Supporting information for: Supporting Information for: Periodic MP2, RPA, and Boundary Condition Assessment of Hydrogen Ordering in Ice XV

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Computational Details

CASTEP settings

The CASTEP[S1] reference PBE calculations were undertaken using version 7.0, a cutoff of 800eV, on-the-fly pesudopotentials and k-point sampling at 0.03 Angstroms^{-1} (108 k-points). Under an isotropic external pressure of 1GPa, each of the 18 unit cells, containing 10 molecules, was fully relaxed until mechanical equilibrium was attained. The lattice parameters a,b,c and α, β, γ were treated as independent variables in the cell optimization using the BFGS scheme.

CP2K settings

The calculations performed with the CP2K program[S2] are all based on the Gaussian and Plane-Waves (GPW) method[S3,S4] that makes use of a Gaussian basis to expand molecular orbitals and an auxiliary plane wave basis for the expansion of the electronic density. In the GPW scheme core electrons are replaced by pseudopotentials in order for the electronic density to be efficiently expanded in the plane waves basis. The employed pseudopotentials are of dual-space, Goedecker-Teter-Hutter (GTH) type[S5]. In particular, pseudopotentials have been specifically generated for the Hartree-Fock (HF), PBE and PBE0 methods, for all other DFT calculations the PBE and PBE0 pseudopotentials have been used respectively for methods of GGA or Hybrid type. Pseudopotential parameters can be retrieved from SI of Ref[S6].

The non-local HF exchange energy is calculated by employing a Γ-point method based on the usage of a truncated Coulomb operator to avoid divergences in the energy when periodic boundary conditions (PBC) are considered[S7,S8]. For wide bandgap systems, this allows for stable calculations in the condensed phase, without loss of accuracy, if a truncation radius larger than $5-6$ Å is used[S8,S9]. The employed truncation radius is 5.5 Å.

The calculation of the MP2 and RPA energies within the RI-GPW[S10] approach (RI-MP2,

RI-RPA) is closely related to the original GPW method. In this case, the dual representation of the electronic density is applied to the fitting density arising from the resolution of identity approximation (RI) within the Coulomb metric[S11–S14]. The RI method requires the introduction of an auxiliary Gaussian basis, the RI basis have been specifically generated tailored on the employed primary basis. In the RI-RPA method, the correlation energy is given in term of a frequency integral, the integration is carried out employing the Clenshaw-Curtius quadrature scheme using 40 grid points.

The primary basis employed in this work have been labeled as cc-TZ, cc-QZ and cc-5Z denoting respectively valence-only correlation-consistent type basis[S15,S16] of triple, quadruple and quintuple zeta level, generated for being used with pseudopotentials. These basis contain functions with angular momentum up to f,g and h for Oxygen and d,f and g for Hydrogen respectively for the cc-TZ, cc-QZ and cc-5Z basis. The associated RI auxiliary basis (RI-TZ, RI-QZ and RI-5Z) has been generated following the procedure proposed by Weigend *et al.*[S13]. Primary and auxiliary basis sets are also reported in this SI.

The number of grid points used in the GPW scheme for the representation of the electronic density is kept constant for all calculations. This avoids discontinuities in the energy due to the volume change in the cell relaxations. Additionally, this is a safe choice when comparing the energy computed on structures with different volume. The original grids are constructed for the reference cell with density $1.089\,\mathrm{g/cm^3}$ corresponding to a $2 \times 2 \times 2$ supercell with edge length of $13.00\,\text{Å}$. The wavefunction optimization is performed employing a charge-density cutoffs (E_{cut}) of 800, 1200 and 1600 Ry, respectively for the HF, GGA-DFT and meta-GGA-DFT methods. E_{cut} is progressively increased in order to ensure convergence in the calculation of the Hartree potential, gradients of the density and the kinetic energy density, respectively for the HF, GGA-DFT and meta-GGA-DFT methods at low cost compared to the evaluation of the HF exchange or non-local dynamical correlation energies. For the RI-MP2 and RI-RPA calculations a cutoff of 300 Ry is used while for the non-local part of the van der Waals density functionals $E_{\mathrm{cut}}^{\mathrm{NL}}$ is set to 600 Ry.

For all level of theory considered, each of the 18 cells have been fully relaxed (a,b,c and α, β, γ were treated as independent variables) under 1 GPa isotropic external pressure using the BFGS scheme until mechanical equilibrium was established employing the cc-TZVP basis[S6,S10,S17]. The manuscript with the details about the RI-MP2 forces and stress-tensor in condensed phase is in preparation.

Basis Set Analysis

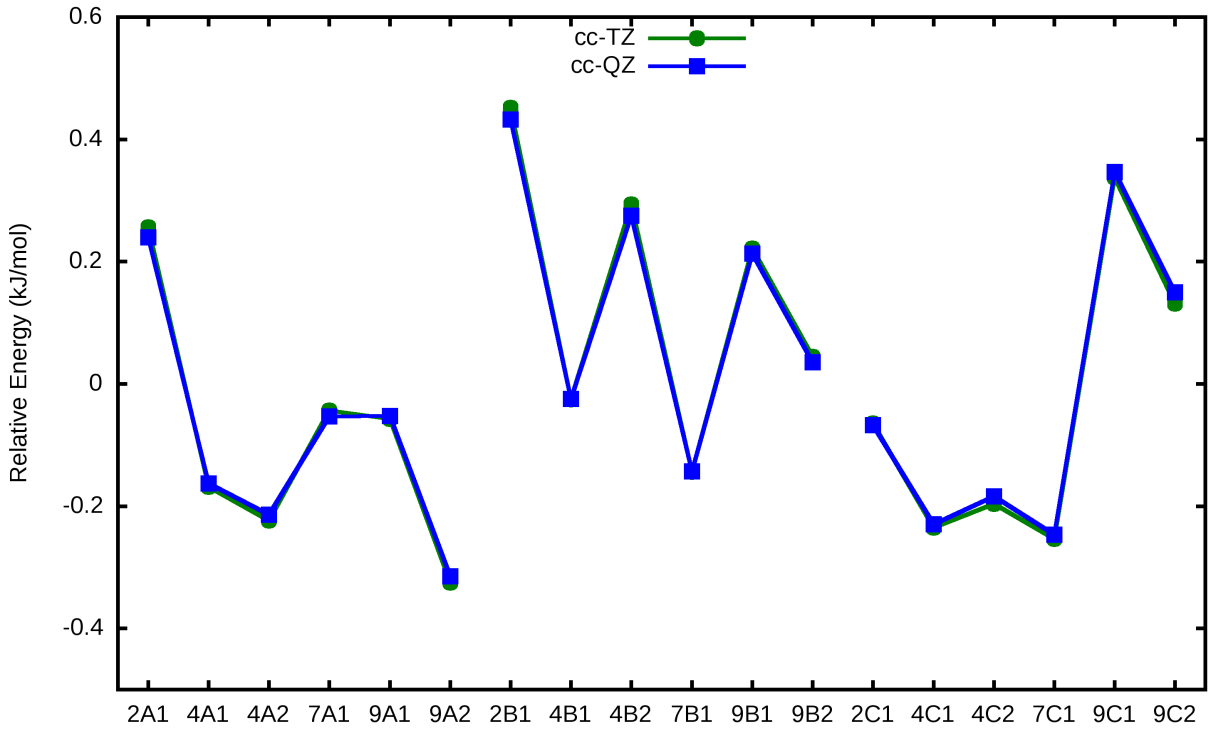

Figure S1: Relative energies in kJ/mol per molecule, with respect to the average, of the 18 symmetry inequivalent structures possible in the ice XV unit cell reported using PBE, cc-TZ and cc-QZ basis.

For all calculations at the DFT level, unless otherwise specified, the cc-TZ basis has been used, that provides converged results at this level of theory. In fact, as shown in S1 for the PBE case, the cc-TZ provides relative stability over the 18 structures of ice XV that are basically identical as those obtained with the cc-QZ basis. In this respect the cc-TZ basis can

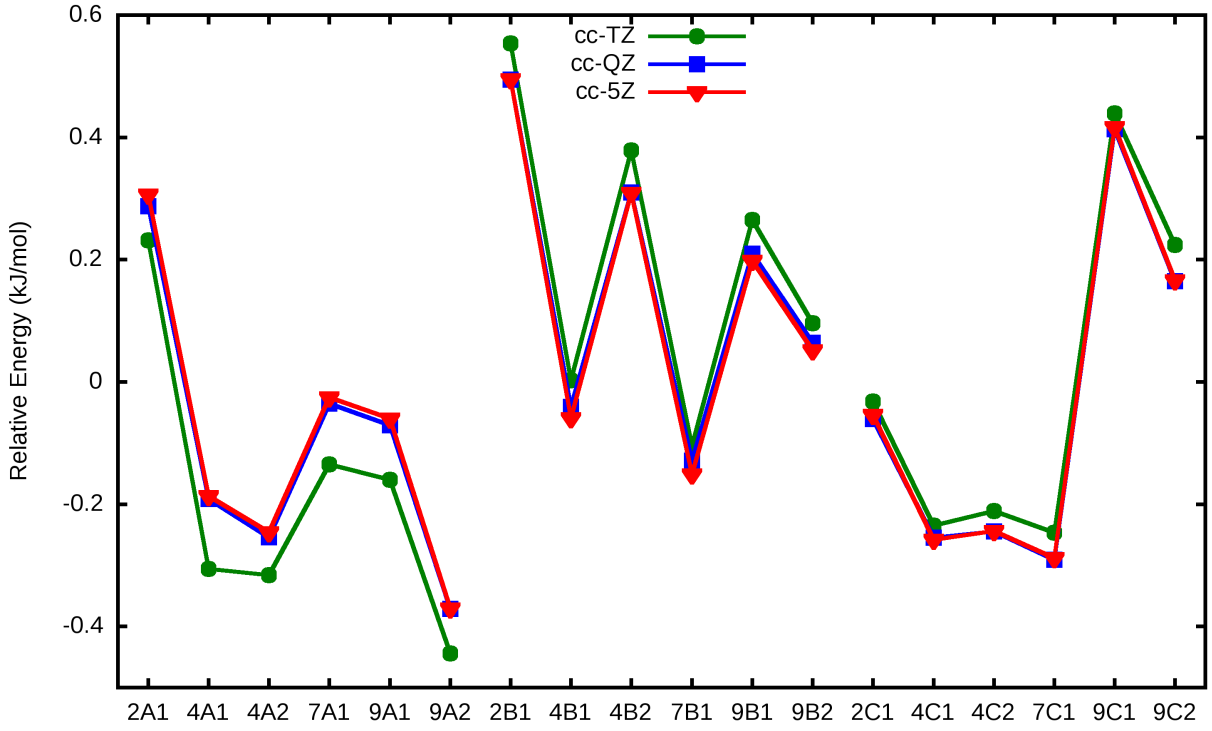

Figure S2: Relative energies in kJ/mol per molecule, with respect to the average, of the 18 symmetry inequivalent structures possible in the ice XV unit cell reported using the cc-TZ, cc-QZ and cc-5Z basis at the RPA level.

be considered of similar quality as the CP2K standard QZV3P basis, that has been shown to provide very well converged results at the DFT level[S18,S19] for liquid water in the condensed phase.

Different is the case for the calculation of the RI-MP2 and RI-RPA correlation energies. In this case, due to the electron coalescence cusp[S20–S22], the convergence of the correlation energies with respect to the basis set is significantly slower compared the the DFT cases. This problem has been investigated by analyzing the convergence of the relative energies of the ice XV structures with respect of the basis set quality over the series cc-TZ, cc-QZ and cc-5Z. This analysis has been focused on the RPA correlation energy that shows essentially the same basis set convergence behavior as the MP2 energy[S21,S23]. This choice is motivated by the favorable scaling of RPA compared to MP2, that is $O(N^4)$ *vs* $O(N^5)$.

Table S1: Representative timings for the evaluation of the correlation energies (2C1 structure) with the various basis employed in this work. The system is made of 80 H_2O molecules ($2\times2\times2$ supercell) resulting in 320 occupied molecular orbitals. Timing measured on a CRAY-XC30 machine, each hybrid node mounts one graphical processing unit (NVIDIA-Tesla-K20X) and 8 processors (Intel-Xeon-E5).

	cc-TZ	cc-QZ	cc-5Z
Number of Basis Functions	4560	9120	16000
Number of RI Basis Functions	10880	19040	29600
Number of Hybrid Nodes	1024	2048	4096
Time for RI-RPA Energy (s)	216.9	347.6	1165.4
Time for RI-MP2 Energy (s)	279.1	523.8	-

In general, for correlation-consistent type basis the correlation energies show an inverse cubic dependence $E^c \propto X^{-3}$ with respect to the basis quality cc-XZ[S20]. The results for the relative stability of the 18 structures of ice XV as obtained using the cc-TZ, cc-QZ and cc-5Z basis at the RPA level are shown in S2. From the plot it appears that the usage of the cc-TZ basis provides results qualitatively in agreement with the higher quality basis while the cc-QZ and cc-5Z give basically the same profiles. These results shows that for the relative stability of ice XV structures the usage of the cc-QZ basis provides essentially converged results for the correlation energies evaluation.

Representative timings for the correlation energies evaluations are reported in S1 for the different calculations reported here.

Supplementary Calculations

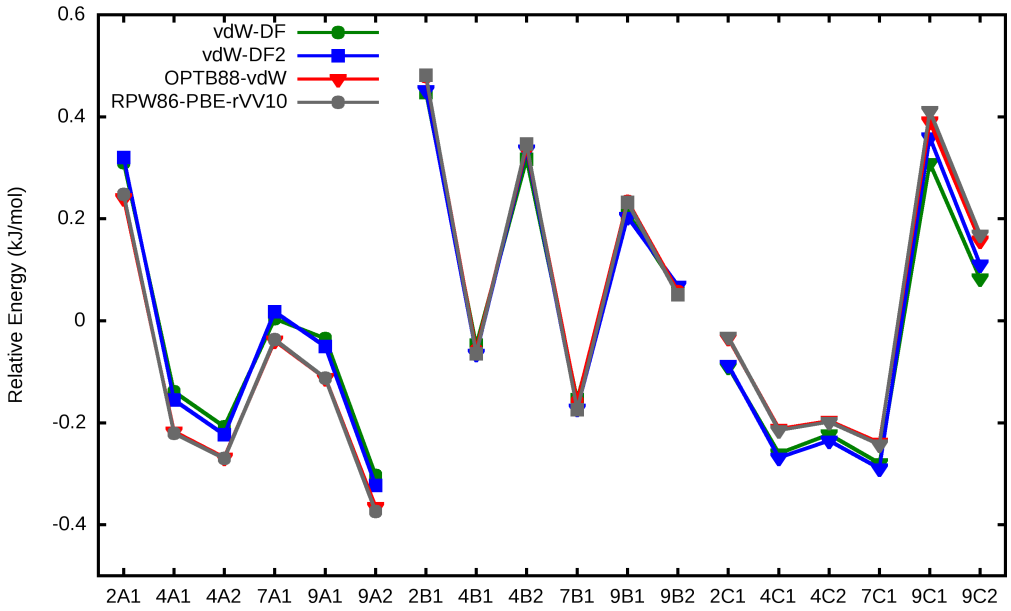

Figure S3: Relative energies in kJ/mol per molecule, with respect to the average, of the 18 symmetry inequivalent structures possible in the ice XV unit cell reported using van der Waals density based functionals.

The results in S3 shows that various selected VdWDF's yield the same qualitative order of energies for the ice XV structures as PBE based approaches. The tested functionals are vdw-DF[S25,S26], vdw-DF2[S27], optPBE-B88vdw[S28,S29] and rVV10[S30].

In S4 it is shown that despite substantial variation in the proportion of HF exchange used between the different formulations of M06 functionals[S31], these methods consistently yield the same overall structure/energy relationship. In the plot, the D3 label stands for Grimme's van der Waals correction[S32].

The dipole moment of the different cells is reported in S5 showing that only four structures are anti-ferroelectric (apolar): 2A1, 2B1, 2C1 and 9A1. More precisely, 2A1, 2B1 and 2C1 have exactly 0 dipole while 9A1 and 9B2 have very small residual dipoles.

To assess whether the initial geometries influence the optimized structures and energy differences, we performed full cell and coordinate optimisations using the MP2 geometries

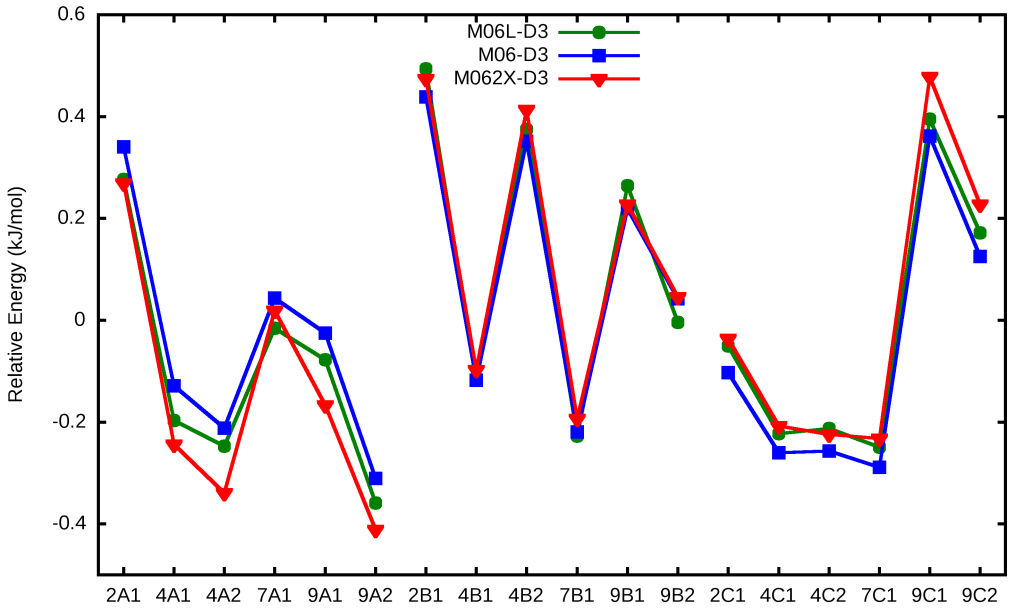

Figure S4: Relative energies in kJ/mol per molecule, with respect to the average, of the 18 symmetry inequivalent structures possible in the ice XV unit cell reported using M06 approaches.

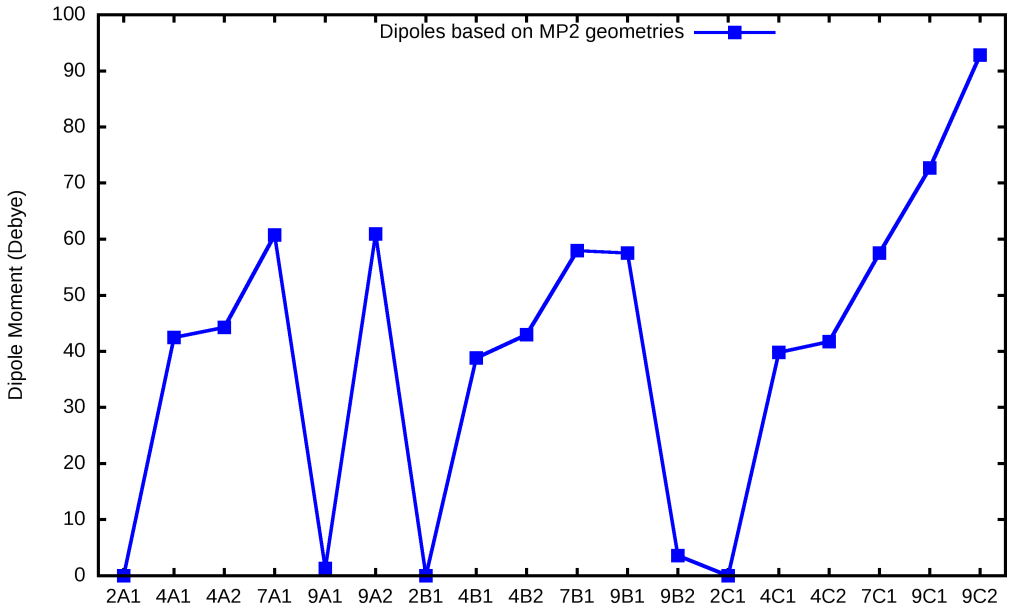

Figure S5: The dipole moments of the 18 symmetry inequivalent structures possible in the ice XV unit cell.

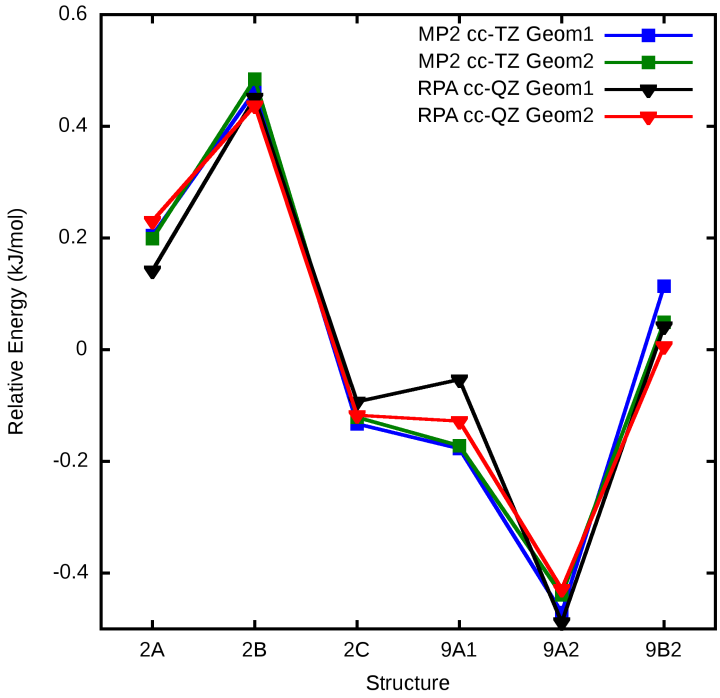

Figure S6: Optimized energies (in kJ/mol per molecule) of five XV structures at the MP2 and RPA level calculated using initial geometries from ref.[S24] (Geom1) and those obtained here (Geom2).

obtained in this work and those reported in the supporting information of ref.[S24]. Figure S6 shows a very minor influence of the starting geometry on the final RPA and MP2 relative energies obtained. The MP2 and RPA absolute energies obtained from MP2 geometries obtained in this work are found to have lower absolute energy than those obtained using structures from ref.[S24].

Because the energy differences between structures reported here are small, the zero point energy of each structure could, in principle, affect the order of stability. To examine this we calculated the vibrational frequencies numerically for all 18 structures using the triple zeta basis (otherwise the settings are as above, except the self-consistent field tolerance was reduced to 1e-7) and a displacement step size of 0.01 Å. Prior to the vibrational calculation, each structure was fully optimised using the MP2 geometries as the starting configuration, at the PBE-D3 level. Because of the high degree of correlation between PBE-D3 and MP2/RPA

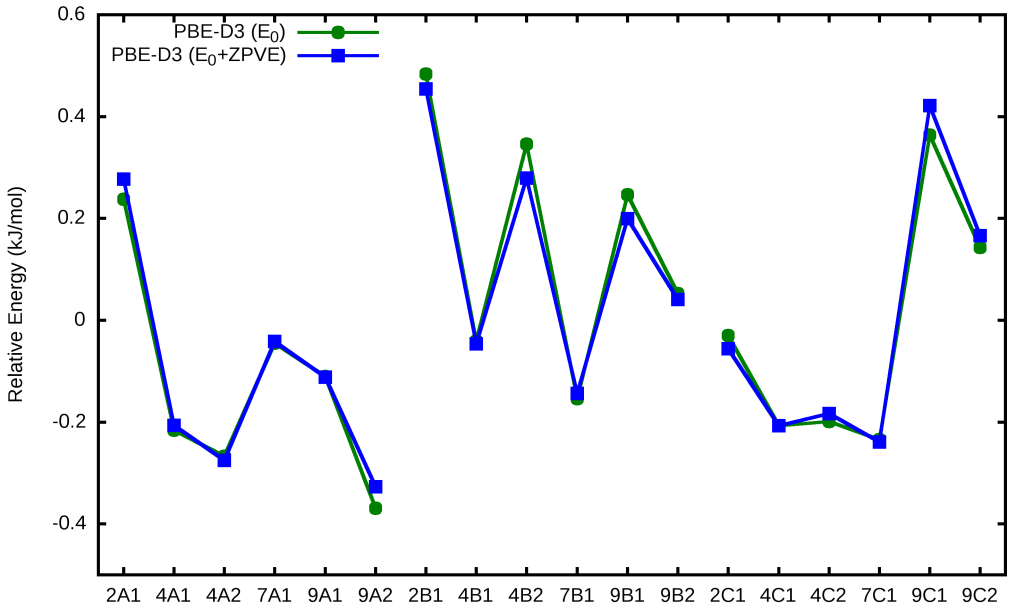

Figure S7: Relative energies (in kJ/mol per molecule) with respect to the average energy, of the 18 possible structures in the ice XV unit cell reported with and without zero point vibrational energy contributions.

Table S2: Absolute energies of ice XV structures computed with CASTEP.

struc.	CASTEP/PBE(eV)
2A	-4736.08985
2B	-4736.071262
2C	-4736.115536
4A1	-4736.13072
4A2	-4736.135906
4B1	-4736.115366
4B2	-4736.084097
4C1	-4736.132146
4C2	-4736.129156
7A	-4736.11849
7B	-4736.125927
7C	-4736.133526
9A1	-4736.121164
9A2	-4736.145393
9B1	-4736.092387
9B2	-4736.109724
9C1	-4736.072654
9C2	-4736.093205

results, PBE-D3 offers an accurate estimate of zero point vibrational energies but at a lower computational cost than the higher level methods. In figure S7 the relative energies (in kJ/mol per molecule) of each of the 18 structures possible in the ice XV unit cell are reported with and without zero point vibrational energy contributions. The order of stability is unchanged and ferroelectric 9A2 structure remains the global minimum energy structure.

For reference, the total energies computed using CP2K of 2x2x2 super cells, containing 80 water molecules are reported in table S3. Total energies of the single unit cell (10 molecules) of ice XV computed with CASTEP with the parameters described earlier are reported in table S2.

Table S3: Absolute energies of ice XV structures computed with CP2K in Hartrees

struc.	PBE	PBE-D3	PBE0	PBE0-D3	vdW-DF	vdW-DF2	OPTB88	rVV10	M06L-D3	M06-D3	M062X-D3	MP2	RPA
2A	-1379.340862	-1379.845349	-1379.007256	-1379.500248	-1389.621058	-1393.884224	-1385.829636	-1382.542395	-1380.332949	-1380.459527	-1380.723938	-1377.679637	-1390.00588
2B	-1379.334927	-1379.837732	-1379.002481	-1379.494431	-1389.616872	-1393.880199	-1385.822373	-1382.535274	-1380.326323	-1380.456537	-1380.717689	-1377.673201	-1389.999573
2C	-1379.350646	-1379.854345	-1379.018773	-1379.512124	-1389.633237	-1393.896613	-1385.837983	-1382.550912	-1380.342911	-1380.473033	-1380.733237	-1377.690639	-1390.016481
4A1	-1379.353791	-1379.859273	-1379.0205	-1379.513865	-1389.634739	-1393.898701	-1385.843569	-1382.556688	-1380.347373	-1380.473821	-1380.739573	-1377.693125	-1390.020472
4A2	-1379.355466	-1379.860974	-1379.02277	-1379.516301	-1389.636838	-1393.900781	-1385.845142	-1382.558169	-1380.348899	-1380.476373	-1380.742466	-1377.695292	-1390.022375
4B1	-1379.349418	-1379.854219	-1379.016827	-1379.509972	-1389.631949	-1393.895957	-1385.83872	-1382.551925	-1380.344818	-1380.473503	-1380.735111	-1377.688868	-1390.015899
4B2	-1379.339711	-1379.842423	-1379.006584	-1379.498168	-1389.620841	-1393.883744	-1385.82658	-1382.539388	-1380.329961	-1380.459192	-1380.719546	-1377.676921	-1390.005193
4C1	-1379.355816	-1379.859573	-1379.023818	-1379.516985	-1389.63843	-1393.90216	-1385.843404	-1382.5565	-1380.348154	-1380.477839	-1380.738459	-1377.695833	-1390.022397
4C2	-1379.354621	-1379.859185	-1379.022873	-1379.516689	-1389.637288	-1393.901132	-1385.84294	-1382.555985	-1380.347856	-1380.477743	-1380.738963	-1377.695037	-1390.022104
7A	-1379.350019	-1379.854281	-1379.016497	-1379.509005	-1389.630377	-1393.89343	-1385.838132	-1382.551079	-1380.341855	-1380.46858	-1380.731553	-1377.688428	-1390.015726
7B	-1379.353063	-1379.857675	-1379.020385	-1379.513197	-1389.635215	-1393.899218	-1385.841764	-1382.555261	-1380.348311	-1380.476596	-1380.73804	-1377.692129	-1390.018557
7C	-1379.356378	-1379.860391	-1379.024342	-1379.517727	-1389.63901	-1393.902794	-1385.844243	-1382.557345	-1380.348964	-1380.478716	-1380.739219	-1377.696632	-1390.023512
9A1	-1379.350413	-1379.855945	-1379.017307	-1379.510915	-1389.631555	-1393.895514	-1385.84038	-1382.553372	-1380.343733	-1380.47067	-1380.737214	-1377.69002	-1390.016806
9A2	-1379.358561	-1379.864044	-1379.025682	-1379.519028	-1389.639742	-1393.903809	-1385.84809	-1382.56134	-1380.352315	-1380.479365	-1380.744676	-1377.698199	-1390.025956
9B1	-1379.341933	-1379.845224	-1379.00953	-1379.50149	-1389.624061	-1393.887765	-1385.829823	-1382.542875	-1380.333316	-1380.463236	-1380.725202	-1377.680295	-1390.008255
9B2	-1379.34732	-1379.851388	-1379.014429	-1379.50688	-1389.628704	-1393.891885	-1385.835223	-1382.548388	-1380.34149	-1380.468631	-1380.73075	-1377.685831	-1390.012702
9C1	-1379.338394	-1379.842098	-1379.005707	-1379.498463	-1389.621077	-1393.883008	-1385.825037	-1382.537425	-1380.329341	-1380.45888	-1380.717571	-1377.674613	-1390.002045
9C2	-1379.344669	-1379.84892	-1379.011932	-1379.504916	-1389.627969	-1393.890604	-1385.832168	-1382.544813	-1380.336142	-1380.466091	-1380.72521	-1377.681463	-1390.009624

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Primary Basis Set

Table S4

Hydrogen cc-TZ		
Shell Type	Exponents	Contraction Coefficients
s	11.3712543500	-0.0151413400
	3.4629589600	-0.0541843100
	1.0118375000	-0.2027920700
s	0.4472818100	1.0000000000
s	0.1581053500	1.0000000000
p	1.4070000000	1.0000000000
p	0.3880000000	1.0000000000
d	1.0570000000	1.0000000000

Table S5

Hydrogen cc-QZ		
Shell Type	Exponents	Contraction Coefficients
s	12.2465222200	0.0086315300
	4.1584420900	0.0308852300
	1.1684633400	0.1290200100
s	0.4753264700	1.0000000000
s	0.1920368500	1.0000000000
s	0.1210243700	1.0000000000
p	2.2920000000	1.0000000000
p	0.8380000000	1.0000000000
p	0.2920000000	1.0000000000
d	2.0620000000	1.0000000000
d	0.6620000000	1.0000000000
f	1.3970000000	1.0000000000

Table S6

Hydrogen cc-5Z		
Shell Type	Exponents	Contraction Coefficients
s	11.3230660100	0.0143963000
	3.7547123600	0.0434588300
	1.3431125300	0.0997000300
s	0.6729200300	1.0000000000
s	0.3924206700	1.0000000000
s	0.2061829000	1.0000000000
s	0.1030253900	1.0000000000
p	4.5160000000	1.0000000000
p	1.7120000000	1.0000000000
p	0.6490000000	1.0000000000
p	0.2460000000	1.0000000000
d	2.9500000000	1.0000000000
d	1.2060000000	1.0000000000
d	0.4930000000	1.0000000000
f	2.5060000000	1.0000000000
f	0.8750000000	1.0000000000
g	2.3580000000	1.0000000000

Table S7

Oxygen cc-TZ		
Shell Type	Exponents	Contraction Coefficients
s	11.1326087700	0.0923503400
	4.8526957700	0.1145513200
	1.1605198700	-0.4686761400
s	0.4176552500	1.0000000000
s	0.1225121100	1.0000000000
p	10.0690207700	-0.0548547800
	3.6112306000	-0.1641600100
	1.3283444800	-0.3000944500
p	0.5007932700	1.0000000000
p	0.1599541600	1.0000000000
d	2.3140000000	1.0000000000
d	0.6450000000	1.0000000000
f	1.4280000000	1.0000000000

Table S8

Oxygen cc-QZ		
Shell Type	Exponents	Contraction Coefficients
s	13.5388233100	-0.0462606600
	5.7451332200	-0.1325990100
	1.5623292200	0.1869179400
s	0.6486941700	1.0000000000
s	0.2412313400	1.0000000000
s	0.1131262300	1.0000000000
p	10.6362976000	0.0476577300
	4.1480952900	0.1371405500
	1.6488908900	0.2564559300
p	0.6618878400	1.0000000000
p	0.2573803800	1.0000000000
p	0.1031229600	1.0000000000
d	3.7750000000	1.0000000000
d	1.3000000000	1.0000000000
d	0.4440000000	1.0000000000
f	2.6660000000	1.0000000000
f	0.8590000000	1.0000000000
g	1.8460000000	1.0000000000

Table S9

Oxygen cc-5Z		
Shell Type	Exponents	Contraction Coefficients
s	13.5169408300	-0.0619110800
	5.6612593700	-0.1804075500
	1.8205415400	0.1696496400
s	0.7719013600	1.0000000000
s	0.3511787100	1.0000000000
s	0.2139283900	1.0000000000
s	0.1034874100	1.0000000000
p	10.8617026900	0.0548352000
	4.3906615000	0.1549286100
	1.7920331100	0.2947797400
p	0.7406042500	1.0000000000
p	0.3518189300	1.0000000000
p	0.2122757100	1.0000000000
p	0.1030280800	1.0000000000
d	5.8790000000	1.0000000000
d	2.3070000000	1.0000000000
d	0.9050000000	1.0000000000
d	0.3550000000	1.0000000000
f	4.0160000000	1.0000000000
f	1.5540000000	1.0000000000
f	0.6010000000	1.0000000000
g	3.3500000000	1.0000000000
g	1.1890000000	1.0000000000
h	2.3190000000	1.0000000000

RI Basis Set

Table S10

Hydrogen RI-TZ		
Shell Type	Exponents	Contraction Coefficients
s	8.5115919477	1.0000000000
s	1.8744684124	1.0000000000
s	0.5632515938	1.0000000000
s	0.3698300166	1.0000000000
p	2.3711712241	1.0000000000
p	1.1794161377	1.0000000000
p	0.6050431475	1.0000000000
d	1.8092525712	1.0000000000
d	1.1433220620	1.0000000000
f	1.8065804521	1.0000000000

Table S11

Hydrogen RI-QZ		
Shell Type	Exponents	Contraction Coefficients
s	21.8834409875	1.0000000000
s	4.2830335923	1.0000000000
s	1.0170620853	1.0000000000
s	0.4071335622	1.0000000000
s	0.3070340255	1.0000000000
p	3.1910516304	1.0000000000
p	1.2144411593	1.0000000000
p	0.5086644570	1.0000000000
p	0.2274376610	1.0000000000
d	2.7576481445	1.0000000000
d	0.9966907612	1.0000000000
d	0.6057979365	1.0000000000
f	1.9816638869	1.0000000000
f	0.6338443522	1.0000000000
g	2.0611299810	1.0000000000

Table S12

Hydrogen RI-5Z		
Shell Type	Exponents	Contraction Coefficients
s	23.3214999994	1.0000000000
s	4.9229700008	1.0000000000
s	1.7751000135	1.0000000000
s	0.9942180008	1.0000000000
s	0.5060539832	1.0000000000
s	0.2369110057	1.0000000000
p	5.9745799999	1.0000000000
p	2.0521700001	1.0000000000
p	1.2486600068	1.0000000000
p	0.8055450233	1.0000000000
p	0.3478920205	1.0000000000
d	3.8581600020	1.0000000000
d	1.7106300287	1.0000000000
d	0.9792370223	1.0000000000
d	0.6253660257	1.0000000000
f	3.1015099915	1.0000000000
f	1.1981099700	1.0000000000
f	0.5728730025	1.0000000000
g	2.9877999906	1.0000000000
g	1.2319200174	1.0000000000
h	3.2473900016	1.0000000000

Table S13

Oxygen RI-TZ		
Shell Type	Exponents	Contraction Coefficients
s	24.5594495349	1.0000000000
s	8.3250684789	1.0000000000
s	2.8879519493	1.0000000000
s	1.3357882803	1.0000000000
s	0.8784857769	1.0000000000
s	0.2852875185	1.0000000000
p	15.0341061141	1.0000000000
p	3.9834306690	1.0000000000
p	2.2146661069	1.0000000000
p	0.8931426289	1.0000000000
p	0.3941471896	1.0000000000
d	15.8667825802	1.0000000000
d	5.3839851670	1.0000000000
d	2.5152728061	1.0000000000
d	1.1605484149	1.0000000000
d	0.4323316874	1.0000000000
f	4.6817668259	1.0000000000
f	2.1670491586	1.0000000000
f	1.0348711157	1.0000000000
g	2.3488140479	1.0000000000

Table S14

Oxygen RI-QZ		
Shell Type	Exponents	Contraction Coefficients
s	25.1166381174	1.0000000000
s	10.9969529050	1.0000000000
s	5.2098292520	1.0000000000
s	2.5072146705	1.0000000000
s	1.3441778513	1.0000000000
s	0.4775866923	1.0000000000
s	0.2625499180	1.0000000000
p	22.2927841601	1.0000000000
p	6.5610002752	1.0000000000
p	3.3096584856	1.0000000000
p	1.7213385147	1.0000000000
p	0.5801200078	1.0000000000
p	0.3660206732	1.0000000000
d	20.3901984179	1.0000000000
d	8.6266510092	1.0000000000
d	3.8173660034	1.0000000000
d	1.8467737268	1.0000000000
d	0.8218865052	1.0000000000
d	0.3041507090	1.0000000000
f	10.4973280288	1.0000000000
f	4.3991608142	1.0000000000
f	2.8173017053	1.0000000000
f	1.4414924865	1.0000000000
f	0.8359670711	1.0000000000
g	4.9519648192	1.0000000000
g	2.4902662088	1.0000000000
g	1.0970858350	1.0000000000
h	2.7897777526	1.0000000000

Table S15

Oxygen RI-5Z		
Shell Type	Exponents	Contraction Coefficients
s	24.7049187963	1.0000000000
s	14.8171767724	1.0000000000
s	5.7780857357	1.0000000000
s	3.4643606955	1.0000000000
s	1.7082256389	1.0000000000
s	0.9751946925	1.0000000000
s	0.4924318744	1.0000000000
s	0.2355189502	1.0000000000
p	21.4607787249	1.0000000000
p	11.0344479402	1.0000000000
p	4.6310664067	1.0000000000
p	2.5324252011	1.0000000000
p	1.0033465804	1.0000000000
p	0.5704236732	1.0000000000
p	0.2935691569	1.0000000000
d	15.9734030464	1.0000000000
d	7.2140017137	1.0000000000
d	4.3539548395	1.0000000000
d	2.4086172256	1.0000000000
d	1.4234640236	1.0000000000
d	0.6607113268	1.0000000000
d	0.3786252487	1.0000000000
f	12.0995680579	1.0000000000
f	6.4411773501	1.0000000000
f	3.7119777364	1.0000000000
f	2.1051548714	1.0000000000
f	1.2318672903	1.0000000000
f	0.7140972916	1.0000000000
g	6.9041367232	1.0000000000
g	3.5918911104	1.0000000000
g	2.5069059481	1.0000000000
g	0.9915374024	1.0000000000
h	5.4051561258	1.0000000000
h	3.2349098361	1.0000000000
h	1.6166546379	1.0000000000
i	3.2340138149	1.0000000000

CP2K Input File and Optimized RI-MP2 Geometries

```
&FORCE_EVAL
  METHOD         Quickstep
  &DFT
    BASIS_SET_FILE_NAME    ./BASIS
    POTENTIAL_FILE_NAME    ./POTENTIALS
    &MGRID
      CUTOFF       800
      REL_CUTOFF    50
    &END MGRID
    &QS
      EPS_DEFAULT  1.0E-20
      EPS_PGF_ORB  1.0E-25
    &END QS
    &SCF
      SCF_GUESS ATOMIC
      EPS_SCF 1.0E-6
      MAX_SCF 20
      &OT
        MINIMIZER       CG
        PRECONDITIONER  FULL_SINGLE_INVERSE
      &END
      &OUTER_SCF
        EPS_SCF  1.0E-6
        MAX_SCF  20
      &END
      &PRINT
        &RESTART OFF
        &END
      &END
    &END SCF
    &XC
      &XC_FUNCTIONAL NONE
      &END XC_FUNCTIONAL
      &HF
        FRACTION  1.0
        &SCREENING
          EPS_SCHWARZ          1.0E-8
          SCREEN_ON_INITIAL_P  FALSE
        &END SCREENING
        &INTERACTION_POTENTIAL
          POTENTIAL_TYPE  TRUNCATED
          CUTOFF_RADIUS   5.5
          T_C_G_DATA      ./t_c_g.dat
        &END
        &MEMORY
          MAX_MEMORY  6000
        &END
      &END HF
      &WF_CORRELATION
        METHOD  RI_MP2_GPW
        &RI_MP2
          BLOCK_SIZE    1
        &END
        &WFC_GPW
          CUTOFF      300
          REL_CUTOFF  50
          EPS_FILTER  1.0E-12
          EPS_GRID    1.0E-8
        &END
        MEMORY    4800
        NUMBER_PROC  1
      &END
    &END XC
  &END DFT
    ⋮
    ⋮
  &SUBSYS
   &CELL
      A     1.204149E+01  0.000000E+00  0.000000E+00
      B     1.153442E-01  1.204087E+01  0.000000E+00
      C     3.368764E-03 -3.385323E-03  1.107183E+01
      MULTIPLE_UNIT_CELL  1 1 1
      &CELL_REF
        A     1.300000E+01  0.000000E+00  0.000000E+00
        B     0.000000E+00  1.300000E+01  0.000000E+00
        C     0.000000E+00  0.000000E+00  1.300000E+01
        MULTIPLE_UNIT_CELL  1 1 1
      &END CELL_REF
    &END CELL
    &TOPOLOGY
       NUMBER_OF_ATOMS  240
       MULTIPLE_UNIT_CELL  1 1 1
       COORD_FILE_NAME   ./9A2.xyz
       COORD_FILE_FORMAT XYZ
    &END TOPOLOGY
    &KIND H
      BASIS_SET          cc-TZ
      RI_AUX_BASIS_SET   RI-TZ
      POTENTIAL      GTH-HF-q1
    &END KIND
    &KIND O
      BASIS_SET          cc-TZ
      RI_AUX_BASIS_SET   RI-TZ
      POTENTIAL      GTH-HF-q6
    &END KIND
  &END SUBSYS
&END FORCE_EVAL
&GLOBAL
  PROJECT     9A2_MP2-cc-TZ
  RUN_TYPE    ENERGY
  PRINT_LEVEL MEDIUM
&END GLOBAL
```

Figure S8: Input example for calculation of the RI-MP2 energy relative to the 9A2 Structure. Additionally the following files are needed: BASIS, containing the (TZ) basis parameters; POTENTIALS, containing the (HF) pseudopotential parameters; t_c_g.dat, data file for the usage of the coulomb truncated potential (retrievable from the CP2K release); 9A2.xyz, coordinate file with the geometry of the 9A2 structure.

```
&FORCE_EVAL
  METHOD         Quickstep
  &DFT
    BASIS_SET_FILE_NAME    ./BASIS
    POTENTIAL_FILE_NAME    ./POTENTIALS
    &MGRID
      CUTOFF       800
      REL_CUTOFF    50
    &END MGRID
    &QS
      EPS_DEFAULT  1.0E-20
      EPS_PGF_ORB  1.0E-25
    &END QS
    &SCF
      SCF_GUESS ATOMIC
      EPS_SCF 1.0E-6
      MAX_SCF 20
      &OT
        MINIMIZER       CG
        PRECONDITIONER  FULL_SINGLE_INVERSE
      &END
      &OUTER_SCF
        EPS_SCF  1.0E-6
        MAX_SCF  20
      &END
      &PRINT
        &RESTART OFF
        &END
      &END
    &END SCF
    &XC
      &XC_FUNCTIONAL PBE
      &END XC_FUNCTIONAL
      &WF_CORRELATION
        METHOD  RI_RPA_GPW
        &RI_RPA
          RPA_NUM_QUAD_POINTS    40
          &HF
            FRACTION  1.0
            &SCREENING
              EPS_SCHWARZ          1.0E-8
              SCREEN_ON_INITIAL_P  FALSE
            &END SCREENING
            &INTERACTION_POTENTIAL
              POTENTIAL_TYPE TRUNCATED
              CUTOFF_RADIUS  5.5
              T_C_G_DATA     ./t_c_g.dat
            &END
            &MEMORY
              MAX_MEMORY 0
            &END
          &END HF
        &END
        &WFC_GPW
          CUTOFF      300
          REL_CUTOFF  50
          EPS_FILTER  1.0E-12
          EPS_GRID    1.0E-8
        &END
        MEMORY    4800
        NUMBER_PROC  1
      &END
    &END XC
  &END DFT
    ⋮
    ⋮
  &SUBSYS
   &CELL
      A     1.204149E+01  0.000000E+00  0.000000E+00
      B     1.153442E-01  1.204087E+01  0.000000E+00
      C     3.368764E-03 -3.385323E-03  1.107183E+01
      MULTIPLE_UNIT_CELL  1 1 1
      &CELL_REF
        A     1.300000E+01  0.000000E+00  0.000000E+00
        B     0.000000E+00  1.300000E+01  0.000000E+00
        C     0.000000E+00  0.000000E+00  1.300000E+01
        MULTIPLE_UNIT_CELL  1 1 1
      &END CELL_REF
    &END CELL
    &TOPOLOGY
       NUMBER_OF_ATOMS  240
       MULTIPLE_UNIT_CELL  1 1 1
       COORD_FILE_NAME   ./9A2.xyz
       COORD_FILE_FORMAT XYZ
    &END TOPOLOGY
    &KIND H
      BASIS_SET          cc-TZ
      RI_AUX_BASIS_SET   RI-TZ
      POTENTIAL     GTH-PBE-q1
    &END KIND
    &KIND O
      BASIS_SET          cc-TZ
      RI_AUX_BASIS_SET   RI-TZ
      POTENTIAL     GTH-PBE-q6
    &END KIND
  &END SUBSYS
&END FORCE_EVAL
&GLOBAL
  PROJECT     9A2_RPA-cc-TZ
  RUN_TYPE    ENERGY
  PRINT_LEVEL MEDIUM
&END GLOBAL
```

Figure S9: Input example for calculation of the (EXX+RPA)@PBE energy relative to the 9A2 Structure. Additionally the following files are needed: BASIS, containing the (TZ) basis parameters; POTENTIALS, containing the (PBE) pseudopotential parameters; t_c_g.dat, data file for the usage of the coulomb truncated potential (retrievable from the CP2K release); 9A2.xyz, coordinate file with the geometry of the 9A2 structure.

Table S16: 2A1 Structure

				A	1.20201535E+01	0.00000000E+00	0.00000000E+00				
				B	-2.72112603E-02	1.19904493E+01	0.00000000E+00				
				C	-4.22301189E-02	-1.02302211E-01	1.11421686E+01				
H	4.463189	3.239621	2.922362	O	1.445438	7.517599	1.389865	H	10.104319	1.401089	10.457169
H	1.512744	2.705893	2.651849	O	4.501435	10.416863	4.181219	H	7.850930	4.437093	6.256697
H	0.268245	1.507090	0.141159	O	1.486341	9.170473	3.512946	H	8.175398	0.124050	9.543188
H	5.708482	4.435328	5.430445	O	4.459508	8.765321	2.056395	H	9.779722	5.715783	7.168728
H	4.485649	5.183669	3.559556	O	4.548636	6.109388	2.110946	H	6.751231	2.696637	9.565650
H	1.488633	0.762213	2.012145	O	1.398805	11.825409	3.458618	H	11.204321	3.143135	7.148550
H	2.215647	1.443878	0.768061	O	5.771876	7.483350	4.848896	H	9.178288	3.709333	6.733226
H	3.759722	4.500996	4.804051	O	0.175168	10.453689	0.721504	H	8.777740	2.129816	9.980411
H	1.451837	4.846980	3.470809	O	3.116335	7.399732	4.886611	H	11.771367	5.131562	6.802282
H	4.522259	1.098155	2.103445	O	2.829902	10.537714	0.684057	H	6.183521	0.707693	9.910088
H	4.114567	1.452327	4.886331	H	10.459313	9.233664	2.919255	O	7.449312	1.471258	6.960898
H	1.861101	4.487925	0.685948	H	7.509277	8.700127	2.649329	O	10.505224	4.370600	9.752312
H	2.185434	0.175402	3.972556	H	6.263494	7.504415	0.140260	O	7.491169	3.122773	9.085766
H	3.789775	5.767585	1.597103	H	11.703378	10.431804	5.429612	O	10.464412	2.717680	7.629156
H	0.761830	2.748434	3.995376	H	10.483209	11.177155	3.558915	O	10.551932	0.062693	7.683527
H	5.214562	3.194312	1.578903	H	7.486585	6.756709	2.010932	O	7.402108	5.778758	9.031199
H	3.188487	3.760575	1.163196	H	8.212348	7.439347	0.766460	O	11.775514	1.434438	10.420642
H	2.787915	2.181260	4.410144	H	9.756123	10.495244	4.802806	O	6.178879	4.404817	6.293188
H	5.782529	5.183027	1.231979	H	7.449893	10.841458	3.468318	O	9.120829	1.350423	10.458127
H	0.194631	0.759625	4.339709	H	10.519786	7.092887	2.099646	O	8.834357	4.488413	6.255523
O	1.459775	1.522922	1.390462	H	10.110753	7.450810	4.886151	H	4.426604	9.182661	8.490760
O	4.515573	4.423231	4.181474	H	7.857347	10.487333	0.685008	H	1.476427	8.648998	8.220326
O	1.501578	3.174838	3.515328	H	8.182079	6.172477	3.973574	H	0.232222	7.452939	5.712602
O	4.474347	2.769431	2.059459	H	9.786484	11.764115	1.598908	H	5.672204	10.381312	11.001565
O	4.561738	0.114288	2.113103	H	6.757856	8.744965	3.992764	H	4.450699	11.126090	9.130665
O	1.411829	5.830765	3.459748	H	11.210368	9.191114	1.575827	H	1.454383	6.704897	7.583099
O	5.786532	1.485749	4.849098	H	9.183958	9.758269	1.161120	H	2.180431	7.387550	6.338635
O	0.189809	4.455857	0.722150	H	8.783639	8.178628	4.408991	H	3.724137	10.444313	10.374854
O	3.131089	1.401743	4.887605	H	11.777221	11.179998	1.231760	H	1.416730	10.790178	9.039079
O	2.844548	4.539316	0.684932	H	6.189445	6.756518	4.339062	H	4.487159	7.041280	7.671420
H	10.474304	3.239086	2.921834	O	7.456642	7.517279	1.389220	H	4.078595	7.400380	10.456260
H	7.524078	2.705504	2.651412	O	10.512083	10.416359	4.180530	H	1.825103	10.435652	6.255426
H	6.278526	1.506882	0.140545	O	7.498114	9.169981	3.512403	H	2.149955	6.120828	9.544998
H	11.718454	4.435168	5.429588	O	10.470533	8.764748	2.055743	H	3.753965	11.712535	7.169667
H	10.496380	5.183271	3.559072	O	10.559662	6.109067	2.110883	H	0.725009	8.693955	9.563720
H	7.499964	0.762024	2.011442	O	7.410440	11.825303	3.458349	H	5.177813	9.139919	7.147409
H	8.226546	1.443846	0.767233	O	11.782055	7.483408	4.849803	H	3.151636	9.706896	6.732118
H	9.770311	4.500576	4.803575	O	6.185372	10.454119	0.721927	H	2.751138	8.127872	9.979554
H	7.463565	4.846888	3.470697	O	9.127313	7.399520	4.886832	H	5.746023	11.128708	6.803147
H	10.534018	1.097941	2.103111	O	8.840829	10.537836	0.683705	H	0.158356	6.705326	9.910363
H	10.125613	1.452441	4.886790	H	4.441428	3.188014	8.492763	O	1.424620	7.465387	6.961210
H	7.872110	4.487788	0.685847	H	1.491449	2.654500	8.222918	O	4.479946	10.365425	9.752336
H	8.196786	0.175594	3.972518	H	0.247305	1.456358	5.712531	O	1.465057	9.119258	9.083192
H	9.800754	5.767280	1.597092	H	5.687222	4.383707	11.001928	O	4.437789	8.713821	7.627224
H	6.772929	2.748194	3.994769	H	4.464119	5.131479	9.131274	O	4.527433	6.057542	7.682538
H	11.225687	3.194195	1.578422	H	1.467546	0.710953	7.583189	O	1.377587	11.774092	9.029286
H	9.199627	3.760236	1.162606	H	2.194578	1.392910	6.339271	O	5.750667	7.432165	10.419783
H	8.799072	2.181211	4.410038	H	3.738370	4.448737	10.375779	O	0.153904	10.402027	6.292293
H	11.792375	5.182838	1.231788	H	1.430864	4.795285	9.042469	O	3.095160	7.349054	10.457624
H	6.204689	0.759377	4.339030	H	4.500850	1.046641	7.673849	O	2.808587	10.486405	6.254560
O	7.470763	1.522718	1.389794	H	4.093408	1.400785	10.457172	H	10.437979	9.182272	8.490321
O	10.526100	4.422765	4.180957	H	1.839929	4.437310	6.256023	H	7.487430	8.648431	8.219892
O	7.512918	3.174334	3.514946	H	2.164201	0.123994	9.543294	H	6.242191	7.452854	5.711664
O	10.485669	2.768862	2.058957	H	3.768677	5.715681	7.168543	H	11.682436	10.381060	11.000994
O	10.573118	0.114028	2.112886	H	0.740342	2.697018	9.566351	H	10.462033	11.125915	9.130005
O	7.423302	5.830624	3.459596	H	5.192872	3.143188	7.149343	H	7.465341	6.704365	7.582615
O	11.796796	1.486088	4.849844	H	3.167032	3.709575	6.733194	H	8.191068	7.387143	6.338081
O	6.200050	4.455991	0.722405	H	2.766805	2.129792	9.980999	H	9.735028	10.444277	10.374049
O	9.142128	1.401720	4.887622	H	5.761332	5.131684	6.802995	H	7.428487	10.789995	9.038821
O	8.855545	4.539040	0.684545	H	0.173478	0.708083	9.910453	H	10.498907	7.041186	7.671252
H	4.448384	9.234206	2.919923	O	1.438651	1.471774	6.961608	H	10.089617	7.400196	10.456146
H	1.497417	8.700569	2.649895	O	4.494051	4.370888	9.752964	H	7.836157	10.435785	6.255884
H	0.253210	7.504531	0.140713	O	1.480177	3.123400	9.086436	H	8.160973	6.120549	9.545044
H	5.693443	10.432095	5.430384	O	4.452608	2.718153	7.629695	H	9.765271	11.712716	7.169625
H	4.472245	11.177546	3.559521	O	4.540345	0.062798	7.683806	H	6.736171	8.693850	9.563240
H	1.475052	6.757008	2.011609	O	1.390988	5.779106	9.031252	H	11.188896	9.139752	7.146764
H	2.201312	7.439751	0.767342	O	5.765327	1.434015	10.420194	H	9.162765	9.706773	6.732016
H	3.745480	10.495645	4.803544	O	0.168679	4.404717	6.292359	H	8.762253	8.127583	9.978958
H	1.437909	10.841512	3.468668	O	3.109918	1.350266	10.458478	H	11.756061	11.128447	6.802468
H	4.508559	7.093165	2.099910	O	2.823373	4.488649	6.255295	H	6.168247	6.705222	9.910141
H	4.099758	7.451043	4.885412	H	10.453262	3.187537	8.492221	O	7.435268	7.464814	6.960715
H	1.846415	10.487022	0.685015	H	7.502347	2.653937	8.222218	O	10.490922	10.365214	9.751689
H	2.170913	6.172421	3.973395	H	6.257314	1.456091	5.711708	O	7.476377	9.118761	9.082719
H	3.775321	11.764060	1.599018	H	11.697461	4.383580	11.001496	O	10.449177	8.713334	7.626836
H	0.746407	8.745073	3.993564	H	10.475628	5.131203	9.130581	O	10.538839	6.057402	7.682350
H	5.199477	9.191450	1.576547	H	7.478503	0.710538	7.582551	O	7.388992	11.773857	9.029068
H	3.173033	9.758296	1.161714	H	8.205238	1.392512	6.338512	O	11.760901	7.432286	10.420027
H	2.772370	8.178836	4.408967	H	9.749373	4.448460	10.374874	O	6.164186	10.402366	6.293021
H	5.767200	11.180407	1.232120	H	7.442102	4.794982	9.042206	O	9.106174	7.348834	10.457219
H	0.179342	6.756599	4.339792	H	10.512870	1.046588	7.673428	O	8.819632	10.486326	6.254582

Table S17: 2B1 Structure

				A	1.20480492E+01	0.00000000E+00	0.00000000E+00				
				B	-7.98933516E-02	1.19517115E+01	0.00000000E+00				
				C	-4.66384170E-02	-1.77146542E-01	1.11890145E+01				
H	4.468881	3.178958	2.954588	O	1.419053	7.436075	1.388300	H	10.101272	1.370849	10.498661
H	1.491977	2.685095	2.671167	O	4.461567	10.380226	4.237041	H	7.860146	4.315836	6.317521
H	0.231193	1.473169	0.141463	O	1.431745	9.035425	3.574787	H	8.204139	0.105796	9.593965
H	5.729367	4.390518	5.484814	O	4.447595	8.780138	2.050801	H	9.756797	5.581049	7.223023
H	4.451340	5.163403	3.622943	O	4.504469	6.101019	2.097811	H	11.273663	5.589646	7.255310
H	1.509512	0.700398	2.002579	O	1.375905	11.714268	3.527318	H	6.687284	0.097298	9.561173
H	2.207264	1.392911	0.754465	O	5.733962	7.416506	4.871170	H	9.217866	3.617655	6.778751
H	3.752955	4.471164	4.870819	O	0.145033	10.400081	0.755746	H	8.743733	2.069368	10.037478
H	4.514554	1.826081	2.112928	O	3.079552	7.354373	4.902105	H	6.224123	2.079080	10.003200
H	1.446884	4.038119	3.512651	O	2.799705	10.462428	0.724431	H	11.737304	3.608234	6.812983
H	4.100144	1.458426	4.904208	H	10.452529	9.154578	2.953971	O	7.459424	1.370881	6.982471
H	1.859076	4.405355	0.722463	H	7.475598	8.660710	2.672714	O	10.501823	4.315692	9.833524
H	2.203507	0.193425	3.997681	H	6.214199	7.451208	0.142703	O	7.472126	2.971613	9.169145
H	3.756432	5.670184	1.627888	H	11.712071	10.365628	5.483577	O	10.489346	2.715502	7.646887
H	5.273398	5.678368	1.659886	H	10.434705	11.138623	3.621594	O	10.544947	0.036196	7.691104
H	0.686594	0.185087	3.964905	H	7.491953	6.676801	2.004930	O	7.414758	5.650929	9.125243
H	3.216852	3.707085	1.183032	H	8.190623	7.368865	0.757007	O	11.774556	1.350341	10.464137
H	2.742621	2.156752	4.443093	H	9.736433	10.446135	4.869515	O	6.186840	4.336424	6.351458
H	0.223575	2.166871	4.408063	H	10.498488	7.801118	2.113396	O	9.120254	1.289271	10.495155
H	5.736239	3.697063	1.216813	H	7.430115	10.013914	3.513719	O	8.841124	4.397699	6.321173
O	1.458851	1.459771	1.387388	H	10.084806	7.434477	4.904361	H	4.404413	9.066877	8.547926
O	4.501898	4.404315	4.238483	H	7.843530	10.379460	0.721000	H	1.426299	8.572419	8.266166
O	1.472026	3.059562	3.574365	H	8.186549	6.169254	4.000077	H	0.168014	7.360757	5.735636
O	4.488219	2.804607	2.051326	H	9.740172	11.645786	1.626781	H	5.665064	10.277000	11.077965
O	4.544632	0.125000	2.095911	H	11.256956	11.653644	1.658831	H	4.387324	11.051370	9.215789
O	1.417344	5.739026	3.528859	H	6.669710	6.162532	3.968349	H	1.444541	6.588476	7.598344
O	5.773826	1.438604	4.869720	H	9.201454	9.681820	1.181927	H	2.143321	7.281365	6.350944
O	0.185540	4.425277	0.757345	H	8.726884	8.132507	4.444022	H	3.688656	10.358997	10.463633
O	3.119186	1.376547	4.900540	H	6.207724	8.144344	4.410468	H	4.450516	7.713925	7.706417
O	2.840059	4.487201	0.725597	H	11.719822	9.671814	1.216388	H	1.380760	9.925552	9.107400
H	10.493367	3.178845	2.955693	O	7.441681	7.435852	1.389325	H	4.036451	7.348185	10.498245
H	7.514474	2.685132	2.671388	O	10.485288	10.379470	4.237066	H	1.795608	10.292514	6.315253
H	6.254263	1.473738	0.141165	O	7.456369	9.035395	3.575864	H	2.139237	6.081355	9.592910
H	11.752668	4.390768	5.485990	O	10.472336	8.779634	2.050931	H	3.693758	11.558761	7.220114
H	10.475649	5.163372	3.624462	O	10.528882	6.100956	2.099453	H	5.210502	11.565895	7.252489
H	7.532380	0.700359	2.003186	O	7.399325	11.714269	3.528301	H	0.622404	6.073309	9.561633
H	8.230644	1.392898	0.755359	O	11.758471	7.414515	4.869009	H	3.153456	9.594964	6.776362
H	9.777137	4.470536	4.871963	O	6.169638	10.399675	0.755330	H	2.678152	8.045248	10.037044
H	10.538466	1.825766	2.114187	O	9.103836	7.352557	4.901686	H	0.159259	8.054746	10.004351
H	7.468503	4.038036	3.513081	O	8.824428	10.461745	0.724366	H	5.672587	9.584138	6.810731
H	10.124567	1.458683	4.902836	H	4.445398	3.091618	8.549773	O	1.394045	7.347677	6.982944
H	7.883619	4.405059	0.723255	H	1.466552	2.596651	8.265507	O	4.437622	10.292259	9.831320
H	8.227114	0.193586	3.998286	H	0.207575	1.383996	5.734865	O	1.406718	8.947009	9.169355
H	9.780857	5.669986	1.629694	H	5.705858	4.302996	11.079134	O	4.424099	8.692474	7.644696
H	11.297609	5.678156	1.661232	H	4.427467	5.076711	9.216922	O	4.481144	6.013549	7.690868
H	6.710364	0.185238	3.966320	H	1.484249	0.611674	7.597799	O	1.350945	11.625759	9.122656
H	9.241262	3.706806	1.184436	H	2.182961	1.303771	6.349963	O	5.710032	7.328548	10.465130
H	8.766728	2.156980	4.442300	H	3.729269	4.384483	10.465059	O	0.121860	10.311445	6.350038
H	6.247261	2.166739	4.409225	H	4.491443	1.738439	7.708289	O	3.055576	7.265384	10.494444
H	11.760428	3.696860	1.217782	H	1.421127	3.949722	9.106975	O	2.776530	10.374941	6.318742
O	7.481714	1.459504	1.387722	H	4.076754	1.370677	10.497098	H	10.428948	9.065340	8.547632
O	10.525981	4.403873	4.239507	H	1.835715	4.316876	6.317252	H	7.452466	8.572623	8.266941
O	7.495259	3.059515	3.574632	H	2.179022	0.104951	9.592201	H	6.191924	7.362112	5.737552
O	10.512848	2.804296	2.052506	H	3.733195	5.582445	7.221019	H	11.688821	10.276848	11.078185
O	10.568027	0.124830	2.096795	H	5.250068	5.590499	7.253315	H	10.411560	11.049419	9.215271
O	7.438117	5.739038	3.530264	H	0.662162	0.096917	9.560882	H	7.469445	6.588255	7.599626
O	11.798236	1.438415	4.868186	H	3.193492	3.618892	6.778341	H	8.168248	7.279926	6.351493
O	6.210017	4.425216	0.756677	H	2.718893	2.068638	10.036180	H	9.713175	10.357249	10.463263
O	9.143588	1.376932	4.899841	H	0.199817	2.078586	10.003563	H	10.474388	7.712236	7.706484
O	8.864570	4.487057	0.727206	H	5.712896	3.608693	6.812126	H	7.406843	9.925788	9.108164
H	4.428219	9.154928	2.953898	O	1.433966	1.370722	6.982170	H	10.060942	7.346362	10.499995
H	1.451902	8.660629	2.671690	O	4.478202	4.317841	9.832696	H	7.820028	10.291497	6.315747
H	0.191216	7.449552	0.142389	O	1.447190	2.971179	9.168682	H	8.162942	6.081383	9.595288
H	5.688751	10.366189	5.483695	O	4.464762	2.716945	7.646647	H	9.717030	11.557272	7.221063
H	4.411083	11.139157	3.621300	O	4.521719	0.037504	7.690291	H	11.233804	11.564942	7.253040
H	1.470349	6.676835	2.003575	O	1.391073	5.650460	9.123348	H	6.646040	6.074389	9.562805
H	2.167429	7.369723	0.755239	O	5.750270	1.351070	10.463502	H	9.177916	9.593505	6.776433
H	3.712627	10.447233	4.869380	O	0.162347	4.336691	6.352532	H	8.703312	8.044561	10.038897
H	4.473934	7.801625	2.112988	O	3.095810	1.288539	10.493514	H	6.184105	8.056249	10.004537
H	1.405901	10.013949	3.512586	O	2.816717	4.398625	6.320211	H	11.696719	9.583037	6.810525
H	4.060468	7.436746	4.905665	H	10.469496	3.089875	8.550111	O	7.419306	7.347124	6.983804
H	1.818764	10.380285	0.721325	H	7.491731	2.597296	8.265912	O	10.462098	10.290427	9.830981
H	2.164840	6.170260	3.999199	H	6.231703	1.384253	5.736142	O	7.432828	8.947247	9.170090
H	3.716537	11.646084	1.626116	H	11.729017	4.302494	11.079956	O	10.448608	8.690808	7.644444
H	5.233391	11.653490	1.658013	H	10.451163	5.074797	9.217998	O	10.504543	6.012298	7.693002
H	0.648020	6.161506	3.966318	H	7.510257	0.612055	7.598305	O	7.376573	11.626283	9.123761
H	3.176719	9.682545	1.182119	H	8.208136	1.303986	6.349879	O	11.734370	7.326383	10.465160
H	2.702467	8.134058	4.444143	H	9.753269	4.382675	10.466247	O	6.146535	10.311968	6.350172
H	0.183456	8.142997	4.408508	H	10.515266	1.736965	7.708372	O	9.079954	7.264528	10.496635
H	5.695912	9.671796	1.215992	H	7.445182	3.950158	9.107706	O	8.800953	10.373580	6.319027

Table S18: 2C1 Structure

				A	1.19919835E+01	0.00000000E+00	0.00000000E+00				
				B	1.37514485E-01	1.20098461E+01	0.00000000E+00				
				C	-2.09809577E-02	-8.24582421E-03	1.11935134E+01				
H	2.714252	1.497216	0.102494	O	1.583598	7.486527	1.362039	H	10.863836	1.540546	10.497369
H	3.346251	4.548951	5.529988	O	4.611653	10.570957	4.270742	H	7.167391	4.497990	6.328340
H	0.276561	1.527011	0.098015	O	1.630054	9.154544	3.457176	H	8.224404	0.217176	9.566419
H	5.783580	4.520236	5.534556	O	4.564395	8.903003	2.175304	H	9.805873	5.820561	7.257056
H	1.546298	2.230633	1.997790	O	4.591499	6.238054	2.103318	H	11.320429	5.749313	7.272523
H	4.514256	3.816203	3.634689	O	1.604681	11.819160	3.529193	H	6.709898	0.290031	9.551728
H	4.555474	5.337201	3.668600	O	5.924931	7.545313	4.803929	H	6.770901	2.780984	9.525133
H	1.504176	0.709697	1.964196	O	0.269978	10.510863	0.826913	H	11.260050	3.257487	7.299786
H	4.546048	1.917378	2.135628	O	3.264030	7.504242	4.848616	H	9.279911	3.820764	6.887642
H	1.514098	4.129852	3.496591	O	2.931128	10.554286	0.783966	H	8.751336	2.217106	9.936681
H	4.877908	1.543517	4.900573	H	8.778506	7.503407	0.101497	O	7.500194	1.477154	6.958291
H	1.181371	4.502924	0.730786	H	9.408270	10.555056	5.529570	O	10.529734	4.562223	9.866184
H	2.238807	0.220485	3.970394	H	6.340807	7.531257	0.097263	O	7.547834	3.145736	9.053349
H	3.820256	5.826272	1.661978	H	11.845729	10.525470	5.533490	O	10.483104	2.892954	7.771762
H	5.334776	5.754434	1.677253	H	7.609525	8.236013	1.996915	O	10.507234	0.228442	7.699575
H	0.724378	0.293624	3.955418	H	10.576161	9.821277	3.634152	O	7.522619	5.810627	9.125436
H	0.785802	2.784765	3.929036	H	10.618086	11.342258	3.667474	O	11.842062	1.537877	10.401518
H	5.274266	3.262660	1.703139	H	7.569315	6.715035	1.962910	O	6.189198	4.501047	6.424528
H	3.293867	3.826403	1.291587	H	10.609182	7.921973	2.134905	O	9.180952	1.494896	10.444986
H	2.766172	2.220317	4.340979	H	7.576867	10.134770	3.496268	O	8.850119	4.542877	6.379314
O	1.515344	1.481016	1.362238	H	10.943048	7.548859	4.900910	H	2.772543	7.498730	5.698830
O	4.545146	4.565744	4.270356	H	7.244453	10.508843	0.731640	H	3.401968	10.551215	11.127488
O	1.562877	3.149304	3.457341	H	8.304683	6.225667	3.969406	H	0.334931	7.526751	5.694812
O	4.497296	2.897934	2.174942	H	9.883519	11.831786	1.661499	H	5.839506	10.521931	11.131463
O	4.521764	0.233240	2.103997	H	11.397975	11.758643	1.676495	H	1.604044	8.231809	7.594141
O	1.537566	5.814092	3.528929	H	6.790227	6.297701	3.954317	H	4.570575	9.816791	9.232330
O	5.856100	1.541055	4.804255	H	6.849432	8.789041	3.928651	H	4.612237	11.337746	9.265523
O	0.203169	4.505645	0.826792	H	11.336778	9.267445	1.702693	H	1.563548	6.710800	7.561033
O	3.195338	1.497821	4.849205	H	9.356297	9.831669	1.291158	H	4.603363	7.917927	7.732383
O	2.864215	4.548631	0.783318	H	8.830249	8.226066	4.339989	H	1.570737	10.131414	9.093266
H	8.710067	1.497522	0.101453	O	7.579247	7.486493	1.361178	H	4.936072	7.545285	10.496855
H	9.341682	4.548434	5.529124	O	10.606986	10.571008	4.269528	H	1.237631	10.503875	6.327453
H	6.272512	1.526562	0.097517	O	7.626073	9.154266	3.456671	H	2.298321	6.222972	9.567728
H	11.779539	4.519698	5.533567	O	10.559859	8.902467	2.174321	H	3.877269	11.827296	7.259550
H	7.541543	2.230719	1.996910	O	10.587060	6.237580	2.102301	H	5.391728	11.754024	7.274411
H	10.509837	3.815917	3.633712	O	7.600668	11.819169	3.528372	H	0.783790	6.294257	9.552089
H	10.551012	5.336917	3.667664	O	11.921246	7.545645	4.804866	H	0.842926	8.785857	9.525417
H	7.499955	0.709747	1.963135	O	6.266278	10.511472	0.827885	H	5.330671	9.263584	7.300409
H	10.541827	1.916932	2.134810	O	9.260131	7.504074	4.848356	H	3.350029	9.827261	6.888784
H	7.509412	4.129669	3.495751	O	8.927139	10.554269	0.783048	H	2.823502	8.223067	9.937329
H	10.874100	1.544092	4.900944	H	2.703607	1.492576	5.699299	O	1.573818	7.481945	6.958847
H	7.177620	4.503190	0.731564	H	3.335114	4.545981	11.126856	O	4.601328	10.566569	9.867670
H	8.234774	0.220589	3.969470	H	0.265958	1.522501	5.694880	O	1.619742	9.150899	9.053609
H	9.815940	5.825431	1.661020	H	5.772776	4.517123	11.131353	O	4.553873	8.898397	7.772110
H	11.330454	5.754131	1.676288	H	1.535924	2.226853	7.594338	O	4.581278	6.233285	7.699650
H	6.720333	0.293569	3.954629	H	4.503637	3.812200	9.232223	O	1.594555	11.815559	9.126239
H	6.781229	2.784503	3.928302	H	4.544906	5.333226	9.265011	O	5.914256	7.542080	10.400769
H	11.270169	3.262143	1.702290	H	1.493937	0.705857	7.561476	O	0.259437	10.506322	6.423430
H	9.289897	3.825821	1.290703	H	4.535879	1.912662	7.733219	O	3.253306	7.501043	10.445751
H	8.761680	2.220472	4.340072	H	1.504052	4.126399	9.093637	O	2.920688	10.549612	6.380468
O	7.510919	1.481125	1.361280	H	4.867589	1.539865	10.497304	H	8.768297	7.498449	5.698354
O	10.540546	4.565455	4.269417	H	1.171382	4.497768	6.327499	H	9.397678	10.551183	11.126373
O	7.558179	3.149124	3.456443	H	2.228645	0.217026	9.567410	H	6.330450	7.526309	5.693957
O	10.493222	2.897503	2.174189	H	3.810072	5.821296	7.258443	H	11.835353	10.521527	11.130452
O	10.517657	0.233060	2.102758	H	5.324595	5.749498	7.273845	H	7.599074	8.231951	7.593147
O	7.533372	5.813982	3.528155	H	0.714150	0.289983	9.552363	H	10.565878	9.816807	9.231205
O	11.852305	1.541408	4.804934	H	0.775639	2.781297	9.525702	H	10.607795	11.337797	9.264148
O	6.199434	4.506216	0.827789	H	5.264119	3.257837	7.300703	H	7.558882	6.710931	7.560156
O	9.191199	1.498308	4.848486	H	3.284053	3.821259	6.888440	H	10.598785	7.917484	7.731202
O	8.860226	4.548167	0.782624	H	2.755893	2.216900	9.937720	H	7.566252	10.131257	9.092751
H	2.782626	7.503738	0.102362	O	1.504895	1.476938	6.959182	H	10.932216	7.545569	10.497151
H	3.412646	10.555043	5.530546	O	4.534379	4.562196	9.867327	H	7.233932	10.504273	6.328035
H	0.344911	7.531748	0.097797	O	1.552783	3.145870	9.054143	H	8.293899	6.222519	9.566594
H	5.849887	10.525846	5.534445	O	4.487180	2.893207	7.772614	H	9.873036	11.827235	7.258369
H	1.613892	8.236024	1.997806	O	4.511456	0.228393	7.700818	H	11.387482	11.754031	7.273195
H	4.580927	9.821346	3.635195	O	1.527294	5.810708	9.126374	H	6.779387	6.294402	9.551425
H	4.622517	11.342327	3.668866	O	5.845786	1.537490	10.401106	H	6.838683	8.785583	9.524982
H	1.573434	6.714994	1.963697	O	0.193184	4.500470	6.423519	H	11.326264	9.263080	7.299404
H	4.613945	7.922518	2.135834	O	3.185038	1.494356	10.445938	H	9.345924	9.827136	6.887803
H	1.580899	10.135059	3.496750	O	2.854351	4.543316	6.379965	H	8.819240	8.222814	9.936561
H	4.946737	7.548525	4.899956	H	8.699296	1.492938	5.698453	O	7.568923	7.482028	6.957929
H	1.248181	10.508349	0.731003	H	9.330784	4.545560	11.125949	O	10.596713	10.566688	9.866393
H	2.308820	6.226032	3.970115	H	6.261880	1.522083	5.694163	O	7.615343	9.150759	9.053012
H	3.887672	11.831977	1.662694	H	11.768582	4.516693	11.130341	O	10.549446	8.897958	7.771093
H	5.402144	11.758944	1.677712	H	7.530888	2.227016	7.593564	O	10.576954	6.232967	7.698155
H	0.794347	6.297674	3.955085	H	10.499204	3.812248	9.231032	O	7.590262	11.815661	9.125450
H	0.853465	8.789383	3.929271	H	10.540394	5.333256	9.263878	O	11.910421	7.542377	10.401280
H	5.341230	9.268180	1.703660	H	7.489399	0.706005	7.560470	O	6.255760	10.506741	6.424332
H	3.360426	9.831951	1.292342	H	10.531637	1.912383	7.732290	O	9.249247	7.500881	10.444950
H	2.834233	8.226395	4.340420	H	7.498994	4.126265	9.092869	O	8.916690	10.549715	6.379729

Table S19: 4A1 Structure

				A	1.20114893E+01	0.00000000E+00	0.00000000E+00				
				B	-1.12316551E-04	1.20740930E+01	0.00000000E+00				
				C	-7.75835461E-02	-3.91924241E-04	1.10641691E+01				
H	4.442305	3.295522	0.118265	O	1.450258	7.515968	4.144292	H	10.092855	1.563374	7.610708
H	1.517272	0.274872	5.388883	O	4.509161	10.536343	1.361507	H	7.799990	4.582390	8.961092
H	0.261687	1.507392	2.899734	O	1.533121	11.881238	0.720159	H	8.161961	2.860206	6.720652
H	5.697247	4.527884	2.607801	O	4.426386	8.864130	4.786043	H	9.730867	5.876806	9.851452
H	4.495679	5.260001	0.739582	O	4.522487	6.205286	4.842290	H	6.759070	0.240931	6.724218
H	1.463116	2.239431	4.767733	O	1.435374	9.222337	0.664219	H	11.133631	3.258267	9.847554
H	2.207696	1.576919	3.526415	O	5.792854	7.540471	2.037957	H	8.770060	0.838580	7.120788
H	3.751146	4.596875	1.980648	O	0.165936	10.556324	3.468038	H	9.122215	3.856122	9.450702
H	1.465803	4.168773	0.671875	O	3.141653	7.647441	2.078741	H	6.167552	2.241235	7.074684
H	4.492375	1.151579	4.834654	O	2.817254	10.665847	3.426651	H	11.725396	5.258359	9.497610
H	4.125609	1.563222	2.078265	H	10.447414	9.330957	0.117333	O	7.417233	1.480634	9.677269
H	1.833145	4.581783	3.428722	H	7.521519	6.313488	5.389096	O	10.476011	4.498140	6.894750
H	2.194487	2.858509	1.188223	H	6.267112	7.546875	2.899551	O	7.499068	5.845705	6.252746
H	3.763866	5.878381	4.318779	H	11.703101	10.563089	2.606472	O	10.392326	2.825745	10.318816
H	0.791963	0.239503	1.191617	H	10.501626	11.295449	0.738752	O	10.490027	0.166888	10.374192
H	5.166948	3.259459	4.315570	H	7.468975	8.277961	4.767676	O	7.403249	3.186891	6.197147
H	2.803230	0.837455	1.588273	H	8.213102	7.614557	3.526536	O	11.760533	1.500802	7.570040
H	3.155814	3.856756	3.918825	H	9.757108	10.632856	1.980073	O	6.132475	4.521683	9.001403
H	0.200154	2.239366	1.542550	H	7.472353	10.207456	0.672355	O	9.109203	1.611021	7.611921
H	5.758492	5.259620	3.965106	H	10.498947	7.187388	4.834986	O	8.783711	4.628966	8.959803
O	1.450350	1.479042	4.144844	H	10.130851	7.599396	2.078205	H	4.403853	9.332098	5.649595
O	4.508736	4.499582	1.362413	H	7.839254	10.619229	3.428392	H	1.477774	6.311604	10.920345
O	1.533060	5.844204	0.719808	H	8.200728	8.896840	1.188456	H	0.222984	7.544740	8.430917
O	4.425716	2.827029	4.787017	H	9.770584	11.914139	4.318486	H	5.658310	10.565660	8.138920
O	4.522539	0.168107	4.841788	H	6.796378	6.278477	1.191527	H	4.456756	11.296499	6.270632
O	1.435790	3.185293	0.664730	H	11.172886	9.295006	4.314401	H	1.423630	8.276623	10.299346
O	5.793136	1.502585	2.038364	H	8.807815	6.874880	1.588157	H	2.168692	7.614469	9.058157
O	0.165583	4.519659	3.469088	H	9.161533	9.893197	3.918216	H	3.712384	10.633594	7.511894
O	3.141899	1.610077	2.079424	H	6.205766	8.278874	1.542349	H	1.427463	10.205751	6.203560
O	2.816815	4.629216	3.427621	H	11.764984	11.294935	3.963720	H	4.454047	7.189010	10.366827
H	10.447510	3.293773	0.118373	O	7.455550	7.517521	4.144854	H	4.087017	7.601436	7.610086
H	7.522524	0.276716	5.389089	O	10.514341	10.534950	1.361524	H	1.794626	10.618707	8.960336
H	6.267300	1.509287	2.900013	O	7.538761	11.882851	0.720603	H	2.155886	8.895256	6.719533
H	11.702757	4.526305	2.607530	O	10.431670	8.862733	4.786027	H	3.725116	11.915558	9.850619
H	10.501128	5.258530	0.739885	O	10.528900	6.203908	4.842696	H	0.753620	6.276547	6.723661
H	7.468760	2.241096	4.768217	O	7.442288	9.223991	0.664840	H	5.128771	9.296763	9.846398
H	8.213368	1.578275	3.527016	O	11.798616	7.537600	2.037687	H	2.764999	6.874901	7.120304
H	9.756696	4.595756	1.981175	O	6.171697	10.558566	3.468488	H	3.117508	9.893883	9.450164
H	7.471134	4.170389	0.672339	O	9.147218	7.647091	2.079475	H	0.161321	8.276474	7.073604
H	10.499317	1.150309	4.834880	O	8.822967	10.665924	3.427170	H	5.719866	11.297356	9.496294
H	10.131240	1.563382	2.078748	H	4.403331	3.294906	5.650613	O	1.411188	7.516319	9.676326
H	7.838843	4.581961	3.429626	H	1.478000	0.274612	10.920723	O	4.469987	10.536248	6.893687
H	8.200287	2.860354	1.188710	H	0.223255	1.507467	8.431668	O	1.495014	11.881162	6.252534
H	9.770099	5.876904	4.319474	H	5.658238	4.528362	8.139804	O	4.387596	8.864314	10.317918
H	6.797552	0.241013	1.192073	H	4.456709	5.259721	6.271398	O	4.483726	6.205520	10.374745
H	11.172799	3.258248	4.315485	H	1.424218	2.239409	10.299871	O	1.397352	9.222280	6.195912
H	8.808431	0.838620	1.588758	H	2.169158	1.577193	9.058601	O	5.754447	7.540914	7.570004
H	9.161223	3.856003	3.919352	H	3.712177	4.597081	7.512701	O	0.126924	10.556432	9.000815
H	6.205822	2.241117	1.542743	H	1.427506	4.168719	6.204114	O	3.103284	7.647807	7.611241
H	11.764430	5.258179	3.964784	H	4.453694	1.151920	10.366879	O	2.778274	10.666354	8.959138
O	7.455790	1.480787	4.145236	H	4.087321	1.563575	7.610460	H	10.409570	9.330638	5.649616
O	10.513908	4.497990	1.362587	H	1.794348	4.582246	8.961322	H	7.482604	6.313381	10.920744
O	7.537485	5.845794	0.720104	H	2.156146	2.858377	6.720222	H	6.228807	7.547516	8.431542
O	10.431721	2.825737	4.787108	H	3.725133	5.878568	9.851216	H	11.664334	10.563271	8.139119
O	10.529470	0.166829	4.841865	H	0.753797	0.239317	6.724003	H	10.463612	11.295290	6.270728
O	7.441559	3.186900	0.665153	H	5.128239	3.259739	9.847323	H	7.430422	8.278178	10.299986
O	11.798927	1.500831	2.038133	H	2.765023	0.837625	7.120594	H	8.174762	7.615295	9.058670
O	6.171305	4.521138	3.469494	H	3.117108	3.857093	9.450957	H	9.718612	10.633006	7.511864
O	9.147590	1.611031	2.079938	H	0.161791	2.239300	7.074420	H	7.433795	10.207483	6.203981
O	8.822556	4.628725	3.428368	H	5.719672	5.260080	9.497158	H	10.459331	7.187392	10.367185
H	4.442834	9.332645	0.117336	O	1.411674	1.479137	9.676826	H	10.092498	7.599962	7.609970
H	1.517271	6.311711	5.388654	O	4.469774	4.499545	6.894529	H	7.800211	10.619772	8.959979
H	0.261513	7.544270	2.899213	O	1.494994	5.844130	6.252404	H	8.162243	8.896890	6.719992
H	5.697492	10.565234	2.606860	O	4.387032	2.827295	10.318801	H	9.731360	11.914178	9.850498
H	4.495901	11.296824	0.738735	O	4.483755	0.168434	10.374220	H	6.758014	6.278443	6.724204
H	1.462967	8.276467	4.767059	O	1.397484	3.185234	6.196709	H	11.133434	9.294892	9.846491
H	2.207483	7.613951	3.525740	O	5.754766	1.502763	7.570329	H	8.769496	6.875170	7.120381
H	3.751535	10.633411	1.979743	O	0.126768	4.519957	9.001917	H	9.122323	9.893486	9.449764
H	1.465512	10.205805	0.671639	O	3.103599	1.610355	7.611631	H	6.167348	8.279160	7.074142
H	4.492790	7.188768	4.834577	O	2.778014	4.629641	8.959956	H	11.725776	11.294956	9.496474
H	4.125375	7.600915	2.077632	H	10.409602	3.293503	5.650767	O	7.417110	7.518023	9.676810
H	1.833603	10.618228	3.427680	H	7.483627	0.276319	10.921212	O	10.476138	10.534957	6.893710
H	2.194086	8.895368	1.187602	H	6.228942	1.509396	8.431973	O	7.500224	11.882797	6.252635
H	3.763965	11.915209	4.318105	H	11.664199	4.526660	8.140221	O	10.392001	8.862725	10.317869
H	0.791754	6.276538	1.191241	H	10.463419	5.258473	6.271782	O	10.489338	6.203914	10.375100
H	5.167622	9.296578	4.314619	H	7.430045	2.240857	10.300359	O	7.403798	9.224007	6.196353
H	2.803213	6.874720	1.587606	H	8.174892	1.578247	9.059184	O	11.760270	7.537914	7.569289
H	3.156413	9.893461	3.917863	H	9.718461	4.596048	7.512886	O	6.132691	10.559057	9.000453
H	0.199549	8.276262	1.542060	H	7.432790	4.170390	6.204664	O	9.108864	7.647608	7.611352
H	5.758866	11.296937	3.964207	H	10.459941	1.150376	10.366979	O	8.783934	10.666315	8.958763

Table S20: 4A2 Structure

				A	1.20200588E+01	0.00000000E+00	0.00000000E+00				
				B	4.48061571E-05	1.20782289E+01	0.00000000E+00				
				C	7.62667724E-02	3.82223571E-04	1.10567714E+01				
H	1.575212	2.785798	5.397815	O	1.588157	7.623212	4.150535	H	10.969568	1.541113	7.615336
H	4.487569	5.803808	0.126897	O	4.476002	10.641099	1.372946	H	7.190341	4.560117	8.966338
H	2.778689	1.486818	2.901884	O	1.481362	11.945195	0.674409	H	9.854331	3.209506	9.883460
H	3.284289	4.506048	2.622541	O	4.583121	8.925663	4.850995	H	8.306088	0.191035	6.699062
H	1.515974	0.824887	4.771913	O	4.511346	6.267640	4.788636	H	11.281629	5.828383	9.818280
H	4.547696	3.842769	0.752952	O	1.551473	9.286928	0.734328	H	6.878363	2.809968	6.764617
H	0.828757	1.544854	3.531022	O	5.905230	7.613995	2.091739	H	9.285150	5.252594	9.497248
H	5.234713	4.563221	1.993705	O	0.159486	10.633947	3.432607	H	8.874699	2.233726	7.085315
H	4.553720	1.903242	4.840409	O	3.254968	7.539410	2.040793	H	11.880657	3.829571	9.468781
H	1.509420	4.922437	0.682611	O	2.809541	10.559898	3.482825	H	6.279367	0.810712	7.113827
H	4.921776	1.540686	2.087268	H	7.585986	8.824602	5.396450	O	7.638292	1.582919	9.681919
H	1.141766	4.560298	3.438180	H	10.499595	11.842788	0.128131	O	10.522452	4.602731	6.900657
H	3.806218	3.210235	4.354808	H	8.788594	7.524954	2.900892	O	7.529570	5.906345	6.201586
H	2.257158	0.190579	1.169961	H	9.296824	10.544384	2.623424	O	10.630153	2.885958	10.379080
H	5.233202	5.829142	4.289781	H	7.525768	6.863084	4.770584	O	10.561503	0.227824	10.318021
H	0.829711	2.809426	1.234760	H	10.559539	9.881491	0.753869	O	7.600155	3.248349	6.265589
H	3.236691	5.253281	3.968613	H	6.838438	7.582849	3.529671	O	11.953757	1.575987	7.621819
H	2.826592	2.233483	1.555629	H	11.246720	10.601693	1.994764	O	6.206143	4.594875	8.959667
H	5.832708	3.830421	3.940119	H	10.564080	7.941819	4.841271	O	9.304008	1.500957	7.571696
H	0.230721	0.810590	1.584879	H	7.521248	10.961343	0.684644	O	8.856005	4.520004	9.010464
O	1.589255	1.584373	4.152656	H	10.930850	7.579401	2.084764	H	1.613549	8.824701	10.924084
O	4.474236	4.602351	1.372042	H	7.153987	10.598825	3.438798	H	4.528110	11.843958	5.656052
O	1.480482	5.905912	0.672083	H	9.817828	9.249453	4.355619	H	2.816294	7.525968	8.428201
O	4.582161	2.886720	4.850261	H	8.266926	6.229726	1.168527	H	3.324944	10.545137	8.151682
O	4.513731	0.228531	4.789143	H	11.245022	11.868137	4.290752	H	1.553178	6.863349	10.297678
O	1.551422	3.247936	0.735712	H	6.840161	8.847870	1.233600	H	4.587552	9.882659	6.281964
O	5.905941	1.575371	2.094309	H	9.248941	11.291865	3.969356	H	0.866192	7.583646	9.056875
O	0.157578	4.595006	3.431532	H	8.836253	8.271940	1.554728	H	5.274991	10.602416	7.522874
O	3.255650	1.500960	2.042571	H	11.844449	9.868950	3.941554	H	4.591961	7.941686	10.369113
O	2.807511	4.520650	3.481934	H	6.240528	6.848997	1.582913	H	1.548402	10.962521	6.211894
H	7.585826	2.785292	5.398809	O	7.598885	7.622567	4.151320	H	4.959210	7.580040	7.613161
H	10.497715	5.803671	0.127129	O	10.486295	10.641052	1.373039	H	1.182187	10.599025	8.967544
H	8.789193	1.486344	2.902989	O	7.492326	11.944808	0.675369	H	3.846020	9.249594	9.883646
H	9.294587	4.505928	2.622515	O	10.593383	8.925292	4.851290	H	2.294243	6.230825	6.696221
H	7.526805	0.824357	4.773030	O	10.521553	6.267324	4.788842	H	5.273895	11.867523	9.819120
H	10.557585	3.842586	0.753001	O	7.562121	9.286516	0.735028	H	0.867677	8.849066	6.761451
H	6.839264	1.544260	3.532266	O	11.915035	7.614364	2.091069	H	3.277380	11.292181	9.497788
H	11.244775	4.562854	1.993823	O	6.169816	10.633653	3.432176	H	2.864251	8.273138	7.082190
H	10.563184	1.902983	4.840857	O	9.265268	7.539201	2.041418	H	5.872946	9.868361	9.469410
H	7.520408	4.922091	0.683409	O	8.819838	10.559143	3.482727	H	0.268217	6.850202	7.110614
H	10.931437	1.540883	2.087135	H	1.613408	2.785184	10.925734	O	1.626580	7.622993	9.678682
H	7.152065	4.560735	3.437952	H	4.525590	5.804689	5.655481	O	4.514561	10.642184	6.901197
H	9.815956	3.210043	4.354997	H	2.816783	1.486774	8.430278	O	1.519627	11.946002	6.202510
H	8.268003	0.190259	1.171081	H	3.322481	4.505661	8.150988	O	4.621453	8.925147	10.379327
H	11.243388	5.828769	4.289995	H	1.553993	0.824151	10.300239	O	4.549627	6.267100	10.316795
H	6.840298	2.809246	1.235569	H	4.585737	3.843561	6.281172	O	1.589460	9.287824	6.262699
H	9.247057	5.253098	3.968649	H	0.866836	1.544185	9.059268	O	5.943374	7.614802	7.620051
H	8.836595	2.233200	1.556724	H	5.272848	4.563528	7.522120	O	0.198014	10.633676	8.960983
H	11.842445	3.829996	3.940388	H	4.592098	1.902639	10.369109	O	3.293182	7.540348	7.568850
H	6.241255	0.810272	1.585687	H	1.547431	4.923226	6.211473	O	2.848091	10.559639	9.011052
O	7.599901	1.583804	4.153670	H	4.959912	1.540937	7.615788	H	7.624157	8.824273	10.924795
O	10.484332	4.602171	1.372126	H	1.180042	4.559763	8.966613	H	10.537511	11.843662	5.656416
O	7.491356	5.905551	0.672876	H	3.844639	3.209566	9.883340	H	8.826719	7.525575	8.429275
O	10.591785	2.886457	4.850582	H	2.295397	0.191355	6.698138	H	9.335168	10.544513	8.151865
O	10.523009	0.228294	4.789535	H	5.271481	5.828549	9.817981	H	7.563835	6.862803	10.298690
O	7.562173	3.247560	0.736603	H	0.867793	2.810168	6.763617	H	10.597687	9.882305	6.282166
O	11.915631	1.575723	2.093571	H	3.274869	5.252619	9.497146	H	6.876527	7.582917	9.057925
O	6.167870	4.595499	3.431345	H	2.864708	2.234138	7.084396	H	11.285035	10.602215	7.523088
O	9.265861	1.500669	2.043508	H	5.870951	3.829795	9.468417	H	10.602446	7.941493	10.369529
O	8.817765	4.520573	3.481899	H	0.268929	0.811101	7.112801	H	7.559333	10.962093	6.212693
H	1.575132	8.825125	5.395734	O	1.627344	1.583556	9.680900	H	10.968965	7.580324	7.613256
H	4.489932	11.842826	0.127948	O	4.512357	4.602963	6.900493	H	7.192421	10.598560	8.967342
H	2.778041	7.525338	2.900125	O	1.518496	5.906702	6.200820	H	9.856348	9.249211	9.883932
H	3.286386	10.544943	2.623462	O	4.620552	2.886120	10.378883	H	8.305170	6.230592	6.697152
H	1.514770	6.863675	4.769670	O	4.552039	0.227956	10.317887	H	11.283516	11.867628	9.819266
H	4.549118	9.881557	0.753749	O	1.589487	3.248786	6.264634	H	6.878301	8.848755	6.762044
H	0.827889	7.583565	3.528607	O	5.944073	1.575564	7.622838	H	9.287369	11.291575	9.497981
H	5.236513	10.601625	1.994553	O	0.195857	4.594576	8.959955	H	8.874359	8.272849	7.083225
H	4.553635	7.942203	4.840915	O	3.293791	1.501409	7.570997	H	11.882983	9.868595	9.469802
H	1.510228	10.961719	0.683757	O	2.845791	4.519943	9.010440	H	6.278685	6.849835	7.111182
H	4.921072	7.579143	2.084972	H	7.624267	2.784738	10.926665	O	7.637006	7.622385	9.679556
H	1.143658	10.599326	3.439230	H	10.535764	5.804364	5.655688	O	10.524588	10.641813	6.901418
H	3.807549	9.250035	4.355478	H	8.827392	1.486152	8.431204	O	7.530383	11.945558	6.203396
H	2.256109	6.229958	1.167715	H	9.332769	4.505650	8.151039	O	10.631825	8.924965	10.379672
H	5.235524	11.868102	4.290281	H	7.565186	0.823617	10.301454	O	10.559783	6.267011	10.317049
H	0.829632	8.848083	1.232912	H	10.595635	3.843289	6.281347	O	7.600250	9.287336	6.263394
H	3.238907	11.292558	3.969306	H	6.877532	1.543479	9.060655	O	11.953157	7.615230	7.619540
H	2.826184	8.272183	1.553984	H	11.282909	4.563170	7.522323	O	6.208248	10.633406	8.960684
H	5.834532	9.868748	3.941130	H	10.601628	1.902477	10.369329	O	9.303458	7.540107	7.569835
H	0.230145	6.849321	1.582202	H	7.558558	4.922887	6.212296	O	8.858274	10.558925	9.011226

Table S21: 4B1 Structure

				A	1.19518068E+01	0.00000000E+00	0.00000000E+00				
				B	-3.67679543E-03	1.21339886E+01	0.00000000E+00				
				C	-5.19662201E-02	1.36809586E-03	1.10853681E+01				
H	4.443329	3.273863	0.146135	O	1.427427	7.574165	4.144891	H	10.030927	1.550831	7.596873
H	1.492019	0.237323	5.381974	O	4.502199	10.607408	1.383652	H	7.801287	4.585336	9.015683
H	0.231465	1.574851	2.883550	O	1.497877	12.005832	0.747177	H	8.151929	2.854823	6.699446
H	5.701457	4.612767	2.642650	O	4.431366	8.975728	4.781106	H	9.678096	5.889426	9.912320
H	4.458094	5.287425	0.750162	O	4.472440	6.302698	4.856088	H	11.196971	5.909535	9.947285
H	1.472367	2.251683	4.776504	O	1.458291	9.333204	0.671428	H	6.633008	2.871151	6.665447
H	2.179852	1.594318	3.516054	O	5.747418	7.609743	2.017116	H	8.677069	0.852808	7.141355
H	3.752055	4.629375	2.011203	O	0.182240	10.645052	3.510777	H	9.155234	3.886848	9.471512
H	4.454436	1.928914	4.841373	O	3.097849	7.692798	2.060879	H	11.642342	3.857006	9.523973
H	1.478187	4.959073	0.685973	O	2.831925	10.731157	3.467753	H	6.190466	0.819321	7.089354
H	4.081113	1.547658	2.054979	H	10.415134	9.342394	0.146930	O	7.381091	1.506007	9.687921
H	1.850980	4.581706	3.472497	H	7.464496	6.307488	5.380701	O	10.451501	4.542451	6.925013
H	2.203551	2.852001	1.156232	H	6.205086	7.643777	2.885330	O	7.447227	5.941637	6.288355
H	3.727026	5.886796	4.369973	H	11.676035	10.678301	2.642742	O	10.383143	2.910998	10.323417
H	5.245799	5.906817	4.404553	H	10.433469	11.356290	0.750295	O	10.428498	0.238261	10.398413
H	0.684785	2.868363	1.121497	H	7.447874	8.322411	4.778365	O	7.405288	3.268759	6.213606
H	2.727235	0.849539	1.598848	H	8.154649	7.665580	3.517098	O	11.699395	1.543298	7.558574
H	3.205201	3.883519	3.928660	H	9.726497	10.700001	2.011588	O	6.133403	4.581170	9.054090
H	5.693562	3.856153	3.981219	H	10.424699	7.997406	4.841849	O	9.049650	1.631762	7.602388
H	0.239652	0.817804	1.545309	H	7.456017	11.027083	0.687795	O	8.782672	4.665478	9.009981
O	1.429319	1.504100	4.144293	H	10.055593	7.615823	2.055087	H	4.414222	9.341017	5.689005
O	4.502517	4.540204	1.382735	H	7.826352	10.652325	3.473441	H	1.461921	6.305888	10.924582
O	1.496269	5.939118	0.747045	H	8.178140	8.919069	1.158778	H	0.203071	7.643486	8.427076
O	4.434702	2.908919	4.780388	H	9.704798	11.956420	4.370130	H	5.674823	10.678175	8.186290
O	4.478331	0.236051	4.856768	H	11.223723	11.975009	4.404980	H	4.432575	11.354829	6.293743
O	1.457260	3.266201	0.670092	H	6.659166	8.937754	1.123720	H	1.446827	8.320127	10.319696
O	5.749661	1.542183	2.016647	H	8.701639	6.917197	1.599770	H	2.152153	7.661327	9.058746
O	0.182891	4.579411	3.510694	H	9.180401	9.954606	3.929543	H	3.725780	10.697806	7.554719
O	3.099800	1.628272	2.060341	H	11.667160	9.921963	3.981551	H	4.423945	7.996656	10.385384
O	2.832383	4.661867	3.466855	H	6.214348	6.886170	1.547088	H	1.453874	11.026746	6.230229
H	10.417529	3.275093	0.145895	O	7.404080	7.575660	4.145249	H	4.053131	7.612309	7.597602
H	7.468730	0.238776	5.382257	O	10.476563	10.609132	1.382952	H	1.825200	10.651116	9.016151
H	6.207406	1.575388	2.884848	O	7.474136	12.007181	0.748085	H	2.177054	8.918104	6.701377
H	11.677174	4.612007	2.642380	O	10.406215	8.977438	4.781275	H	3.703517	11.955946	9.913515
H	10.433992	5.288537	0.749758	O	10.448761	6.304442	4.855191	H	5.222385	11.973736	9.948313
H	7.448536	2.253284	4.777400	O	7.432386	9.334545	0.672775	H	0.658197	8.937512	6.666647
H	8.156569	1.596734	3.516842	O	11.723590	7.611375	2.016094	H	2.698751	6.914868	7.140668
H	9.727529	4.631320	2.010884	O	6.158440	10.645192	3.511975	H	3.179060	9.953334	9.472936
H	10.428818	1.930445	4.841907	O	9.074220	7.695972	2.061030	H	5.666503	9.921802	9.525031
H	7.455115	4.960684	0.686400	O	8.807692	10.733229	3.468010	H	0.211100	6.886690	7.088464
H	10.057225	1.549431	2.054537	H	4.416870	3.274324	5.688242	O	1.401804	7.572702	9.687420
H	7.826798	4.584295	3.472237	H	1.467026	0.237918	10.924459	O	4.475922	10.607366	6.926055
H	8.178913	2.853534	1.157217	H	0.205389	1.575961	8.426764	O	1.471116	12.006892	6.290170
H	9.703382	5.888589	4.368930	H	5.675916	4.613232	8.185747	O	4.406002	8.976696	10.324617
H	11.222219	5.908555	4.403979	H	4.432182	5.287633	6.292916	O	4.446979	6.303757	10.399056
H	6.660030	2.870162	1.122569	H	1.447619	2.252244	10.319072	O	1.431492	9.334252	6.215699
H	8.703121	0.851515	1.599602	H	2.154442	1.595043	9.058157	O	5.721373	7.609531	7.560062
H	9.180690	3.885895	3.928476	H	3.726460	4.629609	7.554067	O	0.156731	10.645337	9.054105
H	11.667939	3.856189	3.981471	H	4.429163	1.929740	10.384692	O	3.071786	7.692816	7.603012
H	6.216250	0.818606	1.546371	H	1.451679	4.960161	6.226995	O	2.806549	10.731747	9.010904
O	7.406118	1.505837	4.145018	H	4.055118	1.548646	7.597168	H	10.389242	9.342729	5.689192
O	10.477807	4.541336	1.382353	H	1.825588	4.582653	9.015491	H	7.439544	6.307536	10.925012
O	7.474032	5.940692	0.747450	H	2.176987	2.853214	6.698392	H	6.179142	7.642809	8.428220
O	10.408459	2.910414	4.780877	H	3.701646	5.887837	9.912828	H	11.650693	10.678356	8.185987
O	10.454318	0.237569	4.856251	H	5.220459	5.907903	9.947712	H	10.408093	11.356404	6.293363
O	7.432565	3.267765	0.671162	H	0.658167	2.869654	6.664411	H	7.422768	8.321728	10.320498
O	11.725610	1.542026	2.015275	H	2.701182	0.850724	7.140871	H	8.128823	7.664066	9.059367
O	6.159066	4.580511	3.510961	H	3.179682	3.884413	9.471878	H	9.701060	10.699880	7.554416
O	9.075951	1.630412	2.060539	H	5.667880	3.856905	9.524476	H	10.399105	7.998153	10.385365
O	8.808202	4.664370	3.466618	H	0.213364	0.819103	7.088478	H	7.429469	11.028084	6.230453
H	4.440905	9.340798	0.147078	O	1.404316	1.504679	9.686873	H	10.029085	7.615424	7.597029
H	1.487335	6.306034	5.380618	O	4.476701	4.540329	6.925365	H	7.800613	10.652677	9.015951
H	0.229415	7.644754	2.884375	O	1.469940	5.940181	6.288267	H	8.151488	8.919875	6.701973
H	5.700711	10.678021	2.643732	O	4.409272	2.909730	10.323690	H	9.679044	11.957113	9.912203
H	4.458999	11.354693	0.751106	O	4.453164	0.236882	10.399542	H	11.197992	11.975338	9.947590
H	1.472312	8.320954	4.777933	O	1.430463	3.267278	6.212507	H	6.632447	8.938601	6.667399
H	2.178150	7.662928	3.516697	O	5.723707	1.542635	7.559892	H	8.675012	6.917535	7.140854
H	3.751729	10.697774	2.011931	O	0.157282	4.580315	9.053333	H	9.154558	9.955042	9.472400
H	4.449348	7.995676	4.841809	O	3.073826	1.629538	7.602144	H	11.641539	9.922387	9.524984
H	1.480734	11.025710	0.686821	O	2.806985	4.662736	9.009958	H	6.188327	6.886511	7.089178
H	4.079197	7.612350	2.055254	H	10.390848	3.276024	5.688664	O	7.378753	7.574361	9.688141
H	1.850553	10.650587	3.472783	H	7.443612	0.239294	10.925381	O	10.451200	10.609098	6.925839
H	2.203696	8.917214	1.157496	H	6.181488	1.575716	8.428047	O	7.447807	12.008199	6.290404
H	3.728733	11.955094	4.370671	H	11.651501	4.613142	8.185088	O	10.380447	8.978157	10.324510
H	5.247586	11.972976	4.405531	H	10.407442	5.289506	6.292284	O	10.423487	6.305249	10.398605
H	0.684921	8.936859	1.122606	H	7.423818	2.253604	10.320089	O	7.405556	9.335552	6.216421
H	2.724766	6.914407	1.599305	H	8.130985	1.597072	9.059092	O	11.697194	7.610841	7.558814
H	3.204378	9.952553	3.929499	H	9.701499	4.632554	7.553849	O	6.132611	10.645540	9.054476
H	5.692363	9.921229	3.982207	H	10.403400	1.931015	10.384272	O	9.047741	7.695808	7.602833
H	0.237252	6.886576	1.546535	H	7.428012	4.961649	6.227219	O	8.781946	10.733497	9.010513

Table S22: 4B2 Structure

				A	1.19068005E+01	0.00000000E+00	0.00000000E+00				
				B	2.21402390E-04	1.20733096E+01	0.00000000E+00				
				C	-1.08360492E-01	7.97439979E-04	1.12095171E+01				
H	4.393730	3.275563	0.127779	O	1.403275	7.514881	4.255608	H	10.688411	1.534085	7.725844
H	1.445765	0.258166	5.513666	O	4.435360	10.531667	1.385021	H	6.951125	4.548090	9.124836
H	0.188070	1.543116	2.965235	O	1.446113	11.884046	0.781318	H	11.038559	5.831620	10.057614
H	5.653116	4.559654	2.677081	O	4.391988	8.867482	4.859828	H	6.597729	2.812339	6.792750
H	4.380662	5.248860	0.758258	O	4.369767	6.204445	4.926022	H	6.611372	0.285729	6.836332
H	1.461405	2.231313	4.883627	O	1.471817	9.221042	0.715358	H	11.029037	3.305000	10.015989
H	2.160178	1.546450	3.636321	O	5.766032	7.565458	2.060676	H	8.562858	0.790711	7.264205
H	3.681205	4.564929	2.005575	O	0.072386	10.584729	3.580544	H	9.078193	3.806244	9.586990
H	1.398220	4.165559	0.725851	O	3.091156	7.580461	2.110433	H	9.065956	5.322784	9.598036
H	4.439570	1.147855	4.915257	O	2.746780	10.602732	3.529556	H	8.571276	2.307253	7.252054
H	4.787859	1.530898	2.121345	H	10.347981	9.314252	0.128345	O	7.304688	1.478229	9.860238
H	1.051914	4.553259	3.519502	H	7.398523	6.295640	5.513510	O	10.334450	4.497257	6.990227
H	5.142018	5.831088	4.452964	H	6.139434	7.579952	2.964522	O	7.346401	5.848614	6.385884
H	0.699393	2.810796	1.189424	H	11.605477	10.598627	2.676773	O	10.294180	2.830559	10.465683
H	0.710813	0.284461	1.231286	H	10.333938	11.287919	0.757605	O	10.267728	0.168335	10.530122
H	5.127206	3.303545	4.410283	H	7.412020	8.268895	4.883377	O	7.369784	3.185950	6.319525
H	2.661912	0.787565	1.659627	H	8.111225	7.584653	3.636089	O	11.667621	1.529851	7.664999
H	3.176623	3.809123	3.981822	H	9.634147	10.604057	2.004915	O	5.971891	4.545985	9.185768
H	3.168801	5.325742	3.992997	H	7.351847	10.202828	0.725017	O	8.992601	1.549263	7.714488
H	2.672053	2.304185	1.648323	H	10.392289	7.186013	4.916256	O	8.646678	4.563456	9.136015
O	1.405578	1.477266	4.255995	H	10.740262	7.571624	2.122318	H	4.339376	9.314507	5.732174
O	4.435407	4.494450	1.385520	H	7.004958	10.588142	3.519374	H	1.387342	6.295434	11.118142
O	1.442941	5.847888	0.781082	H	11.094850	11.867258	4.452204	H	0.132522	7.581181	8.568615
O	4.391394	2.830074	4.859434	H	6.650766	8.848866	1.188146	H	5.598149	10.598755	8.281616
O	4.367780	0.167250	4.924871	H	6.664915	6.322208	1.231760	H	4.325365	11.287372	6.362483
O	1.471377	3.185047	0.716464	H	11.081665	9.341898	4.411082	H	1.405804	8.268391	10.487402
O	5.767093	1.528112	2.060364	H	8.615901	6.827068	1.660599	H	2.104133	7.582186	9.240463
O	0.072704	4.549729	3.580732	H	9.130779	9.845563	3.981534	H	3.626015	10.603222	7.609794
O	3.092559	1.545452	2.110221	H	9.121354	11.362058	3.992864	H	1.346767	10.202439	6.330193
O	2.747457	4.567600	3.530797	H	8.623612	8.343615	1.648444	H	4.387032	7.184669	10.520964
H	10.349795	3.276610	0.128580	O	7.356784	7.514695	4.255923	H	4.733038	7.566245	7.725930
H	7.398679	0.258251	5.514108	O	10.388854	10.533983	1.385480	H	0.997150	10.588712	9.124808
H	6.140359	1.542133	2.964283	O	7.401297	11.885011	0.781544	H	5.086584	11.866878	10.057279
H	11.605991	4.562823	2.676897	O	10.346328	8.868442	4.861007	H	0.646019	8.848441	6.793212
H	10.332614	5.250030	0.757991	O	10.320290	6.205398	4.925264	H	0.654546	6.322281	6.834631
H	7.412619	2.231375	4.883016	O	7.423219	9.222186	0.715323	H	5.073104	9.340616	10.014579
H	8.112010	1.546894	3.636000	O	11.719474	7.567570	2.060873	H	2.606013	6.822464	7.263369
H	9.634107	4.564807	2.005284	O	6.025748	10.584319	3.580487	H	3.121909	9.845202	9.586008
H	7.351907	4.166052	0.725632	O	9.045002	7.585811	2.111205	H	3.113486	11.361716	9.597984
H	10.395856	1.148939	4.915803	O	8.700665	10.603599	3.530681	H	2.618200	8.338952	7.252473
H	10.741885	1.533341	2.122932	H	4.339022	3.276477	5.732092	O	1.349370	7.514174	9.860068
H	7.005519	4.547988	3.520018	H	1.389803	0.258634	11.118548	O	4.380640	10.533378	6.990195
H	11.092873	5.832293	4.452478	H	0.133967	1.544066	8.568978	O	1.393499	11.884628	6.386086
H	6.651634	2.811563	1.188400	H	5.598749	4.559697	8.281830	O	4.337596	8.866942	10.463972
H	6.665520	0.285392	1.230891	H	4.326099	5.249661	6.363235	O	4.315465	6.204043	10.530737
H	11.084258	3.305642	4.411061	H	1.405863	2.232103	10.488805	O	1.418650	9.221840	6.320618
H	8.616653	0.789966	1.660167	H	2.105466	1.547425	9.241866	O	5.712277	7.565040	7.664951
H	9.132963	3.806077	3.982369	H	3.626693	4.565257	7.610388	O	0.017915	10.584991	9.185953
H	9.120509	5.322659	3.993096	H	1.345238	4.165917	6.329272	O	3.037504	7.579614	7.714488
H	8.624880	2.306537	1.648789	H	4.386044	1.147916	10.520802	O	2.692320	10.603685	9.135432
O	7.357567	1.476937	4.255818	H	4.734226	1.531862	7.726630	H	10.294160	9.315754	5.733234
O	10.388748	4.496015	1.385617	H	0.997293	4.552312	9.124801	H	7.344534	6.295816	11.119357
O	7.400480	5.848520	0.782439	H	5.087615	5.830523	10.057615	H	6.085526	7.579255	8.568844
O	10.349632	2.830879	4.860819	H	0.646463	2.811175	6.792902	H	11.551301	10.599422	8.282087
O	10.322732	0.168421	4.925150	H	0.657869	0.285032	6.835525	H	10.279917	11.289177	6.362580
O	7.423861	3.185466	0.715666	H	5.073168	3.303341	10.015288	H	7.358420	8.268670	10.487491
O	11.721058	1.529176	2.061523	H	2.608516	0.788413	7.265235	H	8.057621	7.583995	9.240460
O	6.026304	4.546158	3.581018	H	3.122437	3.808329	9.586979	H	9.579845	10.605052	7.609709
O	9.046046	1.548360	2.111046	H	3.114152	5.324925	9.598243	H	7.297697	10.203315	6.330386
O	8.701288	4.563158	3.531319	H	2.618715	2.304980	7.253551	H	10.338152	7.185515	10.521229
H	4.393665	9.312947	0.126932	O	1.350429	1.478190	9.861003	H	10.686692	7.571172	7.725834
H	1.441759	6.295293	5.512271	O	4.380843	4.495076	6.990247	H	6.950742	10.588036	9.124448
H	0.186420	7.581691	2.964619	O	1.389186	5.847988	6.384482	H	11.040016	11.867350	10.057307
H	5.652329	10.597909	2.676618	O	4.337571	2.829795	10.464715	H	6.596938	8.849070	6.793349
H	4.380273	11.285940	0.757608	O	4.314224	0.167301	10.530371	H	6.610952	6.322089	6.835625
H	1.459916	8.268827	4.883286	O	1.418667	3.185401	6.320292	H	11.027227	9.341402	10.015878
H	2.157935	7.583113	3.635888	O	5.713434	1.529029	7.665289	H	8.561907	6.826791	7.263899
H	3.680711	10.601556	2.004609	O	0.018073	4.548965	9.185797	H	9.076408	9.845256	9.586295
H	1.399748	10.201612	0.724999	O	3.038863	1.546382	7.715988	H	9.066819	11.361767	9.598116
H	4.441304	7.185070	4.916521	O	2.692970	4.566699	9.136045	H	8.570139	8.343346	7.252602
H	4.786817	7.567043	2.121848	H	10.296577	3.277817	5.733167	O	7.303275	7.514193	9.860402
H	1.051595	10.588051	3.519076	H	7.345209	0.259109	11.118550	O	10.334745	10.535264	6.990482
H	5.140327	11.866928	4.452020	H	6.087046	1.543360	8.569057	O	7.346932	11.885187	6.386784
H	0.699315	8.847587	1.188151	H	11.551619	4.562676	8.281879	O	10.291886	8.867801	10.465621
H	0.708262	6.322388	1.230952	H	10.278373	5.251319	6.362660	O	10.266040	6.204903	10.530363
H	5.127538	9.341082	4.410425	H	7.359578	2.232422	10.487692	O	7.369272	9.222672	6.320569
H	2.660028	6.822780	1.659903	H	8.059105	1.548367	9.240424	O	11.665927	7.567488	7.664734
H	3.176426	9.844638	3.980744	H	9.579714	4.565854	7.609782	O	5.971509	10.584401	9.185475
H	3.167496	11.361151	3.991831	H	7.297944	4.166578	6.329039	O	8.991363	7.585144	7.714852
H	2.671401	8.339266	1.647929	H	10.340626	1.148883	10.520810	O	8.646242	10.603381	9.135662

Table S23: 4C1 Structure

				A	1.19546657E+01	0.00000000E+00	0.00000000E+00				
				B	9.42898901E-04	1.20456296E+01	0.00000000E+00				
				C	8.09881422E-02	-5.63594105E-04	1.11930758E+01				
H	2.695169	1.560452	2.895388	O	1.498765	7.559499	4.153141	H	10.888586	1.511817	7.687664
H	3.309368	4.570666	2.727981	O	4.506498	10.571369	1.469260	H	7.152023	4.522499	9.129454
H	0.274549	1.519613	2.889163	O	1.549036	11.928666	0.661529	H	8.267452	2.840481	6.728154
H	5.729987	4.530959	2.734543	O	4.459741	8.917181	4.962629	H	9.772379	5.851730	10.086734
H	1.535296	0.770128	4.769384	O	4.528453	6.252306	4.933776	H	11.288772	5.783596	10.088513
H	4.469664	3.782302	0.854215	O	1.475364	9.264121	0.688950	H	6.751054	2.772035	6.726806
H	4.490900	5.302995	0.844730	O	5.845978	7.539567	1.995497	H	6.802686	0.267532	6.736233
H	1.512397	2.290741	4.779357	O	0.159538	10.550812	3.626982	H	11.238924	3.279583	10.079228
H	4.530187	1.914761	4.931563	O	3.186171	7.576095	2.045512	H	8.781354	0.831349	7.133254
H	1.471619	4.926583	0.691045	O	2.819237	10.588962	3.577044	H	9.260235	3.842434	9.682617
H	4.870412	1.513021	2.091011	H	8.669619	7.582811	2.892977	O	7.520773	1.535258	9.749845
H	1.133727	4.523708	3.531286	H	9.290438	10.595042	2.729245	O	10.519551	4.548269	7.065731
H	2.248896	2.841734	1.133587	H	6.249434	7.542987	2.886890	O	7.562408	5.905858	6.254173
H	3.754085	5.851705	4.488924	H	11.710709	10.554336	2.735616	O	10.476778	2.894784	10.560480
H	5.270504	5.783063	4.491037	H	7.510185	6.794173	4.766895	O	10.549766	0.230011	10.531819
H	0.732458	2.772093	1.132277	H	10.449401	9.806191	0.855245	O	7.492944	3.240892	6.283402
H	0.785131	0.267363	1.141807	H	10.472220	11.326852	0.845601	O	11.867061	1.516017	7.594125
H	5.219693	3.279052	4.482102	H	7.488811	8.314891	4.776554	O	6.173578	4.526927	9.222913
H	2.763211	0.832570	1.538901	H	10.508323	7.937984	4.931589	O	9.207145	1.554318	7.640703
H	3.241061	3.842796	4.084563	H	7.452577	10.949117	0.691133	O	8.833675	4.565001	9.175197
O	1.501294	1.535837	4.154568	H	10.845004	7.535903	2.089688	H	2.732399	7.581109	8.491243
O	4.503017	4.547933	1.469247	H	7.115220	10.546570	3.532833	H	3.354107	10.593514	8.324470
O	1.543860	5.906250	0.659522	H	8.225036	8.862303	1.132735	H	0.312383	7.542982	8.484183
O	4.457165	2.894380	4.962901	H	9.735979	11.874526	4.490316	H	5.774849	10.553351	8.331601
O	4.531211	0.229892	4.934169	H	11.252437	11.807209	4.492504	H	1.572445	6.793964	10.365288
O	1.474057	3.241630	0.688953	H	6.708529	8.795809	1.129810	H	4.513177	9.805445	6.450408
O	5.848765	1.517107	1.996373	H	6.759114	6.290216	1.139394	H	4.535394	11.326074	6.441027
O	0.155363	4.528462	3.625707	H	11.200234	9.301450	4.482958	H	1.552027	8.314652	10.374805
O	3.188878	1.555731	2.046177	H	8.737404	6.854635	1.536514	H	4.571616	7.936998	10.528559
O	2.815135	4.565539	3.576910	H	9.222652	9.866669	4.085628	H	1.516995	10.948433	6.288347
H	8.672645	1.559870	2.893515	O	7.476963	7.559870	4.151967	H	4.908538	7.534126	7.686968
H	9.286586	4.570915	2.729267	O	10.483403	10.571825	1.470179	H	1.178403	10.546062	9.128870
H	6.252498	1.519758	2.887669	O	7.525876	11.928720	0.659989	H	2.289557	8.861262	6.729896
H	11.706344	4.531837	2.734369	O	10.436998	8.917701	4.963247	H	3.798897	11.873446	10.085757
H	7.513205	0.770084	4.767742	O	10.505794	6.252899	4.934338	H	5.315311	11.806305	10.088303
H	10.446824	3.783253	0.854483	O	7.451379	9.264122	0.687554	H	0.773093	8.795330	6.727295
H	10.467866	5.303949	0.845348	O	11.823431	7.540493	1.996009	H	0.821983	6.290013	6.736230
H	7.490522	2.290731	4.777231	O	6.136760	10.550612	3.626586	H	5.263395	9.300361	10.079445
H	10.508647	1.915185	4.932124	O	9.163586	7.577510	2.043850	H	2.800197	6.852995	7.134690
H	7.450311	4.926568	0.690075	O	8.796551	10.589670	3.578401	H	3.285991	9.865395	9.680998
H	10.847695	1.512604	2.091210	H	2.735837	1.559607	8.492046	O	1.539260	7.559570	9.750292
H	7.111374	4.523032	3.532603	H	3.350326	4.570246	8.324415	O	4.547462	10.570932	7.065462
H	8.226650	2.841015	1.132371	H	0.315286	1.519044	8.485788	O	1.589715	11.928054	6.257377
H	9.731542	5.851896	4.489568	H	5.770820	4.530633	8.331180	O	4.500216	8.916711	10.559914
H	11.247976	5.783892	4.491640	H	1.575959	0.770162	10.366682	O	4.568931	6.251689	10.530816
H	6.710247	2.772630	1.130468	H	4.510526	3.782233	6.450348	O	1.516042	9.263301	6.284768
H	6.762136	0.267899	1.140141	H	4.531704	5.302931	6.440942	O	5.886860	7.538812	7.592379
H	11.197955	3.279584	4.482367	H	1.553057	2.290680	10.376207	O	0.200027	10.550414	9.223520
H	8.740838	0.832206	1.536962	H	4.570666	1.914271	10.528610	O	3.226701	7.575442	7.642328
H	9.219222	3.842844	4.085842	H	1.512367	4.925950	6.286918	O	2.859967	10.588202	9.173474
O	7.479640	1.535658	4.152692	H	4.911484	1.512453	7.688057	H	8.710324	7.581723	8.489448
O	10.479326	4.548772	1.469731	H	1.174301	4.523586	9.127373	H	9.331178	10.593810	8.326063
O	7.522020	5.906273	0.658705	H	2.289665	2.840874	6.729664	H	6.290452	7.542150	8.483715
O	10.435635	2.894797	4.963370	H	3.794677	5.851090	10.085764	H	11.751138	10.553708	8.332185
O	10.509063	0.230204	4.935221	H	5.311104	5.782592	10.088168	H	7.551021	6.793651	10.364222
O	7.452301	3.241565	0.687389	H	0.773317	2.771248	6.728595	H	10.489691	9.805416	6.451357
O	11.826171	1.516742	1.997549	H	0.825910	0.266652	6.737874	H	10.512399	11.326064	6.442019
O	6.132932	4.527470	3.626198	H	5.260292	3.278438	10.079142	H	7.529729	8.314383	10.373342
O	9.166483	1.555327	2.044337	H	2.804027	0.831719	7.135546	H	10.549521	7.937717	10.529289
O	8.792830	4.565546	3.578462	H	3.281777	3.842284	9.680981	H	7.492773	10.948769	6.286832
H	2.691959	7.581644	2.894484	O	1.542042	1.535643	9.751580	H	10.885851	7.535085	7.686041
H	3.313290	10.594326	2.727978	O	4.543999	4.547827	7.065394	H	7.155925	10.545629	9.129822
H	0.271661	7.543429	2.887661	O	1.584622	5.905594	6.255479	H	8.265634	8.861908	6.728807
H	5.733941	10.554087	2.734917	O	4.497702	2.893882	10.559914	H	9.776589	11.874345	10.087120
H	1.532008	6.793786	4.768009	O	4.571782	0.229227	10.530865	H	11.293080	11.806911	10.089131
H	4.472273	9.805782	0.854298	O	1.514810	3.240755	6.285058	H	6.749147	8.795122	6.726262
H	4.494577	11.326370	0.844638	O	5.889814	1.516652	7.593346	H	6.799658	6.289642	6.735202
H	1.511590	8.314424	4.777858	O	0.195950	4.528356	9.221834	H	11.241194	9.301142	10.080306
H	4.531230	7.937471	4.931086	O	3.229645	1.554813	7.642915	H	8.777859	6.853879	7.132692
H	1.476343	10.949032	0.692673	O	2.855978	4.565053	9.173270	H	9.263662	9.865865	9.682749
H	4.867622	7.534817	2.089954	H	8.713437	1.559027	8.489931	O	7.517943	7.559140	9.749050
H	1.137931	10.546493	3.532404	H	9.327258	4.570339	8.325907	O	10.523741	10.570912	7.066429
H	2.248856	8.861965	1.134036	H	6.293659	1.519307	8.484592	O	7.566134	11.928342	6.255653
H	3.758218	11.874181	4.489178	H	11.746864	4.531637	8.330532	O	10.478120	8.917419	10.560838
H	5.274676	11.807013	4.491434	H	7.554175	0.769803	10.365025	O	10.546718	6.252545	10.531462
H	0.732363	8.796100	1.131352	H	10.486948	3.782746	6.450523	O	7.491806	9.263530	6.283814
H	0.781225	6.290774	1.140220	H	10.507887	5.303471	6.441397	O	11.864277	7.539803	7.592474
H	5.222853	9.301048	4.482211	H	7.531579	2.290474	10.374190	O	6.177452	10.549779	9.223359
H	2.759572	6.853648	1.537920	H	10.549759	1.915189	10.529120	O	9.204156	7.576517	7.640254
H	3.245295	9.866075	4.084433	H	7.490766	4.926167	6.285505	O	8.837411	10.588597	9.175280

Table S24: 4C2 Structure

				A	1.20320175E+01	0.00000000E+00	0.00000000E+00				
				B	-7.28313148E-04	1.20062496E+01	0.00000000E+00				
				C	-4.20172722E-02	6.50327680E-03	1.11463537E+01				
H	1.521075	2.708053	5.486786	O	1.540209	7.523465	4.227507	H	10.893781	1.503314	7.681511
H	4.501150	5.704213	0.088002	O	4.481216	10.519395	1.345394	H	7.116556	4.503777	9.041807
H	4.534804	3.265073	0.093085	O	1.493817	11.869073	0.803505	H	11.218079	5.792419	9.888395
H	1.485363	0.269857	5.484152	O	4.524599	8.868820	4.771457	H	6.793323	2.790271	6.833323
H	0.788033	1.537559	3.594267	O	4.496308	6.208948	4.816581	H	8.737350	0.751749	7.218631
H	5.232750	4.535120	1.982536	O	1.526048	9.208962	0.755265	H	9.273169	3.754740	9.506526
H	2.310135	1.512361	3.628761	O	5.881120	7.561751	2.139582	H	9.222040	5.270992	9.512628
H	3.710745	4.510894	1.947589	O	0.139477	10.567202	3.433713	H	8.788009	2.267977	7.211137
H	4.530895	1.886861	4.872020	O	3.217557	7.498004	2.070162	H	11.781198	3.793854	9.483506
H	1.490263	4.886805	0.704980	O	2.803249	10.503411	3.502159	H	6.228951	0.791719	7.240721
H	4.899644	1.500101	2.105781	H	7.538572	8.712038	5.482142	O	7.531751	1.523927	9.802656
H	1.121453	4.500613	3.472416	H	10.514201	11.707550	0.092126	O	10.477636	4.524240	6.920800
H	5.225017	5.786998	4.313280	H	10.549568	9.268528	0.091829	O	7.493301	5.870119	6.373543
H	0.796640	2.784391	1.261235	H	7.504866	6.272481	5.481731	O	10.518916	2.869978	10.350006
H	2.742524	0.747383	1.645978	H	6.804990	7.538942	3.590637	O	10.488090	0.210846	10.394623
H	3.278943	3.749840	3.932980	H	11.248806	10.538584	1.982630	O	7.523015	3.210619	6.330197
H	3.228499	5.266126	3.938670	H	8.326986	7.515306	3.624868	O	11.873816	1.563184	7.717591
H	2.792863	2.263608	1.637325	H	9.726812	10.514439	1.947716	O	6.136502	4.563141	9.004600
H	5.787702	3.788992	3.908444	H	10.543531	7.891865	4.867955	O	9.210339	1.499203	7.648418
H	0.232348	0.787213	1.670627	H	7.507331	10.891402	0.705575	O	8.799761	4.501679	9.076305
O	1.538115	1.521711	4.230408	H	10.916214	7.502690	2.105391	H	1.500429	8.714225	11.056872
O	4.482916	4.518743	1.346174	H	7.136280	10.506977	3.467274	H	4.477847	11.709014	5.663440
O	1.495634	5.865095	0.800816	H	11.236908	11.793565	4.317203	H	4.511911	9.270372	5.663544
O	4.526028	2.865128	4.775817	H	6.814236	8.788376	1.257101	H	1.465708	6.274141	11.055500
O	4.495043	0.205659	4.819542	H	8.759854	6.751837	1.641955	H	0.768644	7.542929	9.164613
O	1.525715	3.205284	0.757611	H	9.292406	9.756622	3.929830	H	5.209394	10.540551	7.554402
O	5.879674	1.560428	2.141951	H	9.242115	11.272826	3.937990	H	2.290588	7.518347	9.198996
O	0.141435	4.561232	3.435743	H	8.810163	8.268172	1.633303	H	3.687321	10.517236	7.520482
O	3.216026	1.495214	2.074464	H	11.801444	9.795579	3.908918	H	4.509435	7.893725	10.439571
O	2.805192	4.496847	3.503280	H	6.251658	6.790064	1.664853	H	1.467921	10.894781	6.278808
H	7.538496	2.708854	5.485726	O	7.555105	7.523848	4.226702	H	4.879510	7.505789	7.675734
H	10.515917	5.705768	0.090274	O	10.498972	10.520780	1.346190	H	1.098062	10.511539	9.043114
H	10.550340	3.266911	0.095010	O	7.511599	11.869582	0.802353	H	5.202525	11.794070	9.888172
H	7.502448	0.270790	5.483258	O	10.538297	8.870221	4.772637	H	0.775975	8.791200	6.831156
H	6.802578	1.538314	3.593428	O	10.509210	6.210421	4.817992	H	2.721722	6.754629	7.215026
H	11.250553	4.536473	1.984241	O	7.543064	9.210013	0.753752	H	3.255014	9.759072	9.503888
H	8.324561	1.512983	3.627875	O	11.896278	7.561844	2.142357	H	3.205932	11.275403	9.512523
H	9.728558	4.511731	1.949072	O	6.156192	10.565788	3.430891	H	2.772955	8.270907	7.206383
H	10.543832	1.888266	4.873838	O	9.232899	7.499747	2.070816	H	5.765618	9.797054	9.478804
H	7.509562	4.887269	0.703714	O	8.819648	10.504315	3.500344	H	0.212332	6.794591	7.240244
H	10.914623	1.499778	2.108894	H	1.499825	2.709828	11.059620	O	1.518667	7.526885	9.800719
H	7.137968	4.500029	3.468764	H	4.479792	5.707849	5.661427	O	4.459120	10.522925	6.918542
H	11.238809	5.789274	4.315393	H	4.513779	3.268200	5.667285	O	1.472370	11.872929	6.375630
H	6.814584	2.786288	1.259118	H	1.464486	0.272303	11.058324	O	4.503586	8.872046	10.344236
H	8.758348	0.748046	1.646263	H	0.767033	1.539961	9.167049	O	4.475184	6.211913	10.389587
H	9.294677	3.750856	3.932788	H	5.210844	4.538996	7.555684	O	1.504609	9.213101	6.327709
H	9.243330	5.267094	3.937962	H	2.289055	1.514840	9.201747	O	5.859524	7.566025	7.712754
H	8.809298	2.264235	1.637413	H	3.688801	4.514757	7.520763	O	0.118013	10.570761	9.006213
H	11.802567	3.790384	3.911569	H	4.509879	1.890205	10.444469	O	3.195912	7.502226	7.643184
H	6.249884	0.788184	1.667852	H	1.468863	4.891089	6.278855	O	2.781908	10.507251	9.075749
O	7.552606	1.522427	4.229647	H	4.878488	1.503068	7.678869	H	7.516943	8.715058	11.055440
O	10.500824	4.520109	1.347690	H	1.099758	4.504621	9.044330	H	10.491382	11.710374	5.664773
O	7.514202	5.865566	0.799810	H	5.203717	5.789957	9.886035	H	10.526279	9.272028	5.664643
O	10.539539	2.866532	4.777485	H	0.775800	2.788735	6.834654	H	7.483155	6.274945	11.054595
O	10.508125	0.207171	4.820936	H	2.721026	0.750776	7.218118	H	6.782993	7.542680	9.164055
O	7.544311	3.206285	0.755758	H	3.256759	3.753520	9.505592	H	11.226249	10.541980	7.555238
O	11.894692	1.559441	2.145108	H	3.206937	5.269826	9.511781	H	8.304946	7.519172	9.198676
O	6.157935	4.559908	3.432206	H	2.771755	2.267031	7.210241	H	9.704303	10.517855	7.521997
O	9.231378	1.495777	2.075497	H	5.766334	3.792100	9.480702	H	10.523753	7.894683	10.441774
O	8.821395	4.497488	3.501837	H	0.211570	0.791156	7.242816	H	7.486110	10.895494	6.277724
H	1.521413	8.711455	5.483233	O	1.516985	1.523746	9.803308	H	10.894748	7.507395	7.678820
H	4.499981	11.705604	0.090238	O	4.460977	4.522601	6.919334	H	7.115290	10.509943	9.040641
H	4.533637	9.267153	0.089950	O	1.473886	5.869421	6.374316	H	11.216353	11.797100	9.890232
H	1.486525	6.271575	5.482445	O	4.504412	2.868440	10.347993	H	6.792937	8.792285	6.829653
H	0.790176	7.539001	3.591370	O	4.474870	0.208760	10.392711	H	8.738577	6.756312	7.216262
H	5.231152	10.537170	1.981648	O	1.504924	3.209794	6.331234	H	9.272128	9.759535	9.504704
H	2.312242	7.514471	3.625917	O	5.858501	1.563553	7.715301	H	9.221289	11.275826	9.513165
H	3.709118	10.513555	1.946929	O	0.119729	4.564889	9.007673	H	8.788694	8.272625	7.207635
H	4.530488	7.890459	4.866636	O	3.194760	1.498305	7.646935	H	11.780373	9.799002	9.481541
H	1.489407	10.890922	0.706774	O	2.783303	4.500829	9.076176	H	6.230234	6.794412	7.238046
H	4.901099	7.501591	2.102732	H	7.517714	2.710618	11.057831	O	7.532920	7.527170	9.800347
H	1.119532	10.507598	3.470479	H	10.493125	5.709411	5.662925	O	10.475786	10.524149	6.919608
H	5.223044	11.791185	4.315320	H	10.527955	3.269891	5.668844	O	7.490536	11.873626	6.374663
H	0.797481	8.786956	1.258703	H	7.481505	0.272976	11.057204	O	10.518780	8.873033	10.346240
H	2.743596	6.750365	1.641887	H	6.781784	1.540127	9.166356	O	10.489024	6.213534	10.391836
H	3.276446	9.755380	3.930516	H	11.227774	4.540645	7.556828	O	7.521993	9.213819	6.326563
H	3.227075	11.271640	3.939003	H	8.303794	1.514909	9.200981	O	11.874817	7.566583	7.715226
H	2.794487	8.266661	1.633389	H	9.705807	4.516039	7.522726	O	6.135237	10.568645	9.003218
H	5.786878	9.794115	3.906575	H	10.523409	1.891720	10.446615	O	9.211375	7.504273	7.645316
H	0.233999	6.790003	1.667304	H	7.488368	4.891795	6.277964	O	8.798814	10.507190	9.075769

Table S25: 7A1 Structure

				A	1.19946520E+01	0.00000000E+00	0.00000000E+00				
				B	1.24487823E-03	1.11719825E+01	0.00000000E+00				
				C	9.68704496E-02	8.63219581E-04	1.19931545E+01				
H	4.268812	2.729249	3.267508	O	6.050546	6.790292	0.176443	H	7.341172	2.469490	12.262081
H	6.055278	5.532016	4.990156	O	1.757402	8.925225	6.256142	H	9.076138	-0.332735	7.987717
H	2.319267	3.368193	3.220375	O	1.389952	7.508706	3.189879	H	11.339480	1.834655	6.218794
H	5.975041	0.582017	0.933205	O	6.066054	10.246977	4.536635	H	9.042483	4.614274	9.926777
H	3.382723	3.290207	0.225208	O	-0.048242	10.306338	1.876520	H	6.450325	1.906943	9.218655
H	-0.004633	4.710963	2.859369	O	3.075738	9.580388	3.175728	H	9.064899	0.489313	11.854004
H	1.312140	3.825173	5.530757	O	4.731562	7.448978	3.260744	H	10.330733	1.376311	8.528559
H	4.699322	3.782724	0.962424	O	4.367073	8.864109	0.193761	H	7.766643	1.414361	9.956669
H	3.739138	0.979897	4.540322	O	3.042225	6.127242	1.538054	H	6.764225	4.221045	7.536583
H	2.308890	1.029218	1.973065	O	2.970725	6.066605	4.875513	H	11.377798	4.170277	10.968010
H	1.294505	2.472882	6.263926	H	10.266181	8.314761	3.266518	O	12.095400	1.208286	6.173105
H	3.031845	-0.330734	1.992473	H	12.053162	11.119575	4.989669	O	7.803771	3.336028	12.255160
H	5.294965	1.830424	0.223309	H	8.317561	8.953522	3.220892	O	7.433764	1.919406	9.187680
H	2.998136	4.616307	3.931723	H	11.973057	6.169607	0.931697	O	12.109245	4.658382	10.531788
H	0.405500	1.911526	3.221155	H	9.380697	8.874116	0.225344	O	5.995588	4.720436	7.873690
H	3.013777	0.490998	5.858380	H	5.996235	10.295892	2.860239	O	9.118111	3.992436	9.169934
H	4.286544	1.376918	2.534413	H	7.310970	9.408816	5.531072	O	10.774474	1.862618	9.254377
H	1.721180	1.417842	3.958869	H	10.697033	9.368662	0.961869	O	10.409636	3.279279	6.188368
H	0.719383	4.220941	1.540872	H	9.738233	6.564615	4.538578	O	9.084516	0.539113	7.534001
H	5.332050	4.172237	4.971911	H	8.307009	6.614345	1.971720	O	9.018376	0.478707	10.871470
O	6.050909	1.204277	0.176712	H	7.292126	8.056142	6.263665	H	4.316117	8.314260	9.262076
O	1.756522	3.339678	6.256751	H	9.029667	5.254376	1.991052	H	6.106532	11.115463	10.986411
O	1.388999	1.923183	3.189732	H	11.293786	7.417911	0.221296	H	2.366706	8.953204	9.218920
O	6.064151	4.660101	4.536511	H	8.997054	10.201975	3.931519	H	6.020990	6.171111	6.930217
O	-0.049621	4.720602	1.876709	H	6.404476	7.495944	3.221949	H	3.430362	8.878794	6.219768
O	3.075379	3.994311	3.175233	H	9.013494	6.076217	5.857282	H	0.043351	10.295775	8.855246
O	4.730678	1.862382	3.260586	H	10.284852	6.962738	2.532644	H	1.362938	9.409711	11.527858
O	4.366119	3.277090	0.193888	H	7.720915	7.002269	3.958455	H	4.746643	9.371081	6.957813
O	3.041040	0.540898	1.538312	H	6.719249	9.804625	1.541576	H	3.789416	6.564056	10.534374
O	2.969522	0.480927	4.875707	H	11.329521	9.759853	4.970766	H	2.353709	6.615386	7.971724
H	10.264672	2.730249	3.266110	O	12.049571	6.791446	0.174961	H	1.345358	8.057427	12.260656
H	12.051824	5.532787	4.989531	O	7.755081	8.922463	6.256676	H	3.076436	5.255227	7.987895
H	8.315379	3.366957	3.220248	O	7.387892	7.507923	3.189850	H	5.342077	7.419748	6.219230
H	11.972530	0.583684	0.931914	O	12.061650	10.247854	4.535646	H	3.047541	10.201294	9.928361
H	9.379579	3.288796	0.225253	O	5.950797	10.304987	1.877630	H	0.452884	7.495082	9.220857
H	5.993887	4.709685	2.860266	O	9.073670	9.579593	3.175243	H	3.067390	6.075541	11.854405
H	7.309618	3.823051	5.531248	O	10.728616	7.448152	3.259054	H	4.333010	6.962093	8.528725
H	10.695974	3.783039	0.961796	O	10.364130	8.862964	0.193265	H	1.769077	7.001790	9.958518
H	9.738317	0.979978	4.538875	O	9.039006	6.125982	1.536825	H	0.766780	9.807660	7.535910
H	8.306893	1.027484	1.972145	O	8.968824	6.065729	4.874614	H	5.383316	9.755921	10.968482
H	7.291280	2.470813	6.264613	H	4.315554	2.728074	9.261102	O	6.097509	6.792877	6.173474
H	9.030908	-0.331776	1.991599	H	6.104480	5.529323	10.986384	O	1.807287	8.924286	12.253878
H	11.292851	1.832031	0.221886	H	2.366183	3.367199	9.217502	O	1.436365	7.507703	9.190033
H	8.994061	4.615813	3.931038	H	6.021407	0.584730	6.930901	O	6.115371	10.243595	10.532790
H	6.403534	1.908720	3.222028	H	3.429395	3.292369	6.220416	O	-0.002170	10.306804	7.872658
H	9.014542	0.490066	5.857575	H	0.042185	4.710101	8.855365	O	3.122924	9.579024	9.171870
H	10.284231	1.377966	2.532845	H	1.362316	3.823861	11.528092	O	4.778069	7.447395	9.254406
H	7.720180	1.415638	3.958734	H	4.745595	3.784900	6.958281	O	4.413789	8.866293	6.188595
H	6.717562	4.219450	1.541646	H	3.788746	0.978669	10.534671	O	3.084774	6.127344	7.534701
H	11.328370	4.172949	4.971142	H	2.353104	1.028466	7.971740	O	3.021102	6.064449	10.871880
O	12.048812	1.205804	0.175385	H	1.344336	2.471798	12.261272	H	10.312179	8.314068	9.262452
O	7.753892	3.337323	6.257164	H	3.075884	-0.331648	7.988414	H	12.101714	11.116694	10.985581
O	7.386959	1.920731	3.189876	H	5.341760	1.833329	6.220458	H	8.363725	8.952634	9.218611
O	12.060300	4.660976	4.535669	H	3.047002	4.614877	9.927508	H	12.018987	6.172164	6.929051
O	5.948710	4.719232	1.877628	H	0.452338	1.909660	9.220253	H	9.427415	8.876415	6.219444
O	9.070882	3.993757	3.174522	H	3.066615	0.490027	11.854647	H	6.043301	10.294647	8.856182
O	10.727745	1.863970	3.259025	H	4.332127	1.375420	8.528594	H	7.361237	9.406858	11.528960
O	10.363016	3.277109	0.193356	H	1.768352	1.416366	9.958219	H	10.743393	9.370410	6.956826
O	9.039443	0.539827	1.537381	H	0.765600	4.222288	7.535952	H	9.786579	6.562996	10.533619
O	8.969508	0.480183	4.874932	H	5.381796	4.169421	10.968531	H	8.352530	6.614208	7.969947
H	4.269459	8.315722	3.267943	O	6.097597	1.206962	6.174494	H	7.341845	8.054590	12.261881
H	6.057211	11.118747	4.990577	O	1.806377	3.338603	12.254395	H	9.075141	5.254186	7.986756
H	2.319803	8.954068	3.220982	O	1.435831	1.921770	9.189321	H	11.340273	7.420504	6.217770
H	5.974204	6.168232	0.933038	O	6.113560	4.657458	10.532752	H	9.044460	10.201003	9.928166
H	3.383681	8.876918	0.225077	O	-0.003363	4.721374	7.872767	H	6.451078	7.493557	9.219493
H	-0.003033	10.297062	2.859146	O	3.122378	3.993070	9.170651	H	9.064412	6.074336	11.853593
H	1.312870	9.411148	5.530519	O	4.777386	1.861151	9.253888	H	10.331116	6.962147	8.528492
H	4.700280	9.369457	0.962463	O	4.412833	3.279542	6.189385	H	7.767413	7.000255	9.956974
H	3.740214	6.565751	4.540082	O	3.084205	0.540306	7.534906	H	6.765707	9.805939	7.536461
H	2.309998	6.615384	1.972881	O	3.020313	0.479221	10.872119	H	11.378628	9.756811	10.968018
H	1.295428	8.058411	6.262980	H	10.311323	2.728907	9.261162	O	12.095994	6.793872	6.172332
H	3.033122	5.255563	1.992132	H	12.100814	5.530202	10.985523	O	7.804870	8.920903	12.255069
H	5.295089	7.417049	0.222937	H	8.362353	3.366035	9.216528	O	7.434508	7.506236	9.188589
H	2.998346	10.202573	3.932061	H	12.018572	0.586156	6.929490	O	12.110131	10.244871	10.531862
H	0.406470	7.496308	3.221167	H	9.426158	3.290821	6.219901	O	5.997282	10.305612	7.873639
H	3.014627	6.077285	5.858196	H	6.041414	4.709173	8.856251	O	9.119960	9.578431	9.171898
H	4.287599	6.963637	2.534402	H	7.359955	3.821674	11.528951	O	10.774951	7.447586	9.254819
H	1.722402	7.003149	3.958776	H	10.742083	3.784803	6.957294	O	10.410880	8.865276	6.187681
H	0.720696	9.806648	1.540575	H	9.786416	0.978724	10.533895	O	9.083950	6.126262	7.533481
H	5.333641	9.759226	4.971598	H	8.352574	1.026718	7.969963	O	9.018232	6.063342	10.871036

Table S26: 7B1 Structure

				A	1.21008420E+01	0.00000000E+00	0.00000000E+00				
				B	-3.65648998E-04	1.10895813E+01	0.00000000E+00				
				C	2.54870619E-02	1.54458318E-03	1.19857768E+01				
H	4.355574	2.740480	3.184865	O	6.098106	6.714653	0.127968	H	7.387032	2.402950	6.180958
H	-0.010549	5.454455	4.912590	O	1.685961	8.855047	0.177489	H	9.071496	-0.314449	7.910665
H	2.341507	3.332802	3.196912	O	1.337513	7.434054	3.188632	H	11.423306	1.808728	6.192186
H	6.024934	0.540535	0.879504	O	0.017405	10.122982	4.470277	H	9.068985	4.601613	9.869212
H	5.698687	1.887509	3.177077	O	-0.029192	10.182868	1.813537	H	8.730395	3.255358	6.172451
H	0.045365	4.624452	2.794299	O	3.079551	9.518395	3.124595	H	9.140931	0.517052	11.785206
H	1.749474	1.431318	2.427146	O	4.717884	7.376224	3.172956	H	10.831586	3.710344	5.422405
H	4.760944	3.730405	0.949625	O	4.355933	8.799205	0.192793	H	7.805624	1.411792	9.940031
H	3.767936	0.986347	4.437809	O	3.034746	6.107570	1.474341	H	6.799530	4.156674	7.433647
H	0.745826	4.118489	4.940783	O	3.002617	6.049104	4.810390	H	9.827804	1.021410	7.938781
H	1.323593	2.401453	0.188642	H	10.406156	8.283520	3.184410	O	12.161311	1.168049	6.120836
H	3.007431	-0.312545	1.916995	H	6.039875	11.000785	4.913148	O	7.749760	3.311919	6.169679
H	5.360658	1.810585	0.199984	H	8.392984	8.876567	3.196678	O	7.400549	1.887844	9.182863
H	3.005300	4.603187	3.876271	H	12.074487	6.083315	0.878976	O	6.079483	4.580830	10.463566
H	2.666750	3.254491	0.180724	H	11.749527	7.431124	3.176284	O	6.034172	4.638962	7.806507
H	3.077111	0.516924	5.791396	H	6.096320	10.171264	2.794765	O	9.142947	3.972059	9.118086
H	4.767673	3.711870	-0.569514	H	7.800033	6.975062	2.427140	O	10.781176	1.830221	9.167381
H	1.742606	1.412777	3.946325	H	10.811406	9.273563	0.949299	O	10.419450	3.252539	6.184448
H	0.735779	4.155358	1.440458	H	9.818855	6.530273	4.437672	O	9.099035	0.561631	7.468229
H	3.764293	1.023065	1.944630	H	6.796646	9.665059	4.941072	O	9.066366	0.503068	10.804381
O	6.098823	1.170139	0.128385	H	7.373720	7.947564	0.188722	H	4.367346	8.285226	9.178465
O	1.686094	3.310515	0.177567	H	9.058183	5.230422	1.917486	H	0.001364	11.001016	10.905848
O	1.337555	1.889112	3.189328	H	11.410678	7.353508	0.199388	H	2.353653	8.877470	9.190320
O	0.017151	4.578351	4.470186	H	9.057328	10.146417	3.876451	H	6.037150	6.084851	6.872073
O	-0.029354	4.637892	1.813506	H	8.717319	8.799732	0.180703	H	5.710602	7.432417	9.170785
O	3.079483	3.973480	3.125317	H	9.128132	6.061507	5.791556	H	0.057837	10.169945	8.787512
O	4.718061	1.831431	3.173730	H	10.818229	9.255234	-0.569855	H	1.761170	6.976137	8.420450
O	4.355919	3.253961	0.192682	H	7.792925	6.957205	3.946233	H	4.774427	9.275113	6.942496
O	3.035117	0.563540	1.474488	H	6.786759	9.701949	1.441027	H	3.779808	6.530788	10.430618
O	3.002790	0.503673	4.810577	H	9.815003	6.566010	1.944785	H	0.758013	9.665284	10.934162
H	10.406100	2.739241	3.185268	O	12.148660	6.712841	0.127843	H	1.336834	7.946116	6.181544
H	6.039004	5.455855	4.912856	O	7.736698	8.856437	0.177947	H	3.019465	5.232249	7.909437
H	8.392641	3.331700	3.197644	O	7.388109	7.433344	3.189020	H	5.373451	7.355277	6.192729
H	12.074932	0.538751	0.879392	O	6.067606	10.124672	4.470784	H	3.017585	10.147867	9.869455
H	11.749522	1.886824	3.177145	O	6.021702	10.184688	1.813967	H	2.679872	8.799233	6.173679
H	6.095611	4.626204	2.794634	O	9.131256	9.516924	3.125275	H	3.089050	6.061749	11.784295
H	7.800299	1.430212	2.427880	O	10.768875	7.374546	3.173256	H	4.781062	9.256879	5.423301
H	10.811446	3.728811	0.949239	O	10.406446	8.797236	0.192257	H	1.754620	6.957275	9.939623
H	9.819096	0.985219	4.438282	O	9.085784	6.106386	1.474770	H	0.748696	9.700312	7.434068
H	6.795786	4.120182	4.940833	O	9.053631	6.047952	4.810759	H	3.776329	6.567850	7.937956
H	7.373881	2.403226	0.188881	H	4.367792	2.740404	9.177656	O	6.111340	6.714514	6.121073
H	9.059060	-0.313836	1.917561	H	0.001218	5.455596	10.905332	O	1.699228	8.855208	6.170608
H	11.410866	1.808923	0.199889	H	2.353856	3.332392	9.189084	O	1.349446	7.433809	9.182787
H	9.056720	4.602078	3.876772	H	6.037905	0.540186	6.872374	O	0.029183	10.124856	10.463561
H	8.717373	3.255469	0.180647	H	5.710992	1.887478	9.170282	O	-0.016614	10.182844	7.806686
H	9.128591	0.515690	5.791967	H	0.057838	4.624530	8.787198	O	3.091623	9.518132	9.118497
H	10.818315	3.710110	-0.569921	H	1.761457	1.430700	8.420211	O	4.729978	7.376218	9.167295
H	7.793172	1.411814	3.946996	H	4.773649	3.729799	6.942294	O	4.369283	8.798947	6.185463
H	6.786506	4.157237	1.440984	H	3.780346	0.986613	10.430627	O	3.047335	6.108515	7.467367
H	9.815396	1.022030	1.945492	H	0.758066	4.120016	10.933949	O	3.014679	6.048121	10.803465
O	12.149030	1.168455	0.128379	H	1.336041	2.400940	6.181149	H	10.418016	8.283733	9.178882
O	7.736746	3.312154	0.177865	H	3.019905	-0.313200	7.909991	H	6.052126	11.002390	10.905855
O	7.388305	1.888144	3.189932	H	5.373570	1.810233	6.192838	H	8.404936	8.876475	9.191446
O	6.066637	4.579685	4.470601	H	3.017555	4.602637	9.868576	H	12.087552	6.083147	6.871877
O	6.021174	4.639619	1.813822	H	2.679341	3.253754	6.173357	H	11.761460	7.431336	9.170759
O	9.130689	3.972271	3.125861	H	3.089674	0.517980	11.784532	H	6.109453	10.171182	8.787642
O	10.768875	1.830293	3.174194	H	4.780327	3.711559	5.423125	H	7.811917	6.975362	8.421024
O	10.406412	3.252367	0.192291	H	1.755113	1.412628	9.939435	H	10.824745	9.273483	6.941837
O	9.086389	0.562320	1.475216	H	0.748461	4.154940	7.433608	H	9.830814	6.529726	10.430918
O	9.054117	0.502356	4.811165	H	3.776662	1.022497	7.937848	H	6.808745	9.666679	10.934627
H	4.355345	8.285258	3.184049	O	6.111782	1.169829	6.121306	H	7.387301	7.947423	6.181161
H	-0.010739	10.999086	4.912648	O	1.698703	3.309938	6.170196	H	9.070678	5.231087	7.909843
H	2.341548	8.877721	3.195969	O	1.349825	1.888728	9.182385	H	11.423931	7.353500	6.192373
H	6.024045	6.085176	0.879146	O	0.029125	4.579345	10.463256	H	9.069290	10.146813	9.870338
H	5.698508	7.432420	3.176254	O	-0.016673	4.637642	7.806387	H	8.730763	8.799671	6.172815
H	0.045569	10.169278	2.794324	O	3.091694	3.973227	9.117371	H	9.140253	6.060765	11.784742
H	1.749451	6.975905	2.426661	O	4.730363	1.831374	9.166817	H	10.831984	9.254895	5.422620
H	4.760922	9.275488	0.949829	O	4.368659	3.253495	6.185267	H	7.805194	6.956424	9.940145
H	3.767835	6.531505	4.437423	O	3.047702	0.562868	7.467498	H	6.800182	9.701562	7.434075
H	0.746249	9.663453	4.940928	O	3.015257	0.504050	10.803699	H	9.827292	6.566754	7.938468
H	1.323518	7.945970	0.188328	H	10.418409	2.739188	9.178129	O	12.161973	6.712876	6.120949
H	3.007020	5.231644	1.917160	H	6.051555	5.457188	10.905393	O	7.750139	8.856339	6.170088
H	5.360223	7.355415	0.199645	H	8.404988	3.331389	9.189900	O	7.400163	7.433063	9.183317
H	3.005383	10.147803	3.875809	H	12.087075	0.538492	6.871939	O	6.079887	10.126090	10.463881
H	2.666614	8.799156	0.180720	H	11.761830	1.886672	9.170502	O	6.034950	10.184121	7.806837
H	3.076981	6.062629	5.791196	H	6.108772	4.625948	8.787296	O	9.143134	9.516853	9.119529
H	4.767722	9.257207	-0.569319	H	7.812363	1.429677	8.420878	O	10.780812	7.374777	9.167576
H	1.742491	6.958006	3.945849	H	10.824295	3.728802	6.941603	O	10.419928	8.797123	6.184731
H	0.735776	9.700138	1.440411	H	9.831324	0.985756	10.431183	O	9.098355	6.107357	7.467809
H	3.763993	6.567227	1.944239	H	6.808547	4.121726	10.934304	O	9.065745	6.047057	10.803915

Table S27: 7C1 Structure

				A	1.20368671E+01	0.00000000E+00	0.00000000E+00				
				B	7.11934133E-06	1.11956928E+01	0.00000000E+00				
				C	6.88577946E-02	6.43884153E-03	1.19560344E+01				
H	-0.007593	5.492603	1.388805	O	6.030283	6.755287	0.209258	H	9.069598	-0.265454	10.354993
H	0.047974	5.496240	4.949847	O	1.700341	8.862239	6.231102	H	9.091430	-0.265454	7.937375
H	6.796381	1.771448	0.224594	O	1.335938	7.533873	3.173615	H	9.856964	3.454187	9.193022
H	2.281939	3.438080	3.187294	O	0.059939	10.201016	4.548224	H	11.326956	1.787663	6.175758
H	5.672192	1.931916	3.170286	O	-0.005161	10.245629	1.888401	H	8.733906	3.298500	12.136806
H	0.049939	4.698199	3.569942	O	3.036485	9.662118	3.199446	H	9.093881	0.531266	6.557068
H	1.800677	1.492855	2.426788	O	4.692191	7.558685	3.241543	H	10.844748	3.733706	5.418277
H	1.316559	3.744933	5.467816	O	4.330096	8.883222	0.183298	H	10.360590	1.484916	8.454936
H	4.735699	3.733358	0.957256	O	3.051458	6.219598	1.559616	H	7.795564	1.493575	9.921880
H	3.746311	1.083277	4.459075	O	3.017990	6.174227	4.877081	H	6.772198	4.141810	7.449895
H	3.017148	-0.269911	4.377483	H	6.010945	11.089539	1.385764	O	12.081236	1.161990	6.186759
H	3.041247	-0.270744	1.961201	H	6.066154	11.090706	4.944912	O	7.754036	3.268104	12.208048
H	3.802486	3.450055	3.215426	H	12.814618	7.369324	0.225910	O	7.389555	1.941390	9.151008
H	5.275766	1.783800	0.198069	H	8.299264	9.037334	3.189449	O	6.111936	4.605679	10.525707
H	2.680056	3.294769	6.158855	H	11.689805	7.530988	3.169023	O	6.043589	4.648979	7.866147
H	3.042623	0.525417	0.580396	H	6.067920	10.291698	3.566040	O	9.090997	4.069261	9.177784
H	4.792483	3.728586	-0.559589	H	7.818187	7.091310	2.429334	O	10.744628	1.964105	9.217909
H	4.309500	1.481497	2.477713	H	7.335129	9.340870	5.467037	O	10.381044	3.291220	6.163539
H	1.741345	1.487979	3.943437	H	10.754784	9.332642	0.957061	O	9.102992	0.626633	7.535450
H	0.721697	4.139529	1.472508	H	9.767067	6.682962	4.459653	O	9.070829	0.580531	10.854439
O	6.029605	1.157474	0.208411	H	9.038735	5.329236	4.378439	H	0.027136	11.095299	7.366087
O	1.700137	3.265181	6.230671	H	9.059630	5.329204	1.961797	H	0.084307	11.095881	10.927306
O	1.336300	1.935166	3.171731	H	9.819844	9.049752	3.215612	H	6.829659	7.372624	6.205853
O	0.059581	4.603860	4.548433	H	11.294061	7.381559	0.199009	H	2.318021	9.040192	9.165441
O	-0.006624	4.647049	1.888920	H	8.698157	8.893729	6.160797	H	5.707632	7.532010	9.150449
O	3.035823	4.064291	3.199849	H	9.061340	6.125098	0.580887	H	0.085558	10.298484	9.547272
O	4.692185	1.961342	3.240936	H	10.812977	9.327321	-0.559743	H	1.835801	7.095227	8.405735
O	4.329659	3.285978	0.186180	H	10.326088	7.081865	2.477514	H	1.352554	9.344190	11.445509
O	3.052940	0.621191	1.558701	H	7.762007	7.086074	3.946152	H	4.769135	9.335710	6.932632
O	3.017946	0.576429	4.876266	H	6.740657	9.736612	1.468050	H	3.781461	6.684485	10.439342
H	6.011129	5.492712	1.387607	O	12.047837	6.755262	0.209849	H	3.051776	5.331593	10.356491
H	6.066038	5.496152	4.949040	O	7.718195	8.862962	6.231265	H	3.075786	5.331789	7.939308
H	12.814447	1.771849	0.225040	O	7.354982	7.533047	3.175311	H	3.838568	9.052298	9.193429
H	8.301843	3.440697	3.188174	O	6.077441	10.197876	4.544581	H	5.309092	7.384519	6.177722
H	11.689898	1.930387	3.166187	O	6.012063	10.243379	1.884956	H	2.715898	8.894562	12.137007
H	6.067927	4.698330	3.568973	O	9.052965	9.663748	3.200365	H	3.076817	6.127718	6.558582
H	7.817492	1.495436	2.427566	O	10.709917	7.561707	3.240226	H	4.825796	9.327765	5.415761
H	7.334194	3.745021	5.467239	O	10.349038	8.885417	0.185773	H	4.344937	7.083183	8.457252
H	10.754165	3.733666	0.956697	O	9.070092	6.221112	1.559212	H	1.777200	7.089991	9.922523
H	9.766070	1.084597	4.458034	O	9.039456	6.175469	4.877416	H	0.756415	9.742145	7.449534
H	9.035682	-0.267977	4.377366	H	0.025959	5.496584	7.366880	O	6.063088	6.758403	6.189298
H	9.055906	-0.269749	1.960828	H	0.084045	5.498353	10.927925	O	1.735986	8.864847	12.208684
H	9.822433	3.451259	3.214083	H	6.829432	1.774019	6.200257	O	1.372022	7.537480	9.151062
H	11.293880	1.783455	0.197445	H	2.316752	3.442476	9.165863	O	0.095761	10.203568	10.525697
H	8.697549	3.295570	6.158981	H	5.706407	1.935326	9.147867	O	0.028304	10.249753	7.866229
H	9.057989	0.525930	0.579689	H	0.085418	4.700820	9.547859	O	3.071886	9.666419	9.177145
H	10.812398	3.729340	-0.560059	H	1.834726	1.496994	8.405502	O	4.727647	7.562487	9.220740
H	10.325626	1.481487	2.475324	H	1.352521	3.746974	11.446367	O	4.363029	8.886749	6.162439
H	7.761653	1.490996	3.944375	H	4.768787	3.735332	6.933266	O	3.087491	6.223701	7.536865
H	6.740198	4.139601	1.471708	H	3.781524	1.086899	10.438191	O	3.052762	6.177598	10.855843
O	12.047918	1.157448	0.208479	H	3.052365	-0.266201	10.355790	H	6.042382	11.094945	7.362803
O	7.717656	3.264705	6.229813	H	3.075458	-0.266116	7.938474	H	6.101090	11.096377	10.925390
O	7.355120	1.938234	3.173438	H	3.837311	3.454257	9.193491	H	12.847302	7.373793	6.204484
O	6.077215	4.603881	4.547448	H	5.308942	1.786235	6.172053	H	8.335080	9.040277	9.166181
O	6.011851	4.647218	1.887911	H	2.715489	3.297228	12.138652	H	11.725483	7.533831	9.146560
O	9.056310	4.066197	3.199809	H	3.076106	0.529858	6.557727	H	6.101208	10.299767	9.544985
O	10.710064	1.961298	3.237724	H	4.826002	3.732249	5.416462	H	7.853433	7.094434	8.407598
O	10.348520	3.286844	0.185130	H	4.343345	1.485465	8.455693	H	7.371655	9.345075	11.442206
O	9.067628	0.621987	1.557984	H	1.776667	1.491607	9.922274	H	10.788070	9.336916	6.935601
O	9.037637	0.578486	4.876001	H	0.755594	4.143715	7.450114	H	9.803090	6.685548	10.438308
H	-0.006442	11.091061	1.388081	O	6.062783	1.159920	6.182870	H	9.074320	5.332013	10.356522
H	0.048709	11.093477	4.949485	O	1.735525	3.267300	12.209540	H	9.094400	5.332355	7.939119
H	6.797065	7.369260	0.224793	O	1.371045	1.939030	9.151006	H	9.855572	9.053612	9.193050
H	2.282338	9.036232	3.187681	O	0.095772	4.606068	10.526296	H	11.326713	7.385684	6.177502
H	5.672181	7.528306	3.171122	O	0.027237	4.650909	7.866826	H	8.734735	8.896500	12.135450
H	0.050512	10.295488	3.569767	O	3.070726	4.068530	9.177857	H	9.095478	6.128677	6.558529
H	1.799510	7.091411	2.428285	O	4.726463	1.964876	9.218952	H	10.844812	9.331313	5.418823
H	1.316957	9.341612	5.467925	O	4.363011	3.288758	6.161594	H	10.361625	7.084721	8.455522
H	4.736445	9.330934	0.954065	O	3.086481	0.625801	7.536023	H	7.798108	7.089374	9.924557
H	3.746452	6.680847	4.459757	O	3.053173	0.579830	10.855091	H	6.772223	9.742446	7.448357
H	3.016706	5.327932	4.378241	H	6.043039	5.494844	7.366427	O	12.080637	6.759567	6.188192
H	3.039998	5.327677	1.962155	H	6.101073	5.498233	10.926681	O	7.754766	8.865751	12.205505
H	3.802957	9.047656	3.215218	H	12.847550	1.776693	6.203039	O	7.390787	7.536294	9.153855
H	5.276490	7.381678	0.197522	H	8.336386	3.443950	9.166063	O	6.112325	10.204315	10.523341
H	2.680315	8.891947	6.159589	H	11.724476	1.933660	9.146393	O	6.043241	10.249814	7.863818
H	3.041272	6.123645	0.581329	H	6.101424	4.699722	9.547210	O	9.088425	9.667152	9.177098
H	4.792668	9.325600	-0.562732	H	7.852243	1.499203	8.404978	O	10.745640	7.564425	9.218184
H	4.309165	7.079011	2.478389	H	7.370358	3.747561	11.445088	O	10.381456	8.889646	6.164762
H	1.741397	7.086533	3.945014	H	10.787059	3.737848	6.935018	O	9.104730	6.224363	7.536877
H	0.722977	9.738059	1.471748	H	9.799648	1.087146	10.437830	O	9.075377	6.178059	10.855825

Table S28: 9A1 Structure

				A	1.20516335E+01	0.00000000E+00	0.00000000E+00				
				B	3.12007271E-02	1.20518809E+01	0.00000000E+00				
				C	-8.35922468E-02	8.48292618E-02	1.10464684E+01				
H	3.073214	4.807838	1.234869	O	3.008280	6.002062	-0.009473	H	11.623637	0.090637	8.976576
H	1.232023	3.011764	3.996896	O	0.049460	9.109117	2.751979	H	5.985060	0.433971	6.214149
H	1.756607	0.013529	4.269137	O	2.956819	7.698448	2.045325	H	10.318879	5.386577	8.501370
H	0.048479	4.276320	1.510256	O	4.379080	9.155988	4.805054	H	6.726260	1.751472	5.738038
H	3.016361	0.739681	0.608375	O	3.059525	10.352182	2.089090	H	7.687567	0.775304	8.426433
H	5.300654	3.058944	3.369331	O	1.724910	9.060180	4.852747	H	11.341960	4.372686	5.668298
H	3.711231	0.097083	4.895314	O	4.670083	6.121372	3.456403	H	8.290333	4.793151	8.090975
H	-0.044130	2.320666	2.134426	O	-0.031548	7.403999	0.696128	H	7.276120	3.826978	10.851299
H	2.989132	2.656085	2.050223	O	1.297080	6.022008	3.409514	H	9.690071	1.376803	8.080727
H	3.383637	3.091244	4.811397	O	0.076832	10.776392	0.646705	H	10.688327	2.420567	10.844841
H	5.639634	0.046532	3.452640	H	9.110668	10.836714	1.230109	O	8.976473	0.022944	5.510117
H	-0.001240	0.393901	0.693095	H	7.269855	9.042226	3.992197	O	6.020364	3.124202	8.272765
H	4.334433	5.339631	2.977653	H	7.796460	6.039391	4.268559	O	8.931955	1.718556	7.566119
H	0.738413	1.711298	0.215379	H	6.083582	10.300261	1.506112	O	10.351387	3.180922	10.330340
H	1.703814	0.728538	2.905387	H	9.053531	6.768920	0.609500	O	9.033810	4.372728	7.613233
H	5.356353	4.329923	0.143831	H	11.338319	9.088707	3.371781	O	7.697386	3.084479	10.372695
H	2.305113	4.747186	2.569197	H	9.750613	6.128134	4.896029	O	10.639957	0.136496	8.977814
H	1.293948	3.779803	5.331154	H	5.994350	8.345846	2.131736	O	5.943864	1.417867	6.216893
H	3.705502	1.330764	2.559389	H	9.023912	8.685887	2.048619	O	7.267439	0.045747	8.928925
H	4.707169	2.371682	5.320287	H	9.420608	9.123422	4.810464	O	6.044939	4.790928	6.167649
O	2.992620	-0.023072	-0.011317	H	11.679556	6.077374	3.457153	H	3.042869	10.875752	6.755844
O	0.038623	3.080413	2.752082	H	6.042100	6.417850	0.691140	H	1.201274	9.082591	9.518357
O	2.947356	1.672269	2.044622	H	10.377066	11.364427	2.974816	H	1.729551	6.080191	9.794648
O	4.367500	3.130579	4.805346	H	6.780310	7.736173	0.212854	H	0.017943	10.343158	7.030773
O	3.048583	4.326634	2.091586	H	7.742026	6.754700	2.905153	H	2.986708	6.807198	6.132573
O	1.712956	3.035292	4.853789	H	11.396642	10.359365	0.145014	H	5.268668	9.127683	8.892755
O	4.655921	0.090723	3.455486	H	8.343997	10.779390	2.565441	H	3.685048	6.167623	10.419926
O	-0.044164	1.377760	0.694162	H	7.328788	9.809281	5.327201	H	-0.076364	8.389704	7.659240
O	1.283074	-0.000918	3.407478	H	9.742521	7.362914	2.559895	H	2.955417	8.724703	7.572187
O	0.064084	4.750709	0.649070	H	10.741452	8.401205	5.321854	H	3.352918	9.160795	10.334685
H	9.098858	4.811208	1.232704	O	9.031486	6.006527	-0.010755	H	5.611931	6.118275	8.977538
H	7.258462	3.015369	3.994040	O	6.074106	9.106381	2.748835	H	-0.030996	6.460431	6.219176
H	7.783350	0.016586	4.266854	O	8.983287	7.701939	2.045220	H	4.309552	11.404333	8.499227
H	6.071665	4.275010	1.507414	O	10.404624	9.161266	4.806889	H	0.707752	7.777584	5.740931
H	9.042828	0.743990	0.607604	O	9.085194	10.355747	2.086890	H	1.675109	6.795193	8.430943
H	11.327108	3.060631	3.371404	O	7.750688	9.066802	4.849078	H	5.325994	10.397980	5.664700
H	9.737403	0.100431	4.893266	O	10.695893	6.123952	3.457516	H	2.275949	10.817587	8.091050
H	5.983277	2.320301	2.132791	O	5.998674	7.401706	0.692352	H	1.263573	9.850153	10.852890
H	9.015579	2.660003	2.049207	O	7.322983	6.024046	3.406889	H	3.674096	7.401466	8.082585
H	9.409594	3.096177	4.810871	O	6.099344	10.774437	0.644804	H	4.676289	8.440774	10.843721
H	11.665730	0.047849	3.453072	H	3.030272	4.850329	6.758030	O	2.965776	6.043865	5.513462
H	6.028381	0.392307	0.690578	H	1.189828	3.056827	9.519849	O	0.005953	9.150911	8.275138
H	10.360408	5.342694	2.977910	H	1.714920	0.056358	9.792484	O	2.914789	7.740735	7.568094
H	6.768553	1.710137	0.213380	H	0.005076	4.317264	7.032184	O	4.336829	9.200108	10.329386
H	7.729186	0.731717	2.903362	H	2.973981	0.781829	6.131448	O	3.017426	10.394506	7.612517
H	11.384593	4.333110	0.146827	H	5.257758	3.102729	8.892671	O	1.682523	9.105849	10.375072
H	8.331586	4.750762	2.567345	H	3.669739	0.140145	10.418277	O	4.628248	6.163882	8.979326
H	7.318701	3.782934	5.328621	H	-0.086705	2.362857	7.659471	O	-0.074720	7.444292	6.219995
H	9.731720	1.334606	2.558613	H	2.946253	2.698719	7.573264	O	1.255154	6.065557	8.933468
H	10.731054	2.374558	5.321774	H	3.341712	3.135231	10.335023	O	0.035100	10.816703	6.169150
O	9.018135	-0.018316	-0.012639	H	5.597830	0.090022	8.975483	H	9.068376	10.879270	6.753598
O	6.063695	3.080589	2.750003	H	-0.042968	0.434255	6.217627	H	7.227674	9.086212	9.515135
O	8.973504	1.676147	2.044030	H	4.292379	5.382113	8.500798	H	7.754860	6.082591	9.791395
O	10.393602	3.134256	4.806602	H	0.697081	1.751627	5.740836	H	6.040496	10.342335	7.028533
O	9.074959	4.330193	2.089549	H	1.661606	0.770992	8.428593	H	9.011411	6.810934	6.132120
O	7.739603	3.039762	4.850777	H	5.314552	4.372092	5.665320	H	11.295162	9.131306	8.895425
O	10.682032	0.093433	3.454407	H	2.262523	4.790124	8.092620	H	9.708866	6.171796	10.419265
O	5.986644	1.376188	0.692785	H	1.252481	3.824557	10.854436	H	5.951319	8.388828	7.656220
O	7.309261	0.001810	3.405492	H	3.663044	1.373631	8.082314	H	8.980846	8.728838	7.571344
O	6.086978	4.748699	0.645846	H	4.665094	2.415051	10.843726	H	9.378595	9.167709	10.334177
H	3.085236	10.833418	1.232438	O	2.950412	0.018829	5.512066	H	11.637700	6.121606	8.980700
H	1.244002	9.037831	3.995808	O	-0.004071	3.123774	8.275615	H	5.999460	6.460087	6.214698
H	1.771074	6.036651	4.270929	O	2.904703	1.714892	7.567678	H	10.334835	11.407298	8.498659
H	0.060628	10.302741	1.508282	O	4.325599	3.174317	10.329262	H	6.738377	7.778294	5.737640
H	3.029415	6.765129	0.609964	O	3.005711	4.369286	7.614859	H	7.699947	6.797349	8.427703
H	5.311478	9.083860	3.368686	O	1.671122	3.080169	10.376551	H	11.355105	10.399918	5.666957
H	3.726225	6.124619	4.896504	O	4.614100	0.133896	8.978190	H	8.301576	10.822784	8.088957
H	-0.032604	8.348620	2.135089	O	-0.085554	1.418130	6.219535	H	7.286789	9.852716	10.850509
H	2.997425	8.682415	2.049284	O	1.241041	0.041651	8.931021	H	9.699899	7.406103	8.082245
H	3.395173	9.116241	4.810884	O	0.020907	4.791119	6.170691	H	10.699503	8.445638	10.845699
H	5.653777	6.075903	3.454658	H	9.057448	4.853658	6.756310	O	8.989635	6.048035	5.512518
H	0.012919	6.420190	0.696124	H	7.215867	3.060146	9.516163	O	6.031038	9.149924	8.272545
H	4.351104	11.361354	2.976364	H	7.741597	0.060643	9.790247	O	8.940538	7.744860	7.567597
H	0.750480	7.737775	0.216637	H	6.028850	4.317569	7.029369	O	10.362607	9.205858	10.331054
H	1.716813	6.752038	2.907406	H	9.000992	0.785705	6.129766	O	9.042597	10.398636	7.610581
H	5.368193	10.356569	0.142800	H	11.284407	3.105229	8.895016	O	7.708722	9.110546	10.371901
H	2.317844	10.775210	2.567376	H	9.695536	0.144189	10.417113	O	10.654026	6.168227	8.980556
H	1.306193	9.804602	5.330565	H	5.939932	2.363244	7.656449	O	5.956461	7.443952	6.216754
H	3.716003	7.359237	2.560040	H	8.974180	2.702391	7.571675	O	7.281233	6.066744	8.929824
H	4.718954	8.397147	5.319917	H	9.367375	3.142677	10.333681	O	6.056760	10.816157	6.167053

Table S29: 9A2 Structure

				A	1.20414868E+01	0.00000000E+00	0.00000000E+00				
				B	1.15344222E-01	1.20408699E+01	0.00000000E+00				
				C	3.36876418E-03	-3.38532321E-03	1.10718251E+01				
H	3.100056	4.798114	1.238346	O	3.146762	5.998116	-0.007045	H	6.427761	0.004732	8.997873
H	1.279230	2.993198	4.006558	O	0.135305	8.978590	2.761783	H	6.096926	5.641883	6.229817
H	4.290615	0.062096	4.280001	O	3.040475	7.700182	2.053570	H	10.387425	5.339608	8.467880
H	-0.018242	1.760911	1.510525	O	4.455174	9.100010	4.823966	H	6.746161	1.731259	5.701343
H	3.003638	0.733149	0.618013	O	3.162243	10.355811	2.106412	H	7.736823	0.745805	8.494754
H	5.345106	3.050437	3.386411	O	1.798519	9.006227	4.874136	H	11.364182	4.342010	5.724724
H	2.333540	0.009655	4.907404	O	4.811377	6.066550	3.412989	H	8.395519	4.769047	8.132168
H	0.052442	3.717282	2.137969	O	0.049133	7.316405	0.645674	H	7.337051	3.716721	10.901804
H	3.028053	2.662747	2.060649	O	1.444889	6.003679	3.472824	H	9.772689	1.345362	8.095636
H	3.415183	3.044724	4.828795	O	0.146323	10.681870	0.705230	H	10.748700	2.310173	10.861835
H	0.405392	0.006068	3.462101	H	9.180411	10.820337	1.239600	O	9.113896	-0.022339	5.531084
H	0.074194	5.645565	0.693002	H	7.356204	9.012014	4.007913	O	6.100895	2.954427	8.298694
H	4.365351	5.339684	2.931811	H	10.367377	6.084620	4.278675	O	9.006439	1.679219	7.591652
H	0.724241	1.735123	0.163761	H	6.058226	7.779408	1.512364	O	10.421213	3.079279	10.358031
H	1.714652	0.746513	2.958650	H	9.079852	6.754701	0.616296	O	9.125726	4.334854	7.641403
H	5.342283	4.341453	0.190971	H	11.422534	9.073456	3.384671	O	7.764519	2.982771	10.410771
H	2.372670	4.770118	2.596313	H	8.410380	6.031572	4.906038	O	10.777809	0.046037	8.950539
H	1.314333	3.720397	5.364454	H	6.129529	9.735797	2.139767	O	6.015079	1.292260	6.182594
H	3.750257	1.345803	2.559548	H	9.105755	8.684448	2.059548	O	7.411531	-0.018386	9.010839
H	4.725101	2.309902	5.327731	H	9.492587	9.066198	4.827870	O	6.111194	4.657938	6.242524
O	3.091228	-0.021504	-0.005418	H	6.482054	6.026711	3.460628	H	3.160893	10.817153	6.775886
O	0.078692	2.957905	2.761423	H	6.152926	11.663697	0.693980	H	1.337592	9.011100	9.542351
O	2.984026	1.679727	2.055574	H	10.445412	11.361775	2.933275	H	4.348013	6.080204	9.813929
O	4.398584	3.079280	4.823733	H	6.801066	7.753454	0.165864	H	0.038787	7.779658	7.046677
O	3.102637	4.335463	2.105608	H	7.790824	6.768041	2.957243	H	3.060798	6.752084	6.152145
O	1.741900	2.986236	4.873783	H	11.420299	10.364148	0.189329	H	5.403392	9.068820	8.922251
O	4.755493	0.046204	3.414559	H	8.453219	10.791318	2.597629	H	2.391091	6.028289	10.441266
O	-0.006728	1.295948	0.645047	H	7.392020	9.738806	5.366037	H	0.110688	9.735905	7.674200
O	1.389166	-0.017662	3.474649	H	9.826699	7.366917	2.557972	H	3.086664	8.681533	7.595957
O	0.088504	4.661617	0.705365	H	10.803142	8.332612	5.326194	H	3.473782	9.062834	10.364437
H	9.121296	4.799441	1.238634	O	9.167408	5.999574	-0.006569	H	0.462511	6.025250	8.996401
H	7.299754	2.991171	4.007835	O	6.155400	8.976416	2.763193	H	0.133796	11.664301	6.228911
H	10.311571	0.063656	4.279964	O	9.060708	7.701471	2.054014	H	4.426412	11.358805	8.468841
H	6.001780	1.758761	1.511907	O	10.475942	9.101794	4.822308	H	0.781602	7.753958	5.700149
H	9.024233	0.734714	0.618318	O	9.183106	10.357015	2.106515	H	1.771710	6.765692	8.492808
H	11.366028	3.052575	3.384446	O	7.819360	9.004856	4.874874	H	5.400889	10.360389	5.727264
H	8.354682	0.010820	4.907802	O	10.832112	6.068601	3.413157	H	2.433667	10.788689	8.133903
H	6.072906	3.715139	2.139816	O	6.069986	7.314292	0.646972	H	1.373364	9.738306	10.900200
H	9.049034	2.664030	2.060885	O	7.465824	6.003719	3.473300	H	3.807673	7.363689	8.093816
H	9.436026	3.045223	4.827816	O	6.166702	10.679769	0.706829	H	4.783685	8.328341	10.863735
H	6.426276	0.006072	3.462337	H	3.101374	4.796771	6.773822	O	3.148312	5.997209	5.528989
H	6.095277	5.643426	0.694664	H	1.280897	2.991832	9.542082	O	0.136685	8.976449	8.297537
H	10.386108	5.341609	2.932136	H	4.292320	0.060854	9.815433	O	3.041687	7.698554	7.590056
H	6.744399	1.733102	0.165254	H	-0.016963	1.759453	7.046581	O	4.457169	9.097655	10.359632
H	7.735162	0.747345	2.959164	H	3.004903	0.731270	6.154018	O	3.163478	10.354094	7.642926
H	11.362733	4.343571	0.189286	H	5.347022	3.049347	8.922020	O	1.800473	9.003932	10.409468
H	8.394072	4.771001	2.596654	H	2.335290	0.008501	10.443222	O	4.812837	6.064386	8.948455
H	7.335336	3.718324	5.365750	H	0.053856	3.715891	7.673509	O	0.050397	7.314821	6.181130
H	9.771027	1.347081	2.559804	H	3.029313	2.661225	7.596127	O	1.446285	6.001481	9.008777
H	10.746805	2.311826	5.326048	H	3.417047	3.043257	10.364263	O	0.147400	10.680352	6.241571
O	9.111875	-0.020071	-0.004978	H	0.406795	0.004660	8.998167	H	9.182060	10.818310	6.776057
O	6.098935	2.955571	2.763022	H	0.075604	5.644075	6.228402	H	7.358176	9.009518	9.543695
O	9.004721	1.681028	2.055965	H	4.366642	5.337722	8.467111	H	10.368714	6.082363	9.814551
O	10.419380	3.080828	4.822035	H	0.725657	1.733389	5.699968	H	6.059800	7.777493	7.047749
O	9.124186	4.336698	2.105850	H	1.715997	0.745085	8.494470	H	9.081788	6.753233	6.152593
O	7.762810	2.984284	4.874845	H	5.343967	4.339720	5.726506	H	11.424103	9.071282	8.920670
O	10.776316	0.047628	3.414454	H	2.373953	4.768429	8.131756	H	8.411702	6.029380	10.441788
O	6.013360	1.293899	0.646382	H	1.316181	3.718823	10.900080	H	6.131378	9.733672	7.675818
O	7.410038	-0.017023	3.475076	H	3.751636	1.344393	8.095113	H	9.107240	8.682644	7.596125
O	6.109466	4.659478	0.707172	H	4.726900	2.308355	10.863179	H	9.494543	9.064008	10.363917
H	3.159690	10.819014	1.239442	O	3.092654	-0.023579	5.530840	H	6.483431	6.024484	8.996179
H	1.335793	9.013522	4.006937	O	0.080142	2.956626	8.297095	H	6.154562	11.662156	6.230507
H	4.346435	6.082635	4.278403	O	2.985282	1.678204	7.591263	H	10.446915	11.360061	8.469516
H	0.037626	7.781464	1.511099	O	4.400441	3.077842	10.359320	H	6.802472	7.752035	5.701140
H	3.059388	6.753206	0.615855	O	3.103884	4.333840	7.640934	H	7.792248	6.765977	8.493164
H	5.401426	9.071378	3.386414	O	1.743678	2.984750	10.409244	H	11.421451	10.362683	5.725524
H	2.389323	6.030829	4.905404	O	4.757109	0.044838	8.949944	H	8.454688	10.789679	8.134001
H	0.109406	9.737880	2.138237	O	-0.005424	1.294327	6.181191	H	7.393899	9.736688	10.901600
H	3.085467	8.683159	2.059345	O	1.390577	-0.018971	9.010685	H	9.828228	7.365050	8.094362
H	3.471782	9.065250	4.828959	O	0.089899	4.660125	6.240837	H	10.805185	8.330685	10.862448
H	0.461123	6.027505	3.460450	H	9.123009	4.797781	6.774286	O	9.169451	5.998308	5.529495
H	0.132698	11.665818	0.692517	H	7.301565	2.989898	9.543707	O	6.157315	8.974035	8.298928
H	4.424760	11.360360	2.933218	H	10.312992	0.062317	9.816016	O	9.062228	7.699670	7.590464
H	0.780266	7.755402	0.164460	H	6.003610	1.757358	7.047997	O	10.477890	9.099727	10.358404
H	1.770416	6.767705	2.956646	H	9.026233	0.732563	6.154228	O	9.184603	10.355195	7.643069
H	5.399376	10.361822	0.190814	H	11.367557	3.051369	8.920197	O	7.821268	9.002590	10.410695
H	2.432317	10.790201	2.597381	H	8.356024	0.009727	10.443567	O	10.833539	6.066430	8.949073
H	1.371231	9.740451	5.364962	H	6.074866	3.713872	7.675341	O	6.071440	7.312702	6.182180
H	3.806347	7.365395	2.557565	H	9.050705	2.662223	7.596432	O	7.467206	6.001513	9.008997
H	4.781714	8.330465	5.327703	H	9.437865	3.043649	10.363852	O	6.168266	10.678220	6.243285

Table S30: 9B1 Structure

				A	1.19974220E+01	0.00000000E+00	0.00000000E+00				
				B	-2.29412074E-02	1.19974705E+01	0.00000000E+00				
				C	-6.37953252E-02	6.57461098E-02	1.11874269E+01				
H	2.997116	4.748531	1.272597	O	2.960046	5.996247	0.008678	H	11.563807	0.031795	9.107511
H	1.247392	3.028866	4.071016	O	-0.009750	9.062369	2.807285	H	6.003085	0.438218	6.309608
H	1.747082	0.053964	4.341383	O	2.941193	7.696425	2.127669	H	6.714855	4.317218	5.808738
H	-0.025012	4.255173	1.545347	O	4.288458	9.079176	4.925685	H	7.675441	5.310195	8.606270
H	3.016938	0.740463	0.644266	O	2.978157	10.376144	2.178480	H	10.682810	3.886659	10.957396
H	5.254363	3.016426	3.441505	O	1.608799	9.036569	4.977488	H	8.146539	1.312834	8.160082
H	3.698976	0.104603	4.987483	O	4.604519	6.077585	3.516610	H	10.192556	5.342635	8.637226
H	-0.072562	2.302620	2.190983	O	-0.056937	7.385261	0.720945	H	6.688958	1.800680	5.839514
H	2.972841	3.398099	2.112221	O	1.256872	6.007596	3.485301	H	9.664975	1.306575	8.197420
H	2.597385	3.054489	4.911117	O	0.007869	10.733871	0.691023	H	10.690899	2.368303	10.994514
H	5.596733	0.000443	3.513602	H	8.984360	10.748378	1.273837	O	8.938268	0.031661	5.602273
H	0.036116	0.405839	0.716721	H	7.235586	9.027389	4.070732	O	5.966601	3.096851	8.398651
H	0.750328	4.284146	0.215527	H	7.735360	6.053076	4.341984	O	8.917822	1.730773	7.722387
H	1.708915	5.276962	3.011275	H	5.962290	10.254446	1.545621	O	10.265612	3.114929	10.519638
H	4.714612	3.851942	5.362870	H	9.005160	6.740409	0.645229	O	8.956008	4.410748	7.772064
H	2.179569	1.279066	2.564415	H	11.244190	9.014538	3.443642	O	7.586007	3.072349	10.567702
H	4.225348	5.307692	3.043020	H	9.688906	6.103667	4.986588	O	10.582334	0.113001	9.111124
H	0.722383	1.767934	0.246618	H	5.915515	8.301085	2.190424	O	5.920120	1.419529	6.313306
H	3.697946	1.273863	2.601823	H	8.961495	9.398305	2.113979	O	7.233329	0.041761	9.080667
H	4.724189	2.333573	5.399502	H	8.585476	9.053473	4.911053	O	5.983453	4.767720	6.283045
O	2.970551	-0.003519	0.008365	H	11.585796	5.998456	3.511667	H	2.952201	10.779773	6.866963
O	0.000199	3.064497	2.806312	H	6.023595	6.403990	0.715873	H	1.206225	9.060267	9.665014
O	2.950595	1.697271	2.126387	H	6.738105	10.283588	0.216092	H	1.704658	6.085791	9.936254
O	4.298267	3.079962	4.924770	H	7.695116	11.276283	3.013129	H	-0.069846	10.286356	7.140557
O	2.988509	4.376789	2.177390	H	10.702872	9.851442	5.363946	H	2.973121	6.771127	6.238509
O	1.618699	3.037678	4.975965	H	8.168220	7.279113	2.565962	H	5.213492	9.047791	9.036140
O	4.615260	0.081124	3.517134	H	10.212535	11.308559	3.043152	H	3.657642	6.135648	10.580260
O	-0.046734	1.387125	0.720254	H	6.710613	7.766171	0.246709	H	-0.115617	8.332999	7.785661
O	1.267663	0.008651	3.485487	H	9.686687	7.272964	2.602657	H	2.929504	9.429436	7.706689
O	0.019067	4.735029	0.689662	H	10.712358	8.333105	5.401209	H	2.556337	9.086961	10.504897
H	8.996017	4.749170	1.273200	O	8.958485	5.996894	0.008847	H	5.553815	6.029793	9.105746
H	7.245385	3.030387	4.069364	O	5.988046	9.062863	2.805905	H	-0.007811	6.436322	6.310749
H	7.746404	0.054983	4.342417	O	8.939293	7.697150	2.127977	H	0.706128	10.316373	5.811321
H	5.971977	4.255510	1.544244	O	10.286713	9.079335	4.925971	H	1.663677	11.306951	8.606898
H	9.015753	0.741541	0.645102	O	8.976446	10.377017	2.178786	H	4.673972	9.884823	10.956606
H	11.253903	3.017106	3.442435	O	7.606804	9.036372	4.975699	H	2.136894	7.310375	8.159326
H	9.699922	0.105628	4.986809	O	10.604284	6.079289	3.515838	H	4.180796	11.339826	8.636407
H	5.925872	2.302972	2.189714	O	5.941390	7.385386	0.720174	H	0.679243	7.798513	5.841908
H	8.972435	3.399054	2.113245	O	7.255281	6.007914	3.486501	H	3.655293	7.304350	8.195266
H	8.595596	3.056886	4.909363	O	6.006790	10.734495	0.690075	H	4.682948	8.366448	10.994122
H	11.596650	0.000092	3.511947	H	2.963429	4.780040	6.867241	O	2.926648	6.027420	5.602307
H	6.035846	0.405964	0.715994	H	1.216407	3.061936	9.663891	O	-0.042628	9.094898	8.400923
H	6.747818	4.284608	0.214654	H	1.715146	0.085225	9.936510	O	2.907721	7.728345	7.720738
H	7.707472	5.277450	3.012414	H	-0.058555	4.287720	7.139648	O	4.257451	9.112771	10.518861
H	10.713625	3.853767	5.363032	H	2.982826	0.773553	6.239037	O	2.944368	10.408149	7.771794
H	8.178775	1.280069	2.565894	H	5.223369	3.048656	9.035315	O	1.577686	9.069610	10.569864
H	10.224771	5.309300	3.042687	H	3.668010	0.136368	10.579792	O	4.572341	6.110434	9.109436
H	6.721737	1.768429	0.245891	H	-0.105688	2.335294	7.785169	O	-0.090248	7.417685	6.314895
H	9.697253	1.274055	2.602536	H	2.939207	3.430174	7.707567	O	1.224494	6.040508	9.080779
H	10.721674	2.335475	5.400089	H	2.566752	3.087763	10.503606	O	-0.025673	10.766650	6.285107
O	8.968975	-0.002062	0.008826	H	5.564455	0.031886	9.106210	H	8.952386	10.781501	6.867152
O	5.997756	3.064923	2.805077	H	0.002228	0.438534	6.311110	H	7.204701	9.060738	9.664070
O	8.949800	1.698029	2.127726	H	0.717079	4.316815	5.810059	H	7.702744	6.085967	9.935775
O	10.296724	3.082085	4.924931	H	1.676141	5.309497	8.606994	H	5.930116	10.286824	7.139216
O	8.987798	4.377747	2.178113	H	4.683955	3.885294	10.955625	H	8.973877	6.773137	6.238475
O	7.616942	3.039395	4.974213	H	2.146125	1.310734	8.160415	H	11.211818	9.047048	9.037895
O	10.615156	0.081116	3.516202	H	4.192884	5.340238	8.636580	H	9.656135	6.136811	10.580550
O	5.952826	1.387273	0.719589	H	0.688733	1.800472	5.841214	H	5.883726	8.333591	7.784149
O	7.266019	0.009421	3.487102	H	3.664550	1.305816	8.196340	H	8.928690	9.431260	7.707017
O	6.016309	4.735356	0.688564	H	4.693289	2.366956	10.993122	H	8.554410	9.086920	10.504766
H	2.986365	10.747332	1.273458	O	2.937024	0.030093	5.602492	H	11.553265	6.031826	9.106933
H	1.237736	9.027429	4.072469	O	-0.032343	3.097134	8.400477	H	5.990622	6.436063	6.310350
H	1.736314	6.052130	4.341209	O	2.916665	1.729388	7.721928	H	6.705311	10.316041	5.809432
H	-0.036162	10.253824	1.546587	O	4.267518	3.113141	10.517904	H	7.662682	11.308866	8.606555
H	3.007072	6.739860	0.644944	O	2.955209	4.408895	7.772254	H	10.671947	9.884539	10.958000
H	5.244727	9.014752	3.442429	O	1.588082	3.070972	10.568682	H	8.135618	7.311841	8.159298
H	3.688532	6.101286	4.987126	O	4.582944	0.112468	9.109681	H	10.179820	11.340730	8.637534
H	-0.082424	8.300559	2.191896	O	-0.080605	1.419815	6.314593	H	6.677784	7.798001	5.840740
H	2.963340	9.397400	2.113830	O	1.234744	0.040052	9.081132	H	9.654056	7.306220	8.196513
H	2.587486	9.053639	4.912714	O	-0.014380	4.767607	6.283961	H	10.681142	8.366173	10.995561
H	5.586008	5.997150	3.512875	H	8.964580	4.781945	6.867069	O	8.927431	6.029509	5.602239
H	0.025555	6.403913	0.716646	H	7.214740	3.062913	9.662746	O	5.956619	9.095582	8.399338
H	0.739268	10.283284	0.216908	H	7.713364	0.087012	9.936189	O	8.906703	7.730014	7.721471
H	1.697053	11.275386	3.011926	H	5.939716	4.287539	7.138621	O	10.255438	9.112420	10.520377
H	4.705089	9.851119	5.363532	H	8.984894	0.774950	6.238903	O	8.943840	10.409955	7.771998
H	2.169804	7.278547	2.565328	H	11.221840	3.049844	9.037193	O	7.575711	9.069941	10.569111
H	4.213296	11.308378	3.043866	H	9.666728	0.137479	10.580578	O	10.571764	6.112713	9.110469
H	0.712273	7.766156	0.247548	H	5.894236	2.334911	7.783310	O	5.908564	7.417488	6.314383
H	3.688154	7.271888	2.602726	H	8.940600	3.432051	7.707418	O	7.222952	6.040607	9.080147
H	4.713847	8.332711	5.400819	H	8.564701	3.089681	10.503242	O	5.974091	10.766895	6.283625

Table S31: 9B2 Structure

				A	1.20479498E+01	0.00000000E+00	0.00000000E+00				
				B	-6.66802739E-02	1.20473402E+01	0.00000000E+00				
				C	1.73279874E-03	-5.27712979E-03	1.10863948E+01				
H	2.973692	4.737610	1.240967	O	3.033419	6.004495	-0.014790	H	6.403701	-0.025769	8.992302
H	1.283668	3.041532	4.014467	O	-0.013954	9.000417	2.759869	H	6.030452	5.660967	6.221529
H	4.293923	0.029449	4.286406	O	2.954213	7.720464	2.099748	H	6.740795	4.314554	5.769007
H	-0.026158	1.752163	1.514514	O	4.293442	9.064017	4.872308	H	7.720234	5.296853	8.539505
H	2.999327	0.720269	0.625759	O	2.948966	10.393559	2.148872	H	10.766746	3.803826	10.877761
H	5.303133	3.038374	3.397356	O	1.620287	9.057128	4.921196	H	8.252566	1.272867	8.107234
H	2.318924	0.053186	4.900700	O	4.692678	6.025338	3.403165	H	10.229273	5.306661	8.484682
H	-0.061955	3.726472	2.129991	O	-0.029709	7.343005	0.634303	H	6.744158	1.803529	5.714187
H	2.989930	3.389709	2.085681	O	1.325199	6.067328	3.472602	H	9.773274	1.282655	8.102902
H	2.632384	3.032734	4.857983	O	-0.085393	10.708792	0.703470	H	10.769107	2.283197	10.873197
H	0.379012	-0.021299	3.449094	H	8.967407	10.763397	1.245567	O	9.093436	-0.021967	5.533258
H	0.005033	5.666995	0.677140	H	7.275586	9.062438	4.017101	O	6.043970	2.969883	8.303172
H	0.716258	4.321176	0.224327	H	10.282315	6.055148	4.287401	O	9.011088	1.694978	7.646136
H	1.693865	5.298179	2.993288	H	5.965430	7.772735	1.514896	O	10.350238	3.042124	10.416974
H	4.742761	3.803874	5.334039	H	8.989606	6.744613	0.626265	O	9.005774	4.367693	7.693580
H	2.230780	1.274284	2.562996	H	11.293451	9.066698	3.397852	O	7.677091	3.030348	10.464935
H	4.205533	5.308114	2.938910	H	8.307443	6.078222	4.902161	O	10.751419	0.003493	8.951078
H	0.720795	1.810417	0.169993	H	5.931838	9.746444	2.131301	O	6.028929	1.312614	6.177538
H	3.751291	1.282363	2.558371	H	8.983151	9.414810	2.089050	O	7.384673	0.040631	9.019876
H	4.742966	2.283248	5.328952	H	8.623838	9.056689	4.861184	O	5.969568	4.679585	6.247850
O	3.068412	-0.019599	-0.012731	H	6.369443	6.001384	3.446775	H	2.942670	10.760194	6.786704
O	0.018044	2.976030	2.759175	H	5.996458	11.686590	0.678295	H	1.251926	9.061374	9.558044
O	2.989577	1.695911	2.101981	H	6.707059	10.340421	0.225615	H	4.259045	6.053103	9.827282
O	4.325770	3.042897	4.872432	H	7.688174	11.320801	2.997699	H	-0.060066	7.773932	7.058141
O	2.981173	4.369586	2.147057	H	10.734068	9.831743	5.334990	H	2.965659	6.741599	6.166406
O	1.652528	3.035858	4.920278	H	8.220447	7.301129	2.562337	H	5.270341	9.060056	8.941458
O	4.727740	0.000226	3.405674	H	10.197515	11.334619	2.944293	H	2.284608	6.075853	10.442111
O	0.006206	1.318786	0.633670	H	6.711617	7.830611	0.170167	H	-0.092332	9.748311	7.673000
O	1.360141	0.043513	3.474767	H	9.740826	7.307175	2.558594	H	2.957382	9.411640	7.630059
O	-0.054968	4.685557	0.703523	H	10.734736	8.311193	5.330083	H	2.600444	9.051801	10.401920
H	8.998291	4.738055	1.243675	O	9.058359	6.004598	-0.012101	H	0.345132	5.999924	8.989082
H	7.307485	3.038939	4.016829	O	6.012226	8.995741	2.760170	H	-0.023376	11.687841	6.219732
H	10.317622	0.033975	4.288931	O	8.979928	7.721735	2.101692	H	0.686524	10.340809	5.767528
H	5.997397	1.748915	1.515286	O	10.316781	9.070673	4.873896	H	1.662220	11.319891	8.538674
H	9.021328	0.721440	0.628082	O	8.975503	10.394701	2.151422	H	4.710310	9.824043	10.878437
H	11.325445	3.041178	3.397220	O	7.643938	9.056956	4.923132	H	2.196156	7.297267	8.102845
H	8.342693	0.052938	4.903791	O	10.715760	6.025799	3.406503	H	4.173699	11.329160	8.485054
H	5.964854	3.723268	2.130697	O	5.996841	7.339457	0.633942	H	0.687216	7.830341	5.713795
H	9.012430	3.389982	2.088359	O	7.350349	6.067873	3.474397	H	3.716636	7.304840	8.098808
H	8.655703	3.031456	4.860900	O	5.936134	10.705190	0.705189	H	4.711829	8.303485	10.872912
H	6.403598	-0.024950	3.449574	H	2.974867	4.735452	6.784675	O	3.034811	6.001281	5.528455
H	6.030718	5.663522	0.677117	H	1.284873	3.039436	9.557970	O	-0.013345	8.998022	8.302548
H	6.740933	4.316974	0.224799	H	4.294096	0.028498	9.829682	O	2.955234	7.718573	7.642048
H	7.720220	5.299024	2.995447	H	-0.025240	1.749848	7.057827	O	4.293708	9.062893	10.416776
H	10.765471	3.806364	5.334575	H	3.000398	0.717287	6.168123	O	2.949671	10.391495	7.692594
H	8.252103	1.275004	2.565041	H	5.303417	3.035462	8.941214	O	1.620563	9.054890	10.463929
H	10.228298	5.308500	2.942618	H	2.319508	0.051727	10.444261	O	4.693113	6.023929	8.946658
H	6.743839	1.806029	0.170704	H	-0.060595	3.724108	7.673185	O	-0.028374	7.340123	6.177469
H	9.772648	1.284789	2.560203	H	2.990651	3.387503	7.629162	O	1.326156	6.065814	9.015221
H	10.767964	2.285802	5.330033	H	2.633444	3.030510	10.401738	O	-0.084146	10.706460	6.246675
O	9.091934	-0.018401	-0.010308	H	0.379712	-0.022725	8.992212	H	8.967908	10.760960	6.789676
O	6.044179	2.972751	2.759886	H	0.006139	5.664128	6.220315	H	7.275214	9.061560	9.559079
O	9.010367	1.697259	2.103731	H	0.716973	4.318172	5.767277	H	10.283704	6.053488	9.829284
O	10.348959	3.044661	4.873832	H	1.694969	5.296465	8.536320	H	5.965082	7.770761	7.059490
O	9.005699	4.369961	2.149732	H	4.744486	3.801249	10.878047	H	8.988740	6.742103	6.169701
O	7.675840	3.033175	4.922874	H	2.231159	1.272593	8.104941	H	11.293985	9.064299	8.940432
O	10.750922	0.005223	3.407912	H	4.206325	5.306358	8.482585	H	8.309110	6.076060	10.445361
O	6.028871	1.315244	0.634553	H	0.721689	1.807898	5.713166	H	5.930479	9.745153	7.673831
O	7.384549	0.041793	3.477139	H	3.751626	1.280505	8.100669	H	8.982934	9.412502	7.633266
O	5.970077	4.682148	0.704149	H	4.744134	2.280623	10.873247	H	8.624048	9.055172	10.402462
H	2.941825	10.762447	1.243084	O	3.069528	-0.023047	5.530188	H	6.369671	5.999704	8.990825
H	1.251618	9.063618	4.015326	O	0.019474	2.973758	8.302488	H	5.996727	11.683951	6.220425
H	4.258743	6.054415	4.283830	O	2.990080	1.693904	7.643856	H	6.707800	10.337619	5.768551
H	-0.061039	7.776727	1.515026	O	4.326860	3.040318	10.416891	H	7.688070	11.319265	8.540889
H	2.964208	6.744409	0.623626	O	2.982111	4.367387	7.690766	H	10.734912	9.829325	10.877635
H	5.271239	9.060247	3.397858	O	1.653582	3.033659	10.463840	H	8.220188	7.298762	8.105991
H	2.284125	6.077534	4.899095	O	4.727832	-0.000865	8.948897	H	10.198116	11.332596	8.487814
H	-0.093053	9.750641	2.130292	O	0.007081	1.316403	6.177013	H	6.712596	7.827862	5.715396
H	2.956634	9.413721	2.086321	O	1.360843	0.042079	9.017882	H	9.740642	7.305263	8.101171
H	2.600161	9.053490	4.858961	O	-0.054059	4.682704	6.246674	H	10.734696	8.308677	10.872808
H	0.344177	6.001397	3.446925	H	8.997817	4.735950	6.787568	O	9.057822	6.001681	5.531842
H	-0.024518	11.690162	0.676454	H	7.308374	3.035989	9.559035	O	6.010989	8.995061	8.303447
H	0.685193	10.343151	0.224152	H	10.318128	0.032678	9.832079	O	8.979270	7.719617	7.644868
H	1.661506	11.321531	2.995217	H	5.997012	1.745980	7.058395	O	10.317358	9.068390	10.416491
H	4.709602	9.825619	5.333581	H	9.022887	0.718355	6.171100	O	8.975735	10.392418	7.695606
H	2.195252	7.299058	2.560628	H	11.326829	3.038871	8.940483	O	7.644208	9.055479	10.464850
H	4.173489	11.330607	2.941404	H	8.342906	0.051627	10.446722	O	10.716735	6.024238	8.948156
H	0.685759	7.833194	0.170465	H	5.964200	3.720457	7.674090	O	5.997407	7.336957	6.178836
H	3.715728	7.306587	2.556178	H	9.012799	3.387725	7.631959	O	7.350631	6.065854	9.018405
H	4.711434	8.305114	5.329429	H	8.656934	3.028783	10.402769	O	5.936366	10.702546	6.247171

Table S32: 9C1 Structure

				A	1.20650438E+01	0.00000000E+00	0.00000000E+00				
				B	-1.21605335E-02	1.20656462E+01	0.00000000E+00				
				C	-5.10700267E-02	4.51657026E-02	1.10750017E+01				
H	4.235163	0.054293	4.285411	O	3.033432	6.069104	-0.022695	H	6.384400	0.020832	9.016786
H	-0.017579	1.819522	1.516195	O	-0.029553	9.072254	2.746900	H	6.046129	5.697069	6.247174
H	1.759587	0.016824	4.271747	O	2.977486	7.756716	2.117160	H	10.799712	3.867659	10.850331
H	0.021998	4.294762	1.503756	O	4.315434	9.120902	4.884977	H	8.241340	1.277544	8.080825
H	3.014752	0.799572	0.590627	O	3.048209	10.426512	2.066943	H	10.279638	5.363650	8.477655
H	5.246900	3.059756	3.357916	O	1.645960	9.048356	4.836042	H	6.743158	1.797059	5.708893
H	3.058523	5.319677	0.613568	O	4.708969	6.070072	3.426412	H	8.296766	4.791200	8.081500
H	0.726502	3.014659	3.383695	O	-0.004282	7.373036	0.656927	H	7.281899	3.805998	10.849741
H	2.996230	3.412826	2.111788	O	1.349182	6.034474	3.381574	H	9.756670	1.324516	8.102656
H	2.632968	3.074779	4.880527	O	0.028791	10.732618	0.614562	H	10.750202	2.352364	10.871219
H	0.376878	-0.003227	3.479405	H	10.262030	6.091494	4.284855	O	9.045316	0.058540	5.515043
H	0.040918	5.677082	0.710583	H	6.010757	7.849577	1.513510	O	5.985586	3.060843	8.282922
H	4.791371	3.839649	5.311710	H	7.787908	6.048000	4.271680	O	8.994111	1.746412	7.654375
H	2.232749	1.253828	2.543519	H	6.045476	10.325036	1.503017	O	10.329518	3.115847	10.423518
H	4.272844	5.338098	2.939799	H	9.039689	6.833673	0.591293	O	9.065110	4.415991	7.603968
H	0.733532	1.776096	0.172163	H	11.271432	9.095705	3.360005	O	7.660228	3.039023	10.372239
H	2.288595	4.768370	2.543438	H	9.081910	11.353312	0.613753	O	10.720750	0.058749	8.965686
H	1.277609	3.782066	5.313479	H	6.752399	9.046602	3.381781	O	6.011736	1.360133	6.195623
H	3.748103	1.301269	2.565283	H	9.017581	9.448029	2.111601	O	7.361567	0.027135	8.918801
H	4.745117	2.324249	5.332707	H	8.656576	9.112298	4.881206	O	6.041341	4.719774	6.149768
O	3.038401	0.035598	-0.022657	H	6.405034	6.028015	3.479430	H	4.204364	6.111726	9.821252
O	-0.022463	3.040298	2.746819	H	6.065366	11.708048	0.710519	H	-0.049398	7.873293	7.053080
O	2.985389	1.722968	2.117130	H	10.816956	9.876299	5.313808	H	1.729104	6.071526	9.809604
O	4.322813	3.086849	4.884940	H	8.256949	7.286462	2.543965	H	-0.011631	10.348504	7.041570
O	3.056851	4.392511	2.066299	H	10.297414	11.369918	2.940927	H	2.982480	6.855113	6.128265
O	1.653279	3.014076	4.835667	H	6.761511	7.808244	0.169406	H	5.213435	9.116104	8.895167
O	4.714172	0.035866	3.427734	H	8.312544	10.805078	2.543537	H	3.024448	11.374902	6.151499
O	0.001468	1.340103	0.658698	H	7.298741	9.816107	5.312471	H	0.694110	9.070876	8.921035
O	1.354057	0.002888	3.381339	H	9.771958	7.338844	2.564966	H	2.960280	9.469739	7.649910
O	0.037373	4.699796	0.613215	H	10.767773	8.361056	5.333949	H	2.600139	9.133522	10.418546
H	10.267644	0.054002	4.285459	O	9.065337	6.070137	-0.022468	H	0.346316	6.053310	9.017267
H	6.018057	1.817135	1.514690	O	6.003505	9.070407	2.744735	H	0.007008	11.731448	6.249249
H	7.793153	0.017694	4.271702	O	9.007815	7.758119	2.117075	H	4.759219	9.896445	10.849351
H	6.053266	4.292434	1.503032	O	10.346735	9.124616	4.886765	H	2.199797	7.308604	8.081223
H	9.048006	0.800842	0.591137	O	9.079905	10.427560	2.066035	H	4.239768	11.392560	8.477740
H	11.278385	3.064397	3.359783	O	7.677151	9.049166	4.834928	H	0.701680	7.831828	5.709057
H	9.091138	5.320617	0.613700	O	10.740768	6.073970	3.427040	H	2.254304	10.826559	8.081360
H	6.760115	3.013621	3.382270	O	6.030374	7.370532	0.655871	H	1.244169	9.840069	10.851231
H	9.031169	3.414124	2.111507	O	7.382208	6.033287	3.381340	H	3.714948	7.359490	8.101680
H	8.664499	3.079147	4.881158	O	6.059761	10.730795	0.612747	H	4.711763	8.381068	10.869119
H	6.410158	-0.002103	3.479685	H	4.209446	0.076781	9.822373	O	3.007737	6.091216	5.514936
H	6.072411	5.674955	0.709865	H	-0.042811	1.840902	7.053179	O	-0.054925	9.095083	8.284220
H	10.824617	3.844201	5.313571	H	1.734106	0.039522	9.809634	O	2.951053	7.779598	7.654229
H	8.267037	1.255283	2.543876	H	-0.003297	4.315764	7.041469	O	4.289902	9.144327	10.422156
H	10.305405	5.341532	2.940473	H	2.988553	0.822568	6.128202	O	3.021983	10.449311	7.604174
H	6.768852	1.774890	0.170415	H	5.221350	3.083564	8.895854	O	1.620496	9.072461	10.373354
H	8.322801	4.769011	2.543558	H	3.032769	5.341911	6.151384	O	4.683081	6.093527	8.963459
H	7.306633	3.782772	5.312450	H	0.701727	3.036416	8.921246	O	-0.029813	7.394469	6.195367
H	9.782309	1.302043	2.565382	H	2.970522	3.435536	7.649708	O	1.323480	6.057316	8.919239
H	10.775323	2.328975	5.333628	H	2.607660	3.098647	10.418580	O	0.003127	10.754227	6.151290
O	9.070447	0.037177	-0.022583	H	0.351218	0.019956	9.017502	H	10.236518	6.113868	9.821982
O	6.011266	3.037668	2.745151	H	0.015196	5.698425	6.248831	H	5.984623	7.871463	7.051792
O	9.019729	1.724226	2.117403	H	4.766436	3.863462	10.849419	H	7.761901	6.070731	9.809513
O	10.354419	3.092613	4.886389	H	2.206926	1.276674	8.081450	H	6.019556	10.347131	7.040470
O	9.091250	4.393831	2.066133	H	4.247038	5.361473	8.476894	H	9.013473	6.855848	6.129299
O	7.685074	3.015675	4.835199	H	0.707787	1.797855	5.708811	H	11.246018	9.119181	8.897258
O	10.746517	0.035697	3.427677	H	2.262912	4.791168	8.081242	H	9.056780	11.374746	6.151490
O	6.037397	1.337969	0.657045	H	1.251927	3.805515	10.850937	H	6.726647	9.069652	8.918939
O	7.387305	0.004180	3.381414	H	3.722310	1.324083	8.102621	H	8.991995	9.470344	7.650019
O	6.067700	4.697672	0.612542	H	4.719742	2.348058	10.869780	H	8.631432	9.136080	10.417707
H	4.230244	6.088391	4.284193	O	3.012386	0.058566	5.514956	H	6.379091	6.050995	9.017025
H	-0.023775	7.851544	1.514834	O	-0.047210	3.061583	8.284316	H	6.039554	11.730345	6.248350
H	1.754884	6.048576	4.271918	O	2.959424	1.745819	7.654795	H	10.791702	9.900465	10.851083
H	0.013936	10.326670	1.504727	O	4.297519	3.110968	10.422498	H	8.231125	7.308699	8.082021
H	3.008377	6.832785	0.590911	O	3.031126	4.415234	7.604101	H	10.271865	11.392759	8.479082
H	5.239297	9.092996	3.357672	O	1.628014	3.037429	10.373616	H	6.735654	7.830150	5.707771
H	3.050681	11.352130	0.614086	O	4.688346	0.058549	8.964625	H	8.287074	10.827611	8.081510
H	0.719520	9.047509	3.383647	O	-0.024118	1.361765	6.195543	H	7.273462	9.839408	10.849195
H	2.986566	9.446951	2.112770	O	1.328380	0.025890	8.919318	H	9.746183	7.360942	8.102452
H	2.625601	9.109540	4.881176	O	0.011699	4.721188	6.151084	H	10.742418	8.385230	10.870768
H	0.372044	6.030805	3.479828	H	10.241657	0.077539	9.823359	O	9.039383	6.092344	5.515489
H	0.032702	11.709821	0.712731	H	5.992205	1.839487	7.053156	O	5.977548	9.093140	8.282108
H	4.784446	9.873276	5.312045	H	7.767208	0.041230	9.809162	O	8.981909	7.780385	7.654961
H	2.226073	7.285837	2.543982	H	6.027185	4.314595	7.040294	O	10.321491	9.148937	10.423754
H	4.265678	11.369722	2.941004	H	9.022770	0.822500	6.128392	O	9.054485	10.449868	7.604298
H	0.727190	7.810653	0.170824	H	11.253550	3.086079	8.897150	O	7.652016	9.072684	10.371442
H	2.280349	10.803749	2.543880	H	9.065015	5.342647	6.151476	O	10.715208	6.096030	8.964131
H	1.269634	9.816099	5.313727	H	6.734645	3.036962	8.919802	O	6.004411	7.392444	6.194140
H	3.741296	7.336410	2.564595	H	9.005123	3.436255	7.649275	O	7.356284	6.055951	8.919152
H	4.737390	8.357860	5.332257	H	8.639675	3.102426	10.418145	O	6.033910	10.753120	6.150291

Table S33: 9C2 Structure

				A	1.20645786E+01	0.00000000E+00	0.00000000E+00				
				B	-8.59702480E-02	1.20647442E+01	0.00000000E+00				
				C	-6.65345502E-02	6.44517368E-02	1.10693410E+01				
H	4.253413	0.029884	4.287896	O	2.971963	6.055242	-0.027104	H	11.632361	0.048669	9.023211
H	-0.006928	1.788486	1.518204	O	-0.082800	9.091362	2.739878	H	6.021420	0.439958	6.257004
H	1.783717	0.071239	4.266091	O	2.979505	7.756028	2.088663	H	6.694890	4.375172	5.699803
H	-0.062100	4.256676	1.498385	O	4.249153	9.071050	4.857157	H	7.660816	5.377152	8.468178
H	3.024087	0.771322	0.607145	O	2.877201	10.426885	2.071387	H	10.698880	3.845229	10.836958
H	5.244050	3.042846	3.374628	O	1.577823	9.154293	4.837410	H	8.253119	1.346200	8.070825
H	2.945848	5.291208	0.591370	O	4.612522	6.050884	3.395282	H	7.235236	2.400000	10.860706
H	0.724923	3.089410	3.358061	O	-0.032884	7.418401	0.626556	H	9.673006	4.819572	8.092768
H	3.002966	3.415423	2.110159	O	1.247676	6.087314	3.415714	H	9.769147	1.298962	8.068535
H	2.600065	3.044165	4.877090	O	-0.093718	10.783016	0.649354	H	10.754201	2.329364	10.834081
H	5.634157	0.015317	3.489800	H	10.242803	6.064586	4.286163	O	9.014603	0.055320	5.508079
H	0.019043	0.408075	0.720060	H	5.983129	7.820876	1.520294	O	5.962633	3.091683	8.274934
H	0.698825	4.341338	0.165579	H	7.774185	6.104552	4.267065	O	9.022286	1.757025	7.622734
H	1.661745	5.342602	2.932243	H	5.922727	10.290083	1.499401	O	10.292010	3.073963	10.388859
H	4.697694	3.808798	5.304484	H	9.012371	6.804815	0.607068	O	8.919370	4.427619	7.605850
H	2.254365	1.311571	2.536629	H	11.233136	9.078303	3.373608	O	7.620803	3.157263	10.374397
H	1.233792	2.363656	5.324069	H	8.933521	11.324645	0.591330	O	10.653950	0.051352	8.929661
H	3.674788	4.785699	2.557746	H	6.712592	9.124506	3.358744	O	6.012676	1.418242	6.162628
H	3.770471	1.264390	2.534610	H	8.988584	9.450018	2.110102	O	7.289007	0.091559	8.952342
H	4.757460	2.293137	5.302805	H	8.588217	9.083094	4.876766	O	5.947131	4.783335	6.183599
O	3.014366	0.022832	-0.026952	H	11.622563	6.047656	3.486830	H	4.177361	6.096468	9.821519
O	-0.038778	3.058651	2.739317	H	6.009198	6.440563	0.721588	H	-0.081406	7.852374	7.053189
O	3.023644	1.722603	2.088876	H	6.684582	10.375579	0.167390	H	1.707850	6.136273	9.800439
O	4.293044	3.036060	4.856961	H	7.650167	11.377008	2.934567	H	-0.138538	10.321323	7.034154
O	2.921411	4.393432	2.070844	H	10.687773	9.844746	5.304309	H	2.946478	6.836060	6.141332
O	1.621638	3.119521	4.837292	H	8.242066	7.345370	2.536981	H	5.169868	9.108644	8.909216
O	4.655821	0.017317	3.395561	H	7.224075	8.399477	5.324736	H	2.868543	11.354767	6.127009
O	0.009097	1.386296	0.625805	H	9.661713	10.819529	2.557637	H	0.649900	9.154890	8.893960
O	1.290263	0.055858	3.416337	H	9.758089	7.299675	2.533568	H	2.924664	9.481296	7.646123
O	-0.048768	4.750483	0.648801	H	10.743323	8.329000	5.300996	H	2.523990	9.111044	10.412802
H	10.285832	0.031222	4.286770	O	9.004056	6.056366	-0.027012	H	5.557690	6.081023	9.022941
H	6.027116	1.788854	1.519338	O	5.948526	9.091880	2.740594	H	-0.055260	6.472735	6.253615
H	7.816740	0.072706	4.267691	O	9.010526	7.757326	2.088623	H	0.620974	10.406428	5.700634
H	5.965541	4.257149	1.498895	O	10.280986	9.073554	4.855955	H	1.584148	11.408964	8.467946
H	9.055339	0.772441	0.607657	O	8.907627	10.428038	2.071078	H	4.621536	9.874597	10.837760
H	11.276987	3.045603	3.372868	O	7.609625	9.156522	4.838007	H	2.176911	7.376871	8.071108
H	8.976901	5.292107	0.591217	O	10.644188	6.051034	3.393428	H	1.158427	8.429610	10.860499
H	6.756268	3.091428	3.358558	O	6.000739	7.418882	0.627841	H	3.597199	10.851237	8.093772
H	9.032358	3.416647	2.109564	O	7.280148	6.089035	3.417584	H	3.692974	7.330740	8.068414
H	8.631944	3.050440	4.876221	O	5.936051	10.783862	0.649807	H	4.680717	8.358974	10.836021
H	11.665755	0.015226	3.487494	H	4.219721	0.063519	9.822365	O	2.938110	6.087094	5.507850
H	6.053071	0.408323	0.721235	H	-0.039238	1.820600	7.053321	O	-0.113538	9.123298	8.274910
H	6.727265	4.343224	0.166730	H	1.750181	0.105405	9.800701	O	2.945702	7.788590	7.623157
H	7.693505	5.344177	2.933763	H	-0.094576	4.289577	7.032103	O	4.216692	9.102090	10.390031
H	10.731565	3.812643	5.302619	H	2.991097	0.802739	6.141058	O	2.843281	10.459325	7.607306
H	8.285424	1.312500	2.537313	H	5.213551	3.075778	8.908138	O	1.545482	9.185954	10.373849
H	7.267997	2.366830	5.324743	H	2.912139	5.323284	6.126629	O	4.579365	6.083234	8.929045
H	9.705011	4.786466	2.556887	H	0.692785	3.122758	8.892609	O	-0.065987	7.451072	6.160438
H	9.801477	1.266262	2.534014	H	2.969593	3.447788	7.644886	O	1.214462	6.120032	8.950684
H	10.786981	2.296770	5.300524	H	2.567234	3.077070	10.411356	O	-0.126426	10.815134	6.184538
O	9.046677	0.024226	-0.026778	H	5.600490	0.048748	9.024256	H	10.209435	6.097752	9.821128
O	5.992239	3.058623	2.740331	H	-0.013846	0.439969	6.255319	H	5.952416	7.852970	7.054730
O	9.054085	1.724090	2.088914	H	0.665512	4.373695	5.698837	H	7.740373	6.138060	9.801153
O	10.324803	3.041116	4.854868	H	1.628468	5.374974	8.467630	H	5.892355	10.321638	7.035026
O	8.951178	4.394687	2.070272	H	4.664091	3.841293	10.836976	H	8.979612	6.837297	6.141492
O	7.653328	3.123798	4.837720	H	2.221124	1.344400	8.070232	H	11.202054	9.109917	8.908215
O	10.687349	0.018037	3.394065	H	1.201111	2.396434	10.858796	H	8.901256	11.356414	6.127074
O	6.044571	1.386609	0.626984	H	3.641559	4.817978	8.092718	H	6.682155	9.156364	8.894950
O	7.322758	0.057273	3.418167	H	3.737184	1.297071	8.068248	H	8.955556	9.483162	7.646030
O	5.978574	4.750994	0.649368	H	4.724162	2.325651	10.834846	H	8.555958	9.114899	10.413350
H	4.210303	6.063772	4.287673	O	2.981502	0.053520	5.507828	H	11.589559	6.081046	9.022178
H	-0.049615	7.820157	1.519109	O	-0.070794	3.091861	8.273742	H	5.977156	6.473000	6.255571
H	1.741111	6.103264	4.265472	O	2.990410	1.755090	7.622224	H	6.651945	10.407168	5.701629
H	-0.106885	10.289386	1.499070	O	4.259900	3.068646	10.388921	H	7.616415	11.411008	8.469210
H	2.980820	6.803895	0.606741	O	2.887882	4.425802	7.606127	H	10.655410	9.876209	10.837840
H	5.200354	9.077388	3.374931	O	1.588751	3.152639	10.372444	H	8.209237	7.378468	8.071162
H	2.901770	11.323492	0.591467	O	4.622135	0.050399	8.930060	H	7.191715	8.431697	10.861788
H	0.681035	9.123122	3.358413	O	-0.023975	1.418217	6.161015	H	9.628444	10.852719	8.093997
H	2.958459	9.448876	2.110499	O	1.256639	0.089531	8.951019	H	9.725219	7.332945	8.068277
H	2.556316	9.079738	4.877057	O	-0.081820	4.783029	6.182327	H	10.711205	8.360475	10.835089
H	5.590812	6.048179	3.489453	H	10.252085	0.064972	9.822192	O	8.971623	6.088355	5.508009
H	-0.022306	6.440097	0.720150	H	5.997045	1.820729	7.054901	O	5.918834	9.123634	8.275841
H	0.654262	10.374121	0.166559	H	7.782762	0.107249	9.801983	O	8.977808	7.790529	7.623108
H	1.618023	11.375743	2.932789	H	5.935460	4.289766	7.033310	O	10.248716	9.104808	10.389753
H	4.654529	9.843121	5.305190	H	9.023535	0.804422	6.141425	O	8.874466	10.461194	7.607280
H	2.210466	7.344364	2.536208	H	11.244890	3.078827	8.907174	O	7.577365	9.188688	10.375092
H	1.190768	8.397879	5.323986	H	8.945092	5.324501	6.126801	O	10.611198	6.084171	8.928581
H	3.630944	10.818784	2.558137	H	6.725810	3.124807	8.894213	O	5.968132	7.451327	6.162101
H	3.726573	7.298197	2.534355	H	9.000772	3.449599	7.644774	O	7.246981	6.122199	8.951318
H	4.712941	8.327484	5.302519	H	8.599449	3.083634	10.412625	O	5.904376	10.815594	6.185493