Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Hydrogen-bonded intermediate and transition states during spontaneous and acid-catalized hydrolysis of the carcinogen (+)-*anti*-BPDE

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Supplementary material

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Table S1: Experimentally determined activation energies for BPDE hydrolysis under various conditions.

Spontaneous	water	22.25 kcal/mol	Whalen [1]
Spontaneous*[a]	water	21.33 kcal/mol	Michaud [2]
Acid catalyzed	Hydronium	13.15 kcal/mol	Whalen [1]
Buffer catalyzed	Sodium cacodylate	14.20 kcal/mol	Geacintov [3]

[a] *BPDE was in the conformation it takes on when intercalated in DNA

Activation barriers of Table were calculated in this work based on their corresponding experimental (kinetic) data [1, 2] using the formula

$$k = \frac{k_B T}{c^0 h} e^{-\Delta G‡/K_B T} \tag{1}$$

which was inverted to find $\Delta G‡$ in terms of k, where k is the reaction rate, c^0 is the standard concentration of 1 M, k_B is Boltzmann's constant, and h is Planck's constant.

Table S2: $\Delta E^{KS}‡$ and $\Delta G‡$ for three predicted transition states associated with (+)-*anti*-BPDE hydrolysis [kcal mol^{-1}]. Energy differences defined in footnote.[a]

	XC	6-311g*						6-311+g*					
		$\Delta E^{KS}‡$[a]	$\Delta Z‡$	$\Delta H‡$	$-T\Delta S‡$	$\Delta G‡$[a]	$\Delta G‡$[s]	$\Delta E^{KS}‡$[a]	$\Delta Z‡$	$\Delta H‡$	$-T\Delta S‡$	$\Delta G‡$[a]	$\Delta G‡$[s]
TS1	BPW91	41.79	-0.06	41.37	8.98	50.36	48.47	36.55	0.03	36.44	8.11	44.55	42.66
	BLYP	35.12	0.69	35.25	9.62	44.87	42.98	28.82	0.11	28.78	8.46	37.24	35.35
	B1LYP	41.78	0.45	41.64	9.78	51.42	49.53	34.65	0.85	34.83	9.95	44.78	42.89
	B3LYP	41.30	0.57	41.21	9.88	51.09	49.20	34.69	0.24	34.74	8.21	42.96	41.07
TS2	BPW91	22.30	0.12	21.32	10.84	32.16	30.27	25.22	-0.34	23.85	10.41	34.25	32.36
	BLYP	17.93	-0.04	16.77	10.75	27.52	25.63	19.52	-1.25	17.48	9.72	27.20	25.31
	B1LYP	25.90	0.32	25.15	10.45	35.60	33.71	26.13	0.72	25.69	10.61	36.31	34.42
	B3LYP	24.75	0.33	23.95	10.59	34.55	32.66	25.27	-0.11	24.05	10.46	34.51	32.62
TS3	BPW91	7.33	-1.80	5.55	12.17	17.72	15.83	10.83	-2.23	8.83	11.48	20.31	18.42
	BLYP	4.28	-1.87	2.60	11.53	14.12	12.23	6.17	-2.27	4.18	11.26	15.44	13.55
	B1LYP	10.02	-2.36	7.97	11.27	19.24	17.39	11.44	-1.94	9.69	11.51	21.20	19.31
	B3LYP	9.04	-2.20	7.08	11.45	18.52	16.63	10.69	-2.51	8.48	11.09	19.56	17.67

[a] $\Delta E^{KS}‡ = \sum(E_e^{KS})_{TS\ Species} - \sum(E_e^{KS})_{Reactants}$, $\Delta G‡ = \sum(E_e^{KS} + G_{corr})_{TS\ Species} - \sum(E_e^{KS} + G_{corr})_{Reactants}$

[s] Includes −1.89 kcal/mol correction to entropy and free energy to account for change in standard conditions in the gas phase to standard conditions in the solvated phase.

The computationally determined values of $\Delta G‡$ reproduced the main trends of the experimental values and, at the same time, were somewhat higher than these. With the 6-311g* basis set, the error was around 1-5 kcal mol^{-1} for cacodylic acid catalyzed hydrolysis and 5-10 kcal mol^{-1} for spontaneous hydrolysis. The error was slightly larger with the 6-311+g* basis set, possibly because of the interaction of the extra diffuse orbitals with the implicit solvation model. In both cases, spontaneous and acid catalized, the BLYP/6-311g* and BLYP/6-311+g* functional/basis set combination (displayed in bold in Table) produced the best agreement with experiment.

Table S3: Energies of **HB...BPDE** relative to those of non-interacting (+)-*anti*-BPDE and cacodylic acid in the solvent phase [kcal mol^{-1}].

	6-311g*						6-311+g*					
	ΔE^{KS}	ΔZ	ΔH	$-T\Delta S$	ΔG	ΔG^s	ΔE^{KS}	ΔZ	ΔH	$-T\Delta S$	ΔG	ΔG^s
BPW91	-6.92	1.31	-5.31	11.48	6.17	4.28	-3.78	0.84	-2.47	10.06	7.59	5.70
BLYP	-8.96	1.31	-7.32	11.37	4.06	2.17	-4.85	0.81	-3.55	9.93	6.39	4.50
B1LYP	-9.47	1.29	-7.80	11.15	3.34	1.45	-5.93	1.70	-3.96	11.39	7.42	5.33
B3LYP	-9.44	1.22	-7.84	10.72	2.88	0.99	-5.83	1.09	-4.37	10.69	6.33	4.44

[s] Includes −1.89 kcal/mol correction to entropy and free energy to account for change in standard conditions in the gas phase to standard conditions in the solvated phase.

Table S4: Energies of **H_2O...BPDE** relative to those of its non-interacting components in the solvent phase [kcal mol^{-1}].

	6-311g*						6-311+g*					
	ΔE^{KS}	ΔZ	ΔH	$-T\Delta S$	ΔG	ΔG^s	ΔE^{KS}	ΔZ	ΔH	$-T\Delta S$	ΔG	ΔG^s
BPW91	-4.42	1.70	-2.83	7.72	4.88	2.99	-2.90	1.17	-1.59	6.10	4.51	2.62
B3LYP	-6.01	1.86	-4.34	7.78	3.44	1.55	-4.06	1.37	-2.63	6.34	3.71	1.82

[s] Includes −1.89 kcal/mol correction to entropy and free energy to account for change in standard conditions in the gas phase to standard conditions in the solvated phase.

Table contains the computed energies of the hydrogen bonded **HB...BPDE** complex relative to its separate components (Fig. 4). The negative value of ΔE^{KS} indicates that the hydrogen bond has the effect of lowering the electronic energy of the system. ΔG is positive because the hydrogen bond also corresponds to a decrease in entropy of the entire complex, and thus the Gibbs free energy of the hydrogen bonded complex is between that of the separate components and the transition state. This result holds for both the gas phase and solvated calculations.

If the hydrogen bonded structure were at a Gibbs free energy lower than that corresponding to the sum of the individual reactants and if it forms before an chemical (as opposed to non-covalent) process takes place, this would correspond to an increase in the activation barrier. However, the decrease in enthalpy of the hydrogen bonded complex is more than compensated by a concomitant decrease in entropy.

When water acts as the proton donor, a hydrogen bonded structure can also be found (**H_2O...BPDE**) where water is interacting with O3 (Fig. 3). Table contains the energies of the water/BPDE hydrogen bonded complex relative to the sum of those corresponding to its non-interacting components.

Table S5: ΔG for BPDE hydrolysis [kcal mol^{-1}].

	6-311g*					6-311+g*				
	ΔE^{KS}	ΔZ	ΔH	-TΔS	ΔG	ΔE^{KS}	ΔZ	ΔH	-TΔS	ΔG
BPW91	-18.09	3.70	-15.38	10.64	-4.74	-14.36	3.43	-11.80	10.27	-1.53
BLYP	-19.36	3.79	-16.57	10.61	-5.96	-14.71	3.55	-12.06	10.40	-1.66
B1LYP	-22.63	3.90	-19.72	10.60	-9.12	-18.82	3.67	-16.05	10.36	-5.69
B3LYP	-22.34	3.92	-19.45	10.62	-8.82	-18.31	3.73	-15.53	10.44	-5.09

Table S6: Energies for BPDE-Cacodylic acid hydrogen bonded structure HB...BPDE [Hartrees].

	E^{KS}	Z	Hcorr	Gcorr	E^{KS}	Z	Hcorr	Gcorr
BPW91	-3463.284512	0.372636	0.400244	0.315383	-3463.310438	0.371251	0.399261	0.312014
BLYP	-3462.855784	0.370282	0.398040	0.312854	-3462.886833	0.368927	0.397116	0.309399
B1LYP	-3462.651524	0.385137	0.411950	0.328501	-3462.678735	0.384032	0.411112	0.326260
B3LYP	-3463.280469	0.382855	0.409868	0.325415	-3463.307736	0.381941	0.409129	0.324216

Table S7: Energies for (+)-*anti*-BPDE [Hartrees].

	E^{KS}	Z	Hcorr	Gcorr	E^{KS}	Z	Hcorr	Gcorr
BPW91	-996.337613	0.281862	0.299739	0.238315	-996.356405	0.281307	0.299311	0.237736
BLYP	-996.090562	0.279969	0.297887	0.236482	-996.113028	0.279548	0.297606	0.235946
B1LYP	-995.959720	0.291546	0.308741	0.248693	-995.979432	0.291016	0.308351	0.248034
B3LYP	-996.449192	0.289861	0.307206	0.246959	-996.469152	0.289271	0.306777	0.246149

Table S8: Energies for H_2O [Hartrees].

	E^{KS}	Z	Hcorr	Gcorr	E^{KS}	Z	Hcorr	Gcorr
BPW91	-76.433735	0.020784	0.024563	0.003114	-76.444243	0.020672	0.024451	0.003002
BLYP	-76.423750	0.020546	0.024325	0.002865	-76.436796	0.020442	0.024221	0.002762
B1LYP	-76.411126	0.021426	0.025205	0.003785	-76.421795	0.021315	0.025094	0.003674
B3LYP	-76.442572	0.021308	0.025087	0.003663	-76.453316	0.021194	0.024973	0.003548

Table S9: Energies for Cacodylic acid [Hartrees].

	E^{KS}	Z	Hcorr	Gcorr	E^{KS}	Z	Hcorr	Gcorr
BPW91	-2466.935873	0.088684	0.097943	0.056207	-2466.948013	0.088605	0.097867	0.056165
BLYP	-996.090562	0.279969	0.297887	0.236482	-996.113028	0.279548	0.297606	0.235946
B1LYP	-2466.676721	0.091543	0.100562	0.059397	-2466.689855	0.091407	0.100468	0.059192
B3LYP	-2466.816236	0.091045	0.100113	0.058824	-2466.829297	0.090938	0.100026	0.058698

Table S10: Energies for (7R,8S,9R,10S)-BPT (tetrol) [Hartrees].

	E^{KS}	Z	Hcorr	Gcorr	E^{KS}	Z	Hcorr	Gcorr
BPW91	-1072.800177	0.308548	0.328628	0.262703	-1072.823533	0.307444	0.327839	0.261185
BLYP	-1072.545171	0.306560	0.326671	0.260714	-1072.573262	0.305650	0.326044	0.259498
B1LYP	-1072.406913	0.319189	0.338586	0.274015	-1072.431223	0.318186	0.337856	0.272631
B3LYP	-1072.927368	0.317418	0.336907	0.272164	-1072.951644	0.316410	0.336178	0.270764

Table S11: Energies for transition states [Hartrees].

		E^{KS}	Z	Hcorr	Gcorr	E^{KS}	Z	Hcorr	Gcorr
TS1	BPW91	-1072.704756	0.302550	0.323642	0.255085	-1072.742406	0.302020	0.323584	0.253484
	BLYP	-1072.458345	0.301620	0.322416	0.254886	-1072.503892	0.300159	0.321766	0.252128
	B1LYP	-1072.304272	0.313686	0.333734	0.267854	-1072.346009	0.312646	0.333532	0.264712
	B3LYP	-1072.825945	0.312073	0.332147	0.266216	-1072.867183	0.310855	0.331831	0.262866
TS2	BPW91	-1072.735803	0.302844	0.322736	0.257132	-1072.760460	0.301437	0.321574	0.255135
	BLYP	-1072.485746	0.300455	0.320370	0.254631	-1072.518721	0.297999	0.318575	0.250948
	B1LYP	-1072.329565	0.313485	0.332753	0.267931	-1072.359592	0.312646	0.333532	0.264712
	B3LYP	-1072.852325	0.311690	0.331023	0.266234	-1072.88220	0.310287	0.329808	0.264420
TS3	BPW91	-3463.261806	0.367683	0.394851	0.311078	-3463.287157	0.366351	0.393984	0.309007
	BLYP	-3462.834697	0.365210	0.392753	0.307809	-3462.869274	0.364025	0.391870	0.306263
	B1LYP	-3462.620479	0.379336	0.406040	0.322785	-3462.651061	0.378173	0.405146	0.320742
	B3LYP	-3463.251015	0.377400	0.404180	0.320889	-3463.281408	0.376212	0.403270	0.318983

Table S12: Mulliken and NBO charges for (+)-*anti*-BPDE, **TS1** (Triol), and (7R,8S,9R,10S)-BPT (Tetrol).

	6-311g*						6-31+g*					
	Mulliken			NBO			Mulliken			NBO		
B1LYP	BPDE	Transition	Tetrol	BPDE	Transition	Tetrol	BPDE	Transition	Tetrol	BPDE	Transition	Tetrol
C9	-0.07	-0.11	+0.04	+0.09	+0.07	+0.12	-0.09	-0.44	+0.08	+0.04	+0.01	+0.05
C9,H	+0.17	+0.13	+0.26	+0.29	+0.27	+0.30	+0.14	-0.21	+0.29	+0.29	+0.26	+0.28
C10	-0.23	-0.10	-0.10	+0.09	+0.02	+0.12	-0.72	-0.74	-1.30	+0.04	-0.01	+0.05
C10,H	+0.02	+0.15	+0.14	+0.29	+0.30	+0.31	-0.51	-0.39	-1.08	+0.30	+0.30	+0.30
O3	-0.33	-0.61	-0.62	-0.57	-0.75	-0.76	-0.40	-0.76	-0.73	-0.58	-0.79	-0.80
O4,H	NA	-0.63	NA	NA	-0.83	NA	NA	-0.90	NA	NA	-0.93	NA
BPDE/Triol/Tetrol	0.00	+0.63	0.00	0.00	+0.83	0.00	0.00	+0.90	0.00	0.00	+0.93	0.00
Total	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
B3LYP	BPDE	Transition	Tetrol	BPDE	Transition	Tetrol	BPDE	Transition	Tetrol	BPDE	Transition	Tetrol
C9	-0.07	-0.12	+0.04	+0.09	+0.07	+0.12	-0.09	-0.43	+0.07	+0.04	0.00	+0.04
C9,H	+0.17	+0.12	+0.26	+0.29	+0.27	+0.30	+0.13	-0.21	+0.27	+0.29	+0.26	+0.28
C10	-0.23	-0.10	-0.11	+0.09	+0.01	+0.11	-0.71	-0.79	-1.30	+0.04	-0.02	+0.04
C10,H	+0.02	+0.14	+0.13	+0.29	+0.28	+0.31	-0.50	-0.44	-1.08	+0.29	+0.29	+0.30
O3	-0.33	-0.60	-0.62	-0.57	-0.75	-0.76	-0.39	-0.75	-0.72	-0.58	-0.78	-0.80
O4,H	NA	-0.61	NA	NA	-0.81	NA	NA	-0.89	NA	NA	-0.91	NA
BPDE/Triol/Tetrol	0.00	+0.61	0.00	0.00	+0.81	0.00	0.00	+0.89	0.00	0.00	+0.91	0.00
Total	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00

Table S13: Mulliken and NBO charges for (+)-*anti*-BPDE , **TS2**, and (7R,8S,9R,10S)-BPT (Tetrol).

	6-311g*						6-31+g*					
	Mulliken			NBO			Mulliken			NBO		
B1LYP	BPDE	Transition	Tetrol	BPDE	Transition	Tetrol	BPDE	Transition	Tetrol	BPDE	Transition	Tetrol
C9	-0.07	+0.03	+0.04	+0.09	+0.09	+0.12	-0.09	-0.17	+0.08	+0.04	+0.08	+0.05
C9,H	+0.17	+0.2-	+0.26	+0.29	+0.23	+0.30	+0.14	-0.01	+0.29	+0.29	+0.28	+0.28
C10	-0.23	-0.30	-0.10	+0.09	+0.15	+0.12	-0.72	-1.21	-1.30	+0.04	+0.05	+0.05
C10,H	+0.02	-0.04	+0.14	+0.29	+0.35	+0.31	-0.51	-0.97	-1.08	+0.30	+0.31	+0.30
O3	-0.33	-0.67	-0.62	-0.57	-0.91	-0.76	-0.40	-0.82	-0.73	-0.58	-0.93	-0.80
H+	NA	+0.43	NA	NA	+0.47	NA	NA	+0.57	NA	NA	+0.53	NA
H_2O	NA	+0.01	NA	NA	+0.03	NA	NA	+0.06	NA	NA	+0.04	NA
BPDE/TS2/Tetrol	0.00	-0.01	0.00	0.00	-0.03	0.00	0.00	-0.06	0.00	0.00	-0.04	0.00
Total	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
B3LYP	BPDE	Transition	Tetrol	BPDE	Transition	Tetrol	BPDE	Transition	Tetrol	BPDE	Transition	Tetrol
C9	-0.07	+0.02	+0.04	+0.09	+0.08	+0.12	-0.09	-0.19	+0.07	+0.04	+0.02	+0.04
C9,H	+0.17	+0.19	+0.26	+0.29	+0.23	+0.30	+0.13	-0.03	+0.27	+0.29	+0.23	+0.28
C10	-0.23	-0.31	-0.11	+0.09	+0.13	+0.11	-0.71	-1.20	-1.30	+0.04	+0.07	+0.04
C10,H	+0.02	-0.05	+0.13	+0.29	+0.34	+0.31	-0.50	-0.97	-1.08	+0.29	+0.33	+0.3
O3	-0.33	-0.66	-0.62	-0.57	-0.89	-0.76	-0.39	-0.80	-0.72	-0.58	-0.92	-0.8
H+	NA	+0.43	NA	NA	+0.47	NA	NA	+0.56	NA	NA	+0.52	NA
H_2O	NA	+0.01	NA	NA	+0.03	NA	NA	+0.05	NA	NA	+0.03	NA
BPDE/TS2/Tetrol	0.00	-0.01	0.00	0.00	-0.03	0.00	0.00	-0.05	0.00	0.00	-0.03	0.00
Total	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00

Table S14: Mulliken and NBO charges for (+)-*anti*-BPDE , **TS3**, and (7R,8S,9R,10S)-BPT (Tetrol).

	6-311g*						6-31+g*					
6-311g*	Mulliken			NBO			6-31+g*	Mulliken		NBO		
B1LYP	BPDE	Transition	Tetrol	BPDE	Transition	Tetrol	BPDE	Transition	Tetrol	BPDE	Transition	Tetrol
C9	-0.07	-0.09	+0.04	+0.09	+0.07	+0.12	-0.09	-0.11	+0.08	+0.04	+0.00	+0.05
C9,H	+0.17	+0.13	+0.26	+0.29	+0.25	+0.30	+0.14	+0.09	+0.29	+0.29	+0.23	+0.28
C10	-0.23	-0.17	-0.10	+0.09	+0.11	+0.12	-0.72	-0.37	-1.30	+0.04	+0.03	+0.05
C10,H	+0.02	+0.15	+0.14	+0.29	+0.36	+0.31	-0.51	-0.08	-1.08	+0.30	+0.31	+0.3
O3	-0.33	-0.57	-0.62	-0.57	-0.74	-0.76	-0.40	-0.74	-0.73	-0.58	-0.81	-0.8
H+	NA	+0.44	NA	NA	+0.49	NA	NA	+0.61	NA	NA	+0.53	NA
O4	NA	-0.82	NA	NA	-1.13	NA	NA	-0.88	NA	NA	+0.04	NA
As	NA	+1.23	NA	NA	+2.09	NA	NA	+1.16	NA	NA	+0.62	NA
Total	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
B3LYP	BPDE	Transition	Tetrol	BPDE	Transition	Tetrol	BPDE	Transition	Tetrol	BPDE	Transition	Tetrol
C9	-0.07	-0.10	+0.04	+0.09	+0.06	+0.12	-0.09	-0.10	+0.07	+0.04	0	+0.04
C9,H	+0.17	+0.12	+0.26	+0.29	+0.25	+0.30	+0.13	+0.10	+0.27	+0.29	+0.23	+0.28
C10	-0.23	-0.17	-0.11	+0.09	+0.09	+0.11	-0.71	-0.38	-1.30	+0.04	+0.02	+0.04
C10,H	+0.02	+0.14	+0.13	+0.29	+0.35	+0.31	-0.50	-0.10	-1.08	+0.29	+0.30	+0.30
O3	-0.33	-0.56	-0.62	-0.57	-0.72	-0.76	-0.39	-0.72	-0.72	-0.58	-0.79	-0.80
H+	NA	+0.43	NA	NA	+0.49	NA	NA	+0.60	NA	NA	+0.53	NA
O4	NA	-0.81	NA	NA	-1.12	NA	NA	-0.87	NA	NA	-0.02	NA
As	NA	+1.20	NA	NA	+2.08	NA	NA	+1.14	NA	NA	+0.61	NA
Total	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00

Structural information. Angles ϕ_{1-4} are the dihedrals that the hydroxyl groups make with respect to the six membered ring to which they are attached. Dihedral angles are reported in the range -180 to 180. Hydroxyl are numbered starting at the bottom in counterclockwise order. The atoms involved in the dihedral angles (ϕ) are given below. Fig. S1 displays relevant atom labels.

$$\begin{aligned} \phi_1 &: \mathrm{C}'' - \mathrm{C}' - \mathrm{C7} - \mathrm{O1} \\ \phi_2 &: \mathrm{C}' - \mathrm{C7} - \mathrm{C8} - \mathrm{O2} \\ \phi_3 &: \mathrm{C}'' - \mathrm{C10} - \mathrm{C9} - \mathrm{O3} \\ \phi_4 &: \mathrm{C}' - \mathrm{C}'' - \mathrm{C10} - \mathrm{O4} \end{aligned} \tag{2}$$

(3)

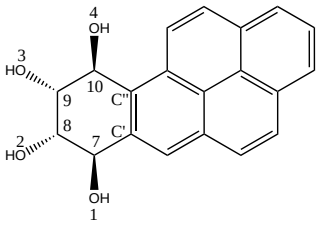

Figure S1: Scheme illustrating labeling convention. Note that only the tetrol has a bound O4 oxygen. For the transition structures, O4 refers to the oxygen that donates a proton to BPDE (either from a water molecule or cacodylic acid). O4 is not present in BPDE by itself.

Table S15: Selected **TS1** geometric parameters. Distances given in Å and angles in degrees.

6-311g*	ϕ_1	ϕ_2	ϕ_3	ϕ_4	C9-C10	C10-O3	C9-03	C10-O4	O4-C10-C9	C10-O4-H
BPW91	-162.769	179.019	-101.589	170.284	1.503	2.407	1.459	2.773	110.278	146.493
BLYP	-162.398	179.502	-93.784	-176.879	1.509	2.429	1.472	2.992	114.644	82.827
B1LYP	164.868	179.603	-98.630	-161.442	1.502	2.376	1.441	2.843	111.667	95.816
B3LYP	-164.529	179.709	-96.572	-164.047	1.502	2.385	1.443	2.867	112.677	92.988
6-311+g*	ϕ_1	ϕ_2	ϕ_3	ϕ_4	C9-C10	C10-O3	C9-03	C10-O4	O4-C10-C9	C10-O4-H
BPW91	-161.897	179.532	-99.477	175.319	1.504	2.409	1.458	2.937	112.519	150.233
BLYP	-162.674	179.600	-93.004	-161.538	15.08	2.428	1.471	2.928	110.457	117.551
B1LYP	-164.698	179.862	-101.977	-160.965	1.507	2.378	1.439	2.871	106.551	149.953
B3LYP	-164.827	179.767	-101.181	-160.511	1.500	2.376	1.442	2.861	107.016	149.070

Table S16: Selected **TS2** geometric parameters. Distances given in Å and angles in degrees.

6-311g*	ϕ_1	ϕ_2	ϕ_3	ϕ_4	C9-C10	C10-O3	C9-03	C10-O4	O4-C10-C9
BPW91	-161.034	-178.101	-80.157	-117.449	1.517	2.354	1.384	2.354	92.690
BLYP	-159.751	-178.295	-82.025	-115.972	1.531	2.384	1.394	2.295	92.926
B1LYP	-158.553	-177.567	-83.442	-114.697	1.530	2.371	1.374	2.281	93.289
B3LYP	-159.055	-177.765	-82.655	-115.550	1.526	2.365	1.376	2.294	93.160
6-311+g*	ϕ_1	ϕ_2	ϕ_3	ϕ_4	C9-C10	C10-O3	C9-03	C10-O4	O4-C10-C9
BPW91	-159.745	-177.189	-85.172	-112.363	1.524	2.381	1.382	2.332	93.304
BLYP	-159.751	-178.295	-82.025	-115.972	1.531	2.384	1.394	2.295	92.926
B1LYP	-157.631	-176.288	-91.659	-108.138	1.539	2.408	1.383	2.215	94.203
B3LYP	-158.049	-176.352	-90.940	-108.560	1.536	2.398	1.384	2.240	94.014

Table S17: Selected **TS3** geometric parameters. Distances given in Å and angles in degrees.

6-311g*	ϕ_1	ϕ_2	ϕ_3	ϕ_4	C9-C10	C10-O3	C9-03	C10-O4	O4-C10-C9	C10-As
BPW91	-168.258	175.424	-96.733	-96.676	1.493	2.226	1.427	3.592	62.003	3.877
BLYP	-163.233	176.348	-93.928	-97.057	1.496	2.141	1.435	3.586	62.679	3.918
B1LYP	-162.478	175.990	-94.134	-96.894	1.483	2.086	1.412	3.542	62.979	3.884
B3LYP	-162.688	176.053	-94.134	-97.233	1.483	2.087	1.414	3.537	63.202	3.879
6-311+g*	ϕ_1	ϕ_2	ϕ_3	ϕ_4	C9-C10	C10-O3	C9-03	C10-O4	O4-C10-C9	C10-As
BPW91	-163.381	176.856	-94.589	-97.475	1.489	2.171	1.426	3.595	63.672	3.954
BLYP	-162.289	176.563	-94.913	-96.247	1.498	2.173	1.431	3.659	62.602	4.026
B1LYP	-161.913	177.255	-94.954	-95.799	1.489	2.157	1.406	3.622	62.339	3.977
B3LYP	-162.159	177.051	-94.888	-96.351	1.488	2.146	1.408	3.610	62.759	3.968

Table S18: Selected (+)-*anti*-BPDE geometric parameters. Distances given in Å and angles in degrees.

6-311g*	ϕ_1	ϕ_2	ϕ_3	C9-C10	C10-O3	C9-03
BPW91	-162.462	177.718	-106.133	1.469	1.468	1.450
BLYP	-161.802	176.822	-106.025	1.462	1.485	1.462
B1LYP	-161.524	176.344	-105.966	1.469	1.454	1.439
B3LYP	-161.652	176.533	-106.015	1.470	1.456	1.440
6-311+g*	ϕ_1	ϕ_2	ϕ_3	C9-C10	C10-O3	C9-03
BPW91	-161.602	176.005	-106.111	1.472	1.472	1.512
BLYP	-160.584	174.697	-105.957	1.491	1.491	1.464
B1LYP	-160.683	174.782	-105.951	1.440	1.458	1.440
B3LYP	-160.804	174.929	-105.993	1.460	1.460	1.441

Table S19: Selected (7R,8S,9R,10S)-BPT (Tetrol) geometric parameters. Distances given in Å and angles in degrees.

6-311g*	ϕ_1	ϕ_2	ϕ_3	ϕ_4	C9-C10	C10-O3	C9-03	C10-O4	O4-C10-C9
BPW91	-149.524	170.982	-81.529	111.275	1.538	2.410	1.434	1.448	109.766
BLYP	-148.611	170.434	-81.942	111.599	1.545	2.421	1.446	1.461	109.467
B1LYP	-147.853	170.857	-80.857	111.222	1.532	2.393	1.426	1.438	109.628
B3LYP	-148.151	170.884	-81.042	111.310	1.533	2.395	1.427	1.439	109.642
6-311+g*	ϕ_1	ϕ_2	ϕ_3	ϕ_4	C9-C10	C10-O3	C9-03	C10-O4	O4-C10-C9
BPW91	-147.100	169.175	-79.147	107.564	1.537	2.404	1.437	1.452	109.613
BLYP	-145.355	154.481	-78.981	107.072	1.544	2.415	1.450	1.467	109.260
B1LYP	-145.704	169.183	-78.750	107.876	1.532	2.389	1.428	1.441	109.442
B3LYP	-145.970	155.240	-78.844	107.866	1.532	2.391	1.429	1.442	109.453

Table S20: As-C10 distances for hydrogen bonded (**HB...BPDE**) and **TS3** structures.

	6-311g*		6-311+g*	
	HB...BPDE	**TS3**	**HB...BPDE**	**TS3**
BPW91	3.985	3.877	4.071	3.954
BLYP	4.018	3.918	4.128	4.026
B1LYP	3.991	3.884	4.073	3.977
B3LYP	4.005	3.879	4.071	3.968

Table S21: BPW91 6-311g* **TS1** coordinates (Å).

Atom	x	y	z
C	-1.916179	0.807790	0.125517
C	-0.921177	1.716607	-0.152883
C	0.439217	1.277392	-0.403596
C	0.721059	-0.157246	-0.421019
C	2.029027	-0.666781	-0.670956
C	2.262788	-2.027226	-0.676767
C	1.222765	-2.972686	-0.425532
C	1.448664	-4.370483	-0.427361
C	0.409506	-5.263612	-0.160255
C	-0.877636	-4.788220	0.115002
C	-1.149738	-3.402567	0.128042
C	-2.454284	-2.886436	0.409228
C	-2.698602	-1.530505	0.415702
C	-1.660474	-0.592952	0.142545
C	-0.337481	-1.074681	-0.142449
C	-0.089577	-2.480265	-0.147675
C	1.456378	2.206292	-0.593047
C	1.236520	3.685830	-0.444312
C	-0.060958	4.033011	0.283669
C	-1.218441	3.187656	-0.281784
O	1.113360	4.276642	-1.772314
O	-0.367615	5.423558	0.174942
O	-2.445890	3.521196	0.359264
H	-2.928642	1.165502	0.316098
H	2.864882	0.032618	-0.840627
H	3.271867	-2.399801	-0.871016
H	2.451884	-4.746078	-0.639848
H	0.600975	-6.337810	-0.165579
H	-1.687280	-5.491217	0.322495
H	-3.263060	-3.588910	0.621632
H	-3.701173	-1.155476	0.630930
H	2.497083	1.896858	-0.816020
H	2.095643	4.139815	0.075025
H	0.041115	3.813731	1.357178
H	-1.286360	3.417010	-1.365781
H	-0.113940	5.670399	-0.738111
H	-2.477516	4.496809	0.346407
H	4.883090	1.028846	-0.459933
O	4.169444	1.644588	-0.707940
H	2.009735	4.401714	-2.128387

Table S22: BPW91 6-311+g* **TS1** coordinates (Å).

Atom	x	y	z
C	-1.919964	0.810197	0.118197
C	-0.927194	1.719413	-0.155458
C	0.439511	1.279244	-0.392963
C	0.721507	-0.160493	-0.412174
C	2.024925	-0.671404	-0.662852
C	2.257408	-2.034509	-0.666191
C	1.216545	-2.976322	-0.416200
C	1.440485	-4.375659	-0.416487
C	0.398925	-5.267436	-0.154540
C	-0.888649	-4.788349	0.114283
C	-1.157503	-3.401287	0.125148
C	-2.461437	-2.884087	0.399567
C	-2.704253	-1.525981	0.404516
C	-1.662977	-0.593015	0.137012
C	-0.339953	-1.076278	-0.140402
C	-0.095039	-2.481518	-0.145076
C	1.454321	2.206806	-0.557450
C	1.227078	3.689490	-0.443321
C	-0.071128	4.039252	0.285506
C	-1.229773	3.191230	-0.275015
O	1.104435	4.250618	-1.783084
O	-0.373456	5.431305	0.182038
O	-2.459940	3.505029	0.376820
H	-2.934603	1.163394	0.304406
H	2.867935	0.017605	-0.834436
H	3.266515	-2.406877	-0.860796
H	2.444194	-4.752750	-0.624337
H	0.588276	-6.341961	-0.158633
H	-1.700994	-5.489370	0.318351
H	-3.273014	-3.584694	0.607726
H	-3.707528	-1.149890	0.614066
H	2.498302	1.900419	-0.743867
H	2.081621	4.160360	0.067109
H	0.039194	3.824118	1.358707
H	-1.317245	3.424714	-1.355774
H	-0.149609	5.693761	-0.734643
H	-2.533997	4.478395	0.355455
H	5.113450	1.130862	-0.490362
O	4.295419	1.523052	-0.849107
H	1.997190	4.433528	-2.125256

Table S23: BLYP 6-311g* **TS1** coordinates (Å).

Atom	x	y	z
C	-1.894233	0.818028	0.112894
C	-0.900967	1.726567	-0.168176
C	0.479365	1.288224	-0.381624
C	0.752748	-0.161993	-0.432637
C	2.045634	-0.688310	-0.731664
C	2.267564	-2.055108	-0.751371
C	1.232503	-2.994477	-0.452224
C	1.449912	-4.398697	-0.449671
C	0.406682	-5.285853	-0.165483
C	-0.876440	-4.799333	0.126549
C	-1.141620	-3.408049	0.133979
C	-2.442271	-2.881944	0.428551
C	-2.679435	-1.520706	0.432059
C	-1.639355	-0.588947	0.137757
C	-0.317395	-1.077954	-0.163660
C	-0.076673	-2.489723	-0.161352
C	1.503561	2.220721	-0.446852
C	1.258296	3.708213	-0.386040
C	-0.069102	4.066328	0.298949
C	-1.208504	3.202771	-0.297811
O	1.148663	4.236588	-1.755213
O	-0.372195	5.463092	0.156981
O	-2.462866	3.519734	0.323102
H	-2.906831	1.174502	0.300553
H	2.885429	-0.012115	-0.958695
H	3.260979	-2.432620	-1.005737
H	2.447634	-4.781396	-0.673173
H	0.591225	-6.360944	-0.167760
H	-1.686098	-5.496063	0.352344
H	-3.253015	-3.578194	0.651840
H	-3.677040	-1.139685	0.657493
H	2.560117	1.931556	-0.658722
H	2.095159	4.213447	0.120040
H	-0.005476	3.869949	1.378845
H	-1.260171	3.437353	-1.379737
H	-0.115657	5.693246	-0.762085
H	-2.525106	4.495211	0.288874
H	4.307432	1.130402	-0.087066
O	4.336878	1.445700	-1.015015
H	2.049654	4.421387	-2.078566

Table S24: BLYP 6-311+g* **TS1** coordinates (Å).

Atom	x	y	z
C	-1.919832	0.802064	0.046401
C	-0.905889	1.705245	-0.184056
C	0.478345	1.251741	-0.299296
C	0.743311	-0.194585	-0.347016
C	2.041118	-0.722014	-0.620370
C	2.261430	-2.089854	-0.631595
C	1.210480	-3.024500	-0.370904
C	1.421074	-4.429924	-0.365517
C	0.364651	-5.312917	-0.115411
C	-0.926982	-4.821121	0.129915
C	-1.185843	-3.428512	0.129533
C	-2.496350	-2.895398	0.365786
C	-2.729920	-1.533078	0.349584
C	-1.671757	-0.605656	0.105286
C	-0.338575	-1.103959	-0.119330
C	-0.105365	-2.515966	-0.119345
C	1.520099	2.166346	-0.243182
C	1.296874	3.657526	-0.198943
C	-0.083758	4.033864	0.362669
C	-1.185877	3.187523	-0.327261
O	1.331424	4.192062	-1.568952
O	-0.351903	5.440041	0.214256
O	-2.486639	3.505484	0.201781
H	-2.940478	1.161303	0.173927
H	2.867724	-0.045325	-0.851104
H	3.261108	-2.471282	-0.851519
H	2.422795	-4.817856	-0.560349
H	0.544462	-6.388777	-0.113001
H	-1.747493	-5.515167	0.322481
H	-3.319246	-3.587564	0.554837
H	-3.737016	-1.149040	0.520930
H	2.575598	1.859329	-0.294204
H	2.089294	4.146703	0.387595
H	-0.108854	3.834606	1.443423
H	-1.166036	3.430336	-1.407105
H	-0.028144	5.701927	-0.674163
H	-2.581732	4.476930	0.135198
H	4.684643	2.266603	-1.712813
O	4.213395	1.563298	-1.221105
H	2.258845	4.180475	-1.876583

Table S25: B1LYP 6-311g* **TS1** coordinates (Å).

Atom	x	y	z
C	-1.903434	0.812822	0.085528
C	-0.912386	1.710165	-0.176268
C	0.460416	1.267158	-0.346615
C	0.737785	-0.166816	-0.406615
C	2.027448	-0.676132	-0.715913
C	2.247042	-2.030950	-0.728343
C	1.217638	-2.968009	-0.428548
C	1.437156	-4.359514	-0.425105
C	0.405045	-5.243841	-0.136486
C	-0.870512	-4.763484	0.150892
C	-1.134760	-3.384020	0.153845
C	-2.431768	-2.860632	0.434583
C	-2.673965	-1.512913	0.422926
C	-1.637589	-0.585265	0.137164
C	-0.321937	-1.072577	-0.135581
C	-0.080537	-2.473606	-0.136049
C	1.486526	2.176567	-0.344649
C	1.265959	3.658008	-0.238079
C	-0.104035	4.028635	0.317012
C	-1.196691	3.177937	-0.344666
O	1.331304	4.206511	-1.568723
O	-0.380752	5.408860	0.142224
O	-2.470277	3.502604	0.180744
H	-2.915884	1.161098	0.238403
H	2.836985	0.014787	-0.983638
H	3.233050	-2.408026	-0.977989
H	2.427001	-4.738004	-0.651962
H	0.591786	-6.310275	-0.136596
H	-1.673185	-5.456741	0.373715
H	-3.236118	-3.552775	0.655044
H	-3.668283	-1.136479	0.629599
H	2.540536	1.887474	-0.567168
H	2.051303	4.109026	0.375497
H	-0.127316	3.840523	1.392496
H	-1.173050	3.391861	-1.423279
H	-0.044671	5.654619	-0.730648
H	-2.545880	4.463353	0.132860
H	4.481151	1.424001	-0.557933
O	4.051349	1.571172	-1.412519
H	2.242534	4.143788	-1.878683

Table S26: B1LYP 6-311+g* **TS1** coordinates (Å).

Atom	x	y	z
C	-1.926684	0.799917	0.066966
C	-0.929046	1.695197	-0.168340
C	0.446011	1.245200	-0.312246
C	0.720656	-0.190677	-0.369564
C	2.011502	-0.706299	-0.648928
C	2.232536	-2.062242	-0.659821
C	1.191701	-2.994001	-0.391866
C	1.406124	-4.387544	-0.390054
C	0.364708	-5.268644	-0.125780
C	-0.914809	-4.783000	0.137377
C	-1.173288	-3.401782	0.140563
C	-2.472983	-2.874971	0.396388
C	-2.710436	-1.524428	0.382986
C	-1.665310	-0.601693	0.123069
C	-0.345439	-1.093493	-0.120542
C	-0.109651	-2.494951	-0.123791
C	1.469827	2.149574	-0.312380
C	1.270970	3.631944	-0.189846
C	-0.111383	4.012420	0.331667
C	-1.200884	3.166520	-0.343523
O	1.406107	4.207613	-1.502533
O	-0.375621	5.396876	0.157780
O	-2.484442	3.491943	0.163698
H	-2.942885	1.146876	0.195661
H	2.832941	-0.031534	-0.869862
H	3.225038	-2.438821	-0.880642
H	2.398799	-4.769272	-0.598261
H	0.546581	-6.335857	-0.126282
H	-1.724936	-5.473605	0.340731
H	-3.284586	-3.564225	0.598598
H	-3.707965	-1.145859	0.568952
H	2.515840	1.865146	-0.457068
H	2.040743	4.049826	0.465357
H	-0.150054	3.827202	1.407007
H	-1.170630	3.377073	-1.422107
H	-0.023027	5.664165	-0.702574
H	-2.588592	4.448984	0.090043
H	5.053819	2.056969	-1.369428
O	4.137789	1.761098	-1.298820
H	2.309941	4.059264	-1.812106

Table S27: B3LYP 6-311g* **TS1** coordinates (Å).

Atom	x	y	z
C	-1.898136	0.814702	0.087722
C	-0.907922	1.712619	-0.182318
C	0.465103	1.270825	-0.357789
C	0.740397	-0.164532	-0.414053
C	2.028099	-0.675957	-0.724887
C	2.247615	-2.031895	-0.738453
C	1.218992	-2.967961	-0.435886
C	1.437834	-4.360367	-0.432185
C	0.405599	-5.244072	-0.140750
C	-0.869291	-4.762660	0.150134
C	-1.133304	-3.382457	0.153097
C	-2.429007	-2.858967	0.438394
C	-2.670343	-1.510127	0.427805
C	-1.634793	-0.583161	0.137346
C	-0.319855	-1.070669	-0.141207
C	-0.078975	-2.471967	-0.140812
C	1.491142	2.183589	-0.356144
C	1.261911	3.665212	-0.265863
C	-0.099398	4.029156	0.315135
C	-1.197139	3.179487	-0.341183
O	1.285511	4.205436	-1.603747
O	-0.381090	5.410100	0.152150
O	-2.467512	3.501359	0.195640
H	-2.909616	1.165773	0.249188
H	2.841654	0.014180	-0.990367
H	3.233950	-2.409430	-0.991323
H	2.428161	-4.739602	-0.661188
H	0.591834	-6.311761	-0.140770
H	-1.672535	-5.455993	0.376248
H	-3.233627	-3.551548	0.662098
H	-3.664618	-1.132641	0.639022
H	2.548763	1.891969	-0.559108
H	2.056672	4.132762	0.324230
H	-0.107564	3.833277	1.390561
H	-1.181196	3.399911	-1.419981
H	-0.061415	5.655976	-0.729281
H	-2.537134	4.465028	0.160426
H	4.439604	1.319730	-0.461928
O	4.100665	1.527076	-1.346316
H	2.199948	4.218508	-1.913180

Table S28: B3LYP 6-311+g* **TS1** coordinates (Å).

Atom	x	y	z
C	-1.919832	0.802064	0.046401
C	-0.905889	1.705245	-0.184056
C	0.478345	1.251741	-0.299296
C	0.743311	-0.194585	-0.347016
C	2.041118	-0.722014	-0.620370
C	2.261430	-2.089854	-0.631595
C	1.210480	-3.024500	-0.370904
C	1.421074	-4.429924	-0.365517
C	0.364651	-5.312917	-0.115411
C	-0.926982	-4.821121	0.129915
C	-1.185843	-3.428512	0.129533
C	-2.496350	-2.895398	0.365786
C	-2.729920	-1.533078	0.349584
C	-1.671757	-0.605656	0.105286
C	-0.338575	-1.103959	-0.119330
C	-0.105365	-2.515966	-0.119345
C	1.520099	2.166346	-0.243182
C	1.296874	3.657526	-0.198943
C	-0.083758	4.033864	0.362669
C	-1.185877	3.187523	-0.327261
O	1.331424	4.192062	-1.568952
O	-0.351903	5.440041	0.214256
O	-2.486639	3.505484	0.201781
H	-2.940478	1.161303	0.173927
H	2.867724	-0.045325	-0.851104
H	3.261108	-2.471282	-0.851519
H	2.422795	-4.817856	-0.560349
H	0.544462	-6.388777	-0.113001
H	-1.747493	-5.515167	0.322481
H	-3.319246	-3.587564	0.554837
H	-3.737016	-1.149040	0.520930
H	2.575598	1.859329	-0.294204
H	2.089294	4.146703	0.387595
H	-0.108854	3.834606	1.443423
H	-1.166036	3.430336	-1.407105
H	-0.028144	5.701927	-0.674163
H	-2.581732	4.476930	0.135198
H	4.684643	2.266603	-1.712813
O	4.213395	1.563298	-1.221105
H	2.258845	4.180475	-1.876583

Table S29: BPW91 6-311g* **TS2** coordinates (Å).

Atom	x	y	z
C	-1.850850	0.819911	-0.178353
C	-0.808219	1.719524	-0.340533
C	0.557066	1.253229	-0.351394
C	0.813071	-0.171591	-0.313041
C	2.126795	-0.713300	-0.456472
C	2.353352	-2.069413	-0.392696
C	1.283584	-2.995998	-0.189233
C	1.492311	-4.392962	-0.110773
C	0.418226	-5.265348	0.071602
C	-0.888002	-4.770998	0.173824
C	-1.144903	-3.386611	0.096930
C	-2.471932	-2.848189	0.189161
C	-2.701011	-1.496889	0.104233
C	-1.623012	-0.571904	-0.072502
C	-0.280132	-1.075872	-0.153888
C	-0.047575	-2.482882	-0.082043
C	1.603185	2.190222	-0.217215
C	1.358391	3.680427	-0.365152
C	-0.004607	3.983291	0.334873
C	-1.076567	3.191136	-0.434778
O	1.310719	3.981891	-1.715508
O	-0.365396	5.363216	0.227774
O	-2.390367	3.510255	0.017381
H	-2.871129	1.199668	-0.118506
H	2.954716	-0.038827	-0.669586
H	3.368379	-2.456071	-0.510161
H	2.508382	-4.784469	-0.195584
H	0.596318	-6.340436	0.132296
H	-1.723363	-5.460610	0.314078
H	-3.308078	-3.537896	0.325241
H	-3.718912	-1.106796	0.169833
H	2.551805	1.845945	0.193075
H	2.144292	4.252414	0.178752
H	0.008698	3.668409	1.392865
H	-0.937551	3.498848	-1.492740
H	-0.118864	5.807250	1.055246
H	-2.392041	4.484430	0.080643
H	3.740299	2.386226	-1.926418
O	2.857192	2.086273	-2.206334
H	2.244710	2.955407	-2.194417

Table S30: BPW91 6-311+g* **TS2** coordinates (Å).

Atom	x	y	z
C	-1.839368	0.822207	-0.204988
C	-0.795638	1.721694	-0.345010
C	0.570581	1.255839	-0.348034
C	0.828776	-0.171273	-0.294326
C	2.144413	-0.717038	-0.392306
C	2.367566	-2.073977	-0.316746
C	1.291395	-2.998670	-0.147698
C	1.497001	-4.396032	-0.059994
C	0.417421	-5.267241	0.095615
C	-0.890294	-4.769996	0.162138
C	-1.142625	-3.384895	0.075483
C	-2.470481	-2.845997	0.135074
C	-2.695417	-1.493381	0.046111
C	-1.612068	-0.571528	-0.105317
C	-0.268273	-1.075550	-0.158347
C	-0.040333	-2.482922	-0.077456
C	1.617886	2.190914	-0.253068
C	1.377375	3.692916	-0.346535
C	0.012801	3.975158	0.352308
C	-1.065377	3.198175	-0.420830
O	1.362178	4.075835	-1.684893
O	-0.346774	5.360910	0.291149
O	-2.380822	3.499484	0.054000
H	-2.861865	1.197553	-0.157556
H	2.990212	-0.051616	-0.558845
H	3.386437	-2.460462	-0.396016
H	2.514813	-4.788625	-0.115624
H	0.592281	-6.342482	0.163829
H	-1.730399	-5.457848	0.282362
H	-3.310931	-3.534246	0.251577
H	-3.713895	-1.101616	0.089818
H	2.586555	1.848436	0.109031
H	2.162905	4.223744	0.235519
H	0.035498	3.639540	1.403531
H	-0.962061	3.519679	-1.476790
H	-0.091009	5.788170	1.125825
H	-2.410840	4.473496	0.120480
H	3.620406	2.272597	-2.197078
O	2.671886	2.093995	-2.331026
H	2.149066	3.045963	-2.234889

Table S31: BLYP 6-311g* **TS2** coordinates (Å).

Atom	x	y	z
C	-1.844480	0.827764	-0.158115
C	-0.797228	1.725559	-0.323693
C	0.569923	1.252603	-0.353748
C	0.820874	-0.178380	-0.321521
C	2.134275	-0.731981	-0.476411
C	2.353212	-2.092058	-0.419035
C	1.277277	-3.017264	-0.211222
C	1.478268	-4.419260	-0.138821
C	0.397850	-5.288008	0.049383
C	-0.907820	-4.785573	0.163722
C	-1.158979	-3.396068	0.093303
C	-2.485927	-2.847878	0.198088
C	-2.708045	-1.492633	0.120013
C	-1.623390	-0.569431	-0.062059
C	-0.279669	-1.081285	-0.156958
C	-0.054177	-2.494688	-0.091607
C	1.628479	2.188828	-0.246327
C	1.388890	3.696112	-0.369608
C	0.027738	3.997528	0.349079
C	-1.066520	3.208815	-0.401431
O	1.335412	4.039977	-1.719160
O	-0.335015	5.390591	0.254737
O	-2.377339	3.521921	0.101931
H	-2.861680	1.211407	-0.084917
H	2.966938	-0.065285	-0.690665
H	3.365300	-2.483503	-0.543895
H	2.490918	-4.816927	-0.232562
H	0.570219	-6.364122	0.105176
H	-1.745210	-5.471449	0.308337
H	-3.324878	-3.533010	0.338168
H	-3.722832	-1.096867	0.195556
H	2.574936	1.845223	0.166639
H	2.186395	4.245111	0.181408
H	0.055741	3.684457	1.406539
H	-0.975022	3.526712	-1.458591
H	-0.050924	5.835481	1.072974
H	-2.382262	4.497787	0.172340
H	3.682186	2.345008	-1.989559
O	2.771254	2.088861	-2.234425
H	2.194291	3.006833	-2.222583

Table S32: BLYP 6-311+g* **TS2** coordinates (Å).

Atom	x	y	z
C	-1.835820	0.819849	-0.211883
C	-0.790107	1.720648	-0.337398
C	0.582766	1.254729	-0.334905
C	0.841812	-0.180121	-0.277776
C	2.160513	-0.732931	-0.358512
C	2.379825	-2.093639	-0.281233
C	1.297564	-3.019719	-0.126797
C	1.499074	-4.421678	-0.038106
C	0.413199	-5.292938	0.104358
C	-0.897304	-4.791716	0.156834
C	-1.147003	-3.402081	0.069153
C	-2.477635	-2.858494	0.114650
C	-2.699087	-1.501995	0.025194
C	-1.609952	-0.579430	-0.112935
C	-0.261970	-1.086219	-0.153016
C	-0.037555	-2.498969	-0.070610
C	1.633034	2.190541	-0.271909
C	1.399287	3.707494	-0.321543
C	0.019006	3.991667	0.352363
C	-1.063560	3.207649	-0.416087
O	1.428984	4.148813	-1.658805
O	-0.345392	5.389766	0.286138
O	-2.387728	3.501870	0.080426
H	-2.858733	1.192647	-0.174561
H	3.013746	-0.073839	-0.505973
H	3.398881	-2.481067	-0.346164
H	2.515964	-4.816846	-0.082326
H	0.584885	-6.368241	0.173082
H	-1.739428	-5.478153	0.266411
H	-3.320817	-3.544412	0.220468
H	-3.716829	-1.108592	0.058436
H	2.617473	1.850166	0.039811
H	2.181134	4.204594	0.291378
H	0.033905	3.667458	1.406222
H	-0.990735	3.526540	-1.472361
H	-0.064857	5.828567	1.110221
H	-2.432223	4.477961	0.140983
H	3.555880	2.248919	-2.319049
O	2.589245	2.143640	-2.419641
H	2.099541	3.168474	-2.234061

Table S33: B1LYP 6-311g* **TS2** coordinates (Å).

Atom	x	y	z
C	-1.835393	0.817059	-0.195811
C	-0.798008	1.712338	-0.334015
C	0.560053	1.247494	-0.339017
C	0.821045	-0.169345	-0.292400
C	2.136088	-0.711923	-0.405781
C	2.357087	-2.057703	-0.337858
C	1.285099	-2.983968	-0.161200
C	1.492168	-4.372799	-0.080561
C	0.419985	-5.241682	0.077452
C	-0.881608	-4.748550	0.152793
C	-1.133652	-3.371965	0.072853
C	-2.460038	-2.833198	0.140035
C	-2.685704	-1.492515	0.055709
C	-1.605119	-0.568926	-0.097865
C	-0.268709	-1.069907	-0.156864
C	-0.039207	-2.473740	-0.081833
C	1.602155	2.183467	-0.236935
C	1.358445	3.688025	-0.365871
C	0.002434	3.971648	0.331441
C	-1.075030	3.187874	-0.414712
O	1.335286	4.034582	-1.695270
O	-0.373311	5.342583	0.249349
O	-2.372092	3.478549	0.086705
H	-2.849288	1.189552	-0.144491
H	2.967606	-0.048509	-0.590992
H	3.366788	-2.441865	-0.429552
H	2.501997	-4.761545	-0.143559
H	0.595186	-6.308681	0.140154
H	-1.713325	-5.433047	0.274161
H	-3.292163	-3.518136	0.257247
H	-3.695858	-1.103454	0.103847
H	2.554347	1.848496	0.145907
H	2.145464	4.215629	0.206767
H	0.023255	3.653282	1.380704
H	-0.993939	3.497234	-1.464236
H	0.015328	5.819517	0.988361
H	-2.404686	4.439474	0.170737
H	3.625809	2.276838	-2.044632
O	2.705258	2.058025	-2.229145
H	2.175228	2.960702	-2.221144

Table S34: B1LYP 6-311+g* **TS2** coordinates (Å).

Atom	x	y	z
C	-1.822329	0.817870	-0.215847
C	-0.783029	1.712201	-0.333769
C	0.574749	1.248318	-0.330329
C	0.836812	-0.169439	-0.266118
C	2.153310	-0.716509	-0.334918
C	2.370821	-2.063105	-0.259761
C	1.293149	-2.988307	-0.119109
C	1.496964	-4.377752	-0.035063
C	0.419595	-5.246043	0.093737
C	-0.882805	-4.750347	0.137375
C	-1.130334	-3.372495	0.053812
C	-2.457119	-2.833164	0.090930
C	-2.678751	-1.491013	0.005046
C	-1.593306	-0.569860	-0.121888
C	-0.256441	-1.070652	-0.153394
C	-0.031285	-2.475354	-0.072836
C	1.623050	2.181741	-0.293655
C	1.384472	3.701350	-0.344392
C	0.021336	3.965141	0.341537
C	-1.059980	3.191957	-0.408154
O	1.419802	4.153451	-1.650503
O	-0.354673	5.340055	0.301384
O	-2.357937	3.471988	0.107308
H	-2.838133	1.186846	-0.180703
H	3.001043	-0.061315	-0.470870
H	3.383265	-2.446999	-0.315418
H	2.507709	-4.767619	-0.072031
H	0.591516	-6.313454	0.158859
H	-1.718626	-5.433503	0.236580
H	-3.292879	-3.516975	0.187438
H	-3.689143	-1.100523	0.032094
H	2.595055	1.849571	0.037045
H	2.164422	4.172247	0.279865
H	0.049538	3.627682	1.384100
H	-1.007865	3.506393	-1.457274
H	0.046394	5.807835	1.041058
H	-2.415947	4.432443	0.191328
H	3.445521	2.148472	-2.287367
O	2.484024	2.084462	-2.331778
H	2.077016	3.075317	-2.253843

Table S35: B3LYP 6-311g* **TS2** coordinates (Å).

Atom	x	y	z
C	-1.837842	0.817124	-0.191065
C	-0.800353	1.712607	-0.335322
C	0.558462	1.247751	-0.341183
C	0.818475	-0.169840	-0.297666
C	2.132251	-0.711563	-0.420491
C	2.354328	-2.058602	-0.354595
C	1.283864	-2.984430	-0.170219
C	1.491259	-4.374017	-0.090783
C	0.419732	-5.243147	0.074246
C	-0.881853	-4.750190	0.157774
C	-1.135039	-3.372932	0.079070
C	-2.460586	-2.834517	0.153789
C	-2.687076	-1.492602	0.069501
C	-1.608074	-0.569228	-0.090848
C	-0.271214	-1.070580	-0.156243
C	-0.040986	-2.474085	-0.082493
C	1.600320	2.183097	-0.228786
C	1.357425	3.683664	-0.364122
C	-0.000763	3.973360	0.328624
C	-1.075810	3.186673	-0.420538
O	1.333425	4.016433	-1.698717
O	-0.373512	5.345228	0.237335
O	-2.375830	3.483264	0.070704
H	-2.852437	1.191070	-0.137273
H	2.961466	-0.045726	-0.614647
H	3.364344	-2.443194	-0.454368
H	2.501755	-4.763094	-0.160448
H	0.595654	-6.311239	0.136013
H	-1.713607	-5.435465	0.284610
H	-3.292867	-3.520141	0.276435
H	-3.698261	-1.103596	0.122849
H	2.550217	1.845946	0.161633
H	2.142950	4.220758	0.203422
H	0.016316	3.659057	1.380140
H	-0.984190	3.493832	-1.471834
H	-0.013275	5.818844	0.994729
H	-2.402718	4.446602	0.151447
H	3.656166	2.296420	-2.007190
O	2.743003	2.060340	-2.214652
H	2.193862	2.957026	-2.208359

Table S36: B3LYP 6-311+g* **TS2** coordinates (Å).

Atom	x	y	z
C	-1.823875	0.818238	-0.215115
C	-0.784598	1.712684	-0.335847
C	0.574657	1.249014	-0.332237
C	0.836013	-0.170344	-0.270228
C	2.151293	-0.716992	-0.343637
C	2.369435	-2.064986	-0.268331
C	1.292507	-2.989226	-0.123059
C	1.496153	-4.379467	-0.037931
C	0.418763	-5.247644	0.095355
C	-0.883831	-4.751688	0.142278
C	-1.131894	-3.373188	0.057685
C	-2.457873	-2.834118	0.097897
C	-2.679788	-1.490585	0.010933
C	-1.595331	-0.570213	-0.119689
C	-0.257759	-1.071467	-0.154119
C	-0.032553	-2.475775	-0.073223
C	1.621385	2.181671	-0.285981
C	1.383480	3.698041	-0.339949
C	0.018766	3.964675	0.343296
C	-1.060031	3.191327	-0.411597
O	1.416327	4.142997	-1.650541
O	-0.355765	5.340699	0.299850
O	-2.361517	3.475416	0.094383
H	-2.840610	1.188227	-0.178745
H	2.998865	-0.060497	-0.484236
H	3.382703	-2.449391	-0.327639
H	2.507821	-4.769840	-0.077645
H	0.590945	-6.316094	0.161419
H	-1.720369	-5.435260	0.244984
H	-3.294425	-3.518326	0.197562
H	-3.691293	-1.099906	0.040164
H	2.594903	1.847157	0.042379
H	2.162875	4.176070	0.281539
H	0.043722	3.627408	1.387095
H	-0.998061	3.506118	-1.461807
H	0.024962	5.803759	1.055212
H	-2.413044	4.437971	0.180978
H	3.471055	2.166263	-2.283415
O	2.509512	2.089082	-2.340368
H	2.085455	3.079101	-2.247194

Table S37: BPW91 6-311g* **TS3** coordinates (Å).

Atom	x	y	z
C	0.457528	4.173041	1.334696
C	0.025677	2.755641	1.576078
C	0.552723	1.739238	0.688729
C	1.688434	2.012423	-0.065183
C	2.343792	3.352229	-0.120336
C	1.969656	4.276250	1.037827
C	-0.029809	0.403428	0.711427
C	-0.972324	0.089204	1.737973
C	-1.379113	1.095377	2.680766
C	-0.884665	2.423718	2.554408
C	-1.523011	-1.223552	1.828390
C	-1.148999	-2.222757	0.877971
C	-0.229604	-1.867161	-0.155009
C	0.315796	-0.603155	-0.237077
C	-2.452466	-1.546112	2.868167
C	-2.978597	-2.853958	2.939874
C	-2.606756	-3.828319	2.006628
C	-1.706164	-3.519409	0.985586
C	-2.308233	0.748955	3.705929
C	-2.821701	-0.524959	3.800495
O	1.754082	3.851567	-1.320115
O	2.298073	5.628384	0.713218
O	0.091896	5.018005	2.419717
O	3.120419	3.061718	-3.187644
As	2.800552	1.446610	-3.736379
O	2.611610	0.302736	-2.509378
C	1.210210	1.516608	-4.879529
C	4.312295	1.014308	-4.897423
H	-1.249034	3.195742	3.232579
H	1.002744	-0.370270	-1.055841
H	0.039384	-2.619644	-0.899688
H	-1.422511	-4.281787	0.256926
H	-3.025254	-4.833436	2.076543
H	-3.685980	-3.099988	3.734524
H	-3.530064	-0.770089	4.594824
H	-2.611456	1.516621	4.420105
H	2.120035	1.257331	-0.736451
H	3.441411	3.275132	-0.211924
H	2.530955	4.018914	1.948858
H	-0.056939	4.500792	0.407007
H	2.054167	5.714348	-0.233176
H	0.492823	5.882681	2.211635
H	1.362114	2.250891	-5.680087
H	0.354398	1.815902	-4.262319
H	1.023483	0.525615	-5.311381
H	4.404021	1.777025	-5.680073
H	2.387514	3.451810	-2.231052
H	4.149909	0.029410	-5.352010
H	5.223859	0.995175	-4.288483

Table S38: BPW91 6-311+g* **TS3** coordinates (Å).

Atom	x	y	z
C	0.530483	4.181033	1.436597
C	0.062397	2.758405	1.616256
C	0.552736	1.753280	0.701981
C	1.656153	2.037097	-0.107213
C	2.280871	3.386161	-0.190657
C	2.011789	4.249012	1.042823
C	-0.038666	0.425258	0.716246
C	-0.986120	0.108467	1.739173
C	-1.380315	1.107866	2.691675
C	-0.857417	2.426125	2.588324
C	-1.553701	-1.198760	1.814932
C	-1.187632	-2.194415	0.857406
C	-0.258876	-1.839566	-0.169014
C	0.298951	-0.581629	-0.238153
C	-2.491362	-1.519678	2.848478
C	-3.033985	-2.821909	2.905681
C	-2.669034	-3.792173	1.965556
C	-1.759063	-3.484973	0.951067
C	-2.318241	0.763966	3.711450
C	-2.850649	-0.502801	3.790314
O	1.526856	3.769074	-1.338799
O	2.303527	5.639530	0.832633
O	0.272357	4.946651	2.614284
O	2.720617	3.101991	-3.371503
As	2.693364	1.435124	-3.874518
O	2.601495	0.320976	-2.602121
C	1.182137	1.219491	-5.099809
C	4.322695	1.199990	-4.925771
H	-1.201560	3.189425	3.286666
H	0.993119	-0.355141	-1.051351
H	0.007115	-2.589289	-0.917976
H	-1.480116	-4.244674	0.217446
H	-3.099476	-4.793285	2.024503
H	-3.747925	-3.066952	3.695177
H	-3.565415	-0.746376	4.579723
H	-2.611625	1.528003	4.434115
H	2.058031	1.295505	-0.808690
H	3.362188	3.346829	-0.405858
H	2.617670	3.856077	1.878639
H	-0.042370	4.606802	0.588145
H	3.243613	5.797894	1.024549
H	0.689861	5.815512	2.458630
H	1.260848	1.952807	-5.911848
H	0.254225	1.383208	-4.538756
H	1.192484	0.202332	-5.510774
H	4.339253	1.931866	-5.742533
H	2.084957	3.410175	-2.304657
H	4.344936	0.182295	-5.334499
H	5.185694	1.355629	-4.267650

Table S39: BLYP 6-311g* **TS3** coordinates (Å).

Atom	x	y	z
C	0.508636	4.193509	1.405595
C	0.047507	2.762264	1.593409
C	0.560057	1.749415	0.691495
C	1.683486	2.032247	-0.098259
C	2.302145	3.391376	-0.185734
C	2.001583	4.271859	1.035519
C	-0.029087	0.414978	0.707983
C	-0.985514	0.099523	1.730207
C	-1.394452	1.106922	2.675681
C	-0.880321	2.431368	2.561665
C	-1.546764	-1.215164	1.813158
C	-1.169811	-2.218226	0.860179
C	-0.238360	-1.860977	-0.169208
C	0.314048	-0.598600	-0.245672
C	-2.490720	-1.535937	2.848060
C	-3.025075	-2.844938	2.911686
C	-2.648887	-3.820916	1.977525
C	-1.735506	-3.514402	0.961732
C	-2.338656	0.761690	3.695361
C	-2.862542	-0.510231	3.782272
O	1.555183	3.760856	-1.354144
O	2.274496	5.672546	0.804054
O	0.231500	4.973358	2.579249
O	2.888384	3.088876	-3.306435
As	2.718351	1.432896	-3.829207
O	2.588192	0.297240	-2.575205
C	1.146496	1.351340	-5.029207
C	4.302987	1.098622	-4.958593
H	-1.234175	3.199663	3.248579
H	1.002323	-0.370702	-1.062481
H	0.031152	-2.612660	-0.914465
H	-1.450157	-4.277408	0.234680
H	-3.072730	-4.824138	2.041824
H	-3.740209	-3.089913	3.699483
H	-3.579522	-0.752588	4.569477
H	-2.641765	1.529563	4.409305
H	2.106554	1.283002	-0.775740
H	3.385320	3.361793	-0.389410
H	2.593525	3.903021	1.891296
H	-0.049201	4.608058	0.542706
H	3.210732	5.841776	1.013479
H	0.662249	5.835563	2.412257
H	1.261768	2.085817	-5.835724
H	0.251369	1.586035	-4.440547
H	1.057087	0.342398	-5.450575
H	4.353232	1.855833	-5.750263
H	2.167693	3.419340	-2.297954
H	4.226493	0.097839	-5.400802
H	5.197779	1.158449	-4.327965

Table S40: BLYP 6-311+g* **TS3** coordinates (Å).

Atom	x	y	z
C	0.526337	4.184340	1.444813
C	0.050763	2.754535	1.625800
C	0.551268	1.739202	0.716574
C	1.657976	2.019726	-0.090611
C	2.283584	3.376576	-0.193195
C	2.012574	4.248954	1.045130
C	-0.044425	0.404766	0.738089
C	-1.000360	0.094513	1.761482
C	-1.402131	1.104659	2.706417
C	-0.877563	2.426950	2.593956
C	-1.569450	-1.216865	1.845899
C	-1.198501	-2.223237	0.894555
C	-0.263979	-1.873739	-0.134005
C	0.294759	-0.612973	-0.210621
C	-2.514833	-1.530951	2.881356
C	-3.057538	-2.837110	2.946762
C	-2.687197	-3.817146	2.013561
C	-1.771587	-3.516954	0.997340
C	-2.347502	0.767075	3.726682
C	-2.880044	-0.502625	3.814782
O	1.558371	3.779731	-1.359548
O	2.310257	5.649970	0.826347
O	0.273578	4.948612	2.641389
O	2.753449	3.122777	-3.403097
As	2.712529	1.445312	-3.933752
O	2.592966	0.312534	-2.669207
C	1.196617	1.274002	-5.189205
C	4.369206	1.224724	-4.978111
H	-1.227608	3.193223	3.284875
H	0.988784	-0.393753	-1.023479
H	0.004839	-2.627959	-0.876798
H	-1.490160	-4.282459	0.271389
H	-3.116920	-4.817754	2.079114
H	-3.774082	-3.076984	3.734877
H	-3.598040	-0.739371	4.602759
H	-2.645695	1.536663	4.440826
H	2.062249	1.272246	-0.778203
H	3.369110	3.325891	-0.387228
H	2.621757	3.865832	1.881725
H	-0.051635	4.623180	0.609170
H	3.255987	5.806352	1.006345
H	0.674601	5.827873	2.487140
H	1.294589	2.026305	-5.981248
H	0.266678	1.435388	-4.631284
H	1.202278	0.266371	-5.622611
H	4.398521	1.978630	-5.773944
H	2.142244	3.410112	-2.367324
H	4.387520	0.217733	-5.412196
H	5.222731	1.357354	-4.303167

Table S41: B1LYP 6-311g* **TS3** coordinates (Å).

Atom	x	y	z
C	0.533080	4.166009	1.416147
C	0.066580	2.743883	1.596641
C	0.555884	1.740226	0.692504
C	1.659218	2.024098	-0.112580
C	2.276598	3.369100	-0.200948
C	2.005306	4.238497	1.019802
C	-0.027557	0.419942	0.707198
C	-0.975646	0.108494	1.721246
C	-1.374186	1.106969	2.661215
C	-0.855863	2.419197	2.557483
C	-1.538646	-1.197038	1.802214
C	-1.167963	-2.191109	0.856888
C	-0.237504	-1.837708	-0.167290
C	0.313531	-0.590309	-0.243521
C	-2.475180	-1.512320	2.827462
C	-3.011204	-2.807621	2.890132
C	-2.641297	-3.777375	1.961791
C	-1.732379	-3.474693	0.954165
C	-2.316206	0.766160	3.677142
C	-2.840838	-0.490373	3.759686
O	1.507499	3.708563	-1.335167
O	2.279218	5.618208	0.793148
O	0.289020	4.917826	2.593069
O	2.755584	3.084546	-3.309208
As	2.672986	1.443643	-3.817200
O	2.546412	0.346366	-2.561900
C	1.163198	1.295295	-5.035835
C	4.284149	1.164571	-4.865600
H	-1.200171	3.179995	3.244778
H	0.998928	-0.366031	-1.052596
H	0.028335	-2.585788	-0.905799
H	-1.451124	-4.232276	0.231742
H	-3.065763	-4.771785	2.024126
H	-3.722168	-3.048897	3.671873
H	-3.553805	-0.730301	4.540257
H	-2.611164	1.529060	4.387513
H	2.064180	1.285585	-0.799810
H	3.348092	3.337905	-0.423649
H	2.606922	3.863581	1.856185
H	-0.038137	4.590107	0.578961
H	3.219141	5.780140	0.918387
H	0.687432	5.783449	2.441801
H	1.265107	2.023697	-5.839525
H	0.248026	1.492902	-4.478701
H	1.124726	0.289229	-5.452427
H	4.332453	1.901453	-5.666336
H	2.101217	3.390131	-2.315641
H	4.273247	0.160489	-5.288133
H	5.147605	1.276545	-4.211371

Table S42: B1LYP 6-311+g* **TS3** coordinates (Å).

Atom	x	y	z
C	0.535348	4.160832	1.429111
C	0.057710	2.741093	1.608173
C	0.555688	1.729065	0.710520
C	1.650404	2.008983	-0.093285
C	2.269015	3.359197	-0.203282
C	2.009501	4.216352	1.034978
C	-0.030295	0.404107	0.733233
C	-0.986663	0.101208	1.740644
C	-1.394148	1.108036	2.667965
C	-0.872264	2.421832	2.560694
C	-1.550900	-1.203048	1.827588
C	-1.170826	-2.205594	0.895730
C	-0.230273	-1.862676	-0.120844
C	0.321181	-0.613564	-0.201564
C	-2.497480	-1.508974	2.846086
C	-3.034680	-2.804174	2.915709
C	-2.655520	-3.783493	2.000103
C	-1.736270	-3.489653	0.999038
C	-2.345318	0.777954	3.676341
C	-2.872180	-0.479463	3.764768
O	1.560648	3.760631	-1.348941
O	2.315532	5.595470	0.835109
O	0.288058	4.910796	2.610875
O	2.719854	3.106045	-3.374800
As	2.675570	1.454915	-3.895839
O	2.555866	0.356333	-2.635522
C	1.175998	1.288451	-5.120812
C	4.309001	1.229622	-4.916449
H	-1.224990	3.184118	3.241977
H	1.017522	-0.398958	-1.002800
H	0.046025	-2.617106	-0.848873
H	-1.447239	-4.253782	0.286625
H	-3.080536	-4.777268	2.067594
H	-3.753489	-3.038191	3.692501
H	-3.593104	-0.711363	4.540463
H	-2.647768	1.546457	4.377395
H	2.046981	1.268850	-0.780893
H	3.348879	3.299024	-0.388175
H	2.608040	3.820065	1.863467
H	-0.035573	4.594895	0.597614
H	3.261198	5.740148	0.945333
H	0.677294	5.783858	2.474821
H	1.268879	2.027934	-5.915326
H	0.254646	1.458018	-4.565116
H	1.168088	0.285639	-5.546691
H	4.347060	1.972896	-5.711802
H	2.144398	3.396215	-2.382995
H	4.331366	0.228087	-5.344323
H	5.156639	1.362416	-4.245807

Table S43: B3LYP 6-311g* **TS3** coordinates (Å).

Atom	x	y	z
C	0.531248	4.168748	1.417050
C	0.066919	2.746698	1.597113
C	0.556374	1.744605	0.690787
C	1.659808	2.029672	-0.114415
C	2.277127	3.374933	-0.199200
C	2.004208	4.243423	1.021720
C	-0.027478	0.423658	0.704113
C	-0.974259	0.109987	1.719839
C	-1.371409	1.106904	2.663326
C	-0.853491	2.419661	2.560157
C	-1.537141	-1.195450	1.798818
C	-1.168173	-2.188027	0.849887
C	-0.239719	-1.832785	-0.174667
C	0.311944	-0.584090	-0.248828
C	-2.472420	-1.513251	2.825649
C	-3.008789	-2.809346	2.885989
C	-2.640681	-3.777159	1.954307
C	-1.733223	-3.472287	0.945445
C	-2.310987	0.763823	3.679922
C	-2.836080	-0.494049	3.760749
O	1.505150	3.715656	-1.334143
O	2.276242	5.624764	0.796710
O	0.284769	4.923098	2.592539
O	2.757391	3.082159	-3.307903
As	2.672979	1.438664	-3.811579
O	2.547783	0.340607	-2.553613
C	1.161133	1.285626	-5.029892
C	4.282722	1.153892	-4.863824
H	-1.196862	3.180564	3.249774
H	0.997448	-0.357959	-1.059323
H	0.025093	-2.579974	-0.916141
H	-1.453122	-4.228951	0.219908
H	-3.065758	-4.772631	2.015063
H	-3.719156	-3.052471	3.669279
H	-3.548266	-0.735926	4.543019
H	-2.605103	1.525785	4.393427
H	2.066069	1.291065	-0.803624
H	3.349129	3.346290	-0.424446
H	2.606119	3.867349	1.858882
H	-0.039461	4.591368	0.576719
H	3.216012	5.788880	0.932557
H	0.690008	5.787397	2.439577
H	1.262340	2.012599	-5.836244
H	0.245560	1.484290	-4.472001
H	1.123427	0.277408	-5.443802
H	4.329280	1.888455	-5.668072
H	2.094191	3.393551	-2.306004
H	4.269416	0.147300	-5.282731
H	5.148562	1.267713	-4.211552

Table S44: B3LYP 6-311+g* **TS3** coordinates (Å).

Atom	x	y	z
C	0.536087	4.164159	1.432566
C	0.060615	2.744242	1.610379
C	0.556045	1.735190	0.708799
C	1.652065	2.016273	-0.095858
C	2.271372	3.365063	-0.199580
C	2.010203	4.223484	1.036682
C	-0.031069	0.410871	0.728139
C	-0.985045	0.104484	1.738072
C	-1.388980	1.108266	2.671323
C	-0.866803	2.421936	2.566056
C	-1.549994	-1.199567	1.821345
C	-1.173783	-2.199138	0.883266
C	-0.236487	-1.852943	-0.134794
C	0.316415	-0.603134	-0.211791
C	-2.493928	-1.509291	2.842401
C	-3.032154	-2.805044	2.908058
C	-2.656853	-3.780823	1.986599
C	-1.740474	-3.483534	0.983272
C	-2.336676	0.774513	3.681448
C	-2.864560	-0.483825	3.766653
O	1.551552	3.758062	-1.344657
O	2.311382	5.604323	0.833738
O	0.288404	4.915254	2.614384
O	2.709566	3.101663	-3.372919
As	2.675529	1.446335	-3.886530
O	2.565932	0.349586	-2.620574
C	1.174086	1.262046	-5.109091
C	4.308565	1.225216	-4.911576
H	-1.217025	3.183666	3.251249
H	1.011616	-0.385559	-1.015215
H	0.036805	-2.605312	-0.867830
H	-1.454268	-4.245624	0.265791
H	-3.082998	-4.775562	2.051279
H	-3.749281	-3.041959	3.687143
H	-3.583645	-0.718754	4.544763
H	-2.636645	1.541070	4.387534
H	2.049502	1.276588	-0.786113
H	3.350980	3.310668	-0.391674
H	2.611459	3.829443	1.865750
H	-0.036105	4.597863	0.599753
H	3.256535	5.753896	0.955828
H	0.681246	5.788448	2.476080
H	1.260474	1.998769	-5.908183
H	0.251789	1.427785	-4.552015
H	1.173442	0.256017	-5.529802
H	4.338790	1.964529	-5.712225
H	2.129375	3.394335	-2.370351
H	4.335852	0.220269	-5.333518
H	5.157963	1.367992	-4.243735

Table S45: BPW91 6-311g* BPDE coordinates (Å).

Atom	x	y	z
C	-1.741332	0.782002	-0.163064
C	-0.669341	1.673722	-0.148745
C	0.662042	1.198808	-0.064202
C	0.914455	-0.201645	-0.029772
C	2.239598	-0.768014	0.014313
C	2.446364	-2.121009	0.057754
C	1.352882	-3.050555	0.065309
C	1.545865	-4.446493	0.116862
C	0.452472	-5.318059	0.117290
C	-0.852887	-4.819899	0.064162
C	-1.095752	-3.431168	0.009392
C	-2.425056	-2.888089	-0.048639
C	-2.635180	-1.536286	-0.102201
C	-1.536784	-0.609572	-0.100903
C	-0.197825	-1.114520	-0.039738
C	0.019806	-2.527336	0.011347
C	1.768232	2.192351	0.038820
C	1.472922	3.601940	0.374985
C	0.036101	3.995890	0.604304
C	-0.918297	3.162596	-0.271253
O	1.837947	3.245596	-0.982379
O	-0.221481	5.397782	0.397461
O	-2.272196	3.476521	0.059887
H	-2.757356	1.174623	-0.216765
H	3.110026	-0.112579	-0.003193
H	3.465902	-2.513544	0.083634
H	2.563407	-4.842435	0.156296
H	0.619072	-6.396502	0.158516
H	-1.701518	-5.508195	0.064287
H	-3.272205	-3.578354	-0.050250
H	-3.651398	-1.137209	-0.147817
H	2.755756	1.825009	0.319743
H	2.230228	4.185939	0.909275
H	-0.214661	3.821817	1.662990
H	-0.719618	3.451711	-1.323137
H	0.085440	5.626005	-0.499346
H	-2.305456	4.451854	0.074952

Table S46: BPW91 6-311+g* BPDE coordinates (Å).

Atom	x	y	z
C	-1.744336	0.780231	-0.149142
C	-0.673186	1.674199	-0.129131
C	0.657803	1.198584	-0.043362
C	0.911933	-0.202196	-0.016014
C	2.237898	-0.767039	0.024693
C	2.446065	-2.120622	0.061251
C	1.353311	-3.051237	0.064344
C	1.547967	-4.447561	0.108332
C	0.455090	-5.320447	0.103169
C	-0.851124	-4.822871	0.051650
C	-1.094873	-3.433750	0.004220
C	-2.424819	-2.891470	-0.052659
C	-2.636124	-1.539117	-0.100062
C	-1.537936	-0.611605	-0.092071
C	-0.198976	-1.115973	-0.031199
C	0.019852	-2.529082	0.012353
C	1.766425	2.187304	0.057410
C	1.477827	3.602005	0.370971
C	0.044251	4.012517	0.589721
C	-0.924958	3.164198	-0.255822
O	1.853057	3.228068	-0.980087
O	-0.193917	5.413921	0.346776
O	-2.279664	3.470369	0.096770
H	-2.761831	1.168816	-0.204771
H	3.108140	-0.111138	0.010563
H	3.466270	-2.512062	0.084645
H	2.566005	-4.842906	0.146079
H	0.622627	-6.399130	0.138438
H	-1.699203	-5.512129	0.047044
H	-3.271678	-3.582334	-0.059119
H	-3.652921	-1.141051	-0.145326
H	2.749437	1.819555	0.352623
H	2.235789	4.186007	0.904285
H	-0.197416	3.873215	1.655520
H	-0.759211	3.443820	-1.315256
H	0.124100	5.630278	-0.549935
H	-2.351505	4.443338	0.063276

Table S47: BLYP 6-311g* BPDE coordinates (Å).

Atom	x	y	z
C	-1.746417	0.781985	-0.155433
C	-0.672748	1.676827	-0.138534
C	0.663199	1.201098	-0.054440
C	0.917309	-0.203721	-0.022360
C	2.246588	-0.773453	0.022045
C	2.453494	-2.128991	0.062272
C	1.357502	-3.062566	0.065553
C	1.550100	-4.462372	0.113049
C	0.454133	-5.336052	0.109318
C	-0.854538	-4.837129	0.056168
C	-1.099196	-3.444914	0.005525
C	-2.432223	-2.898677	-0.052552
C	-2.642844	-1.544346	-0.102058
C	-1.541858	-0.613337	-0.096678
C	-0.198589	-1.120103	-0.035560
C	0.019964	-2.537657	0.011637
C	1.774530	2.197853	0.049688
C	1.482711	3.615195	0.376139
C	0.041352	4.018585	0.599368
C	-0.924798	3.173674	-0.265039
O	1.853537	3.254376	-0.991251
O	-0.207696	5.430274	0.371188
O	-2.286495	3.486359	0.085849
H	-2.762121	1.173600	-0.209774
H	3.116478	-0.118199	0.007862
H	3.472889	-2.521419	0.089112
H	2.567129	-4.859104	0.152501
H	0.620921	-6.414438	0.147206
H	-1.702263	-5.526241	0.053045
H	-3.279364	-3.588677	-0.057467
H	-3.658983	-1.145530	-0.147588
H	2.760601	1.829299	0.329823
H	2.238154	4.203828	0.907239
H	-0.210872	3.866725	1.660470
H	-0.746489	3.461335	-1.319301
H	0.099619	5.645277	-0.531837
H	-2.332550	4.463340	0.074993

Table S48: BLYP 6-311+g* BPDE coordinates (Å).

Atom	x	y	z
C	-1.749712	0.780283	-0.139396
C	-0.677080	1.677980	-0.114637
C	0.658498	1.201198	-0.029408
C	0.914517	-0.204242	-0.006148
C	2.244823	-0.772259	0.034610
C	2.453368	-2.128657	0.066529
C	1.358111	-3.063406	0.064004
C	1.552709	-4.463760	0.102623
C	0.457178	-5.338984	0.092475
C	-0.852624	-4.840611	0.041272
C	-1.098151	-3.447816	-0.000834
C	-2.431993	-2.902463	-0.057615
C	-2.643939	-1.547315	-0.099928
C	-1.543024	-0.615454	-0.086712
C	-0.199771	-1.121652	-0.025849
C	0.020119	-2.539644	0.012475
C	1.772441	2.191827	0.073051
C	1.489013	3.614775	0.371632
C	0.051812	4.038249	0.581507
C	-0.933153	3.176224	-0.245566
O	1.872782	3.233408	-0.989030
O	-0.173185	5.449148	0.309434
O	-2.294870	3.479702	0.136102
H	-2.766990	1.166963	-0.196471
H	3.114494	-0.116782	0.025574
H	3.473362	-2.519646	0.090714
H	2.570100	-4.859742	0.140067
H	0.624963	-6.417420	0.123482
H	-1.699590	-5.530608	0.032771
H	-3.278715	-3.592889	-0.068080
H	-3.660567	-1.149806	-0.145047
H	2.753188	1.822924	0.369411
H	2.245256	4.203213	0.901203
H	-0.189403	3.928348	1.649962
H	-0.797798	3.452424	-1.308084
H	0.146472	5.649240	-0.593571
H	-2.392474	4.449955	0.057656

Table S49: B1LYP 6-311g* BPDE coordinates (Å).

Atom	x	y	z
C	-1.733016	0.776024	-0.154713
C	-0.666335	1.663859	-0.137112
C	0.657226	1.189831	-0.055949
C	0.908197	-0.201385	-0.020669
C	2.233469	-0.768334	0.027396
C	2.437783	-2.110026	0.068297
C	1.345069	-3.039771	0.068500
C	1.538272	-4.427556	0.115692
C	0.450437	-5.295576	0.109329
C	-0.848620	-4.799594	0.054058
C	-1.088956	-3.418547	0.004062
C	-2.417551	-2.875148	-0.056071
C	-2.625927	-1.534620	-0.105130
C	-1.528082	-0.607585	-0.097669
C	-0.197405	-1.109386	-0.035160
C	0.019936	-2.520148	0.012409
C	1.764326	2.184183	0.037537
C	1.472928	3.585909	0.367732
C	0.041988	3.987181	0.596644
C	-0.918794	3.151728	-0.258767
O	1.824831	3.222300	-0.979320
O	-0.197186	5.378551	0.368118
O	-2.261527	3.453275	0.096613
H	-2.741294	1.164779	-0.207614
H	3.096525	-0.117560	0.016888
H	3.448972	-2.500968	0.098356
H	2.547883	-4.820998	0.156995
H	0.615966	-6.366011	0.146853
H	-1.690391	-5.483246	0.048786
H	-3.257454	-3.561211	-0.062404
H	-3.633891	-1.137321	-0.151788
H	2.744778	1.818392	0.308580
H	2.225073	4.174291	0.885789
H	-0.203102	3.830914	1.650255
H	-0.749020	3.438241	-1.305470
H	0.110609	5.603248	-0.518350
H	-2.335544	4.414992	0.077472

Table S50: B1LYP 6-311+g* BPDE coordinates (Å).

Atom	x	y	z
C	-1.735780	0.774781	-0.142433
C	-0.669759	1.664851	-0.119406
C	0.653489	1.190028	-0.037391
C	0.905972	-0.201710	-0.009130
C	2.232096	-0.767301	0.035426
C	2.437731	-2.109843	0.070073
C	1.345561	-3.040459	0.066758
C	1.540408	-4.428744	0.107637
C	0.452847	-5.298063	0.097123
C	-0.847210	-4.802455	0.043640
C	-1.088221	-3.420880	-0.000328
C	-2.417499	-2.878244	-0.059134
C	-2.626954	-1.536921	-0.103039
C	-1.529146	-0.609218	-0.090061
C	-0.198401	-1.110588	-0.028285
C	0.020010	-2.521709	0.012824
C	1.762989	2.179503	0.055534
C	1.477973	3.585680	0.365121
C	0.049911	4.002428	0.583744
C	-0.925178	3.153871	-0.244411
O	1.840634	3.206296	-0.976272
O	-0.171571	5.392856	0.323549
O	-2.267367	3.448849	0.131754
H	-2.745364	1.159726	-0.197001
H	3.095055	-0.116411	0.027845
H	3.449458	-2.499665	0.097402
H	2.550350	-4.821633	0.147136
H	0.619174	-6.368555	0.129761
H	-1.688405	-5.486847	0.034870
H	-3.257128	-3.564645	-0.069237
H	-3.635395	-1.140716	-0.149062
H	2.738840	1.812772	0.340580
H	2.230686	4.173122	0.883147
H	-0.186402	3.877132	1.643256
H	-0.785469	3.431408	-1.297302
H	0.145146	5.609761	-0.562580
H	-2.382911	4.404247	0.058066

Table S51: B3LYP 6-311g* BPDE coordinates (Å).

Atom	x	y	z
C	-1.733640	0.776538	-0.155644
C	-0.666568	1.664563	-0.138635
C	0.657737	1.190638	-0.057073
C	0.908912	-0.201505	-0.021953
C	2.233346	-0.767991	0.025625
C	2.438024	-2.111042	0.066872
C	1.345904	-3.040262	0.068014
C	1.538859	-4.428809	0.115768
C	0.450639	-5.297025	0.110307
C	-0.848871	-4.800982	0.055351
C	-1.089718	-3.419309	0.004729
C	-2.417600	-2.876221	-0.055044
C	-2.626230	-1.534336	-0.104651
C	-1.529045	-0.607808	-0.098050
C	-0.197426	-1.109997	-0.035806
C	0.019878	-2.520266	0.012202
C	1.764230	2.184303	0.037703
C	1.472464	3.587026	0.368585
C	0.041266	3.987123	0.597211
C	-0.918549	3.151889	-0.260262
O	1.826705	3.224658	-0.979682
O	-0.200773	5.379585	0.371564
O	-2.262499	3.455522	0.091673
H	-2.742908	1.166149	-0.208465
H	3.097410	-0.116507	0.014219
H	3.450396	-2.502151	0.096456
H	2.549576	-4.822577	0.156820
H	0.616338	-6.368554	0.148321
H	-1.691560	-5.485322	0.050805
H	-3.258537	-3.562839	-0.060744
H	-3.635378	-1.136873	-0.151114
H	2.745557	1.818205	0.310576
H	2.225122	4.174663	0.889418
H	-0.204691	3.828466	1.651577
H	-0.744656	3.438853	-1.307751
H	0.106837	5.605145	-0.516714
H	-2.330382	4.419752	0.077969

Table S52: B3LYP 6-311+g* BPDE coordinates (Å).

Atom	x	y	z
C	-1.749712	0.780283	-0.139396
C	-0.677080	1.677980	-0.114637
C	0.658498	1.201198	-0.029408
C	0.914517	-0.204242	-0.006148
C	2.244823	-0.772259	0.034610
C	2.453368	-2.128657	0.066529
C	1.358111	-3.063406	0.064004
C	1.552709	-4.463760	0.102623
C	0.457178	-5.338984	0.092475
C	-0.852624	-4.840611	0.041272
C	-1.098151	-3.447816	-0.000834
C	-2.431993	-2.902463	-0.057615
C	-2.643939	-1.547315	-0.099928
C	-1.543024	-0.615454	-0.086712
C	-0.199771	-1.121652	-0.025849
C	0.020119	-2.539644	0.012475
C	1.772441	2.191827	0.073051
C	1.489013	3.614775	0.371632
C	0.051812	4.038249	0.581507
C	-0.933153	3.176224	-0.245566
O	1.872782	3.233408	-0.989030
O	-0.173185	5.449148	0.309434
O	-2.294870	3.479702	0.136102
H	-2.766990	1.166963	-0.196471
H	3.114494	-0.116782	0.025574
H	3.473362	-2.519646	0.090714
H	2.570100	-4.859742	0.140067
H	0.624963	-6.417420	0.123482
H	-1.699590	-5.530608	0.032771
H	-3.278715	-3.592889	-0.068080
H	-3.660567	-1.149806	-0.145047
H	2.753188	1.822924	0.369411
H	2.245256	4.203213	0.901203
H	-0.189403	3.928348	1.649962
H	-0.797798	3.452424	-1.308084
H	0.146472	5.649240	-0.593571
H	-2.392474	4.449955	0.057656

Table S53: BPW91 6-311g* Tetrol coordinates (Å).

Atom	x	y	z
C	12.422420	0.761389	1.400775
C	11.881851	-0.427734	1.897763
C	12.717584	-1.467784	2.319099
C	14.120220	-1.338771	2.254392
C	15.007792	-2.389132	2.676545
C	16.366458	-2.240218	2.605867
C	16.959516	-1.026557	2.110730
C	18.350770	-0.848090	2.047212
C	18.918684	0.343126	1.576021
C	20.426334	0.491908	1.633985
C	20.955321	1.525513	0.645103
C	20.199503	2.847242	0.789195
C	18.691668	2.671486	0.541550
C	18.097069	1.398501	1.125503
C	16.678942	1.253253	1.173659
C	15.778337	2.286812	0.730998
C	14.418286	2.136988	0.804769
C	13.820105	0.937097	1.316859
C	14.685304	-0.119749	1.749755
C	16.104820	0.039247	1.677327
O	21.054522	-0.779003	1.419689
O	22.349753	1.694129	0.981646
O	20.379942	3.375386	2.110592
H	11.763117	1.567725	1.070726
H	10.797958	-0.547388	1.956573
H	12.285599	-2.394783	2.703985
H	14.573973	-3.316674	3.058220
H	17.027924	-3.047062	2.931052
H	19.011391	-1.651143	2.377206
H	20.685671	0.859776	2.646146
H	20.852250	1.132585	-0.381168
H	20.568449	3.568010	0.036003
H	18.205173	3.553040	0.987160
H	16.189064	3.199155	0.301122
H	13.763044	2.942563	0.463654
H	22.011221	-0.595918	1.457842
H	22.807823	2.071090	0.211099
O	18.413405	2.770710	-0.875928
H	18.481483	1.876662	-1.254556
H	21.335113	3.289931	2.294678

Table S54: BPW91 6-311+g* Tetrol coordinates (Å).

Atom	x	y	z
C	12.421511	0.768684	1.412878
C	11.881192	-0.420772	1.910530
C	12.717887	-1.461884	2.328841
C	14.120670	-1.333532	2.259789
C	15.008328	-2.384483	2.680651
C	16.367344	-2.236777	2.605948
C	16.959533	-1.024457	2.105688
C	18.351232	-0.848699	2.038035
C	18.921102	0.337057	1.554451
C	20.432175	0.477027	1.606950
C	20.969018	1.546185	0.659461
C	20.189070	2.854190	0.806897
C	18.695133	2.653728	0.504024
C	18.098278	1.392398	1.104525
C	16.679396	1.254563	1.167108
C	15.777434	2.292131	0.736639
C	14.416960	2.144692	0.816933
C	13.819435	0.942713	1.324641
C	14.685291	-0.115345	1.752733
C	16.104957	0.041642	1.673639
O	21.045154	-0.796289	1.336323
O	22.357095	1.727121	1.019489
O	20.301530	3.372435	2.142113
H	11.761825	1.576457	1.086562
H	10.797234	-0.539652	1.972631
H	12.286322	-2.388799	2.714899
H	14.574882	-3.311297	3.064960
H	17.028886	-3.043929	2.930672
H	19.008592	-1.651958	2.374260
H	20.704288	0.786870	2.634477
H	20.895117	1.183117	-0.380079
H	20.574377	3.594324	0.082481
H	18.181722	3.543872	0.897239
H	16.182243	3.215271	0.323049
H	13.761872	2.954489	0.485226
H	22.006722	-0.654342	1.417858
H	22.833467	2.104672	0.259405
O	18.477976	2.702182	-0.930554
H	18.511127	1.792045	-1.276326
H	21.251481	3.357668	2.367803

Table S55: BLYP 6-311g* Tetrol coordinates (Å).

Atom	x	y	z
C	12.404382	0.758633	1.404444
C	11.863802	-0.431886	1.907311
C	12.702313	-1.473451	2.330798
C	14.108393	-1.345332	2.262649
C	15.000762	-2.397286	2.686986
C	16.361512	-2.248275	2.613035
C	16.956895	-1.032521	2.111759
C	18.351174	-0.853957	2.044714
C	18.920987	0.338611	1.569168
C	20.437306	0.485194	1.627310
C	20.973703	1.532513	0.646649
C	20.211657	2.858460	0.789956
C	18.696869	2.680491	0.541672
C	18.097199	1.397571	1.117745
C	16.674192	1.252653	1.165988
C	15.767717	2.287111	0.719783
C	14.405510	2.136511	0.796972
C	13.805352	0.935341	1.316235
C	14.674606	-0.123674	1.751555
C	16.098708	0.035762	1.675472
O	21.063011	-0.796529	1.389165
O	22.376447	1.703885	0.996963
O	20.386395	3.390902	2.123022
H	11.743798	1.563415	1.073739
H	10.780176	-0.551230	1.968951
H	12.270264	-2.398734	2.719182
H	14.567913	-3.323677	3.072078
H	17.023461	-3.054125	2.939119
H	19.011329	-1.656710	2.374448
H	20.704613	0.831066	2.643392
H	20.883810	1.147321	-0.382686
H	20.582007	3.582591	0.042619
H	18.208663	3.559688	0.986588
H	16.176263	3.195810	0.282328
H	13.749795	2.940398	0.453259
H	22.023474	-0.623764	1.440457
H	22.841830	2.082834	0.228343
O	18.421032	2.795298	-0.888809
H	18.486137	1.903310	-1.279608
H	21.344401	3.319103	2.310100

Table S56: BLYP 6-311+g* Tetrol coordinates (Å).

Atom	x	y	z
C	12.403012	0.764988	1.415947
C	11.863053	-0.426493	1.919039
C	12.703129	-1.468407	2.340850
C	14.109485	-1.339579	2.269807
C	15.002364	-2.391066	2.694891
C	16.363672	-2.242119	2.618215
C	16.957568	-1.027921	2.110170
C	18.352414	-0.851921	2.038350
C	18.924261	0.333211	1.545289
C	20.444907	0.467893	1.593273
C	20.989931	1.558754	0.664042
C	20.197984	2.867593	0.809930
C	18.700330	2.659429	0.495389
C	18.098482	1.391425	1.093440
C	16.674604	1.255345	1.160425
C	15.766157	2.294285	0.728501
C	14.403323	2.145444	0.811879
C	13.804355	0.940981	1.324788
C	14.674750	-0.118572	1.756058
C	16.099091	0.039671	1.673712
O	21.050524	-0.815654	1.280941
O	22.384361	1.747105	1.045072
O	20.291640	3.387898	2.159621
H	11.741859	1.570593	1.088474
H	10.779591	-0.545985	1.982734
H	12.271986	-2.393689	2.730210
H	14.570450	-3.316550	3.083101
H	17.025795	-3.047339	2.945307
H	19.008636	-1.653983	2.377369
H	20.730287	0.740076	2.625642
H	20.937134	1.209379	-0.379921
H	20.587346	3.615100	0.097942
H	18.179655	3.549088	0.874914
H	16.167254	3.217152	0.313028
H	13.747687	2.954023	0.479402
H	22.015669	-0.696850	1.384286
H	22.872864	2.123788	0.288739
O	18.499347	2.709990	-0.956650
H	18.521420	1.798436	-1.307153
H	21.241486	3.397801	2.395796

Table S57: B1LYP 6-311g* Tetrol coordinates (Å).

Atom	x	y	z
C	12.444928	0.755930	1.392443
C	11.907006	-0.425017	1.892668
C	12.739563	-1.456844	2.319710
C	14.133605	-1.326451	2.256642
C	15.021768	-2.372871	2.686758
C	16.368756	-2.224498	2.618002
C	16.962094	-1.013887	2.115844
C	18.344980	-0.838787	2.051094
C	18.910699	0.343757	1.574189
C	20.418463	0.484533	1.620467
C	20.941321	1.526986	0.644804
C	20.187298	2.841267	0.806944
C	18.686749	2.667881	0.550543
C	18.092487	1.391923	1.125807
C	16.682578	1.247319	1.171879
C	15.781411	2.277872	0.722585
C	14.432790	2.127522	0.793961
C	13.834903	0.930490	1.311035
C	14.694882	-0.117034	1.748495
C	16.112071	0.042605	1.677398
O	21.027871	-0.780243	1.372208
O	22.329105	1.691273	0.963934
O	20.351898	3.344812	2.130632
H	11.790105	1.553502	1.059298
H	10.831264	-0.544578	1.949629
H	12.310537	-2.374780	2.706315
H	14.590148	-3.290919	3.070335
H	17.026455	-3.021949	2.946233
H	18.999576	-1.635655	2.379956
H	20.693581	0.821900	2.627552
H	20.829608	1.149716	-0.376817
H	20.558196	3.570746	0.078049
H	18.201219	3.537402	0.997077
H	16.188957	3.181576	0.293230
H	13.781206	2.923434	0.449564
H	21.979687	-0.633336	1.420460
H	22.787231	2.069555	0.206554
O	18.422015	2.774996	-0.858568
H	18.465069	1.897182	-1.252498
H	21.295783	3.305991	2.328439

Table S58: B1LYP 6-311+g* Tetrol coordinates (Å).

Atom	x	y	z
C	12.443472	0.760599	1.402170
C	11.906043	-0.420981	1.903187
C	12.740006	-1.453346	2.328294
C	14.134338	-1.322735	2.261772
C	15.022875	-2.369212	2.691472
C	16.370458	-2.221315	2.619361
C	16.962537	-1.011828	2.112030
C	18.345921	-0.838895	2.042942
C	18.913017	0.338861	1.554461
C	20.423872	0.471825	1.595798
C	20.954300	1.546239	0.657478
C	20.178214	2.848248	0.822856
C	18.689668	2.653162	0.517425
C	18.093398	1.386969	1.106869
C	16.682752	1.248554	1.166323
C	15.779928	2.282381	0.727668
C	14.430643	2.133552	0.804475
C	13.833829	0.934257	1.317518
C	14.694840	-0.113857	1.751313
C	16.112261	0.044620	1.674559
O	21.019683	-0.793540	1.297888
O	22.336510	1.722618	0.998556
O	20.284047	3.342292	2.158358
H	11.788085	1.558928	1.071869
H	10.830407	-0.540370	1.962656
H	12.311739	-2.371173	2.716095
H	14.592027	-3.286533	3.077695
H	17.028315	-3.018643	2.947578
H	18.997679	-1.635536	2.378016
H	20.709194	0.758367	2.615187
H	20.869707	1.196220	-0.375956
H	20.562682	3.594545	0.119748
H	18.180230	3.530466	0.917663
H	16.181587	3.196209	0.313274
H	13.778993	2.932957	0.468394
H	21.974557	-0.688468	1.389708
H	22.814446	2.093295	0.248720
O	18.480083	2.715462	-0.907063
H	18.484767	1.824037	-1.273791
H	21.220754	3.375087	2.390286

Table S59: B3LYP 6-311g* Tetrol coordinates (Å).

Atom	x	y	z
C	12.443316	0.756756	1.394118
C	11.905200	-0.424976	1.893611
C	12.737844	-1.457781	2.319328
C	14.132721	-1.327910	2.255880
C	15.020312	-2.374394	2.684203
C	16.368727	-2.226057	2.615055
C	16.961770	-1.015674	2.114465
C	18.345425	-0.839932	2.049835
C	18.911163	0.343582	1.574387
C	20.418242	0.485764	1.622620
C	20.942060	1.526246	0.645181
C	20.188112	2.841324	0.804105
C	18.686741	2.667789	0.550184
C	18.092772	1.392504	1.125880
C	16.682101	1.247899	1.172039
C	15.781554	2.278304	0.724013
C	14.431558	2.128162	0.795925
C	13.833932	0.931467	1.312068
C	14.694481	-0.117328	1.748492
C	16.111223	0.042034	1.677112
O	21.031026	-0.779479	1.380491
O	22.330456	1.691142	0.967044
O	20.356277	3.349283	2.126564
H	11.787913	1.555675	1.061659
H	10.828345	-0.544435	1.951017
H	12.308409	-2.377012	2.705583
H	14.588424	-3.293844	3.067349
H	17.026874	-3.024975	2.942605
H	19.001088	-1.637659	2.378420
H	20.690744	0.828489	2.630226
H	20.831761	1.146430	-0.376957
H	20.558255	3.568779	0.070763
H	18.201672	3.538738	0.997844
H	16.189679	3.182877	0.294029
H	13.779488	2.925482	0.452105
H	21.983871	-0.627013	1.427665
H	22.789441	2.069474	0.208008
O	18.419021	2.775214	-0.859539
H	18.463535	1.895093	-1.252531
H	21.302325	3.303282	2.322002

Table S60: B3LYP 6-311+g* Tetrol coordinates (Å).

Atom	x	y	z
C	12.441937	0.761590	1.404154
C	11.904347	-0.420879	1.904137
C	12.738386	-1.454272	2.327675
C	14.133526	-1.324147	2.260853
C	15.021510	-2.370737	2.688545
C	16.370466	-2.222811	2.616139
C	16.962238	-1.013441	2.110651
C	18.346372	-0.839831	2.041873
C	18.913528	0.338822	1.554744
C	20.423743	0.473128	1.597960
C	20.955100	1.545913	0.658146
C	20.178753	2.848517	0.819877
C	18.689704	2.652579	0.516039
C	18.093707	1.387650	1.106949
C	16.682292	1.249421	1.166788
C	15.780028	2.283224	0.729812
C	14.429430	2.134574	0.807205
C	13.832894	0.935452	1.318902
C	14.694485	-0.113995	1.751422
C	16.111444	0.044257	1.674405
O	21.022650	-0.793105	1.305426
O	22.337795	1.723227	1.002001
O	20.286724	3.347526	2.154363
H	11.785951	1.561347	1.074737
H	10.827586	-0.540201	1.964009
H	12.309728	-2.373524	2.714880
H	14.590408	-3.289590	3.074088
H	17.028798	-3.021668	2.943513
H	18.999140	-1.637377	2.376700
H	20.706841	0.764019	2.618323
H	20.872189	1.193458	-0.375918
H	20.562896	3.593011	0.112585
H	18.180133	3.531754	0.915767
H	16.182106	3.198354	0.315556
H	13.777255	2.935500	0.472031
H	21.978840	-0.682671	1.396343
H	22.816744	2.093223	0.250257
O	18.478256	2.713263	-0.909551
H	18.484058	1.818907	-1.273862
H	21.225869	3.372851	2.385325

Table S61: BPW91 6-311g* hydrogen bonded structure (Å).

Atom	x	y	z
C	0.583539	4.177554	1.587857
C	0.069264	2.755728	1.666727
C	0.518505	1.801080	0.722626
C	1.597264	2.181878	-0.226470
C	2.377718	3.415933	-0.001085
C	2.072804	4.244785	1.222421
C	-0.023894	0.485381	0.724990
C	-0.985915	0.129476	1.732924
C	-1.402832	1.101537	2.698856
C	-0.871278	2.404135	2.634733
C	-1.532316	-1.191188	1.780458
C	-1.133046	-2.170760	0.813779
C	-0.188133	-1.782586	-0.194990
C	0.344213	-0.520882	-0.240693
C	-2.483041	-1.543838	2.796618
C	-3.002137	-2.855453	2.824017
C	-2.603981	-3.803447	1.876419
C	-1.681308	-3.468423	0.880356
C	-2.357335	0.722536	3.704281
C	-2.873707	-0.544785	3.752982
O	1.364491	3.406138	-1.047154
O	2.357541	5.645808	1.046382
O	0.356282	4.864661	2.819232
O	2.640115	3.088889	-3.502388
As	2.643438	1.355983	-3.982240
O	2.694459	0.329000	-2.666506
C	1.056550	1.137497	-5.091372
C	4.218029	1.331698	-5.118399
H	-1.193452	3.152909	3.359139
H	1.044358	-0.276781	-1.042441
H	0.104494	-2.521176	-0.945861
H	-1.376277	-4.214065	0.142190
H	-3.017488	-4.813476	1.914254
H	-3.724196	-3.125740	3.598285
H	-3.597560	-0.815385	4.525630
H	-2.666223	1.472400	4.436635
H	2.075493	1.398612	-0.818657
H	3.404263	3.460514	-0.379409
H	2.659837	3.838983	2.066208
H	0.040998	4.694407	0.772110
H	3.291477	5.798875	1.265684
H	0.790629	5.730391	2.701056
H	1.069026	1.884331	-5.893554
H	0.170974	1.275830	-4.460667
H	1.056992	0.126631	-5.516339
H	4.135171	2.127335	-5.867723
H	2.109763	3.210402	-2.668947
H	4.283008	0.355254	-5.612252
H	5.100299	1.493649	-4.489380

Table S62: BPW91 6-311+g* hydrogen bonded structure (Å).

Atom	x	y	z
C	0.609157	4.178550	1.617049
C	0.083780	2.758229	1.685293
C	0.548826	1.798028	0.754311
C	1.650956	2.167205	-0.170551
C	2.432381	3.398412	0.063406
C	2.104270	4.241779	1.270641
C	0.000071	0.484636	0.747792
C	-0.988745	0.136631	1.731746
C	-1.424421	1.114017	2.683503
C	-0.883932	2.413794	2.629780
C	-1.541995	-1.181699	1.770779
C	-1.123434	-2.166601	0.817895
C	-0.152492	-1.786443	-0.169173
C	0.386216	-0.526729	-0.205148
C	-2.518926	-1.526183	2.764533
C	-3.043849	-2.835911	2.784978
C	-2.626402	-3.789768	1.850935
C	-1.678379	-3.462185	0.875778
C	-2.406393	0.743917	3.665972
C	-2.929418	-0.521485	3.706882
O	1.448538	3.383196	-1.010094
O	2.398492	5.641203	1.079497
O	0.360218	4.860267	2.851821
O	2.531261	3.098111	-3.567674
As	2.656795	1.358472	-4.031122
O	2.852297	0.364774	-2.698233
C	1.033981	0.993203	-5.042969
C	4.170670	1.438475	-5.242959
H	-1.221894	3.164191	3.345255
H	1.107880	-0.289311	-0.988806
H	0.155454	-2.528781	-0.910265
H	-1.358712	-4.212080	0.147922
H	-3.044749	-4.798195	1.882803
H	-3.785880	-3.100269	3.542498
H	-3.673935	-0.785653	4.462134
H	-2.730313	1.497958	4.387683
H	2.141738	1.377198	-0.741421
H	3.469727	3.431152	-0.285848
H	2.684525	3.849826	2.125297
H	0.074894	4.705008	0.802916
H	3.333552	5.800581	1.294659
H	0.753241	5.747438	2.747119
H	0.943409	1.722874	-5.855952
H	0.177751	1.073348	-4.363621
H	1.095071	-0.022808	-5.451314
H	3.982370	2.205641	-6.003239
H	2.105795	3.190360	-2.671473
H	4.292395	0.458284	-5.718657
H	5.065031	1.689578	-4.662033

Table S63: BLYP 6-311g* hydrogen bonded structure (Å).

Atom	x	y	z
C	0.583395	4.186837	1.604239
C	0.071677	2.754893	1.684416
C	0.523372	1.798123	0.736522
C	1.607336	2.180110	-0.214554
C	2.380957	3.426023	-0.003137
C	2.074192	4.266656	1.219555
C	-0.022527	0.478595	0.735814
C	-0.989038	0.121342	1.746301
C	-1.406184	1.095972	2.716585
C	-0.871712	2.401193	2.653414
C	-1.540188	-1.202582	1.791805
C	-1.141684	-2.184820	0.820454
C	-0.192840	-1.794524	-0.190170
C	0.343330	-0.531727	-0.234610
C	-2.495541	-1.556146	2.810377
C	-3.018474	-2.870133	2.834642
C	-2.620915	-3.819555	1.883265
C	-1.694862	-3.484401	0.885714
C	-2.365140	0.714928	3.723788
C	-2.884994	-0.553564	3.770563
O	1.361821	3.410717	-1.059058
O	2.343267	5.679426	1.020681
O	0.366379	4.869149	2.853875
O	2.666421	3.095796	-3.516107
As	2.654977	1.351219	-4.003977
O	2.687585	0.315103	-2.683898
C	1.055506	1.152772	-5.132969
C	4.251373	1.318741	-5.141933
H	-1.194644	3.148792	3.377739
H	1.042300	-0.289228	-1.036157
H	0.098226	-2.532373	-0.942212
H	-1.391931	-4.230031	0.146944
H	-3.036733	-4.828550	1.919188
H	-3.741549	-3.140830	3.607556
H	-3.609667	-0.823547	4.542431
H	-2.672975	1.464236	4.456905
H	2.085971	1.397779	-0.803350
H	3.406414	3.477459	-0.383104
H	2.676608	3.882269	2.061442
H	0.026986	4.709942	0.803891
H	3.282078	5.844932	1.221882
H	0.777007	5.748269	2.732570
H	1.079535	1.905839	-5.928892
H	0.170309	1.295644	-4.502921
H	1.049454	0.144671	-5.564012
H	4.183668	2.127637	-5.878316
H	2.124648	3.223178	-2.689228
H	4.302576	0.348731	-5.649604
H	5.131106	1.457275	-4.504028

Table S64: BLYP 6-311+g* hydrogen bonded structure (Å).

Atom	x	y	z
C	0.614668	4.191351	1.646440
C	0.091828	2.760099	1.711785
C	0.565410	1.797511	0.780114
C	1.676489	2.168093	-0.141408
C	2.448290	3.412169	0.079595
C	2.111930	4.270099	1.281860
C	0.013185	0.480127	0.766905
C	-0.988631	0.131310	1.744775
C	-1.432228	1.111695	2.696891
C	-0.887109	2.413760	2.649145
C	-1.548111	-1.189921	1.776524
C	-1.122244	-2.177891	0.822812
C	-0.137169	-1.796898	-0.156544
C	0.406293	-0.536136	-0.186183
C	-2.539242	-1.534364	2.763478
C	-3.069863	-2.845934	2.775564
C	-2.645225	-3.801727	1.841304
C	-1.684085	-3.474943	0.873646
C	-2.427887	0.740465	3.672365
C	-2.956262	-0.525750	3.706137
O	1.464647	3.388070	-1.009997
O	2.388994	5.681609	1.061445
O	0.373624	4.863602	2.903483
O	2.544544	3.096490	-3.590613
As	2.666542	1.342038	-4.062566
O	2.874159	0.340645	-2.724946
C	1.016683	0.978773	-5.068673
C	4.185101	1.430752	-5.298099
H	-1.231484	3.162537	3.362033
H	1.135657	-0.301388	-0.961709
H	0.176391	-2.538855	-0.895169
H	-1.360629	-4.224910	0.148111
H	-3.067305	-4.808420	1.866992
H	-3.820196	-3.109852	3.524481
H	-3.708665	-0.788469	4.453536
H	-2.756470	1.493917	4.392037
H	2.171236	1.378518	-0.705191
H	3.486491	3.452144	-0.265231
H	2.707982	3.905541	2.136293
H	0.064768	4.726672	0.851154
H	3.328517	5.856872	1.257259
H	0.723467	5.770827	2.797759
H	0.922188	1.711686	-5.877996
H	0.169319	1.059884	-4.378736
H	1.073952	-0.036487	-5.478824
H	3.988756	2.204653	-6.049240
H	2.125557	3.192237	-2.690314
H	4.299947	0.453636	-5.781379
H	5.083061	1.676400	-4.720779

Table S65: B1LYP 6-311g* hydrogen bonded structure (Å).

Atom	x	y	z
C	0.594154	4.168896	1.596281
C	0.079919	2.747202	1.669151
C	0.537611	1.795518	0.737957
C	1.625515	2.177869	-0.201683
C	2.396572	3.405964	0.027819
C	2.079506	4.240525	1.239572
C	-0.000268	0.488064	0.735292
C	-0.971821	0.136157	1.723827
C	-1.400708	1.104472	2.675391
C	-0.870842	2.399435	2.618876
C	-1.518122	-1.182297	1.766355
C	-1.106553	-2.158050	0.813602
C	-0.147872	-1.771612	-0.182074
C	0.380714	-0.520684	-0.224028
C	-2.478348	-1.530224	2.763069
C	-2.995405	-2.833944	2.786680
C	-2.584793	-3.779926	1.852182
C	-1.651733	-3.448418	0.873948
C	-2.370724	0.727794	3.666360
C	-2.883505	-0.528640	3.710039
O	1.399389	3.386025	-1.016411
O	2.359211	5.629810	1.048076
O	0.361889	4.839966	2.826984
O	2.594760	3.063883	-3.509375
As	2.605966	1.350890	-3.980443
O	2.657027	0.349265	-2.662864
C	1.021854	1.127075	-5.071756
C	4.173700	1.314702	-5.107876
H	-1.200661	3.142940	3.332246
H	1.084128	-0.279639	-1.011149
H	0.151683	-2.507334	-0.921006
H	-1.338440	-4.190505	0.147882
H	-2.995617	-4.782348	1.885946
H	-3.723845	-3.100707	3.544463
H	-3.613887	-0.796343	4.465739
H	-2.687440	1.474782	4.385918
H	2.103576	1.398918	-0.779604
H	3.417434	3.458006	-0.340130
H	2.660238	3.851931	2.084029
H	0.055956	4.688649	0.793613
H	3.290469	5.794543	1.224058
H	0.747085	5.718643	2.727081
H	1.025055	1.865891	-5.871251
H	0.145340	1.264815	-4.440855
H	1.017690	0.122624	-5.492560
H	4.094506	2.096284	-5.861541
H	2.103749	3.207734	-2.673158
H	4.242584	0.340587	-5.589228
H	5.050178	1.483046	-4.485123

Table S66: BPW91 6-311g* hydrogen bonded structure (Å).

Atom	x	y	z
C	0.621056	4.177330	1.629155
C	0.099911	2.755460	1.688219
C	0.583567	1.798508	0.775386
C	1.698563	2.172670	-0.133879
C	2.464080	3.401188	0.106872
C	2.114189	4.249651	1.299713
C	0.043527	0.491550	0.761378
C	-0.963479	0.146515	1.715838
C	-1.422754	1.120435	2.646976
C	-0.885651	2.413544	2.605341
C	-1.514335	-1.170764	1.745380
C	-1.070826	-2.152490	0.813285
C	-0.075569	-1.773740	-0.149159
C	0.456495	-0.523240	-0.177927
C	-2.511178	-1.511035	2.708188
C	-3.032344	-2.813774	2.720239
C	-2.590038	-3.766297	1.806018
C	-1.620851	-3.441867	0.860154
C	-2.430101	0.752014	3.603821
C	-2.948318	-0.503406	3.634744
O	1.501295	3.371111	-0.969316
O	2.399980	5.637723	1.093564
O	0.359242	4.842589	2.860943
O	2.494174	3.054921	-3.560579
As	2.587441	1.334537	-4.018990
O	2.766617	0.359550	-2.686648
C	0.958381	0.999347	-5.009027
C	4.094376	1.372240	-5.224951
H	-1.239163	3.158697	3.305425
H	1.189275	-0.288459	-0.939160
H	0.249549	-2.513810	-0.872716
H	-1.283383	-4.188500	0.149701
H	-3.004312	-4.767604	1.830087
H	-3.788762	-3.074775	3.452245
H	-3.707057	-0.764962	4.364233
H	-2.770643	1.503122	4.308069
H	2.193639	1.387920	-0.688206
H	3.496799	3.446156	-0.227194
H	2.684008	3.876981	2.158230
H	0.094123	4.703876	0.824313
H	3.330186	5.812222	1.271924
H	0.691286	5.744375	2.772500
H	0.871516	1.723887	-5.816905
H	0.115046	1.094856	-4.327279
H	0.993805	-0.010587	-5.415145
H	3.925469	2.131374	-5.987080
H	2.111819	3.181439	-2.665673
H	4.197880	0.393595	-5.690912
H	4.988347	1.608163	-4.650876

Table S67: B3LYP 6-311g* hydrogen bonded structure (Å).

Atom	x	y	z
C	-0.868622	2.405852	2.621295
C	0.087685	2.754647	1.676976
C	0.549522	1.804213	0.745485
C	0.008303	0.497148	0.735614
C	0.391508	-0.508513	-0.224734
C	-0.140230	-1.759792	-0.189299
C	-1.103409	-2.147417	0.800513
C	-1.651482	-3.437620	0.854815
C	-2.589444	-3.770671	1.828448
C	-3.002659	-2.826643	2.764421
C	-2.483418	-1.522915	2.747162
C	-2.890922	-0.524044	3.694849
C	-2.375547	0.733007	3.657116
C	-1.401116	1.110930	2.672093
C	-0.969171	0.143988	1.719035
C	-1.517729	-1.173253	1.755056
C	1.644990	2.185140	-0.184183
C	2.418170	3.411490	0.053466
C	2.093607	4.243593	1.264883
C	0.604993	4.174904	1.610008
O	1.429190	3.397827	-1.001235
O	2.378193	5.634047	1.081267
O	0.364322	4.847190	2.839152
H	-1.200883	3.149050	3.335704
H	1.099565	-0.265833	-1.009088
H	0.161437	-2.494321	-0.930241
H	-1.335973	-4.178685	0.126974
H	-3.002407	-4.773573	1.857447
H	-3.735482	-3.094733	3.519130
H	-3.625814	-0.793014	4.447358
H	-2.694733	1.479027	4.378307
H	2.125871	1.405665	-0.761839
H	3.443953	3.460386	-0.304686
H	2.666871	3.849531	2.113575
H	0.074397	4.696398	0.801393
H	3.309345	5.795414	1.269638
H	0.761618	5.722906	2.742143
H	0.977302	1.761426	-5.880936
H	0.129219	1.130130	-4.442377
H	1.058980	0.022287	-5.485554
C	1.011570	1.030410	-5.073731
As	2.583443	1.347803	-3.986251
H	4.040436	2.118553	-5.885093
O	2.479926	3.069007	-3.549451
H	2.107521	3.185180	-2.646772
H	4.248974	0.371243	-5.588767
C	4.149147	1.350060	-5.120221
O	2.683414	0.377767	-2.645510
H	5.022448	1.557043	-4.503033

Table S68: B3LYP 6-311+g* hydrogen bonded structure (Å).

Atom	x	y	z
C	0.618214	4.178799	1.627824
C	0.098051	2.757215	1.687480
C	0.577703	1.801961	0.769714
C	1.689677	2.176296	-0.141480
C	2.456625	3.405436	0.098010
C	2.110416	4.252082	1.293105
C	0.036434	0.494500	0.754558
C	-0.965221	0.146746	1.714867
C	-1.418836	1.118752	2.652239
C	-0.882274	2.412822	2.609854
C	-1.515636	-1.170218	1.744174
C	-1.078303	-2.149720	0.805465
C	-0.090223	-1.768182	-0.162160
C	0.442621	-0.516525	-0.190357
C	-2.506402	-1.513747	2.713424
C	-3.027261	-2.817361	2.725046
C	-2.591096	-3.767295	1.804584
C	-1.628379	-3.439845	0.852581
C	-2.419024	0.747544	3.614310
C	-2.937071	-0.509394	3.645362
O	1.490926	3.377643	-0.977743
O	2.394835	5.642040	1.089586
O	0.359794	4.845146	2.860709
O	2.499313	3.056406	-3.556004
As	2.592631	1.331901	-4.010221
O	2.767065	0.357074	-2.674767
C	0.966193	0.994988	-5.006368
C	4.103905	1.367464	-5.212576
H	-1.232235	3.157330	3.314286
H	1.171218	-0.279151	-0.956800
H	0.230103	-2.506588	-0.891287
H	-1.295397	-4.185027	0.136752
H	-3.005432	-4.769803	1.828631
H	-3.779219	-3.080911	3.462416
H	-3.691433	-0.773343	4.380228
H	-2.755546	1.497256	4.323740
H	2.184426	1.391214	-0.698626
H	3.489953	3.449129	-0.238360
H	2.683676	3.877085	2.149952
H	0.088348	4.705609	0.823083
H	3.326526	5.816221	1.269644
H	0.700624	5.745534	2.770875
H	0.883221	1.718516	-5.816819
H	0.119702	1.092630	-4.327357
H	1.003232	-0.016837	-5.410189
H	3.937072	2.126912	-5.976206
H	2.108628	3.183129	-2.661602
H	4.207652	0.387419	-5.677732
H	4.997078	1.603383	-4.635523

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