337366
42.Si	13.626509	8.757689	11.158302
43.Si	18.394914	13.382950	11.173361
44.Si	16.138929	12.629178	9.060084
45.Si	15.497812	13.332061	6.205906
46.Si	11.352460	12.506049	9.256607
47.Si	13.788506	13.349736	10.903118
48.H	13.517739	0.678934	5.794769
49.H	6.098897	10.252665	1.093547
50.H	2.003493	7.296008	1.059977
51.H	1.044564	9.693808	2.018387
52.H	2.224515	9.174697	9.425787
53.Si	16.409217	18.696612	4.400185
54.Si	11.533455	3.424614	4.391964
55.Si	13.897058	2.635799	2.441939
56.O	7.273292	13.351034	10.102888
57.O	2.667899	6.710440	3.428856
58.H	2.765969	6.486334	5.899561
59.Si	16.325442	3.448176	4.307543
60.O	3.913491	8.928552	4.177192
61.O	6.249761	7.214945	7.020266
62.O	4.671971	4.890721	7.525922
63.Si	12.417923	1.360842	6.526026
64.H	14.107370	17.278863	12.073781
65.O	5.510834	10.864160	3.517241
66.Si	18.432106	16.481945	11.119327
67.Si	16.143264	17.269802	9.082199
68.Si	15.474584	16.492981	6.149245
69.Si	12.401461	16.470603	6.276625
70.Si	11.434232	17.325825	9.163515
71.Si	13.760634	16.405484	10.941879
72.Si	8.469444	8.841442	8.729002
73.Si	6.083869	9.407682	10.739780
74.O	4.659517	13.090605	10.299580
75.O	6.267597	11.016734	10.868706
76.O	7.674517	4.978387	7.608877
77.Si	3.574759	8.817302	8.956283
78.Si	8.489196	13.354060	9.019152
79.Si	6.086934	12.621809	10.917886
80.O	8.341084	9.944708	7.531950
81.O	3.598692	7.300975	8.459861
82.O	8.090283	12.612158	7.620213
83.Si	3.613346	13.342744	9.077338
84.Si	1.584345	11.080247	2.062649
85.Si	4.011044	10.550753	4.047028
86.Si	4.442242	11.133323	6.981217
87.Si	7.672942	11.251462	6.851209
88.Si	8.667135	10.405590	4.076803
89.Si	6.451587	11.149246	2.218605
90.Si	1.571113	6.515684	2.239395
91.Si	3.946592	7.330895	4.163651
92.Si	7.705558	6.517627	7.043593
93.Si	8.671934	7.343645	4.213698
94.Si	6.385472	6.492637	2.401736
95.O	14.765029	16.664604	9.694536
96.O	8.344184	6.467379	5.530659
97.O	10.270125	10.451012	3.774218
98.O	1.496765	4.964592	1.842067
99.H	2.270860	1.061189	9.624451
100.H	4.655361	0.939754	10.019700
101.O	7.335979	16.662077	10.042700
102.H	6.197169	16.799566	12.278601
103.O	3.930989	9.778755	7.687487
104.O	16.261119	4.973770	4.856986
105.H	2.271432	16.655689	9.564733
106.O	4.678612	16.667795	10.289430
107.H	6.075885	18.725695	10.767342
108.H	2.255728	13.066538	9.567790
109.H	8.535151	2.631422	7.900306

110.H	8.751938	19.528767	6.881281
111.O	8.090665	17.154306	7.532737
112.O	3.753927	2.651674	8.362502
113.H	3.739497	0.138291	7.933294
114.H	3.977237	17.277205	7.919333
115.O	5.352141	6.717430	3.679774
116.H	19.759503	17.007165	10.722096
117.O	2.912154	11.109495	3.003911
118.O	12.249877	16.743323	10.453673
119.H	6.496975	19.137240	7.668564
120.H	7.179850	18.313697	5.492881
121.H	12.858979	1.684447	7.903342
122.H	1.959467	11.505324	0.691247
123.O	2.593429	3.168486	3.504982
124.O	3.842128	3.064591	5.771679
125.O	6.160728	2.740111	7.103896
126.O	8.179620	3.479235	5.522016
127.O	7.832387	3.151907	2.917303
128.O	5.253034	3.224853	3.523474
129.H	3.960903	1.132017	4.122820
130.H	8.280346	1.180220	4.460006
131.H	19.447870	7.850622	10.896350
132.H	6.032356	7.446486	1.342035
133.H	2.002033	2.636298	1.101232
134.H	16.134812	18.737423	9.199013
135.O	17.422762	16.661942	9.869670
136.H	6.065177	2.584649	1.192059
137.O	16.267832	16.832257	7.532609
138.O	10.175060	2.730028	3.852213
139.O	12.846511	10.950619	3.527727
140.H	13.903439	11.154703	1.271726
141.H	17.894068	17.219786	12.288198
142.O	12.342568	14.988441	5.691666
143.H	17.817537	10.825085	4.081237
144.O	15.510061	10.774292	3.184728
145.O	12.695290	6.640941	3.272724
146.H	13.848037	6.721287	1.065211
147.H	6.269429	8.785891	12.055243
148.Al	12.408213	13.415499	6.417179
149.H	17.718435	6.766503	3.813339
150.O	15.336298	6.725347	3.084600
151.O	13.924993	8.865058	2.346002
152.Al	4.690351	6.567440	7.359365
153.O	11.422117	12.434891	5.175956
154.O	11.844971	9.932034	5.861151
155.O	12.014365	7.217069	5.840273
156.O	16.263378	12.613698	4.942232
157.O	16.096665	10.117568	5.770925
158.O	16.099875	7.455758	5.600783
159.H	0.558258	11.994893	2.618677
160.H	0.265470	6.977691	2.760059
161.O	17.172467	8.882743	10.458587
162.O	16.349811	8.631088	7.948954
163.O	14.033336	8.712196	6.613692
164.O	11.840482	8.460639	8.107413
165.O	12.086238	8.953343	10.706229
166.O	14.592194	9.035244	9.874696
167.O	17.265201	13.266806	10.034456
168.O	16.433756	13.097591	7.539167
169.O	14.015229	12.759042	6.433214
170.O	11.598485	13.356968	7.937813
171.O	12.241833	13.013520	10.546484
172.O	14.676783	13.179067	9.541110
173.O	16.190178	11.013946	9.199970
174.O	11.759774	10.945252	8.954778
175.H	18.095322	8.540805	12.785044
176.H	19.141563	10.205874	11.371302
177.H	17.952263	12.661770	12.390005
178.H	13.809360	7.364947	11.624376
179.H	13.939776	9.728092	12.232639
180.H	14.271331	12.440560	11.952319
181.O	9.759225	9.273917	9.620046
182.O	9.767023	12.606428	9.705053
183.O	13.939307	17.080721	6.198682
184.H	6.390841	12.568154	1.803610
185.O	8.176663	8.886377	4.428778
186.O	18.605965	14.934990	11.551222
187.H	17.725827	18.905164	3.748127
188.H	15.331885	18.953762	3.408350
189.O	12.600954	3.240965	3.191353
190.H	13.846035	3.057857	1.026737
191.O	4.582975	9.118697	10.207456
192.H	10.513332	12.793417	5.079759
193.H	17.680855	3.171087	3.780356
194.O	15.260766	3.232902	3.095973
195.H	13.890994	1.159593	2.579063
196.O	7.832387	10.779092	2.817303
197.H	11.561871	17.380901	5.476996
198.H	11.238089	0.458029	6.579060
199.O	12.022904	2.739746	5.774086
200.O	16.336326	17.170908	4.940391
201.H	16.257996	19.658317	5.525503
202.H	15.983161	2.555685	5.438614
203.O	6.060193	11.108958	6.854727
204.H	0.211858	3.002375	2.736576

Figure S12b

Atom	X	Y	Z (Angstrom)
1.H	11.721237	18.759902	8.988107
2.O	7.905434	6.718915	2.918203
3.O	8.769086	14.904732	8.621397
4.O	10.256288	7.300206	3.850785
5.O	3.747943	14.866833	8.541266
6.Si	3.608383	1.178364	8.991497
7.Si	8.510158	16.468016	8.942364
8.Si	6.080702	17.246897	10.874931
9.O	3.927836	12.435724	7.779864
10.H	19.669123	12.824519	10.664157
11.O	11.261974	4.979486	4.760475
12.Si	3.641757	16.399351	9.064493
13.O	8.258402	11.367538	5.329838
14.O	3.757783	11.203355	5.502358
15.O	11.853464	16.505999	7.829272
16.Si	7.623219	18.561818	6.886585
17.O	3.678520	6.804509	5.763359
18.O	8.683827	7.382991	8.034960

19.Si	1.562565	3.409045	2.285621
20.Si	3.925210	2.598888	4.229845
21.Si	4.628036	3.352819	7.183220
22.Si	7.642333	3.445997	7.064690
23.Si	8.606398	2.597838	4.229984
24.Si	6.348566	3.452390	2.343302
25.Si	11.619775	10.889195	4.573893
26.Si	14.052075	10.462394	2.554765
27.O	9.852796	17.164946	9.534970
28.O	7.169574	8.791325	9.704741
29.O	13.920543	14.873119	11.460635
30.Si	16.430657	11.072603	4.498444
31.Si	11.569735	6.533465	4.432283
32.Si	13.938170	7.247473	2.431637
33.O	6.246889	4.989009	1.836310
34.H	6.136159	13.070633	12.314410
35.O	15.509939	14.915550	5.851883
36.Si	16.365481	6.500210	4.326441
37.Si	18.492784	8.870413	11.394933
38.Si	16.093857	9.406061	9.366069
39.Si	15.645651	8.731120	6.480304
40.Si	12.429454	8.587330	6.604200
41.Si	11.354801	9.421519	9.337366
42.Si	13.626509	8.757689	11.158302
43.Si	18.394914	13.382950	11.173361
44.Si	16.138929	12.629178	9.060084
45.Si	15.497812	13.332061	6.205906
46.Si	11.352460	12.506049	9.256607
47.Si	13.788506	13.349736	10.903118
48.H	13.509011	0.670983	5.789642
49.H	6.097626	10.252497	1.093594
50.H	2.000855	7.286451	1.051700
51.H	0.989973	9.717666	2.084444
52.H	2.215534	9.155162	9.413202
53.Si	16.409217	18.696612	4.400185
54.Si	11.533455	3.424614	4.391964
55.Si	13.897058	2.635799	2.441939
56.O	7.273292	13.351034	10.102888
57.O	2.667899	6.710440	3.428856
58.H	2.840925	6.192457	5.854288
59.Si	16.325442	3.448176	4.307543
60.O	3.913491	8.928552	4.177192
61.O	6.247938	7.217416	6.996373
62.O	4.649174	4.901135	7.476958
63.Si	12.417923	1.360842	6.526026
64.H	14.104598	17.279631	12.073779
65.O	5.510834	10.864160	3.517241
66.Si	18.432106	16.481945	11.119327
67.Si	16.143264	17.269802	9.082199
68.Si	15.474584	16.492981	6.149245
69.Si	12.372221	16.556224	6.261201
70.Si	11.434232	17.325825	9.163515
71.Si	13.760634	16.405484	10.941879
72.Si	8.469444	8.841442	8.729002
73.Si	6.083869	9.407682	10.739780
74.O	4.659517	13.090605	10.299580
75.O	6.267597	11.016734	10.868706
76.O	7.674517	4.978387	7.608877
77.Si	3.574759	8.817302	8.956283
78.Si	8.489196	13.354060	9.019152
79.Si	6.086934	12.621809	10.917886
80.O	8.341084	9.944708	7.531950
81.O	3.662121	7.278212	8.512763
82.O	8.090283	12.612158	7.620213
83.Si	3.613346	13.342744	9.077338
84.Si	1.584345	11.080247	2.062649
85.Si	4.011044	10.550753	4.047028
86.Si	4.442242	11.133323	6.981217
87.Si	7.672942	11.251462	6.851209
88.Si	8.667135	10.405590	4.076803
89.Si	6.451587	11.149246	2.218605
90.Si	1.571113	6.515684	2.239395
91.Si	3.942631	7.326353	4.196949
92.Si	7.706523	6.520015	7.040047
93.Si	8.671934	7.343645	4.213698
94.Si	6.385472	6.492637	2.401736
95.O	14.765029	16.664604	9.694536
96.O	8.344184	6.467379	5.530659
97.O	10.270125	10.451012	3.774218
98.O	1.496765	4.964592	1.842067
99.H	2.261680	1.062242	9.604427
100.H	4.643107	0.947191	10.031303
101.O	7.335979	16.662077	10.042700
102.H	6.199528	16.800455	12.278315
103.O	3.930989	9.778755	7.687487
104.O	16.261119	4.973770	4.856986
105.H	2.272557	16.658946	9.564817
106.O	4.678612	16.667795	10.289430
107.H	6.078774	18.725235	10.765164
108.H	2.256214	13.069107	9.570220
109.H	8.527563	2.625579	7.902567
110.H	8.760696	19.517933	6.867758
111.O	8.090665	17.154306	7.532737
112.O	3.753927	2.651674	8.362502
113.H	3.753374	0.142519	7.932195
114.H	3.980260	17.276514	7.919633
115.O	5.352141	6.717430	3.679774
116.H	19.758684	17.008715	10.722129
117.O	2.912154	11.109495	3.003911
118.O	12.249877	16.743323	10.453673
119.H	6.510224	19.145227	7.679586
120.H	7.167884	18.308464	5.498536
121.H	12.869759	1.684330	7.899820
122.H	1.971668	11.424436	0.672788
123.O	2.593429	3.168486	3.504982
124.O	3.842128	3.064591	5.771679
125.O	6.160728	2.740111	7.103896
126.O	8.179620	3.479235	5.522016
127.O	7.832387	3.151907	2.917303
128.O	5.253034	3.224853	3.523474
129.H	3.957905	1.131544	4.142960
130.H	8.279479	1.180105	4.460828
131.H	19.465601	7.876718	10.876421
132.H	6.042407	7.438697	1.331826
133.H	2.011144	2.629045	1.110090
134.H	16.133329	18.737481	9.197181

135.O	17.422762	16.661942	9.869670
136.H	6.060653	2.578198	1.198122
137.O	16.267832	16.832257	7.532609
138.O	10.175060	2.730028	3.852213
139.O	12.846511	10.950619	3.527727
140.H	13.913753	11.151754	1.268558
141.H	17.892637	17.219677	12.287391
142.O	12.191001	15.046835	5.685491
143.H	17.819226	10.828644	4.083763
144.O	15.510061	10.774292	3.184728
145.O	12.695290	6.640941	3.272724
146.H	13.850203	6.718531	1.065851
147.H	6.270520	8.789366	12.056970
148.Al	12.404777	13.465978	6.409419
149.H	17.719404	6.764977	3.814625
150.O	15.336298	6.725347	3.084600
151.O	13.924993	8.865058	2.346002
152.Al	4.677394	6.588171	7.316224
153.O	11.391604	12.429425	5.205479
154.O	11.844971	9.932034	5.861151
155.O	12.014365	7.217069	5.840273
156.O	16.263378	12.613698	4.942232
157.O	16.096665	10.117568	5.770925
158.O	16.099875	7.455758	5.600783
159.H	0.594519	12.060778	2.569226
160.H	0.258561	6.974366	2.744157
161.O	17.172467	8.882743	10.458587
162.O	16.349811	8.631088	7.948954
163.O	14.033336	8.712196	6.613692
164.O	11.840482	8.460639	8.107413
165.O	12.086238	8.953343	10.706229
166.O	14.592194	9.035244	9.874696
167.O	17.265201	13.266806	10.034456
168.O	16.433756	13.097591	7.539167
169.O	13.989086	12.778195	6.376589
170.O	11.582268	13.365935	7.920336
171.O	12.241833	13.013520	10.546484
172.O	14.676783	13.179067	9.541110
173.O	16.190178	11.013946	9.199970
174.O	11.759774	10.945252	8.954778
175.H	18.099739	8.505940	12.778676
176.H	19.121198	10.216905	11.400340
177.H	17.951810	12.663145	12.390194
178.H	13.810527	7.366098	11.626837
179.H	13.939833	9.728833	12.232338
180.H	14.271300	12.443062	11.954082
181.O	9.759225	9.273917	9.620046
182.O	9.767023	12.606428	9.705053
183.O	13.939307	17.080721	6.198682
184.H	6.385467	12.567411	1.801391
185.O	8.176663	8.886377	4.428778
186.O	18.605965	14.934990	11.551222
187.H	17.730467	18.910549	3.761287
188.H	15.337934	18.948817	3.400868
189.O	12.600954	3.240965	3.191353
190.H	13.846531	3.054542	1.025906
191.O	4.582975	9.118697	10.207456
192.H	10.497615	12.958969	5.060444
193.H	17.680652	3.169284	3.780729
194.O	15.260766	3.232902	3.095973
195.H	13.891596	1.159649	2.580971
196.O	7.832387	10.779092	2.817303
197.H	11.557909	17.511998	5.493462
198.H	11.235198	0.462375	6.589971
199.O	12.022904	2.739746	5.774086
200.O	16.336326	17.170908	4.940391
201.H	16.242313	19.656823	5.524487
202.H	15.983720	2.555651	5.438826
203.O	6.060193	11.108958	6.854727
204.H	0.217652	2.990527	2.741944
205.O	1.744177	5.146109	6.090356
206.H	2.202434	4.294573	5.908901
207.H	1.544677	5.131345	7.045942
208.O	9.461235	14.059033	5.115173
209.H	10.048620	14.821061	5.316807
210.H	8.906506	13.921514	5.910967

Figure S12c

Atom	X	Y	Z (Angstrom)
1.H	11.714082	18.761261	8.985441
2.O	7.905434	6.718915	2.918203
3.O	8.769086	14.904732	8.621397
4.O	10.256288	7.300206	3.850785
5.O	3.747943	14.866833	8.541266
6.Si	3.608383	1.178364	8.991497
7.Si	8.510158	16.468016	8.942364
8.Si	6.080702	17.246897	10.874931
9.O	3.927836	12.435724	7.779864
10.H	19.670057	12.825364	10.665272
11.O	11.261974	4.979486	4.760475
12.Si	3.641757	16.399351	9.064493
13.O	8.258402	11.367538	5.329838
14.O	3.757783	11.203355	5.502358
15.O	11.853464	16.505999	7.829272
16.Si	7.623219	18.561818	6.886585
17.O	3.667913	6.787972	5.760543
18.O	8.683827	7.382991	8.034960
19.Si	1.562565	3.409045	2.285621
20.Si	3.925210	2.598888	4.229845
21.Si	4.628036	3.352819	7.183220
22.Si	7.642333	3.445997	7.064690
23.Si	8.606398	2.597838	4.229984
24.Si	6.348566	3.452390	2.343302
25.Si	11.622035	10.905850	4.580427
26.Si	14.052075	10.462394	2.554765
27.O	9.852796	17.164946	9.534970
28.O	7.169574	8.791325	9.704741
29.O	13.920543	14.873119	11.460635
30.Si	16.430657	11.072603	4.498444
31.Si	11.569735	6.533465	4.432283
32.Si	13.938170	7.247473	2.431637
33.O	6.246889	4.989009	1.836310
34.H	6.133651	13.069487	12.314952
35.O	15.509939	14.915550	5.851883
36.Si	16.365481	6.500210	4.326441
37.Si	18.492784	8.870413	11.394933
38.Si	16.093857	9.406061	9.366069

39.Si	15.645651	8.731120	6.480304
40.Si	12.429454	8.587330	6.604200
41.Si	11.354801	9.421519	9.337366
42.Si	13.626509	8.757689	11.158302
43.Si	18.394914	13.382950	11.173361
44.Si	16.138929	12.629178	9.060084
45.Si	15.497812	13.332061	6.205906
46.Si	11.352460	12.506049	9.256607
47.Si	13.788506	13.349736	10.903118
48.H	13.512087	0.672337	5.793003
49.H	6.099594	10.259388	1.088566
50.H	1.984630	7.283257	1.043254
51.H	0.986309	9.719752	2.081889
52.H	2.209952	9.128306	9.412182
53.Si	16.409217	18.696612	4.400185
54.Si	11.533455	3.424614	4.391964
55.Si	13.897058	2.635799	2.441939
56.O	7.273292	13.351034	10.102888
57.O	2.667899	6.710440	3.428856
58.H	2.549061	5.911825	5.876723
59.Si	16.325442	3.448176	4.307543
60.O	3.913491	8.928552	4.177192
61.O	6.249352	7.217411	7.014706
62.O	4.638766	4.897974	7.512456
63.Si	12.417923	1.360842	6.526026
64.H	14.102336	17.282115	12.072672
65.O	5.510834	10.864160	3.517241
66.Si	18.432106	16.481945	11.119327
67.Si	16.143264	17.269802	9.082199
68.Si	15.474584	16.492981	6.149245
69.Si	12.394036	16.512376	6.269623
70.Si	11.434232	17.325825	9.163515
71.Si	13.760634	16.405484	10.941879
72.Si	8.469444	8.841442	8.729002
73.Si	6.083869	9.407682	10.739780
74.O	4.659517	13.090605	10.299580
75.O	6.267597	11.016734	10.868706
76.O	7.674517	4.978387	7.608877
77.Si	3.574759	8.817302	8.956283
78.Si	8.489196	13.354060	9.019152
79.Si	6.086934	12.621809	10.917886
80.O	8.341084	9.944708	7.531950
81.O	3.668250	7.262423	8.515879
82.O	8.090283	12.612158	7.620213
83.Si	3.613346	13.342744	9.077338
84.Si	1.584345	11.080247	2.062649
85.Si	4.011044	10.550753	4.047028
86.Si	4.442242	11.133323	6.981217
87.Si	7.672942	11.251462	6.851209
88.Si	8.667135	10.405590	4.076803
89.Si	6.451587	11.149246	2.218605
90.Si	1.571113	6.515684	2.239395
91.Si	3.937080	7.314139	4.241583
92.Si	7.705302	6.521182	7.040452
93.Si	8.671934	7.343645	4.213698
94.Si	6.385472	6.492637	2.401736
95.O	14.765029	16.664604	9.694536
96.O	8.344184	6.467379	5.530659
97.O	10.270125	10.451012	3.774218
98.O	1.496765	4.964592	1.842067
99.H	2.289379	1.101119	9.666365
100.H	4.687025	0.927123	9.979058
101.O	7.335979	16.662077	10.042700
102.H	6.202169	16.802178	12.278097
103.O	3.930989	9.778755	7.687487
104.O	16.261119	4.973770	4.856986
105.H	2.272321	16.663320	9.560605
106.O	4.678612	16.667795	10.289430
107.H	6.078377	18.724855	10.759983
108.H	2.256033	13.069760	9.570366
109.H	8.522269	2.621407	7.904103
110.H	8.796968	19.224251	6.264616
111.O	8.090665	17.154306	7.532737
112.O	3.753927	2.651674	8.362502
113.H	3.678879	0.152307	7.917887
114.H	3.987843	17.276434	7.920606
115.O	5.352141	6.717430	3.679774
116.H	19.758554	17.009547	10.722455
117.O	2.912154	11.109495	3.003911
118.O	12.249877	16.743323	10.453673
119.H	7.065145	19.432981	7.951253
120.H	6.595114	18.293038	5.856272
121.H	12.864227	1.683376	7.901938
122.H	1.970853	11.427350	0.672984
123.O	2.593429	3.168486	3.504982
124.O	3.842128	3.064591	5.771679
125.O	6.160728	2.740111	7.103896
126.O	8.179620	3.479235	5.522016
127.O	7.832387	3.151907	2.917303
128.O	5.253034	3.224853	3.523474
129.H	3.953743	1.131079	4.150164
130.H	8.278513	1.180387	4.463239
131.H	19.468470	7.880833	10.873603
132.H	6.055010	7.433294	1.322317
133.H	2.009743	2.621721	1.114843
134.H	16.132376	18.737654	9.198088
135.O	17.422762	16.661942	9.869670
136.H	6.058766	2.573065	1.202333
137.O	16.267832	16.832257	7.532609
138.O	10.175060	2.730028	3.852213
139.O	12.846511	10.950619	3.527727
140.H	13.918096	11.149223	1.266343
141.H	17.892579	17.220192	12.287310
142.O	12.249928	15.022875	5.682514
143.H	17.819625	10.827715	4.084389
144.O	15.510061	10.774292	3.184728
145.O	12.695290	6.640941	3.272724
146.H	13.850797	6.716540	1.066355
147.H	6.263370	8.787506	12.057080
148.Al	12.388828	13.432006	6.392916
149.H	17.719874	6.763366	3.814707
150.O	15.336298	6.725347	3.084600
151.O	13.924993	8.865058	2.346002
152.Al	4.656765	6.592713	7.230508
153.O	11.392746	12.437772	5.187994
154.O	11.844971	9.932034	5.861151

155.O	12.014365	7.217069	5.840273
156.O	16.263378	12.613698	4.942232
157.O	16.096665	10.117568	5.770925
158.O	16.099875	7.455758	5.600783
159.H	0.595390	12.062574	2.569219
160.H	0.252063	6.963128	2.741744
161.O	17.172467	8.882743	10.458587
162.O	16.349811	8.631088	7.948954
163.O	14.033336	8.712196	6.613692
164.O	11.840482	8.460639	8.107413
165.O	12.086238	8.953343	10.706229
166.O	14.592194	9.035244	9.874696
167.O	17.265201	13.266806	10.034456
168.O	16.433756	13.097591	7.539167
169.O	13.995033	12.770060	6.389219
170.O	11.591785	13.366396	7.925626
171.O	12.241833	13.013520	10.546484
172.O	14.676783	13.179067	9.541110
173.O	16.190178	11.013946	9.199970
174.O	11.759774	10.945252	8.954778
175.H	18.100856	8.500117	12.777608
176.H	19.118787	10.218143	11.405791
177.H	17.952781	12.664083	12.391256
178.H	13.810167	7.365899	11.627277
179.H	13.939770	9.727874	12.233431
180.H	14.272017	12.445135	11.955868
181.O	9.759225	9.273917	9.620046
182.O	9.767023	12.606428	9.705053
183.O	13.939307	17.080721	6.198682
184.H	6.389188	12.570784	1.809996
185.O	8.176663	8.886377	4.428778
186.O	18.605965	14.934990	11.551222
187.H	17.710696	18.896763	3.717370
188.H	15.308224	18.964396	3.437491
189.O	12.600954	3.240965	3.191353
190.H	13.846435	3.053310	1.025578
191.O	4.582975	9.118697	10.207456
192.H	10.527825	13.043697	4.761349
193.H	17.680690	3.168602	3.780832
194.O	15.260766	3.232902	3.095973
195.H	13.891522	1.159519	2.581746
196.O	7.832387	10.779092	2.817303
197.H	11.571600	17.471322	5.493881
198.H	11.236048	0.460467	6.585902
199.O	12.022904	2.739746	5.774086
200.O	16.336326	17.170908	4.940391
201.H	16.290346	19.657593	5.530204
202.H	15.983675	2.554899	5.438418
203.O	6.060193	11.108958	6.854727
204.H	0.219975	2.989619	2.749827
205.O	1.786557	5.169053	6.098579
206.H	2.178647	4.319407	5.786199
207.H	1.761489	5.132725	7.182204
208.O	9.457528	13.652699	4.310374
209.H	9.362770	14.629451	4.576425
210.H	8.722419	13.163912	4.738659
211.O	9.085396	16.154967	4.999778
212.H	9.920277	16.658011	4.931759
213.H	8.820940	16.231035	5.942234
214.O	1.868630	5.199149	8.623323
215.H	2.459506	5.994948	8.774832
216.H	2.420877	4.437394	8.897476

Figure S12d

Atom	X	Y	Z (Angstrom)
1.H	11.719737	18.759714	8.985496
2.O	7.905434	6.718915	2.918203
3.O	8.769086	14.904732	8.621397
4.O	10.256288	7.300206	3.850785
5.O	3.747943	14.866833	8.541266
6.Si	3.608383	1.178364	8.991497
7.Si	8.510158	16.468016	8.942364
8.Si	6.080702	17.246897	10.874931
9.O	3.927836	12.435724	7.779864
10.H	19.670078	12.825093	10.665557
11.O	11.261974	4.979486	4.760475
12.Si	3.641757	16.399351	9.064493
13.O	8.258402	11.367538	5.329838
14.O	3.757783	11.203355	5.502358
15.O	11.853464	16.505999	7.829272
16.Si	7.623219	18.561818	6.886585
17.O	3.663402	6.842596	5.773808
18.O	8.683827	7.382991	8.034960
19.Si	1.562565	3.409045	2.285621
20.Si	3.925210	2.598888	4.229845
21.Si	4.628036	3.352819	7.183220
22.Si	7.642333	3.445997	7.064690
23.Si	8.606398	2.597838	4.229984
24.Si	6.348566	3.452390	2.343302
25.Si	11.609760	10.942528	4.596049
26.Si	14.052075	10.462394	2.554765
27.O	9.852796	17.164946	9.534970
28.O	7.169574	8.791325	9.704741
29.O	13.920543	14.873119	11.460635
30.Si	16.430657	11.072603	4.498444
31.Si	11.569735	6.533465	4.432283
32.Si	13.938170	7.247473	2.431637
33.O	6.246889	4.989009	1.836310
34.H	6.135383	13.070383	12.314382
35.O	15.509939	14.915550	5.851883
36.Si	16.365481	6.500210	4.326441
37.Si	18.492784	8.870413	11.394933
38.Si	16.093857	9.406061	9.366069
39.Si	15.645651	8.731120	6.480304
40.Si	12.429454	8.587330	6.604200
41.Si	11.354801	9.421519	9.337366
42.Si	13.626509	8.757689	11.158302
43.Si	18.394914	13.382950	11.173361
44.Si	16.138929	12.629178	9.060084
45.Si	15.497812	13.332061	6.205906
46.Si	11.352460	12.506049	9.256607
47.Si	13.788506	13.349736	10.903118
48.H	13.514525	0.673563	5.795369
49.H	6.096219	10.268769	1.082157
50.H	1.978934	7.285483	1.042209
51.H	0.972707	9.725963	2.098557

52.H	2.220498	9.108433	9.434986
53.Si	16.409217	18.696612	4.400185
54.Si	11.533455	3.424614	4.391964
55.Si	13.897058	2.635799	2.441939
56.O	7.273292	13.351034	10.102888
57.O	2.667899	6.710440	3.428856
58.H	2.246195	5.701250	5.903824
59.Si	16.325442	3.448176	4.307543
60.O	3.913491	8.928552	4.177192
61.O	6.253193	7.215680	7.018827
62.O	4.630275	4.897426	7.532803
63.Si	12.417923	1.360842	6.526026
64.H	14.103214	17.281253	12.073143
65.O	5.510834	10.864160	3.517241
66.Si	18.432106	16.481945	11.119327
67.Si	16.143264	17.269802	9.082199
68.Si	15.474584	16.492981	6.149245
69.Si	12.383124	16.539822	6.271249
70.Si	11.434232	17.325825	9.163515
71.Si	13.760634	16.405484	10.941879
72.Si	8.469444	8.841442	8.729002
73.Si	6.083869	9.407682	10.739780
74.O	4.659517	13.090605	10.299580
75.O	6.267597	11.016734	10.868706
76.O	7.674517	4.978387	7.608877
77.Si	3.574759	8.817302	8.956283
78.Si	8.489196	13.354060	9.019152
79.Si	6.086934	12.621809	10.917886
80.O	8.341084	9.944708	7.531950
81.O	3.691023	7.245949	8.526950
82.O	8.090283	12.612158	7.620213
83.Si	3.613346	13.342744	9.077338
84.Si	1.584345	11.080247	2.062649
85.Si	4.011044	10.550753	4.047028
86.Si	4.442242	11.133323	6.981217
87.Si	7.672942	11.251462	6.851209
88.Si	8.667135	10.405590	4.076803
89.Si	6.451587	11.149246	2.218605
90.Si	1.571113	6.515684	2.239395
91.Si	3.937745	7.310625	4.249214
92.Si	7.708796	6.521423	7.039648
93.Si	8.671934	7.343645	4.213698
94.Si	6.385472	6.492637	2.401736
95.O	14.765029	16.664604	9.694536
96.O	8.344184	6.467379	5.530659
97.O	10.270125	10.451012	3.774218
98.O	1.496765	4.964592	1.842067
99.H	2.282554	1.096716	9.652821
100.H	4.677039	0.935312	9.991867
101.O	7.335979	16.662077	10.042700
102.H	6.199243	16.801287	12.278352
103.O	3.930989	9.778755	7.687487
104.O	16.261119	4.973770	4.856986
105.H	2.272017	16.660956	9.561806
106.O	4.678612	16.667795	10.289430
107.H	6.078345	18.725184	10.762830
108.H	2.256060	13.069657	9.570094
109.H	8.520886	2.620563	7.904835
110.H	8.760418	19.516276	6.847847
111.O	8.090665	17.154306	7.532737
112.O	3.753927	2.651674	8.362502
113.H	3.695336	0.152031	7.919950
114.H	3.982675	17.275523	7.918922
115.O	5.352141	6.717430	3.679774
116.H	19.758775	17.009299	10.722722
117.O	2.912154	11.109495	3.003911
118.O	12.249877	16.743323	10.453673
119.H	6.514567	19.150113	7.681582
120.H	7.153188	18.301824	5.502861
121.H	12.860605	1.682628	7.903314
122.H	1.972390	11.407244	0.668379
123.O	2.593429	3.168486	3.504982
124.O	3.842128	3.064591	5.771679
125.O	6.160728	2.740111	7.103896
126.O	8.179620	3.479235	5.522016
127.O	7.832387	3.151907	2.917303
128.O	5.253034	3.224853	3.523474
129.H	3.956354	1.130686	4.150677
130.H	8.279013	1.180300	4.463846
131.H	19.469362	7.881967	10.872987
132.H	6.055611	7.432987	1.321450
133.H	2.010716	2.625744	1.111616
134.H	16.133249	18.737655	9.197914
135.O	17.422762	16.661942	9.869670
136.H	6.060689	2.573228	1.201508
137.O	16.267832	16.832257	7.532609
138.O	10.175060	2.730028	3.852213
139.O	12.846511	10.950619	3.527727
140.H	13.924378	11.150721	1.264346
141.H	17.892790	17.220169	12.287444
142.O	12.282136	15.024361	5.677795
143.H	17.820002	10.829456	4.084135
144.O	15.510061	10.774292	3.184728
145.O	12.695290	6.640941	3.272724
146.H	13.852246	6.716372	1.066049
147.H	6.261987	8.788142	12.057629
148.Al	12.378798	13.397451	6.378485
149.H	17.720213	6.762511	3.814726
150.O	15.336298	6.725347	3.084600
151.O	13.924993	8.865058	2.346002
152.Al	4.662286	6.585072	7.196422
153.O	11.370385	12.456420	5.191409
154.O	11.844971	9.932034	5.861151
155.O	12.014365	7.217069	5.840273
156.O	16.263378	12.613698	4.942232
157.O	16.096665	10.117568	5.770925
158.O	16.099875	7.455758	5.600783
159.H	0.603581	12.077654	2.556329
160.H	0.252285	6.966351	2.742851
161.O	17.172467	8.882743	10.458587
162.O	16.349811	8.631088	7.948954
163.O	14.033336	8.712196	6.613692
164.O	11.840482	8.460639	8.107413
165.O	12.086238	8.953343	10.706229
166.O	14.592194	9.035244	9.874696
167.O	17.265201	13.266806	10.034456

168.O	16.433756	13.097591	7.539167
169.O	13.997607	12.769099	6.389145
170.O	11.577087	13.367719	7.918603
171.O	12.241833	13.013520	10.546484
172.O	14.676783	13.179067	9.541110
173.O	16.190178	11.013946	9.199970
174.O	11.759774	10.945252	8.954778
175.H	18.100877	8.497854	12.777156
176.H	19.117559	10.218718	11.408069
177.H	17.952611	12.664125	12.391265
178.H	13.810144	7.366092	11.628000
179.H	13.939708	9.728014	12.233488
180.H	14.270291	12.444503	11.956033
181.O	9.759225	9.273917	9.620046
182.O	9.767023	12.606428	9.705053
183.O	13.939307	17.080721	6.198682
184.H	6.391445	12.573004	1.808900
185.O	8.176663	8.886377	4.428778
186.O	18.605965	14.934990	11.551222
187.H	17.720488	18.901807	3.737148
188.H	15.322864	18.958432	3.419681
189.O	12.600954	3.240965	3.191353
190.H	13.846947	3.052992	1.025411
191.O	4.582975	9.118697	10.207456
192.H	10.155982	13.248477	5.121781
193.H	17.680735	3.168076	3.780917
194.O	15.260766	3.232902	3.095973
195.H	13.891927	1.159350	2.581382
196.O	7.832387	10.779092	2.817303
197.H	11.564644	17.470679	5.484514
198.H	11.237043	0.458808	6.582941
199.O	12.022904	2.739746	5.774086
200.O	16.336326	17.170908	4.940391
201.H	16.270398	19.657913	5.527535
202.H	15.983974	2.554543	5.438320
203.O	6.060193	11.108958	6.854727
204.H	0.218370	2.987556	2.742771
205.O	1.635528	4.994335	6.252171
206.H	2.065445	4.162704	5.959059
207.H	1.757420	5.183580	7.671561
208.O	9.306956	13.903435	5.163645
209.H	9.440592	14.870734	4.716381
210.H	8.941998	13.908789	6.074758
211.O	9.652767	16.063739	3.968366
212.H	10.511845	15.906715	3.449626
213.H	8.952934	16.290486	3.331336
214.O	1.245865	7.895870	6.999853
215.H	2.047874	7.806367	6.444589
216.H	0.530214	8.136755	6.387858
217.O	12.028194	15.450912	3.012976
218.H	12.184492	14.718648	2.393034
219.H	12.305633	15.129170	3.916284
220.O	2.000022	5.343089	8.723779
221.H	2.608685	6.210527	8.735618
222.H	2.616621	4.606768	8.944885

Figure S12e

Atom	X	Y	Z (Angstrom)
1.H	11.726356	18.758362	8.985058
2.O	7.905434	6.718915	2.918203
3.O	8.769086	14.904732	8.621397
4.O	10.256288	7.300206	3.850785
5.O	3.747943	14.866833	8.541266
6.Si	3.608383	1.178364	8.991497
7.Si	8.510158	16.468016	8.942364
8.Si	6.080702	17.246897	10.874931
9.O	3.927836	12.435724	7.779864
10.H	19.669834	12.825535	10.664222
11.O	11.261974	4.979486	4.760475
12.Si	3.641757	16.399351	9.064493
13.O	8.258402	11.367538	5.329838
14.O	3.757783	11.203355	5.502358
15.O	11.853464	16.505999	7.829272
16.Si	7.623219	18.561818	6.886585
17.O	3.622316	6.871932	5.787807
18.O	8.683827	7.382991	8.034960
19.Si	1.562565	3.409045	2.285621
20.Si	3.925210	2.598888	4.229845
21.Si	4.628036	3.352819	7.183220
22.Si	7.642333	3.445997	7.064690
23.Si	8.606398	2.597838	4.229984
24.Si	6.348566	3.452390	2.343302
25.Si	11.598619	10.954454	4.626075
26.Si	14.052075	10.462394	2.554765
27.O	9.852796	17.164946	9.534970
28.O	7.169574	8.791325	9.704741
29.O	13.920543	14.873119	11.460635
30.Si	16.430657	11.072603	4.498444
31.Si	11.569735	6.533465	4.432283
32.Si	13.938170	7.247473	2.431637
33.O	6.246889	4.989009	1.836310
34.H	6.128946	13.066655	12.315908
35.O	15.509939	14.915550	5.851883
36.Si	16.365481	6.500210	4.326441
37.Si	18.492784	8.870413	11.394933
38.Si	16.093857	9.406061	9.366069
39.Si	15.645651	8.731120	6.480304
40.Si	12.429454	8.587330	6.604200
41.Si	11.354801	9.421519	9.337366
42.Si	13.626509	8.757689	11.158302
43.Si	18.394914	13.382950	11.173361
44.Si	16.138929	12.629178	9.060084
45.Si	15.497812	13.332061	6.205906
46.Si	11.352460	12.506049	9.256607
47.Si	13.788506	13.349736	10.903118
48.H	13.517925	0.677765	5.795822
49.H	6.096945	10.279395	1.075684
50.H	1.993104	7.277760	1.041114
51.H	0.991050	9.718300	2.074408
52.H	2.203154	9.126865	9.394398
53.Si	16.409217	18.696612	4.400185
54.Si	11.533455	3.424614	4.391964
55.Si	13.897058	2.635799	2.441939
56.O	7.273292	13.351034	10.102888
57.O	2.667899	6.710440	3.428856
58.H	2.140262	5.572137	5.666329

59.Si	16.325442	3.448176	4.307543
60.O	3.913491	8.928552	4.177192
61.O	6.234234	7.212528	7.019801
62.O	4.653476	4.900474	7.503090
63.Si	12.417923	1.360842	6.526026
64.H	14.106210	17.280890	12.072630
65.O	5.510834	10.864160	3.517241
66.Si	18.432106	16.481945	11.119327
67.Si	16.143264	17.269802	9.082199
68.Si	15.474584	16.492981	6.149245
69.Si	12.376039	16.537383	6.272392
70.Si	11.434232	17.325825	9.163515
71.Si	13.760634	16.405484	10.941879
72.Si	8.469444	8.841442	8.729002
73.Si	6.083869	9.407682	10.739780
74.O	4.659517	13.090605	10.299580
75.O	6.267597	11.016734	10.868706
76.O	7.674517	4.978387	7.608877
77.Si	3.574759	8.817302	8.956283
78.Si	8.489196	13.354060	9.019152
79.Si	6.086934	12.621809	10.917886
80.O	8.341084	9.944708	7.531950
81.O	3.663767	7.257371	8.531083
82.O	8.090283	12.612158	7.620213
83.Si	3.613346	13.342744	9.077338
84.Si	1.584345	11.080247	2.062649
85.Si	4.011044	10.550753	4.047028
86.Si	4.442242	11.133323	6.981217
87.Si	7.672942	11.251462	6.851209
88.Si	8.667135	10.405590	4.076803
89.Si	6.451587	11.149246	2.218605
90.Si	1.571113	6.515684	2.239395
91.Si	3.934016	7.307403	4.253311
92.Si	7.695303	6.521271	7.042213
93.Si	8.671934	7.343645	4.213698
94.Si	6.385472	6.492637	2.401736
95.O	14.765029	16.664604	9.694536
96.O	8.344184	6.467379	5.530659
97.O	10.270125	10.451012	3.774218
98.O	1.496765	4.964592	1.842067
99.H	2.432546	1.167156	9.897076
100.H	4.822562	0.805803	9.763578
101.O	7.335979	16.662077	10.042700
102.H	6.195600	16.799284	12.278587
103.O	3.930989	9.778755	7.687487
104.O	16.261119	4.973770	4.856986
105.H	2.271279	16.654073	9.564935
106.O	4.678612	16.667795	10.289430
107.H	6.074431	18.725473	10.768164
108.H	2.254844	13.062581	9.565655
109.H	8.530635	2.625296	7.899884
110.H	8.764896	19.512289	6.840452
111.O	8.090665	17.154306	7.532737
112.O	3.753927	2.651674	8.362502
113.H	3.401880	0.165072	7.919716
114.H	3.975902	17.275919	7.918289
115.O	5.352141	6.717430	3.679774
116.H	19.758762	17.008757	10.721904
117.O	2.912154	11.109495	3.003911
118.O	12.249877	16.743323	10.453673
119.H	6.529199	19.160281	7.696796
120.H	7.135350	18.309835	5.509386
121.H	12.859521	1.682591	7.903528
122.H	1.969926	11.439876	0.675908
123.O	2.593429	3.168486	3.504982
124.O	3.842128	3.064591	5.771679
125.O	6.160728	2.740111	7.103896
126.O	8.179620	3.479235	5.522016
127.O	7.832387	3.151907	2.917303
128.O	5.253034	3.224853	3.523474
129.H	3.943369	1.132125	4.118922
130.H	8.282014	1.179013	4.459010
131.H	19.468997	7.881962	10.872337
132.H	6.056039	7.436413	1.323729
133.H	2.007870	2.619426	1.116070
134.H	16.135052	18.737736	9.194761
135.O	17.422762	16.661942	9.869670
136.H	6.062182	2.576735	1.198041
137.O	16.267832	16.832257	7.532609
138.O	10.175060	2.730028	3.852213
139.O	12.846511	10.950619	3.527727
140.H	13.904412	11.169769	1.276543
141.H	17.893279	17.220441	12.287260
142.O	12.335767	15.019514	5.676279
143.H	17.818411	10.833015	4.078656
144.O	15.510061	10.774292	3.184728
145.O	12.695290	6.640941	3.272724
146.H	13.852177	6.723559	1.063634
147.H	6.254813	8.786270	12.057217
148.Al	12.358250	13.383636	6.379800
149.H	17.719037	6.765630	3.813184
150.O	15.336298	6.725347	3.084600
151.O	13.924993	8.865058	2.346002
152.Al	4.634347	6.573494	7.211552
153.O	11.406740	12.454776	5.183139
154.O	11.844971	9.932034	5.861151
155.O	12.014365	7.217069	5.840273
156.O	16.263378	12.613698	4.942232
157.O	16.096665	10.117568	5.770925
158.O	16.099875	7.455758	5.600783
159.H	0.593484	12.057100	2.576910
160.H	0.251182	6.972875	2.727108
161.O	17.172467	8.882743	10.458587
162.O	16.349811	8.631088	7.948954
163.O	14.033336	8.712196	6.613692
164.O	11.840482	8.460639	8.107413
165.O	12.086238	8.953343	10.706229
166.O	14.592194	9.035244	9.874696
167.O	17.265201	13.266806	10.034456
168.O	16.433756	13.097591	7.539167
169.O	13.998585	12.774035	6.371585
170.O	11.603216	13.376281	7.933929
171.O	12.241833	13.013520	10.546484
172.O	14.676783	13.179067	9.541110
173.O	16.190178	11.013946	9.199970
174.O	11.759774	10.945252	8.954778

175.H	18.101467	8.498370	12.777189
176.H	19.117719	10.218609	11.406711
177.H	17.953369	12.663158	12.390736
178.H	13.811452	7.365913	11.626795
179.H	13.941121	9.727606	12.233237
180.H	14.275019	12.445266	11.954885
181.O	9.759225	9.273917	9.620046
182.O	9.767023	12.606428	9.705053
183.O	13.939307	17.080721	6.198682
184.H	6.430903	12.576726	1.813906
185.O	8.176663	8.886377	4.428778
186.O	18.605965	14.934990	11.551222
187.H	17.721852	18.899462	3.739803
188.H	15.324934	18.952599	3.416407
189.O	12.600954	3.240965	3.191353
190.H	13.847920	3.055904	1.025953
191.O	4.582975	9.118697	10.207456
192.H	10.001529	13.523953	5.017549
193.H	17.680830	3.170795	3.779822
194.O	15.260766	3.232902	3.095973
195.H	13.893003	1.159440	2.578545
196.O	7.832387	10.779092	2.817303
197.H	11.555170	17.458766	5.474935
198.H	11.239629	0.456037	6.579090
199.O	12.022904	2.739746	5.774086
200.O	16.336326	17.170908	4.940391
201.H	16.266541	19.656218	5.527357
202.H	15.985224	2.555049	5.438583
203.O	6.060193	11.108958	6.854727
204.H	0.221825	2.989263	2.754590
205.O	1.402075	4.922953	5.591375
206.H	1.796839	4.201774	5.063252
207.H	0.911514	4.325508	7.006721
208.O	9.298430	14.180001	4.769822
209.H	9.252817	13.904129	3.188146
210.H	8.544121	13.955544	5.342939
211.O	9.449578	13.673097	2.212346
212.H	10.844073	13.418054	2.056253
213.H	8.875972	12.917513	1.989072
214.O	0.655572	4.150691	7.977863
215.H	-0.285556	3.903394	7.995525
216.H	0.956400	5.436848	8.522514
217.O	13.299334	14.841137	3.235462
218.H	14.254140	14.659089	3.311941
219.H	12.943799	14.927938	4.186598
220.O	1.230418	6.444229	8.780398
221.H	2.250950	6.551881	8.840372
222.H	1.038731	7.057966	7.973631
223.O	11.905663	13.240285	1.939357
224.H	12.518812	13.957941	2.495588
225.H	12.117738	12.363462	2.335577
226.O	1.192679	7.954299	6.665506
227.H	1.245560	8.911029	6.837020
228.H	2.084749	7.696178	6.304020

Figure S12f

1.H	11.726931	18.758400	8.982632
2.O	7.905434	6.718915	2.918203
3.O	8.769086	14.904732	8.621397
4.O	10.256288	7.300206	3.850785
5.O	3.747943	14.866833	8.541266
6.Si	3.608383	1.178364	8.991497
7.Si	8.510158	16.468016	8.942364
8.Si	6.080702	17.246897	10.874931
9.O	3.927836	12.435724	7.779864
10.H	19.671034	12.827133	10.664045
11.O	11.261974	4.979486	4.760475
12.Si	3.641757	16.399351	9.064493
13.O	8.258402	11.367538	5.329838
14.O	3.757783	11.203355	5.502358
15.O	11.853464	16.505999	7.829272
16.Si	7.623219	18.561818	6.886585
17.O	3.680292	6.789035	5.761447
18.O	8.683827	7.382991	8.034960
19.Si	1.562565	3.409045	2.285621
20.Si	3.925210	2.598888	4.229845
21.Si	4.628036	3.352819	7.183220
22.Si	7.642333	3.445997	7.064690
23.Si	8.606398	2.597838	4.229984
24.Si	6.348566	3.452390	2.343302
25.Si	11.599600	10.950822	4.624056
26.Si	14.052075	10.462394	2.554765
27.O	9.852796	17.164946	9.534970
28.O	7.169574	8.791325	9.704741
29.O	13.920543	14.873119	11.460635
30.Si	16.430657	11.072603	4.498444
31.Si	11.569735	6.533465	4.432283
32.Si	13.938170	7.247473	2.431637
33.O	6.246889	4.989009	1.836310
34.H	6.132007	13.067963	12.316111
35.O	15.509939	14.915550	5.851883
36.Si	16.365481	6.500210	4.326441
37.Si	18.492784	8.870413	11.394933
38.Si	16.093857	9.406061	9.366069
39.Si	15.645651	8.731120	6.480304
40.Si	12.429454	8.587330	6.604200
41.Si	11.354801	9.421519	9.337366
42.Si	13.626509	8.757689	11.158302
43.Si	18.394914	13.382950	11.173361
44.Si	16.138929	12.629178	9.060084
45.Si	15.497812	13.332061	6.205906
46.Si	11.352460	12.506049	9.256607
47.Si	13.788506	13.349736	10.903118
48.H	13.511716	0.673379	5.790083
49.H	6.102622	10.255863	1.089521
50.H	2.000690	7.296030	1.058160
51.H	0.980019	9.721947	2.099218
52.H	14.456488	14.604047	3.517674
53.Si	16.409217	18.696612	4.400185
54.Si	11.533455	3.424614	4.391964
55.Si	13.897058	2.635799	2.441939
56.O	7.273292	13.351034	10.102888
57.O	2.667899	6.710440	3.428856
58.H	2.897103	6.206627	5.812839
59.Si	16.325442	3.448176	4.307543
60.O	3.913491	8.928552	4.177192

61.O	6.252339	7.222989	6.985737
62.O	4.669902	4.902402	7.476006
63.Si	12.417923	1.360842	6.526026
64.H	14.105327	17.281635	12.072929
65.O	5.510834	10.864160	3.517241
66.Si	18.432106	16.481945	11.119327
67.Si	16.143264	17.269802	9.082199
68.Si	15.474584	16.492981	6.149245
69.Si	12.382969	16.531678	6.280500
70.Si	11.434232	17.325825	9.163515
71.Si	13.760634	16.405484	10.941879
72.Si	8.469444	8.841442	8.729002
73.Si	6.083869	9.407682	10.739780
74.O	4.659517	13.090605	10.299580
75.O	6.267597	11.016734	10.868706
76.O	7.674517	4.978387	7.608877
77.Si	3.574759	8.817302	8.956283
78.Si	8.489196	13.354060	9.019152
79.Si	6.086934	12.621809	10.917886
80.O	8.341084	9.944708	7.531950
81.O	3.663893	7.280937	8.512051
82.O	8.090283	12.612158	7.620213
83.Si	3.613346	13.342744	9.077338
84.Si	1.584345	11.080247	2.062649
85.Si	4.011044	10.550753	4.047028
86.Si	4.442242	11.133323	6.981217
87.Si	7.672942	11.251462	6.851209
88.Si	8.667135	10.405590	4.076803
89.Si	6.451587	11.149246	2.218605
90.Si	1.571113	6.515684	2.239395
91.Si	3.949351	7.331050	4.175764
92.Si	7.712128	6.518501	7.040493
93.Si	8.671934	7.343645	4.213698
94.Si	6.385472	6.492637	2.401736
95.O	14.765029	16.664604	9.694536
96.O	8.344184	6.467379	5.530659
97.O	10.270125	10.451012	3.774218
98.O	1.496765	4.964592	1.842067
99.H	2.271864	1.061098	9.627327
100.H	4.657256	0.934768	10.016401
101.O	7.335979	16.662077	10.042700
102.H	6.197559	16.800706	12.279407
103.O	3.930989	9.778755	7.687487
104.O	16.261119	4.973770	4.856986
105.H	2.271455	16.656968	9.566111
106.O	4.678612	16.667795	10.289430
107.H	6.075089	18.726220	10.769447
108.H	2.254567	13.069074	9.568412
109.H	8.533283	2.629224	7.900884
110.H	8.775962	19.497285	6.803910
111.O	8.090665	17.154306	7.532737
112.O	3.753927	2.651674	8.362502
113.H	3.733527	0.138403	7.932206
114.H	3.975392	17.278482	7.919216
115.O	5.352141	6.717430	3.679774
116.H	19.759217	17.008920	10.722025
117.O	2.912154	11.109495	3.003911
118.O	12.249877	16.743323	10.453673
119.H	6.558501	19.183176	7.718009
120.H	7.099688	18.305615	5.523010
121.H	12.869116	1.681131	7.900757
122.H	1.975286	11.404408	0.668842
123.O	2.593429	3.168486	3.504982
124.O	3.842128	3.064591	5.771679
125.O	6.160728	2.740111	7.103896
126.O	8.179620	3.479235	5.522016
127.O	7.832387	3.151907	2.917303
128.O	5.253034	3.224853	3.523474
129.H	3.959179	1.131463	4.120913
130.H	8.281135	1.178709	4.456504
131.H	19.475992	7.892349	10.865048
132.H	6.034124	7.444063	1.338061
133.H	2.000607	2.635259	1.100729
134.H	16.135277	18.738227	9.194059
135.O	17.422762	16.661942	9.869670
136.H	6.065128	2.583769	1.191810
137.O	16.267832	16.832257	7.532609
138.O	10.175060	2.730028	3.852213
139.O	12.846511	10.950619	3.527727
140.H	13.908210	11.172276	1.277835
141.H	17.895127	17.221190	12.288227
142.O	12.327250	15.021970	5.684199
143.H	17.819188	10.835781	4.078015
144.O	15.510061	10.774292	3.184728
145.O	12.695290	6.640941	3.272724
146.H	13.851052	6.724103	1.062993
147.H	6.268254	8.787308	12.056918
148.Al	12.351690	13.383510	6.372652
149.H	17.719799	6.764317	3.812425
150.O	15.336298	6.725347	3.084600
151.O	13.924993	8.865058	2.346002
152.Al	4.703872	6.580267	7.356420
153.O	11.402654	12.452189	5.178030
154.O	11.844971	9.932034	5.861151
155.O	12.014365	7.217069	5.840273
156.O	16.263378	12.613698	4.942232
157.O	16.096665	10.117568	5.770925
158.O	16.099875	7.455758	5.600783
159.H	0.601290	12.073575	2.556454
160.H	0.262955	6.976285	2.755731
161.O	17.172467	8.882743	10.458587
162.O	16.349811	8.631088	7.948954
163.O	14.033336	8.712196	6.613692
164.O	11.840482	8.460639	8.107413
165.O	12.086238	8.953343	10.706229
166.O	14.592194	9.035244	9.874696
167.O	17.265201	13.266806	10.034456
168.O	16.433756	13.097591	7.539167
169.O	13.995506	12.781322	6.359692
170.O	11.605729	13.372521	7.931195
171.O	12.241833	13.013520	10.546484
172.O	14.676783	13.179067	9.541110
173.O	16.190178	11.013946	9.199970
174.O	11.759774	10.945252	8.954778
175.H	18.104160	8.481885	12.773742
176.H	19.112034	10.221094	11.420918

177.H	17.955499	12.661430	12.390851
178.H	13.812698	7.365399	11.627156
179.H	13.942346	9.727213	12.234008
180.H	14.274107	12.445204	11.955841
181.O	9.759225	9.273917	9.620046
182.O	9.767023	12.606428	9.705053
183.O	13.939307	17.080721	6.198682
184.H	6.402689	12.568364	1.804309
185.O	8.176663	8.886377	4.428778
186.O	18.605965	14.934990	11.551222
187.H	17.696478	18.881381	3.686318
188.H	15.287915	18.975021	3.464653
189.O	12.600954	3.240965	3.191353
190.H	13.847995	3.055330	1.025457
191.O	4.582975	9.118697	10.207456
192.H	9.996315	13.451948	4.938555
193.H	17.681195	3.171235	3.778305
194.O	15.260766	3.232902	3.095973
195.H	13.893631	1.158754	2.575629
196.O	7.832387	10.779092	2.817303
197.H	11.563239	17.455503	5.476248
198.H	11.238385	0.457595	6.585897
199.O	12.022904	2.739746	5.774086
200.O	16.336326	17.170908	4.940391
201.H	16.329082	19.655917	5.534658
202.H	15.987701	2.552753	5.437968
203.O	6.060193	11.108958	6.854727
204.H	0.212206	2.999113	2.735758
205.H	12.315645	12.503619	2.424371
206.O	13.548674	14.906054	3.326294
207.H	13.086203	14.986273	4.221041
208.O	9.288425	14.093673	4.659897
209.H	9.282017	13.694654	2.979025
210.H	8.558635	13.963497	5.289658
211.O	9.572686	13.379192	2.074456
212.H	11.066562	13.487061	2.029895
213.H	9.257468	12.459713	2.007331
214.O	12.117289	13.367131	1.992856
215.H	12.705486	14.105514	2.545224
216.H	10.251374	15.547407	3.837875
217.O	10.743925	15.921388	3.077321
218.H	11.172913	16.718825	3.428032
219.H	2.214039	9.153141	9.410150

Figure S12g

1.H	11.725817	18.758791	8.981229
2.O	7.905434	6.718915	2.918203
3.O	8.769086	14.904732	8.621397
4.O	10.256288	7.300206	3.850785
5.O	3.747943	14.866833	8.541266
6.Si	3.608383	1.178364	8.991497
7.Si	8.510158	16.468016	8.942364
8.Si	6.080702	17.246897	10.874931
9.O	3.927836	12.435724	7.779864
10.H	19.671147	12.827382	10.663918
11.O	11.261974	4.979486	4.760475
12.Si	3.641757	16.399351	9.064493
13.O	8.258402	11.367538	5.329838
14.O	3.757783	11.203355	5.502358
15.O	11.853464	16.505999	7.829272
16.Si	7.623219	18.561818	6.886585
17.O	3.680341	6.788972	5.761552
18.O	8.683827	7.382991	8.034960
19.Si	1.562565	3.409045	2.285621
20.Si	3.925210	2.598888	4.229845
21.Si	4.628036	3.352819	7.183220
22.Si	7.642333	3.445997	7.064690
23.Si	8.606398	2.597838	4.229984
24.Si	6.348566	3.452390	2.343302
25.Si	11.600570	10.954616	4.624779
26.Si	14.052075	10.462394	2.554765
27.O	9.852796	17.164946	9.534970
28.O	7.169574	8.791325	9.704741
29.O	13.920543	14.873119	11.460635
30.Si	16.430657	11.072603	4.498444
31.Si	11.569735	6.533465	4.432283
32.Si	13.938170	7.247473	2.431637
33.O	6.246889	4.989009	1.836310
34.H	6.131853	13.067561	12.316176
35.O	15.509939	14.915550	5.851883
36.Si	16.365481	6.500210	4.326441
37.Si	18.492784	8.870413	11.394933
38.Si	16.093857	9.406061	9.366069
39.Si	15.645651	8.731120	6.480304
40.Si	12.429454	8.587330	6.604200
41.Si	11.354801	9.421519	9.337366
42.Si	13.626509	8.757689	11.158302
43.Si	18.394914	13.382950	11.173361
44.Si	16.138929	12.629178	9.060084
45.Si	15.497812	13.332061	6.205906
46.Si	11.352460	12.506049	9.256607
47.Si	13.788506	13.349736	10.903118
48.H	13.511414	0.673094	5.789730
49.H	6.103892	10.254831	1.090071
50.H	2.000961	7.295602	1.057972
51.H	0.983991	9.719959	2.094311
52.H	14.504954	14.615361	3.577016
53.Si	16.409217	18.696612	4.400185
54.Si	11.533455	3.424614	4.391964
55.Si	13.897058	2.635799	2.441939
56.O	7.273292	13.351034	10.102888
57.O	2.667899	6.710440	3.428856
58.H	2.911496	6.187840	5.809259
59.Si	16.325442	3.448176	4.307543
60.O	3.913491	8.928552	4.177192
61.O	6.254327	7.223772	6.984270
62.O	4.669432	4.902255	7.477585
63.Si	12.417923	1.360842	6.526026
64.H	14.105787	17.281718	12.072644
65.O	5.510834	10.864160	3.517241
66.Si	18.432106	16.481945	11.119327
67.Si	16.143264	17.269802	9.082199
68.Si	15.474584	16.492981	6.149245
69.Si	12.380062	16.538805	6.278002
70.Si	11.434232	17.325825	9.163515

71.Si	13.760634	16.405484	10.941879
72.Si	8.469444	8.841442	8.729002
73.Si	6.083869	9.407682	10.739780
74.O	4.659517	13.090605	10.299580
75.O	6.267597	11.016734	10.868706
76.O	7.674517	4.978387	7.608877
77.Si	3.574759	8.817302	8.956283
78.Si	8.489196	13.354060	9.019152
79.Si	6.086934	12.621809	10.917886
80.O	8.341084	9.944708	7.531950
81.O	3.664293	7.281486	8.511672
82.O	8.090283	12.612158	7.620213
83.Si	3.613346	13.342744	9.077338
84.Si	1.584345	11.080247	2.062649
85.Si	4.011044	10.550753	4.047028
86.Si	4.442242	11.133323	6.981217
87.Si	7.672942	11.251462	6.851209
88.Si	8.667135	10.405590	4.076803
89.Si	6.451587	11.149246	2.218605
90.Si	1.571113	6.515684	2.239395
91.Si	3.948879	7.330952	4.176235
92.Si	7.713414	6.517747	7.040786
93.Si	8.671934	7.343645	4.213698
94.Si	6.385472	6.492637	2.401736
95.O	14.765029	16.664604	9.694536
96.O	8.344184	6.467379	5.530659
97.O	10.270125	10.451012	3.774218
98.O	1.496765	4.964592	1.842067
99.H	2.306472	1.090119	9.699298
100.H	4.706403	0.902769	9.955217
101.O	7.335979	16.662077	10.042700
102.H	6.197838	16.801166	12.279568
103.O	3.930989	9.778755	7.687487
104.O	16.261119	4.973770	4.856986
105.H	2.271328	16.655826	9.566635
106.O	4.678612	16.667795	10.289430
107.H	6.073420	18.726091	10.767820
108.H	2.254801	13.068078	9.568399
109.H	8.533521	2.629624	7.900862
110.H	8.751909	19.131757	6.103687
111.O	8.090665	17.154306	7.532737
112.O	3.753927	2.651674	8.362502
113.H	3.649948	0.142598	7.921784
114.H	3.976142	17.279796	7.920442
115.O	5.352141	6.717430	3.679774
116.H	19.759307	17.008382	10.721535
117.O	2.912154	11.109495	3.003911
118.O	12.249877	16.743323	10.453673
119.H	7.258817	19.521194	7.963934
120.H	6.456951	18.348972	5.999756
121.H	12.869645	1.681765	7.900545
122.H	1.974921	11.410298	0.670054
123.O	2.593429	3.168486	3.504982
124.O	3.842128	3.064591	5.771679
125.O	6.160728	2.740111	7.103896
126.O	8.179620	3.479235	5.522016
127.O	7.832387	3.151907	2.917303
128.O	5.253034	3.224853	3.523474
129.H	3.959286	1.131494	4.121419
130.H	8.280925	1.178861	4.456754
131.H	19.473906	7.888876	10.867319
132.H	6.034765	7.444295	1.338151
133.H	2.000670	2.635301	1.100717
134.H	16.135469	18.738222	9.193593
135.O	17.422762	16.661942	9.869670
136.H	6.065149	2.583798	1.191897
137.O	16.267832	16.832257	7.532609
138.O	10.175060	2.730028	3.852213
139.O	12.846511	10.950619	3.527727
140.H	13.909067	11.170426	1.277912
141.H	17.895478	17.221145	12.288404
142.O	12.304868	15.033015	5.674375
143.H	17.819058	10.835950	4.077922
144.O	15.510061	10.774292	3.184728
145.O	12.695290	6.640941	3.272724
146.H	13.850974	6.724155	1.063099
147.H	6.268465	8.786738	12.056540
148.Al	12.349661	13.394791	6.370357
149.H	17.719652	6.764436	3.812303
150.O	15.336298	6.725347	3.084600
151.O	13.924993	8.865058	2.346002
152.Al	4.705735	6.580555	7.356709
153.O	11.408019	12.459027	5.170361
154.O	11.844971	9.932034	5.861151
155.O	12.014365	7.217069	5.840273
156.O	16.263378	12.613698	4.942232
157.O	16.096665	10.117568	5.770925
158.O	16.099875	7.455758	5.600783
159.H	0.598586	12.068866	2.560546
160.H	0.262879	6.976020	2.755752
161.O	17.172467	8.882743	10.458587
162.O	16.349811	8.631088	7.948954
163.O	14.033336	8.712196	6.613692
164.O	11.840482	8.460639	8.107413
165.O	12.086238	8.953343	10.706229
166.O	14.592194	9.035244	9.874696
167.O	17.265201	13.266806	10.034456
168.O	16.433756	13.097591	7.539167
169.O	13.992797	12.788769	6.357250
170.O	11.607373	13.373776	7.931385
171.O	12.241833	13.013520	10.546484
172.O	14.676783	13.179067	9.541110
173.O	16.190178	11.013946	9.199970
174.O	11.759774	10.945252	8.954778
175.H	18.103058	8.486290	12.774759
176.H	19.114737	10.220014	11.417275
177.H	17.955507	12.661512	12.390930
178.H	13.812373	7.365217	11.626853
179.H	13.942133	9.727225	12.234076
180.H	14.274903	12.445161	11.955376
181.O	9.759225	9.273917	9.620046
182.O	9.767023	12.606428	9.705053
183.O	13.939307	17.080721	6.198682
184.H	6.401491	12.568644	1.806317
185.O	8.176663	8.886377	4.428778
186.O	18.605965	14.934990	11.551222

187.H	17.698496	18.882819	3.690223
188.H	15.290808	18.972312	3.459746
189.O	12.600954	3.240965	3.191353
190.H	13.847863	3.056070	1.025645
191.O	4.582975	9.118697	10.207456
192.H	10.048222	13.518966	4.818823
193.H	17.681213	3.171555	3.778133
194.O	15.260766	3.232902	3.095973
195.H	13.893533	1.158754	2.575487
196.O	7.832387	10.779092	2.817303
197.H	11.567834	17.488088	5.500558
198.H	11.238027	0.457947	6.586536
199.O	12.022904	2.739746	5.774086
200.O	16.336326	17.170908	4.940391
201.H	16.322682	19.656756	5.533392
202.H	15.987593	2.553000	5.438158
203.O	6.060193	11.108958	6.854727
204.H	0.212294	2.999324	2.736249
205.H	12.379815	12.499062	2.440464
206.O	13.610581	14.919292	3.333270
207.H	13.104419	15.006725	4.199828
208.O	9.206579	13.975170	4.544014
209.H	9.378280	13.673732	2.848471
210.H	8.517828	13.441122	4.980411
211.O	9.679736	13.345059	1.951246
212.H	11.166419	13.486651	1.948595
213.H	9.385328	12.416821	1.910299
214.O	12.218227	13.348266	1.965702
215.H	12.776452	14.091404	2.513552
216.H	10.362625	16.375575	3.123430
217.O	11.044377	15.953618	2.543335
218.H	11.706537	16.642765	2.374391
219.H	2.214277	9.153298	9.410336
220.H	9.070271	15.790213	4.649102
221.O	9.079613	16.742009	4.386327
222.H	9.530643	17.204159	5.113040

Figure S12h

1.H	11.725906	18.758248	8.978685
2.O	7.905434	6.718915	2.918203
3.O	8.769086	14.904732	8.621397
4.O	10.256288	7.300206	3.850785
5.O	3.747943	14.866833	8.541266
6.Si	3.608383	1.178364	8.991497
7.Si	8.510158	16.468016	8.942364
8.Si	6.080702	17.246897	10.874931
9.O	3.927836	12.435724	7.779864
10.H	19.670681	12.827008	10.663626
11.O	11.261974	4.979486	4.760475
12.Si	3.641757	16.399351	9.064493
13.O	8.258402	11.367538	5.329838
14.O	3.757783	11.203355	5.502358
15.O	11.853464	16.505999	7.829272
16.Si	7.623219	18.561818	6.886585
17.O	3.680575	6.785715	5.760787
18.O	8.683827	7.382991	8.034960
19.Si	1.562565	3.409045	2.285621
20.Si	3.925210	2.598888	4.229845
21.Si	4.628036	3.352819	7.183220
22.Si	7.642333	3.445997	7.064690
23.Si	8.606398	2.597838	4.229984
24.Si	6.348566	3.452390	2.343302
25.Si	11.600978	10.951656	4.624768
26.Si	14.052075	10.462394	2.554765
27.O	9.852796	17.164946	9.534970
28.O	7.169574	8.791325	9.704741
29.O	13.920543	14.873119	11.460635
30.Si	16.430657	11.072603	4.498444
31.Si	11.569735	6.533465	4.432283
32.Si	13.938170	7.247473	2.431637
33.O	6.246889	4.989009	1.836310
34.H	6.132635	13.067900	12.315987
35.O	15.509939	14.915550	5.851883
36.Si	16.365481	6.500210	4.326441
37.Si	18.492784	8.870413	11.394933
38.Si	16.093857	9.406061	9.366069
39.Si	15.645651	8.731120	6.480304
40.Si	12.429454	8.587330	6.604200
41.Si	11.354801	9.421519	9.337366
42.Si	13.626509	8.757689	11.158302
43.Si	18.394914	13.382950	11.173361
44.Si	16.138929	12.629178	9.060084
45.Si	15.497812	13.332061	6.205906
46.Si	11.352460	12.506049	9.256607
47.Si	13.788506	13.349736	10.903118
48.H	13.526799	0.684771	5.802333
49.H	6.105152	10.256284	1.089055
50.H	2.001538	7.295725	1.058347
51.H	0.983837	9.720154	2.096600
52.H	2.214186	9.152872	9.410031
53.Si	16.409217	18.696612	4.400185
54.Si	11.533455	3.424614	4.391964
55.Si	13.897058	2.635799	2.441939
56.O	7.273292	13.351034	10.102888
57.O	2.667899	6.710440	3.428856
58.H	2.919051	6.174284	5.803821
59.Si	16.325442	3.448176	4.307543
60.O	3.913491	8.928552	4.177192
61.O	6.253126	7.223450	6.985274
62.O	4.665690	4.903035	7.474004
63.Si	12.417923	1.360842	6.526026
64.H	14.104879	17.281815	12.072632
65.O	5.510834	10.864160	3.517241
66.Si	18.432106	16.481945	11.119327
67.Si	16.143264	17.269802	9.082199
68.Si	15.474584	16.492981	6.149245
69.Si	12.380890	16.540180	6.279921
70.Si	11.434232	17.325825	9.163515
71.Si	13.760634	16.405484	10.941879
72.Si	8.469444	8.841442	8.729002
73.Si	6.083869	9.407682	10.739780
74.O	4.659517	13.090605	10.299580
75.O	6.267597	11.016734	10.868706
76.O	7.674517	4.978387	7.608877
77.Si	3.574759	8.817302	8.956283
78.Si	8.489196	13.354060	9.019152

79.Si	6.086934	12.621809	10.917886
80.O	8.341084	9.944708	7.531950
81.O	3.665671	7.281303	8.512552
82.O	8.090283	12.612158	7.620213
83.Si	3.613346	13.342744	9.077338
84.Si	1.584345	11.080247	2.062649
85.Si	4.011044	10.550753	4.047028
86.Si	4.442242	11.133323	6.981217
87.Si	7.672942	11.251462	6.851209
88.Si	8.667135	10.405590	4.076803
89.Si	6.451587	11.149246	2.218605
90.Si	1.571113	6.515684	2.239395
91.Si	3.948663	7.330832	4.175951
92.Si	7.712265	6.517978	7.040667
93.Si	8.671934	7.343645	4.213698
94.Si	6.385472	6.492637	2.401736
95.O	14.765029	16.664604	9.694536
96.O	8.344184	6.467379	5.530659
97.O	10.270125	10.451012	3.774218
98.O	1.496765	4.964592	1.842067
99.H	2.317936	1.098663	9.720647
100.H	4.720428	0.893072	9.936035
101.O	7.335979	16.662077	10.042700
102.H	6.198707	16.802189	12.279619
103.O	3.930989	9.778755	7.687487
104.O	16.261119	4.973770	4.856986
105.H	2.271636	16.656747	9.566314
106.O	4.678612	16.667795	10.289430
107.H	6.074421	18.725919	10.765939
108.H	2.254966	13.067946	9.568479
109.H	8.533445	2.629991	7.901235
110.H	8.738540	19.097783	6.061061
111.O	8.090665	17.154306	7.532737
112.O	3.753927	2.651674	8.362502
113.H	3.624625	0.144450	7.919481
114.H	3.977621	17.279278	7.920456
115.O	5.352141	6.717430	3.679774
116.H	19.758911	17.008858	10.721485
117.O	2.912154	11.109495	3.003911
118.O	12.249877	16.743323	10.453673
119.H	7.308460	19.541094	7.960523
120.H	6.429334	18.354656	6.035824
121.H	12.847982	1.679762	7.907891
122.H	1.975323	11.408333	0.669972
123.O	2.593429	3.168486	3.504982
124.O	3.842128	3.064591	5.771679
125.O	6.160728	2.740111	7.103896
126.O	8.179620	3.479235	5.522016
127.O	7.832387	3.151907	2.917303
128.O	5.253034	3.224853	3.523474
129.H	3.959684	1.131557	4.121294
130.H	8.281220	1.178889	4.456936
131.H	19.476938	7.894414	10.863214
132.H	6.035649	7.444682	1.338220
133.H	2.001046	2.635374	1.100909
134.H	16.134493	18.738159	9.192770
135.O	17.422762	16.661942	9.869670
136.H	6.065423	2.584045	1.191735
137.O	16.267832	16.832257	7.532609
138.O	10.175060	2.730028	3.852213
139.O	12.846511	10.950619	3.527727
140.H	13.907448	11.172519	1.279374
141.H	17.894446	17.220966	12.287926
142.O	12.306533	15.032324	5.672949
143.H	17.819053	10.836558	4.078108
144.O	15.510061	10.774292	3.184728
145.O	12.695290	6.640941	3.272724
146.H	13.850575	6.724703	1.063075
147.H	6.269016	8.786962	12.056498
148.Al	12.348081	13.392411	6.370780
149.H	17.719546	6.765250	3.812642
150.O	15.336298	6.725347	3.084600
151.O	13.924993	8.865058	2.346002
152.Al	4.704715	6.581051	7.356962
153.O	11.408731	12.459681	5.167239
154.O	11.844971	9.932034	5.861151
155.O	12.014365	7.217069	5.840273
156.O	16.263378	12.613698	4.942232
157.O	16.096665	10.117568	5.770925
158.O	16.099875	7.455758	5.600783
159.H	0.599551	12.069766	2.560147
160.H	0.263211	6.976429	2.755907
161.O	17.172467	8.882743	10.458587
162.O	16.349811	8.631088	7.948954
163.O	14.033336	8.712196	6.613692
164.O	11.840482	8.460639	8.107413
165.O	12.086238	8.953343	10.706229
166.O	14.592194	9.035244	9.874696
167.O	17.265201	13.266806	10.034456
168.O	16.433756	13.097591	7.539167
169.O	13.991394	12.791186	6.356248
170.O	11.605347	13.373371	7.929948
171.O	12.241833	13.013520	10.546484
172.O	14.676783	13.179067	9.541110
173.O	16.190178	11.013946	9.199970
174.O	11.759774	10.945252	8.954778
175.H	18.103944	8.479525	12.772959
176.H	19.110012	10.221994	11.422722
177.H	17.954765	12.661627	12.390597
178.H	13.812352	7.365466	11.627024
179.H	13.941871	9.727816	12.233525
180.H	14.273956	12.445115	11.955576
181.O	9.759225	9.273917	9.620046
182.O	9.767023	12.606428	9.705053
183.O	13.939307	17.080721	6.198682
184.H	6.404410	12.569421	1.807995
185.O	8.176663	8.886377	4.428778
186.O	18.605965	14.934990	11.551222
187.H	17.693512	18.879505	3.681338
188.H	15.283476	18.973125	3.469003
189.O	12.600954	3.240965	3.191353
190.H	13.847825	3.055818	1.025702
191.O	4.582975	9.118697	10.207456
192.H	10.047952	13.484080	4.815007
193.H	17.681190	3.171667	3.778346
194.O	15.260766	3.232902	3.095973

195.H	13.893407	1.158878	2.576102
196.O	7.832387	10.779092	2.817303
197.H	11.568246	17.483433	5.496120
198.H	11.244219	0.448943	6.566629
199.O	12.022904	2.739746	5.774086
200.O	16.336326	17.170908	4.940391
201.H	16.331865	19.655078	5.535236
202.H	15.987488	2.553412	5.438348
203.O	6.060193	11.108958	6.854727
204.H	0.212460	2.999120	2.736235
205.H	13.116953	15.008556	4.234835
206.O	12.234502	13.355542	1.989148
207.H	12.781333	14.111594	2.536926
208.O	9.209712	13.942973	4.527651
209.H	9.373358	13.627549	2.857713
210.H	8.514354	13.416304	4.964249
211.O	9.677645	13.322585	1.949827
212.H	11.190835	13.479736	1.952305
213.H	9.399395	12.390001	1.889759
214.O	13.593608	14.957411	3.344896
215.H	12.397764	12.509174	2.470435
216.H	14.511698	14.694595	3.545991
217.H	11.817784	16.632666	2.544370
218.O	11.040478	16.050883	2.518637
219.H	10.382469	16.432370	3.160015
220.H	9.098965	15.749120	4.652733
221.O	9.122757	16.700002	4.385665
222.H	9.489022	17.178740	5.148521
223.H	10.306265	15.923980	0.777186
224.O	9.920861	15.678813	-0.093932
225.H	9.436964	14.861337	0.112000

Figure S12i

1.H	11.655629	18.678468	9.783392
2.O	8.077151	6.612770	2.928211
3.O	8.573774	14.868976	8.322711
4.O	10.373706	7.462383	3.963290
5.O	3.969379	15.136905	8.704855
6.Si	3.675546	0.768084	8.666301
7.Si	8.591447	16.495109	8.629606
8.Si	6.515975	17.046316	10.920594
9.O	4.295205	12.765516	7.610599
10.H	19.239259	13.156222	9.469335
11.O	11.121941	4.992844	4.754679
12.Si	3.807986	16.580860	9.507205
13.O	7.764908	11.228407	5.536083
14.O	4.002415	11.229326	5.495863
15.O	12.006983	17.063227	7.878793
16.Si	7.552944	17.669719	5.980798
17.O	3.851011	6.238231	5.638948
18.O	8.632032	7.249208	8.183930
19.Si	1.822750	3.283913	2.250488
20.Si	4.055604	2.596706	4.303092
21.Si	4.567141	3.371403	7.265995
22.Si	7.619837	3.314127	6.952554
23.Si	8.493738	2.369151	4.121673
24.Si	6.365568	3.308454	2.091254
25.Si	11.407297	11.109497	4.878264
26.Si	13.952416	10.501581	3.105177
27.O	9.895085	16.877572	9.538198
28.O	7.130614	8.708926	9.845784
29.O	13.785144	14.501460	11.777092
30.Si	16.512798	10.710781	5.105899
31.Si	11.623910	6.530580	4.491962
32.Si	14.004292	7.378685	2.688994
33.O	6.405013	4.907634	1.695645
34.H	5.924964	12.989958	12.354265
35.O	15.690256	14.682023	5.964931
36.Si	16.023100	6.233982	4.765493
37.Si	19.241625	9.100844	10.011222
38.Si	16.191795	9.282725	9.728926
39.Si	15.560203	8.397888	6.892140
40.Si	12.441029	8.609778	6.632038
41.Si	11.326815	9.464919	9.396099
42.Si	13.600714	8.347902	11.201141
43.Si	18.629179	13.177959	10.815807
44.Si	15.928958	12.355151	9.557423
45.Si	15.508520	13.201071	6.693367
46.Si	11.148966	12.573185	9.479345
47.Si	13.459301	12.923904	11.408951
48.H	13.312110	1.205793	7.220912
49.H	6.014614	11.810831	1.096113
50.H	3.512004	6.816194	0.784966
51.H	0.327919	8.950747	3.358844
52.H	14.477965	14.649869	3.783265
53.Si	16.569426	18.506878	4.421782
54.Si	11.496721	3.464469	4.258263
55.Si	13.707389	3.150421	2.053686
56.O	7.044627	13.697107	10.172547
57.O	2.823862	6.897155	3.249258
58.H	3.834107	5.237537	5.489995
59.Si	15.692208	3.146094	4.449484
60.O	4.194051	8.672111	4.771393
61.O	6.207017	6.945026	7.060114
62.O	4.419158	4.822761	7.941186
63.Si	12.355797	2.314315	6.996712
64.H	14.168580	16.972327	12.102969
65.O	5.118419	10.549774	3.122310
66.Si	17.947286	16.063964	11.738198
67.Si	16.172503	16.935417	9.315147
68.Si	15.794148	16.269565	6.376433
69.Si	12.680155	16.660748	6.447743
70.Si	11.490200	17.263915	9.415049
71.Si	13.801543	15.985302	11.076630
72.Si	8.470908	8.707104	8.908441
73.Si	6.016048	9.556450	10.711884
74.O	4.433702	12.991734	10.314531
75.O	6.413338	11.159510	10.614711
76.O	7.846719	4.848966	7.468277
77.Si	3.338944	9.014284	9.004552
78.Si	8.228120	13.434695	9.063022
79.Si	5.942831	12.709956	10.914916
80.O	8.402914	9.863511	7.729176
81.O	3.593237	7.617768	8.228948
82.O	7.695004	12.472245	7.855077
83.Si	3.687867	13.533712	8.940024

84.Si	0.877402	10.229579	3.869428
85.Si	3.947365	10.214212	4.215238
86.Si	4.364280	11.208185	7.103030
87.Si	7.437323	11.035742	7.131343
88.Si	8.421448	10.564771	4.195456
89.Si	6.136468	11.735829	2.562882
90.Si	2.475685	6.330567	1.718794
91.Si	4.105959	7.143846	4.233959
92.Si	7.738050	6.439634	7.065957
93.Si	8.749764	7.422155	4.197222
94.Si	6.564395	6.416409	2.323450
95.O	14.897535	16.020369	9.837403
96.O	8.430217	6.643728	5.587075
97.O	10.013882	10.900931	4.030732
98.O	2.519844	4.679781	1.685343
99.H	2.301594	0.369246	9.051033
100.H	4.530424	0.890389	9.872333
101.O	7.234028	16.942029	9.425911
102.H	7.112138	16.075418	11.858601
103.O	3.294866	10.287487	7.925023
104.O	15.328643	4.742363	4.745147
105.H	2.463151	16.657166	10.119879
106.O	4.905229	16.703862	10.744057
107.H	6.654390	18.437969	11.404737
108.H	2.249888	13.272598	9.088350
109.H	8.587387	2.425264	7.605007
110.H	8.310469	18.365685	4.914351
111.O	8.648632	17.241544	7.171649
112.O	3.561285	2.241246	7.883437
113.H	4.254410	-0.245158	7.748173
114.H	4.036319	17.649814	8.512017
115.O	5.484850	6.603212	3.567618
116.H	18.841111	17.020783	12.419736
117.O	2.500938	10.312394	3.463876
118.O	12.303805	16.321955	10.482920
119.H	6.531099	18.585653	6.545973
120.H	6.896192	16.458586	5.437052
121.H	12.712320	3.476794	7.844216
122.H	0.183907	11.369641	3.224779
123.O	2.554167	2.791544	3.657054
124.O	4.150336	3.602579	5.630557
125.O	6.102223	2.766561	7.323702
126.O	7.780530	3.262898	5.306998
127.O	7.820072	2.813336	2.681043
128.O	5.182697	3.051240	3.209341
129.H	4.259280	1.207117	4.729001
130.H	8.260553	0.934911	4.348952
131.H	19.585948	8.157471	8.917974
132.H	6.286970	7.390104	1.262615
133.H	2.015379	2.252066	1.210212
134.H	15.790939	18.356848	9.304066
135.O	17.476153	16.743339	10.299366
136.H	6.061559	2.556984	0.869455
137.O	16.600925	16.455316	7.797135
138.O	10.108981	2.613058	4.079697
139.O	12.591426	11.265468	3.698064
140.H	14.317062	11.270304	1.907479
141.H	16.737510	15.756352	12.535490
142.O	12.424832	15.099736	6.043552
143.H	17.704991	10.656081	4.253012
144.O	15.157881	10.516940	4.188851
145.O	12.781092	6.489873	3.327763
146.H	14.236000	6.950025	1.307586
147.H	6.068948	9.114088	12.110573
148.Al	12.368150	13.468571	6.755450
149.H	17.472419	6.138163	4.540649
150.O	15.386898	7.187005	3.571160
151.O	13.555933	8.966131	2.692214
152.Al	4.577721	6.477923	7.415787
153.O	11.315122	12.481001	5.716199
154.O	11.688046	9.783579	5.779271
155.O	12.226940	7.160745	5.886003
156.O	16.479792	12.168910	5.845606
157.O	16.596588	9.457267	6.177740
158.O	15.712035	6.902295	6.237297
159.H	0.720592	10.295649	5.343157
160.H	1.119953	6.814431	1.391267
161.O	17.632376	8.934473	10.426206
162.O	15.913964	8.238894	8.482494
163.O	14.036279	8.972179	6.685621
164.O	11.829468	8.515589	8.142757
165.O	12.308236	9.250137	10.688605
166.O	15.026247	9.130069	10.866834
167.O	17.007685	12.825012	10.700785
168.O	16.097286	13.308039	8.233917
169.O	13.966523	12.754520	6.664302
170.O	11.694081	13.588186	8.358949
171.O	11.894287	12.738321	10.939988
172.O	14.413428	12.431074	10.158377
173.O	16.218841	10.800031	9.098840
174.O	11.347098	11.025957	8.916666
175.H	20.048643	8.801090	11.216109
176.H	19.503573	10.489620	9.557113
177.H	19.254819	12.197778	11.726898
178.H	13.591223	7.036152	10.516918
179.H	13.501789	8.237795	12.668592
180.H	13.706810	12.128736	12.615369
181.O	9.805309	8.997142	9.821821
182.O	9.539019	12.805707	9.796501
183.O	14.306206	16.960525	6.525161
184.H	5.839170	13.010433	3.245625
185.O	8.145136	8.950892	4.201883
186.O	18.818971	14.679408	11.485598
187.H	17.733180	18.581531	3.508051
188.H	15.312961	18.650695	3.641465
189.O	12.279039	3.474408	2.825733
190.H	14.150451	4.399266	1.395560
191.O	4.499521	9.310094	10.150099
192.H	10.253071	15.941155	3.438323
193.H	17.145260	3.022634	4.187150
194.O	14.881559	2.632875	3.101926
195.H	13.478944	2.062681	1.080639
196.O	7.717370	11.288751	2.885541
197.H	12.116869	17.534254	5.405982
198.H	10.976145	1.867842	7.315735
199.O	12.444663	2.740862	5.382480

200.O	16.609336	17.013388	5.164705
201.H	16.642148	19.593381	5.431025
202.H	15.277429	2.343575	5.614686
203.O	5.870982	10.588927	7.327299
204.H	0.396846	3.520628	2.562428
205.H	12.250521	12.540765	2.662240
206.O	13.559335	14.924673	3.605544
207.H	13.127129	14.950025	4.512036
208.O	9.304401	15.681332	3.545063
209.H	9.334210	14.378886	2.561241
210.H	9.210381	15.194585	4.429615
211.O	9.600015	13.597253	1.961218
212.H	11.018853	13.521642	2.063688
213.H	9.117771	12.802852	2.276168
214.O	12.093069	13.381387	2.135799
215.H	12.625883	14.108011	2.648090
216.H	11.032927	17.216089	1.937535
217.O	11.568075	16.471450	2.288934
218.H	12.410945	16.826331	2.618720
219.H	2.039213	9.007244	9.687126
220.H	8.852906	17.144905	2.498623
221.O	9.074015	17.718693	1.724950
222.H	8.591356	18.551981	1.852269
223.H	8.303698	16.281000	0.484195
224.O	7.953814	15.455491	0.092493
225.H	8.541458	14.760313	0.440585
226.H	8.861633	14.419286	6.495744
227.O	9.040764	14.118206	5.582499
228.H	9.798020	13.489033	5.640419

Figure S12j

1.H	11.655006	18.678544	9.783983
2.O	8.077151	6.612770	2.928211
3.O	8.573774	14.868976	8.322711
4.O	10.373706	7.462383	3.963290
5.O	3.969379	15.136905	8.704855
6.Si	3.675546	0.768084	8.666301
7.Si	8.591447	16.495109	8.629606
8.Si	6.515975	17.046316	10.920594
9.O	4.295205	12.765516	7.610599
10.H	19.239163	13.156140	9.469294
11.O	11.121941	4.992844	4.754679
12.Si	3.807986	16.580860	9.507205
13.O	7.764908	11.228407	5.536083
14.O	4.002415	11.229326	5.495863
15.O	12.006983	17.063227	7.878793
16.Si	7.552944	17.669719	5.980798
17.O	3.852480	6.238759	5.639068
18.O	8.632032	7.249208	8.183930
19.Si	1.822750	3.283913	2.250488
20.Si	4.055604	2.596706	4.303092
21.Si	4.567141	3.371403	7.265995
22.Si	7.619837	3.314127	6.952554
23.Si	8.493738	2.369151	4.121673
24.Si	6.365568	3.308454	2.091254
25.Si	11.407474	11.107475	4.875836
26.Si	13.952416	10.501581	3.105177
27.O	9.895085	16.877572	9.538198
28.O	7.130614	8.708926	9.845784
29.O	13.785144	14.501460	11.777092
30.Si	16.512798	10.710781	5.105899
31.Si	11.623910	6.530580	4.491962
32.Si	14.004292	7.378685	2.688994
33.O	6.405013	4.907634	1.695645
34.H	5.924448	12.992241	12.353487
35.O	15.690256	14.682023	5.964931
36.Si	16.023100	6.233982	4.765493
37.Si	19.241625	9.100844	10.011222
38.Si	16.191795	9.282725	9.728926
39.Si	15.560203	8.397888	6.892140
40.Si	12.441029	8.609778	6.632038
41.Si	11.326815	9.464919	9.396099
42.Si	13.600714	8.347902	11.201141
43.Si	18.629179	13.177959	10.815807
44.Si	15.928958	12.355151	9.557423
45.Si	15.508520	13.201071	6.693367
46.Si	11.148966	12.573185	9.479345
47.Si	13.459301	12.923904	11.408951
48.H	13.148820	1.076629	7.181819
49.H	6.031128	11.755649	1.089788
50.H	3.511708	6.815659	0.784549
51.H	0.218061	9.302087	2.918972
52.H	14.436279	14.651701	3.753298
53.Si	16.569426	18.506878	4.421782
54.Si	11.496721	3.464469	4.258263
55.Si	13.707389	3.150421	2.053686
56.O	7.044627	13.697107	10.172547
57.O	2.823862	6.897155	3.249258
58.H	3.836087	5.238199	5.489183
59.Si	15.692208	3.146094	4.449484
60.O	4.194051	8.672111	4.771393
61.O	6.208168	6.945533	7.061215
62.O	4.419158	4.822761	7.941186
63.Si	12.355797	2.314315	6.996712
64.H	14.167675	16.972175	12.103293
65.O	5.118419	10.549774	3.122310
66.Si	17.947286	16.063964	11.738198
67.Si	16.172503	16.935417	9.315147
68.Si	15.794148	16.269565	6.376433
69.Si	12.680252	16.660678	6.447657
70.Si	11.490332	17.264139	9.415330
71.Si	13.801543	15.985302	11.076630
72.Si	8.470908	8.707104	8.908441
73.Si	6.016048	9.556450	10.711884
74.O	4.433702	12.991734	10.314531
75.O	6.413338	11.159510	10.614711
76.O	7.846719	4.848966	7.468277
77.Si	3.338944	9.014284	9.004552
78.Si	8.228120	13.434695	9.063022
79.Si	5.942831	12.709956	10.914916
80.O	8.402914	9.863511	7.729176
81.O	3.593237	7.617768	8.228948
82.O	7.695004	12.472245	7.855077
83.Si	3.687867	13.533712	8.940024
84.Si	0.877402	10.229579	3.869428
85.Si	3.947365	10.214212	4.215238

86.Si	4.364280	11.208185	7.103030
87.Si	7.437323	11.035742	7.131343
88.Si	8.421448	10.564771	4.195456
89.Si	6.136468	11.735829	2.562882
90.Si	2.475685	6.330567	1.718794
91.Si	4.106303	7.145261	4.233671
92.Si	7.738967	6.438860	7.065775
93.Si	8.749764	7.422155	4.197222
94.Si	6.564395	6.416409	2.323450
95.O	14.897535	16.020369	9.837403
96.O	8.430217	6.643728	5.587075
97.O	10.013882	10.900931	4.030732
98.O	2.519844	4.679781	1.685343
99.H	2.299597	0.362004	9.036212
100.H	4.516844	0.894426	9.881530
101.O	7.234028	16.942029	9.425911
102.H	7.111183	16.073439	11.857394
103.O	3.294866	10.287487	7.925023
104.O	15.328643	4.742363	4.745147
105.H	2.463304	16.650206	10.120481
106.O	4.905229	16.703862	10.744057
107.H	6.654517	18.437223	11.405984
108.H	2.251207	13.266403	9.081592
109.H	8.586093	2.425253	7.606039
110.H	8.325498	18.352610	4.913632
111.O	8.648632	17.241544	7.171649
112.O	3.561285	2.241246	7.883437
113.H	4.269755	-0.241506	7.753929
114.H	4.035045	17.648543	8.511436
115.O	5.484850	6.603212	3.567618
116.H	18.841187	17.020725	12.419614
117.O	2.500938	10.312394	3.463876
118.O	12.303805	16.321955	10.482920
119.H	6.560495	18.618865	6.546787
120.H	6.876246	16.465624	5.455127
121.H	12.912109	3.405085	7.831610
122.H	0.281858	11.582406	3.752170
123.O	2.554167	2.791544	3.657054
124.O	4.150336	3.602579	5.630557
125.O	6.102223	2.766561	7.323702
126.O	7.780530	3.262898	5.306998
127.O	7.820072	2.813336	2.681043
128.O	5.182697	3.051240	3.209341
129.H	4.259227	1.207138	4.729119
130.H	8.261257	0.934845	4.349359
131.H	19.585214	8.159074	8.916266
132.H	6.287629	7.389616	1.262271
133.H	2.015609	2.251905	1.210367
134.H	15.790483	18.356677	9.304286
135.O	17.476153	16.743339	10.299366
136.H	6.061867	2.556799	0.869546
137.O	16.600925	16.455316	7.797135
138.O	10.108981	2.613058	4.079697
139.O	12.591426	11.265468	3.698064
140.H	14.316063	11.270585	1.907450
141.H	16.737341	15.756180	12.535311
142.O	12.420056	15.099219	6.047410
143.H	17.704921	10.656074	4.253092
144.O	15.157881	10.516940	4.188851
145.O	12.781092	6.489873	3.327763
146.H	14.235999	6.950295	1.307592
147.H	6.069164	9.115867	12.110973
148.Al	12.370558	13.465964	6.755857
149.H	17.472406	6.138331	4.540763
150.O	15.386898	7.187005	3.571160
151.O	13.555933	8.966131	2.692214
152.Al	4.577877	6.477176	7.414454
153.O	11.311580	12.479224	5.716196
154.O	11.688046	9.783579	5.779271
155.O	12.226940	7.160745	5.886003
156.O	16.479792	12.168910	5.845606
157.O	16.596588	9.457267	6.177740
158.O	15.712035	6.902295	6.237297
159.H	0.728766	9.725372	5.257632
160.H	1.119253	6.813736	1.393119
161.O	17.632376	8.934473	10.426206
162.O	15.913964	8.238894	8.482494
163.O	14.036279	8.972179	6.685621
164.O	11.829468	8.515589	8.142757
165.O	12.308236	9.250137	10.688605
166.O	15.026247	9.130069	10.866834
167.O	17.007685	12.825012	10.700785
168.O	16.097286	13.308039	8.233917
169.O	13.966210	12.752430	6.663801
170.O	11.687968	13.588345	8.356067
171.O	11.894287	12.738321	10.939988
172.O	14.413428	12.431074	10.158377
173.O	16.218841	10.800031	9.098840
174.O	11.347098	11.025957	8.916666
175.H	20.048191	8.798762	11.215931
176.H	19.503856	10.490378	9.559359
177.H	19.254388	12.197985	11.727396
178.H	13.590681	7.036163	10.516980
179.H	13.501422	8.238885	12.668630
180.H	13.706009	12.128337	12.615135
181.O	9.805309	8.997142	9.821821
182.O	9.539019	12.805707	9.796501
183.O	14.306206	16.960525	6.525161
184.H	5.838283	13.024432	3.202090
185.O	8.145136	8.950892	4.201883
186.O	18.818971	14.679408	11.485598
187.H	17.735361	18.582276	3.510876
188.H	15.314205	18.649018	3.639257
189.O	12.279039	3.474408	2.825733
190.H	14.150439	4.399412	1.395797
191.O	4.499521	9.310094	10.150099
192.H	10.202849	15.919869	3.391631
193.H	17.145293	3.021516	4.188269
194.O	14.881559	2.632875	3.101926
195.H	13.478919	2.062583	1.080803
196.O	7.717370	11.288751	2.885541
197.H	12.116847	17.532455	5.404607
198.H	10.939731	2.069519	7.368278
199.O	12.444663	2.740862	5.382480
200.O	16.609336	17.013388	5.164705
201.H	16.638989	19.593065	5.431698

202.H	15.276366	2.343662	5.614819
203.O	5.870982	10.588927	7.327299
204.H	0.396822	3.520131	2.562913
205.H	12.210171	12.526102	2.648403
206.O	13.513061	14.918755	3.590291
207.H	13.095522	14.948399	4.502838
208.O	9.259628	15.645587	3.529539
209.H	9.276785	14.341649	2.552867
210.H	9.198347	15.195335	4.426100
211.O	9.550177	13.566741	1.948262
212.H	10.948073	13.490163	2.053472
213.H	9.057383	12.767872	2.238145
214.O	12.034074	13.363554	2.124757
215.H	12.562279	14.093163	2.629561
216.H	11.002773	17.271948	2.005199
217.O	11.516435	16.495919	2.317323
218.H	12.361198	16.810262	2.681346
219.H	2.039565	9.009195	9.687547
220.H	8.800456	17.211167	2.575901
221.O	9.056459	17.808938	1.833900
222.H	8.536675	18.622232	1.939712
223.H	8.502410	16.417221	0.463743
224.O	8.244516	15.638837	-0.069735
225.H	8.697142	14.889969	0.357284
226.H	9.017532	14.491668	6.570112
227.O	9.065538	14.132079	5.659279
228.H	9.799591	13.469261	5.661435
229.H	5.700679	13.828572	6.373933
230.O	6.135070	13.938507	5.510568
231.H	7.092934	13.818648	5.667839

Optimized Geometry Coordinates for water clusters in Tables S1

TMS

Si	3.59047068	-2.05637602	2.60032555
C	3.20378301	-3.09649773	1.06598144
C	2.29078686	-0.69124551	2.78134664
C	3.56179623	-3.16285550	4.13670301
C	5.30554320	-1.27495830	2.41725960
H	3.94210075	-3.90025309	0.93315883
H	3.21339239	-2.48121855	0.15485320
H	2.21175631	-3.56440392	1.14170580
H	2.48781291	-0.06840874	3.66567294
H	1.28159503	-1.11391092	2.88953705
H	2.28274186	-0.02997095	1.90303510
H	4.30789810	-3.96695901	4.06241243
H	2.57708967	-3.63322021	4.27048329
H	3.78228548	-2.58662390	5.04671844
H	6.08406731	-2.04376457	2.30944769
H	5.56033444	-0.66338800	3.29468375
H	5.35451463	-0.62462834	1.53212756

1H2O

H	5.37363862	-0.23684087	-1.84093179
H	5.20376507	0.86687510	-2.89942295
O	4.80134789	0.50941951	-2.08925525

2H2O

H	3.23584385	1.77450997	-0.53577122
O	2.30633259	1.51507517	-0.66300363
O	4.77489658	0.52013293	-2.07412182
H	5.34601847	-0.22561872	-1.82130311
H	2.38508005	0.84635557	-1.36591794
H	5.17382120	0.87873532	-2.88560542

3H2O

H	3.21102906	1.79464534	-0.52079440
O	-0.16960510	2.50354638	0.74647215
H	0.42083679	1.76339523	0.97392525
H	5.29289126	-0.20481290	-1.78647130
H	2.36287999	0.85371392	-1.34698652
H	5.11656858	0.89089792	-2.86097261
H	0.25868048	2.84022833	-0.06061206
O	4.72223712	0.53951847	-2.04418122
O	2.28355406	1.52833897	-0.64960870

4H2O

H	1.44989475	-0.22718553	-0.05082633
O	0.81696166	1.31502459	0.49068978
H	1.38721046	1.95841706	-0.02189958
H	3.26821268	-0.13609677	-1.16028999
H	3.20642499	2.04262540	-1.20905867
H	4.79143886	0.27236690	-1.30879232
H	-0.09738027	1.53292885	0.24511198
O	3.89786763	0.49657600	-1.61555535
O	2.02064497	-0.97123575	-0.39784756
H	1.48431658	-1.42141740	-1.07116957
O	2.58733441	2.78743974	-0.96120206
H	3.10262871	3.40384465	-0.41606194

5H2O

H	0.74572216	-0.11613862	-1.49213570
O	0.29265789	1.70332369	0.18450447
H	1.21768155	2.06970776	0.04429518
H	2.90548638	-0.27888889	-1.27253731
H	0.44159636	0.19176720	1.12035259
H	4.26736565	0.07634935	-1.99037636
H	-0.20991641	2.41822820	0.60720112
O	3.77288138	0.21042548	-1.16614555
O	1.30693150	-0.89114766	-1.30649695
H	1.11483057	-1.06558579	-0.34655599
O	2.80599319	2.57646586	-0.30807815
O	0.64871087	-0.74630136	1.38033122
H	-0.19941911	-1.14456175	1.63766793
H	3.26675320	1.76070574	-0.66440066
H	2.84643346	3.23089473	-1.02455895

6H2O

H	5.33503182	0.83588616	0.02252398
H	6.68179696	0.56320528	0.76106019
H	-0.49304290	2.23199752	-0.95296005
O	3.59470215	0.43281343	-0.63552446
H	2.91327018	0.16349498	-1.31392788
H	3.34125866	0.04492596	0.23624885

H	2.99010829	1.99812777	-0.13649666
H	1.02793190	0.84707296	-2.15122471
O	3.46426413	0.39900783	2.14849537
H	2.99065485	1.24962894	2.07867609
O	1.61444140	0.10235141	-2.46145064
H	1.05963668	-0.69393997	-2.48696793
O	2.45155754	2.74508050	0.25608244
H	2.97484073	3.55411167	0.12818677
O	5.88426684	1.11735988	0.78921848
O	0.33502037	2.31004198	-1.45471854
H	1.03005317	2.57365041	-0.79256443
H	4.40288817	0.64228226	1.96877149

7H2O

H	4.45411151	0.86362934	-0.08388521
H	5.09286300	0.97534338	1.38837983
H	1.28376123	2.07373172	-0.05619528
O	4.34545439	0.26799077	-1.56037825
H	3.92182489	0.99714497	-2.08436473
H	3.65225142	-0.43539839	-1.47939628
H	4.01721197	3.87717450	-0.94051336
H	1.54769877	-1.63756149	-1.50493126
O	1.75651312	0.50124671	0.99118958
H	1.37989617	0.37566279	1.87776910
O	2.28112367	-1.49907609	-0.88316435
H	1.93679965	-0.88111483	-0.19131332
O	3.83787222	3.95382815	0.01589200
H	4.15442579	3.09505753	0.38282088
O	4.34598188	1.28135178	0.84820870
O	1.32013384	2.88730308	-0.60522200
H	2.05394708	3.41509935	-0.19683669
H	2.71428158	0.76164243	1.12079117
O	3.08207679	2.48393662	-2.62193138
H	2.73185044	2.60006978	-3.52003301
H	2.30752027	2.58480484	-1.99088693

8H2O

H	5.10752769	0.94935476	0.27584156
H	6.12302634	1.03201571	1.48901163
H	1.36851175	3.19499193	-1.46363014
O	4.63301262	0.87765555	-1.38169527
H	4.58454434	1.80315986	-1.68771252
H	3.67678884	0.60510450	-1.33361854
H	3.21900249	3.14629208	-0.07722076
H	1.36283249	1.01773803	-1.20298611
O	2.30226294	0.36621737	1.50446075
H	2.38612364	1.34196968	1.36727903
O	1.92303539	0.20276345	-1.19804867
H	2.02483398	0.01671408	-0.22230026
O	3.15158524	3.03259717	0.89101649
H	4.00632462	2.61098913	1.14314030
O	5.18126417	1.10183331	1.26301644
O	0.54293342	2.66828974	-1.37294479
H	0.15589176	2.92854573	-0.51944835
H	3.22131808	0.11742244	1.72278894
O	2.23701452	1.43237843	-3.73894357
H	2.29400353	0.69681811	-3.08866563
H	1.28136369	1.61431801	-3.79587455
O	3.17508389	3.38417090	-2.12663417
H	2.89243449	2.72419811	-2.83147896
H	3.44136867	4.19776804	-2.58636906

9H2O

O	3.02984967	6.41488757	-1.61523709
H	3.72234672	6.95007742	-1.19249884
H	0.87441462	3.46240877	-3.17675466
O	4.15702588	0.50402337	-0.89537873
H	3.37796525	0.35818611	-1.53125812
H	4.66425692	-0.32337448	-0.86907969
H	4.97237518	3.40889639	-2.12349236
H	0.99899096	0.54986567	0.34465942
O	2.28203681	1.48227460	1.05116642
H	3.04110445	1.09613340	0.55528432
O	0.42548404	-0.04193571	-0.22479998
H	-0.49068270	0.25028744	-0.09389760
O	5.01727853	3.10503193	-1.19396005
H	4.87998997	2.12372257	-1.20281728
H	3.48241980	5.91561680	-2.33803322
O	1.75085347	3.12391002	-2.92837293
H	1.90759692	3.40310223	-1.96408997
H	2.23838255	2.40953387	0.73243366
O	2.00657852	0.31038149	-2.43909305
H	1.31158636	0.14261833	-1.74562347
H	1.85543553	1.23925724	-2.72577374
O	4.00450894	4.55915681	-3.52057195
H	4.22592131	4.71654373	-4.45324858
H	3.16026727	4.03006253	-3.50930046
O	2.52901951	3.90374546	-0.50534829
H	3.48399428	3.61719465	-0.65097658
H	2.57383695	4.88403467	-0.63480287

10H2O

H	4.95786182	0.30622259	0.32506125
H	5.22492893	-1.20819447	0.61694168
H	1.32949134	4.55694402	-1.46815613
O	4.43628238	1.73213763	-0.68121445
H	4.47877854	2.01101566	-1.63239300
H	3.47910892	1.43804185	-0.63171090
H	4.39512329	3.35939653	-0.06095921
H	1.44226412	1.94570501	-0.64856942
O	2.19042843	-0.44738911	1.52538705
H	2.01716780	-0.17482472	2.44111351
O	1.79095481	1.02473820	-0.70873183
H	1.71013599	0.55567661	0.16579587
O	4.17675808	4.32512030	0.09137906
H	4.57576540	4.58015555	0.93903669
O	4.90291567	-0.38890945	1.02844606
O	1.63525072	3.74886675	-0.97182433
H	2.38388167	4.06844700	-0.41871394
H	3.18248585	-0.47157266	1.42673842
O	2.23869201	0.37493561	-3.36712624
H	1.94423352	0.45808665	-2.42526186
H	1.42881843	0.25428734	-3.88967624
O	3.47082214	2.84165695	-3.02007769
H	3.08402713	2.01698429	-3.40906802
H	2.77196144	3.14470821	-2.38922706

O	1.40503114	5.97879554	-2.51079796
H	1.14676669	6.85664549	-2.18596975
H	2.40388458	5.98327520	-2.57244007
O	4.11375320	5.57717871	-2.54779674
H	4.28558066	5.27978777	-1.62703208
H	4.09682602	4.73648773	-3.05454140

12H2O

H	3.77772114	-2.92069238	0.09713669
H	4.32347630	-3.43305197	1.49333183
H	1.47455466	2.53255302	-1.33075447
H	-1.76489575	-4.03435137	1.88742890
H	1.20833510	-1.31752104	2.11973113
H	-0.01039606	-4.35681071	0.49940021
H	-1.38287179	-2.70922492	0.18248801
O	-2.11493411	-2.36728972	0.75126693
H	-2.84716219	-2.14001205	0.15476332
O	0.33292308	-3.55583782	0.04430167
H	0.53684039	-2.96611859	0.82488091
O	0.46012542	-1.95588880	2.26534232
H	-0.36618309	-1.48319797	2.05320132
O	-1.11889309	-4.68001681	2.24515037
H	-0.51267945	-4.11250761	2.75732913
O	0.82538305	1.83648646	-1.63094796
H	0.51395110	2.11624179	-2.50727931
O	4.28832361	-2.64742573	0.92369951
H	4.50381176	1.65656877	0.69186848
H	4.79207366	2.03357753	2.19412169
H	3.59363334	2.92947575	-1.03861613
H	1.84981654	0.42198588	-1.46606784
H	3.34491451	-1.33622617	1.43745391
H	1.89891990	-3.38269700	-0.90147344
H	5.48578088	1.05773818	-1.51272316
O	4.68624892	1.37495833	-1.06270231
H	3.95226006	0.69430901	-1.22185545
O	2.77048104	-3.08221585	-1.25968203
H	2.62323718	-2.13793754	-1.49496757
O	2.68133058	-0.58568995	1.51029186
H	3.17916837	0.23563494	1.74107121
O	2.56760421	-0.22304188	-1.21307654
H	2.47482459	-0.35210432	-0.22744882
O	2.83573298	3.47467801	-0.72685076
H	2.87893198	3.36607175	0.24245461
O	4.07395456	1.83643051	1.57007359

Al(NO3)3 9H2O

1H	1.71058489	4.91496040	8.17321865
2H	1.49988964	2.48101361	5.48492791
3H	0.46144530	5.22160046	9.23448007
4H	-1.13893084	2.20586402	8.60805695
5H	1.18305422	5.29721256	5.34246113
6H	-1.76806873	4.50505391	4.88272389
7H	-0.24270187	6.02534137	5.38184957
8H	-2.64168513	5.39057081	7.67198343
9H	-1.58743736	2.93598695	5.20777205
10H	-1.42598314	5.93230825	8.53461860
11H	1.18214193	2.46229881	7.29303488
12H	-1.76936034	3.57916286	9.22508450
13H	2.36806972	4.06621714	4.12808481
14H	1.96465977	5.42759853	3.48507463
15H	-3.81899289	4.77832201	9.25622103
16H	-4.85075779	5.57584129	8.38094563
17H	3.42995630	4.08771318	7.19134876
18H	3.12729950	5.46434105	6.54841324
19O	0.40110404	5.53913498	5.95494227
20O	0.60598585	2.77679517	6.57421548
21O	3.49799895	2.19209121	6.58266417
22O	4.34739756	1.61697211	4.62559915
23O	2.21543334	2.23744222	4.70836436
24O	-1.66338044	5.64425734	12.14558452
25O	-0.89359370	6.06640531	10.12024464
26O	-2.32745579	4.37244380	10.46692788
27O	0.29256120	5.94570190	2.65157691
28O	-1.48481435	5.58833908	3.93011185
29O	-0.38382772	3.87388389	3.03015846
30O	2.37458651	5.03594436	4.29573575
31O	0.78574087	4.64774110	8.49573997
32O	-1.65765441	5.60819703	7.60561275
33O	-4.11708740	4.93917926	8.33170621
34O	-1.45827975	3.09409573	8.37382733
35O	3.15870156	5.00560773	7.40981434
36O	-1.74711650	3.78132020	5.66842820
37N	-0.50407848	5.11387811	3.16011909
38N	-1.62335749	5.37050573	10.95296337
39N	3.44769033	1.99332413	5.34895214
40Al	-0.46823736	4.18007539	7.05037043

$Al(H_2O)_6^{3+}$

1.Al	0.765464	-1.373416	0.373108
2.H	3.308327	-1.032931	1.049818
3.H	1.293741	1.205355	0.048264
4.H	-1.773906	-1.714480	-0.306681
5.H	0.924502	-1.855552	2.976147
6.H	1.810237	-3.797616	0.630148
7.H	0.768167	-2.456115	-2.048078
8.O	0.705527	-1.604181	-1.556822
9.H	0.607498	-0.890376	-2.229099
10.O	0.962999	-3.295556	0.596994
11.H	0.234858	-3.951710	0.698398
12.O	0.826123	-1.142350	2.303332
13.H	0.764439	-0.290076	2.794081
14.O	-1.168481	-1.563254	0.455936
15.H	-1.728869	-1.524680	1.265572
16.O	0.566199	0.548316	0.148384
17.H	-0.281556	1.049515	0.114853
18.O	2.699380	-1.183128	0.289778
19.H	3.256094	-1.220656	-0.522421

$Al(H_2O)_6^{3+}\cdot 12H_2O$

1Al	0.00000000	0.00000000	0.00000000
2O	0.00000000	1.91743270	0.00000000
3O	-1.91743270	0.00000000	0.00000000
4O	1.91743270	0.00000000	0.00000000
5O	0.00000000	0.00000000	-1.91743270

6O	0.00000000	0.00000000	1.91743270
7O	0.00000000	-1.91743270	0.00000000
8H	0.69659531	-2.49087726	-0.41469785
9H	0.69659531	2.49087726	0.41469785
10H	-0.69659531	2.49087726	-0.41469785
11H	-2.49087726	0.41469785	-0.69659531
12H	2.49087726	0.41469785	0.69659531
13H	2.49087726	-0.41469785	-0.69659531
14H	-2.49087726	-0.41469785	0.69659531
15H	0.41469785	-0.69659531	-2.49087726
16H	-0.41469785	-0.69659531	2.49087726
17H	-0.41469785	0.69659531	-2.49087726
18H	0.41469785	0.69659531	2.49087726
19H	-0.69659531	-2.49087726	0.41469785
20O	1.82513518	-3.47067181	-1.23753561
21O	1.82513518	3.47067181	1.23753561
22O	-1.82513518	3.47067181	-1.23753561
23O	-3.47067181	1.23753561	-1.82513518
24O	3.47067181	1.23753561	1.82513518
25O	3.47067181	-1.23753561	-1.82513518
26O	-3.47067181	-1.23753561	1.82513518
27O	1.23753561	-1.82513518	-3.47067181
28O	-1.23753561	-1.82513518	3.47067181
29O	-1.23753561	1.82513518	-3.47067181
30O	1.23753561	1.82513518	3.47067181
31O	-1.82513518	-3.47067181	1.23753561
32H	1.53592388	-3.29998695	-2.15485711
33H	1.53592388	3.29998695	2.15485711
34H	-1.53592388	3.29998695	-2.15485711
35H	-3.29998695	2.15485711	-1.53592388
36H	3.29998695	2.15485711	1.53592388
37H	3.29998695	-2.15485711	-1.53592388
38H	-3.29998695	-2.15485711	1.53592388
39H	2.15485711	-1.53592388	-3.29998695
40H	-2.15485711	-1.53592388	3.29998695
41H	-2.15485711	1.53592388	-3.29998695
42H	2.15485711	1.53592388	3.29998695
43H	-1.53592388	-3.29998695	2.15485711
44H	1.74718568	-4.42707384	-1.10370605
45H	1.74718568	4.42707384	1.10370605
46H	-1.74718568	4.42707384	-1.10370605
47H	-4.42707384	1.10370605	-1.74718568
48H	4.42707384	1.10370605	1.74718568
49H	4.42707384	-1.10370605	-1.74718568
50H	-4.42707384	-1.10370605	1.74718568
51H	1.10370605	-1.74718568	-4.42707384
52H	-1.10370605	-1.74718568	4.42707384
53H	-1.10370605	1.74718568	-4.42707384
54H	1.10370605	1.74718568	4.42707384
55H	-1.74718568	-4.42707384	1.10370605