Supporting Information for "Molten Plastics Induced Noncovalent Interactions for Tunable Cellulose Fast Pyrolysis"

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Table of Contents

S1. Experimental Section

Materials. Microcrystalline cellulose (CE, Alfa Aesar, degree of polymerization = 219, and bulk density of 0.28 g mL^{-1}), polyethylene (PE, Sigma-Aldrich, $M_w \approx 4000$ g mol^{-1}, $M_n \approx 1700$ g mol^{-1}, and density = 0.92 g mL^{-1}), polystyrene (PS, Sigma-Aldrich, $M_w \approx 192\,000$ g mol^{-1}, and density = 1.04 g mL^{-1}), polyethylene glycol (PEG, Alfa Aesar, $M_w \approx 20\,000$ g mol^{-1} and density = 1.200 g mL^{-1}), and polyketone (PK, Goodfellow PK306310, density = 1.240 g mL^{-1}) were used for the pyrolysis experiments. Methanol (Alfa Aesar, environmental grade, 99.8+%) and dichloromethane (DCM, Alfa Aesar, environmental grade, 99.8+%) were used as solvents for product extraction. The standard chemicals used for gas chromatography (GC) calibration include acetic acid (AA, Alfa Aesar, glacial, 99+%), 2-furaldehyde (Alfa Aesar, 98%), 5-hydroxymethyl-2-furaldehyde (Alfa Aesar, 97%), and levoglucosan (LG, Acros Organics, 99+%) for CE-derived pyrolysis products and o-terphenyl (TCI, 99.0+%) as an external calibration standard.

Sample Preparation. To ensure rapid heating of the biomass samples, micrometer-scale thin-film samples were prepared following the thin-film deposition technique by Paulsen *et al.*[1] Briefly, for neat CE fast pyrolysis, 100 μL of CE suspension in distilled water (5 wt % CE) was transferred into a 6 mm x 3 mm (diameter x height) copper autosampler pan (Shimadzu Scientific Instruments). Water was removed via heating on a hot plate (Fisher Scientific, Isotemp 7.25 x 7.25 in., HP 100 120V) at 120°C, resulting in a CE thin-film of approximately 5 mg and 111.84 μm in the copper holder. For binary samples containing CE and one of PE, PS, PEG, and PK, the thickness of the samples was kept constant by changing mass loadings according to the densities of individual components. The sample thickness is calculated using the following equation:

$$\text{Thickness}_{\,i} = \frac{m_i / \rho_i}{\pi \cdot ID^2/4}$$

where ρ_i and ID are the density of species i and the internal diameter of the reactor, respectively. The thickness of the samples was verified using a digital caliper (the iGaging Cal Digital Calipers). The mass loading of PE, PS, PEG, and PK in the neat and co-pyrolysis experiments were determined to be 3.08, 4.10, 3.48, and 4.03 mg, respectively. Through these steps, the same thickness (223.68 μm) was maintained across all samples to equalize the extent of inhibition of evaporation and thermal ejection.[2]

The sample preparation process of PE, PEG, and PK in the neat and co-pyrolysis experiments is summarized in **Figure S1**. These binary samples were prepared by manually mixing CE powder and each plastic powder homogeneously and

melting the binary samples containing PE, PEG, or PK to 92°C, 75°C, or 200°C, respectively, to allow the plastic phase to be molten.

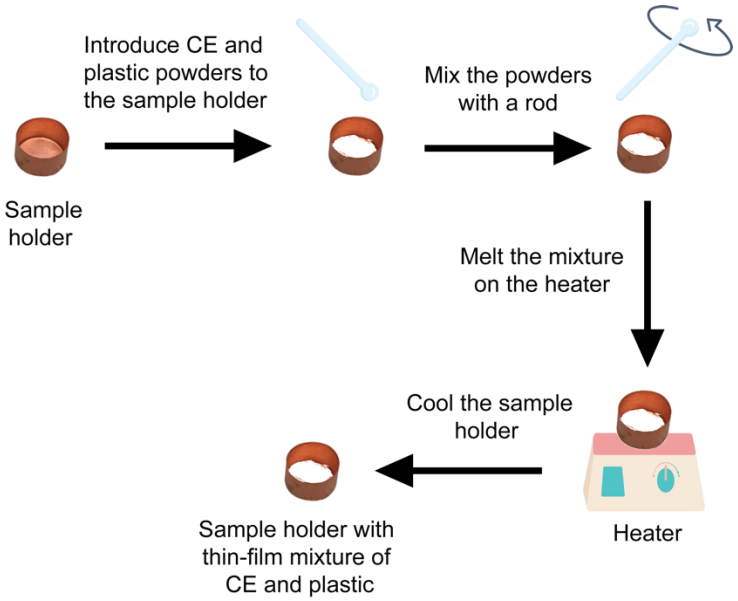

Figure S1. Schematic illustration of sample preparation for PE, PEG, and PK in the neat and co-pyrolysis experiments.

The sample preparation process of PS in the neat and co-pyrolysis experiments is summarized in **Figure S2**. For binary samples containing PS, dilute suspension of CE in DCM solutions dissolving PS were prepared based on target concentrations of CE (35.7 mg g^{-1}) and PS (29.3 mg g^{-1}). Approximately 1 ml of the sample solution was transferred into the copper holder, followed by evaporation of DCM on a hot plate at 100°C. In addition to the co-pyrolysis experiments, neat pyrolysis of PK without CE was performed as controls following the same procedure.

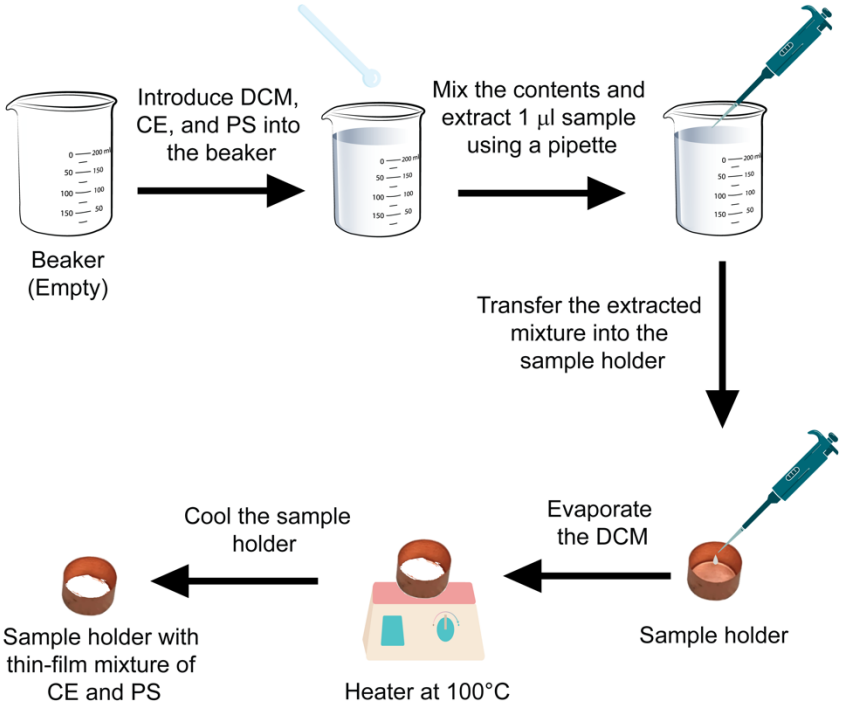

Figure S2. Schematic illustration of sample preparation for PS in the neat and co-pyrolysis experiments.

Pyrolysis Experiments. A custom-made batch reactor used in our previous work[2, 3] was employed for the pyrolysis experiments. The reactor was first evacuated to <0.04 torr before it was closed and placed into a hot furnace of two heating zones, each of which was controlled at the desired reaction temperature with a proportional−integral−derivative (PID) controller (Omega Engineering, CN742). Since measuring temporal evolution of the products was not our interest, we opted a reaction time of 15 min to ensure that cellulose-derived products reach equilibrium. This reaction time is also expected to be sufficiently long to observe the mass transfer effect caused by the molten plastic phase on cellulose pyrolysis, which is expected to slow down cellulose pyrolysis. Finally, we would also like to observe the catalytic effect of cellulose-derived char on thermoplastic pyrolysis, which would not be obvious unless a reaction time of this scale is employed. Since our reactor is designed to mimic semi-batch operations where reaction products are continually removed into the condenser positioned in a liquid nitrogen bath, we do not believe a long reaction time would create interference between the products made from different reaction timescales. The products from cellulose and different thermoplastics are also distinct so that they did not pose a challenge in our product analysis via GC.

The experiments were conducted by beginning with positioning the copper sample holder in the cold zone above the furnace. The sample holder was rapidly dropped into the hot zone to initiate the reaction, ensuring fast heating of the

samples. The condenser placed in the liquid-nitrogen bath was used to collect pyrolysis products throughout the reaction. Between 2 and 6 mg of o-terphenyl was placed inside the condenser prior to the experiments as an external standard. This reactor design mimics semi-batch reactions where volatile products are continuously removed *via* rapid thermal diffusion so that gas-phase reactions are minimized, yet the batch design allows easier mass balance closure. Once the reaction was completed, the reactor was removed from the hot furnace and cooled in a water bath at ambient temperature for 2 min. The condenser was also removed from the liquid-nitrogen bath and thawed to room temperature. The entire reactor assembly was subsequently connected to a vacuum chamber to collect gaseous products. The liquid products in the condenser were then extracted by equal volume of methanol and DCM. Both gaseous and liquid products were analyzed by GC. The experiments were repeated three times to ensure reproducibility. In this work, the average values are reported in the figures, and the standard deviations of the three repeated runs are used as error bars.

Safety Statement. No unexpected or unusually high safety hazards were encountered.

Product Analysis. The identification and quantification of the reaction products were performed using a Shimadzu GC-2010 Plus GC system equipped with a mass spectrometer (MS) and a flame ionization detector (FID) and a Shimadzu GC-2014 system equipped with a thermal conductivity detector (TCD) and FID. For gaseous products, 2 mL of the samples were injected into a Restek packed column (80486-810, 2 m) connected to a TCD. H_2 was used as the carrier gas through the column, with a flow rate set at 12.5 ml min^{-1}. Peak identification and calibration were achieved from results obtained using standard gas mixtures containing CO, CO_2, and C_1−C_4 hydrocarbons (Scotty Specialty Gases). The GC was programmed with an injection temperature of 250°C, and the programmed temperature regime for the GC oven was: start at 35°C, ramp up to 50°C at 7.5°C min^{-1}, hold for 1 min, ramp up to 100°C at 5°C min^{-1}, hold for 3 min, ramp up to 200°C at 10°C min^{-1}, hold for 7 min, ramp up to 250°C at 25°C min^{-1}, and hold at 250°C for 10 min.

Identification of the extracted liquid products was achieved by injecting 3 μL of samples into the GC/MS system equipped with a Shimadzu Rxi-5Sil MS column (30 m). H_2 was used as the carrier gas through the column, with a flow rate set at 1.64 ml min^{-1}. The GC was programmed with an injection temperature of 280°C and a split ratio of 7.0. The programmed temperature regime for the GC oven was: start at 31°C, hold for 5 min, ramp up to 100°C at 4°C min^{-1}, hold for 5 min, ramp up to 150°C at 8°C min^{-1}, hold for 5 min, ramp up to 175°C at 6°C min^{-1}, hold for 5 min, ramp up to 275°C at 5°C min^{-1}, and hold at 275°C for 18 min. Quantification of the extracted liquid products was performed

using the same GC system equipped with a Shimazu Rxi-5Sil MS column (30 m). The GC was programmed with an injection temperature of 280°C and a split ratio of 10.0. H_2 was used as the carrier gas through the column, with a flow rate set at 0.44 ml min^{-1}. The programmed temperature regime for the GC oven was set the same as the GC/MS program described above.

Mixtures of o-terphenyl (external standard), LG, 5-hydroxymethyl-2-furaldehyde, 2-furaldehyde, and AA in four different ratios, dissolved in 40 mL of methanol and 40 mL of DCM, were used as calibration standards for the quantification of CE-derived products in GC analysis.

The mass of the produced char was determined by the difference in weight of the copper sample holder before and after the reaction. The measurement was conducted using a Mettler Toledo XP105 analytical balance with a repeatability of < 0.05 mg.

The mass yields of the CE-derived products are calculated based on their individual mass determined by GC analysis relative to the CE mass initially loaded in the reactor:

$$\text{Mass yield}_i\ (\%) = \frac{m_i}{m_{CE,0}} \times 100$$

where m_i and $m_{CE,0}$ are the mass of species *i* in the product mixture and mass of CE initially loaded in the reactor, respectively.

The carbon yields of the CE-derived products are calculated based on the moles of carbon atoms in the CE sample initially loaded, using the following equation:

$$\text{Carbon yield}_i\ (\%\text{C}) = \frac{\left({m_i}/{MW_i}\right) \cdot N_{C,i}}{\left({m_{CE,0}}/{MW_{glucose}}\right) \cdot N_{C,glucose}} \times 100$$

where MW_i is the molecular weight of species *i* in the product mixture, $N_{C,i}$ is the number of carbon atoms in species *i*, $MW_{glucose}$ is the molecular weight of glucose (which is 180.16 g mol^{-1}), and $N_{C,glucose}$ is the number of carbon atoms in glucose (which is 6). Char is assumed to be pure carbon, where MW_{char} is set as 12.01 g mol^{-1} and $N_{C,char}$ is set as 1.

S2. Computational Methods

Density functional theory (DFT) calculations were performed in the gas phase at the global hybrid meta M06-2X[4] functional coupled with the 6-31+G(2df,p) basis set using the Gaussian 16 package.[5] The functional M06-2X has been reported to accurately predict reaction barriers of carbohydrate systems.[6] The DFT-D3 empirical dispersion correction was included.[7] The D3-M06-2X functional has been shown to accurately estimate conformers, reaction energies, barriers, and noncovalent interactions on large main-group benchmark sets like the GMTKN55.[8] Partial charges were evaluated with the CHelpG scheme.[9]

Frequency calculations were performed to verify that all transition states (TSs) have exactly one negative frequency and all minima have zero imaginary frequency. The TSs were searched by the Berny algorithm.[10] Intrinsic reaction coordinate calculations using the Hessian-based predictor-corrector integration algorithm[11-13] were performed to confirm that each TS connects the reactant(s) and the product(s) of interest. Corrections to the harmonic oscillator approximation at low frequency modes were included using quasi-rigid-rotor-harmonic-oscillator approach proposed by Grimme,[14] which interpolates between the harmonic vibrational and free rotor entropy. The cut-off frequency was set to 150 cm^{-1} (within the usual limits 50–150 cm^{-1}). The exponent of the Head-Gordon damping function[15] was chosen as 4 (same value used by Grimme).

Given the large molecules studied, small changes in structures could lead to large electronic energy differences. In the absence of experimental structures, the geometries associated with the lowest energy levels were identified for each supramolecular system by starting the calculations with a set of different configurations, followed by manual distortion and re-optimization. For each elementary step studied, the Gibbs free energy of activation, $\Delta^{\ddagger}G^{0}$, was determined from the difference between the Gibbs free energy of the TS and that of the lowest-energy conformation found in this study. The rate constants were calculated using the transition-state theory based on the Eyring-Polanyi equation[16, 17] over a temperature range of 300–1500 K with an interval of 100 K. The reported activation energy and pre-exponential factor values were obtained from the Arrhenius plot.

In our DFT calculations, cellobiose, a dimer of CE containing a β-1,4 glycosidic bond, was employed as a model compound to investigate the reaction pathways of CE pyrolysis. Propane (C3), benzene (Bz), dimethyl ether (DME), and acetone (Ace) were used as surrogates for PE, PS, PEG, and PK, respectively.

S3. Supporting Experimental Data

Table S1. Mass yields (in wt%) of cellulose-derived products from neat cellulose (CE) pyrolysis and co-pyrolysis of CE with polyethylene (CE+PE), polystyrene (CE+PS), polyethylene glycol (CE+PEG), or polyketone (CE+PK)[a]

Products	Neat CE	CE+PE	CE+PS	CE+PEG	CE+PK
Levoglucosan (LG)	14.29 ± 5.51	30.62 ± 8.39	34.64 ± 1.25	32.88 ± 6.29	52.20 ± 1.59
Levoglucosenone (LGO)	0.00 ± 0.00	0.00 ± 0.00	0.48 ± 0.11	0.00 ± 0.00	0.00 ± 0.00
Dianhydroglucopyranose (DAGP)	6.48 ± 4.27	2.27 ± 1.36	3.50 ± 2.87	3.37 ± 0.98	0.56 ± 0.49
1,6-Anhydroglucofuranose (AGF)	0.70 ± 0.36	2.49 ± 0.84	2.45 ± 0.19	1.63 ± 0.39	3.04 ± 0.08
Glycolaldehyde (GA)	1.18 ± 0.34	2.75 ± 1.05	2.55 ± 0.75	7.77 ± 2.29	3.41 ± 0.55
Acetic acid (AA)	1.27 ± 0.38	3.86 ± 0.58	3.20 ± 0.58	3.22 ± 1.01	1.19 ± 0.11
5-Hydroxymethylfurfural (5-HMF)	2.30 ± 1.90	0.46 ± 0.80	3.60 ± 2.01	3.16 ± 1.58	1.05 ± 0.77
2-(5H)-Furanone (FO)	0.95 ± 0.50	0.34 ± 0.59	2.19 ± 2.45	0.95 ± 0.62	1.52 ± 0.05
Furfural (FF)	0.16 ± 0.20	0.00 ± 0.00	2.11 ± 1.89	0.08 ± 0.13	0.00 ± 0.00
Carbon monoxide (CO)	1.16 ± 0.79	0.73 ± 0.55	0.43 ± 0.14	0.23 ± 0.07	0.40 ± 0.34
Carbon dioxide (CO_2)	1.93 ± 1.23	1.85 ± 1.54	1.27 ± 1.02	1.38 ± 0.59	0.64 ± 0.17
Char	1.90 ± 0.32	1.33 ± 2.14	0.91 ± 0.79	0.88 ± 0.77	0.93 ± 0.44
Total	**32.33 ± 3.14**	**46.71 ± 6.99**	**57.33 ± 0.65**	**55.54 ± 1.15**	**64.95 ± 0.24**

[a] Some high uncertainties reflected by the large standard deviation values are attributed to the low species yields.

Figure S3a shows the carbon yields of CE-derived products from neat CE pyrolysis as well as binary co-pyrolysis of CE with PE, PS, PEG, or PK, while **Figure S3b** depicts the corresponding selectivity toward CE-derived anhydrosugars, small oxygenates, furans, gases, and char. The same trend was observed comparing the carbon yields with mass yields shown in **Figure 1**. However, the absolute values of carbon yields are higher since the mass of undetected water is excluded in this calculation.

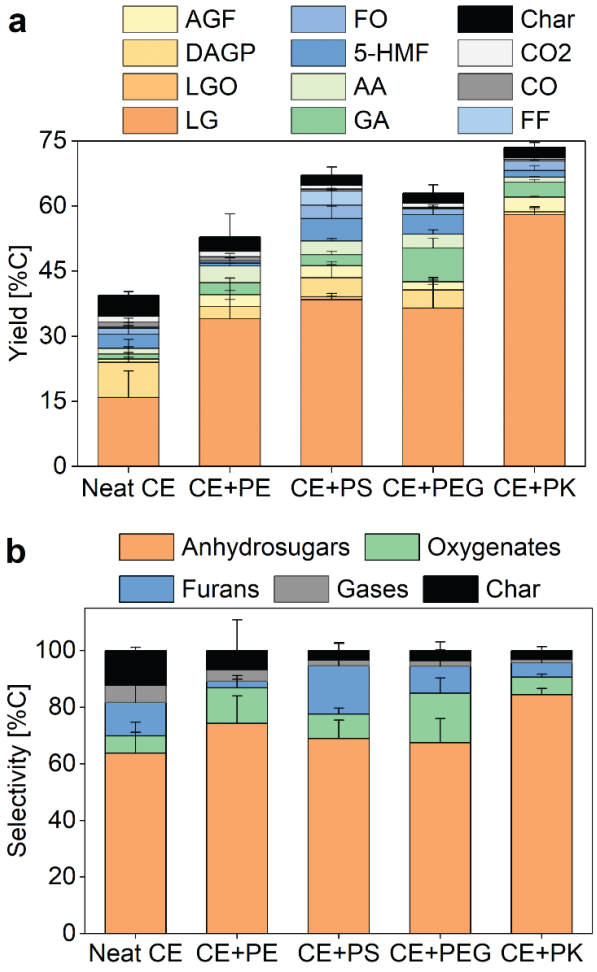

Figure S3. (a) Carbon yields of CE-derived products and (b) selectivity toward CE-derived anhydrosugars, small oxygenates, furans, gases, and char from neat CE pyrolysis and co-pyrolysis of CE with PE (CE+PE), PS (CE+PS), PEG (CE+PEG), or PK (CE+PK). Yields are shown for levoglucosan (LG), levoglucosenone (LGO), dianhydroglucopyranose (DAGP), 1,6-anhydroglucofuranose (AGF), glycolaldehyde (GA), acetic acid (AA), 5-hydroxymethylfurfural (5-HMF), 2-(5H)-furanone (FO), furfural (FF), carbon monoxide (CO), carbon dioxide (CO_2), and char. Reaction condition: 5.0 mg of CE co-pyrolyzed with PE (3.08 mg), PS (4.10 mg), PEG (3.48 mg), or PK (4.03 mg) at 500°C under vacuum (< 0.04 torr). The mass loading of each plastic component was chosen to ensure that the thickness of the samples was kept constant and the extent of inhibition of evaporation and thermal ejection approximately equal.

Table S2. Carbon yields (%C) of CE-derived products from neat CE pyrolysis and co-pyrolysis of CE with PE (CE+PE), PS (CE+PS), PEG (CE+PEG), or PK (CE+PK)[a]

Products	Neat CE	CE+PE	CE+PS	CE+PEG	CE+PK
Levoglucosan (LG)	15.86 ± 6.11	34.02 ± 9.34	38.43 ± 1.45	36.52 ± 6.99	58.01 ± 1.77
Levoglucosenone (LGO)	0.00 ± 0.00	0.00 ± 0.00	0.69 ± 0.16	0.00 ± 0.00	0.00 ± 0.00
Dianhydroglucopyranose (DAGP)	8.10 ± 5.34	2.82 ± 1.66	4.39 ± 3.62	4.21 ± 1.23	0.71 ± 0.62
1,6-Anhydroglucofuranose (AGF)	0.78 ± 0.40	2.77 ± 0.94	2.72 ± 0.22	1.81 ± 0.43	3.38 ± 0.09
Glycolaldehyde (GA)	1.18 ± 0.34	2.75 ± 1.06	2.55 ± 0.77	7.76 ± 2.30	3.41 ± 0.56
Acetic acid (AA)	1.28 ± 0.39	3.86 ± 0.58	3.19 ± 0.58	3.22 ± 1.01	1.19 ± 0.11
5-Hydroxymethylfurfural (5-HMF)	3.28 ± 2.71	0.66 ± 1.14	5.15 ± 2.85	4.51 ± 2.26	1.50 ± 1.09
2-(5H)-Furanone (FO)	1.36 ± 0.70	0.49 ± 0.84	3.13 ± 3.50	1.36 ± 0.88	2.17 ± 0.08
Furfural (FF)	0.25 ± 0.31	0.00 ± 0.00	3.21 ± 2.85	0.11 ± 0.20	0.00 ± 0.00
Carbon monoxide (CO)	1.20 ± 0.85	0.93 ± 0.78	0.46 ± 0.15	0.25 ± 0.08	0.42 ± 0.37
Carbon dioxide (CO_2)	1.28 ± 0.84	1.26 ± 1.05	0.86 ± 0.69	0.96 ± 0.42	0.44 ± 0.12
Char	4.81 ± 0.90	3.34 ± 5.34	2.27 ± 1.98	2.25 ± 1.95	2.33 ± 1.09
Total	**39.39 ± 5.09**	**52.89 ± 4.51**	**67.06 ± 1.52**	**62.97 ± 1.91**	**73.56 ± 0.87**

[a] Some high uncertainties reflected by the large standard deviation values are attributed to the low species yields.

Table S3. Mass yields (in wt%) of polyethylene-derived products (linear alkanes, alkenes, and dienes) from neat polyethylene (PE) pyrolysis and co-pyrolysis of PE with cellulose (CE+PE) [a]

Alkenes	Neat PE	CE+PE	Alkanes	Neat PE	CE+PE	Dienes	Neat PE	CE+PE
C1	-	-	C1	0.02 ± 0.01	0.02 ± 0.01	C1	-	-
C2	0.01 ± 0.00	0.02 ± 0.01	C2	0.01 ± 0.01	0.01 ± 0.00	C2	-	-
C3	0.01 ± 0.01	0.01 ± 0.01	C3	0.01 ± 0.01	0.03 ± 0.02	C3	0.00 ± 0.00	0.00 ± 0.00
C4	0.00 ± 0.00	0.00 ± 0.00	C4	0.00 ± 0.00	0.00 ± 0.00	C4	0.00 ± 0.00	0.00 ± 0.00
C5	0.00 ± 0.00	0.01 ± 0.01	C5	0.01 ± 0.01	0.01 ± 0.01	C5	0.00 ± 0.00	0.00 ± 0.00
C6	0.00 ± 0.00	0.00 ± 0.01	C6	0.00 ± 0.01	0.00 ± 0.01	C6	0.00 ± 0.00	0.00 ± 0.00
C7	0.12 ± 0.06	0.15 ± 0.08	C7	0.05 ± 0.06	0.08 ± 0.04	C7	0.07 ± 0.06	0.13 ± 0.10
C8	0.07 ± 0.01	0.11 ± 0.09	C8	0.08 ± 0.03	0.09 ± 0.05	C8	0.06 ± 0.04	0.06 ± 0.03
C9	0.04 ± 0.01	0.10 ± 0.11	C9	0.04 ± 0.02	0.06 ± 0.03	C9	0.04 ± 0.03	0.04 ± 0.01
C10	0.08 ± 0.02	0.13 ± 0.15	C10	0.04 ± 0.01	0.05 ± 0.04	C10	0.05 ± 0.00	0.05 ± 0.04
C11	0.09 ± 0.01	0.11 ± 0.05	C11	0.07 ± 0.01	0.08 ± 0.07	C11	0.03 ± 0.02	0.11 ± 0.14
C12	0.08 ± 0.02	0.12 ± 0.11	C12	0.06 ± 0.01	0.07 ± 0.05	C12	0.04 ± 0.03	0.04 ± 0.03
C13	0.05 ± 0.03	0.08 ± 0.08	C13	0.05 ± 0.02	0.06 ± 0.03	C13	0.03 ± 0.01	0.03 ± 0.02
C14	0.06 ± 0.04	0.12 ± 0.07	C14	0.03 ± 0.02	0.06 ± 0.02	C14	0.01 ± 0.01	0.03 ± 0.02
C15	0.06 ± 0.04	0.03 ± 0.06	C15	0.05 ± 0.03	0.03 ± 0.05	C15	0.02 ± 0.01	0.01 ± 0.02
C16	0.07 ± 0.02	0.03 ± 0.05	C16	0.06 ± 0.02	0.03 ± 0.05	C16	0.01 ± 0.01	0.01 ± 0.01
C17	0.07 ± 0.02	0.21 ± 0.13	C17	0.07 ± 0.01	0.12 ± 0.07	C17	0.01 ± 0.01	0.05 ± 0.03
C18	0.09 ± 0.01	0.14 ± 0.10	C18	0.08 ± 0.01	0.10 ± 0.07	C18	0.02 ± 0.01	0.07 ± 0.06
C19	0.01 ± 0.02	0.03 ± 0.04	C19	0.00 ± 0.01	0.01 ± 0.02	C19	0.01 ± 0.01	0.01 ± 0.01
C20	0.10 ± 0.02	0.17 ± 0.13	C20	0.08 ± 0.04	0.18 ± 0.13	C20	0.05 ± 0.04	0.04 ± 0.02
C21	0.09 ± 0.03	0.15 ± 0.11	C21	0.09 ± 0.03	0.14 ± 0.11	C21	0.03 ± 0.01	0.09 ± 0.07
C22	0.10 ± 0.04	0.17 ± 0.14	C22	0.08 ± 0.04	0.10 ± 0.07	C22	0.03 ± 0.02	0.09 ± 0.08
C23	0.09 ± 0.05	0.17 ± 0.09	C23	0.08 ± 0.03	0.14 ± 0.05	C23	0.02 ± 0.01	0.04 ± 0.02
C24	0.04 ± 0.01	0.17 ± 0.14	C24	0.04 ± 0.01	0.09 ± 0.04	C24	0.03 ± 0.03	0.11 ± 0.15
C25	0.03 ± 0.03	0.15 ± 0.09	C25	0.03 ± 0.02	0.10 ± 0.05	C25	0.02 ± 0.03	0.06 ± 0.02
C26	0.03 ± 0.03	0.23 ± 0.16	C26	0.03 ± 0.03	0.09 ± 0.04	C26	0.02 ± 0.01	0.08 ± 0.06
C27	0.02 ± 0.04	0.07 ± 0.07	C27	0.00 ± 0.01	0.09 ± 0.08	C27	0.00 ± 0.01	0.04 ± 0.04
Total	**1.41 ± 0.04**	**2.69 ± 1.40**	**Total**	**1.18 ± 0.16**	**1.82 ± 0.88**	**Total**	**0.61 ± 0.20**	**1.20 ± 0.67**

[a] Some high uncertainties reflected by the large standard deviation values are attributed to the low species yields.

Table S4. Mass yields (in wt%) of polystyrene-derived products from neat polystyrene (PS) pyrolysis and co-pyrolysis of PS with cellulose (CE+PS) [a]

Products	Neat PS	CE+PS
Benzene	0.06 ± 0.01	2.17 ± 2.12
Toluene	0.78 ± 0.13	2.86 ± 1.80
Styrene	27.01 ± 7.76	44.34 ± 9.73
α-Methylstyrene	0.02 ± 0.03	0.15 ± 0.05
2,4-Diphenyl-1-butene (styrene dimer)	2.95 ± 0.28	5.20 ± 1.63
2,4,6-Triphenyl-1-hexene (styrene trimer)	9.53 ± 2.62	14.34 ± 2.33
Total	**40.35 ± 7.15**	**69.06 ± 15.24**

[a] Some high uncertainties reflected by the large standard deviation values are attributed to the low species yields.

Table S5. Mass yields (in wt%) of polyethylene glycol-derived products from neat polyethylene glycol (PEG) pyrolysis and co-pyrolysis of PEG with cellulose (CE+PEG) [a]

Products	Neat PEG	CE+PEG
1-Pentanol ($C_5H_{12}O$)	1.06 ± 0.14	1.88 ± 0.78
Ethylene glycol dimethyl ether ($C_4H_{10}O_2$)	1.06 ± 0.34	7.56 ± 3.62
1-Heptanol ($C_7H_{16}O$)	0.00 ± 0.00	0.30 ± 0.45
Diethylene glycol diethyl ether ($C_8H_{18}O_3$)	0.88 ± 0.22	2.60 ± 1.64
Pentaethylene glycol ($C_{10}H_{12}O_6$)	0.00 ± 0.00	0.53 ± 0.32
Tetraethylene glycol dimethyl ether ($C_{10}H_{22}O_5$)	0.00 ± 0.00	0.20 ± 0.09
Hexaethylene glycol monomethyl ether ($C_{13}H_{28}O_7$)	0.00 ± 0.00	0.17 ± 0.15
Triethylene glycol monodecyl ether ($C_{16}H_{34}O_4$)	0.00 ± 0.00	0.29 ± 0.12
Tetrapropylene glycol monopropyl ether ($C_{15}H_{32}O_5$)	0.00 ± 0.00	0.25 ± 0.25
Pentaoxaheneicosanol ($C_{16}H_{34}O_6$)	0.00 ± 0.00	0.12 ± 0.06
Hexaoxatricosane ($C_{17}H_{36}O_6$)	0.00 ± 0.00	1.06 ± 1.68
Total	**3.00 ± 0.13**	**14.96 ± 2.19**

[a] Some high uncertainties reflected by the large standard deviation values are attributed to the low species yields.

S4. Heat Transfer Model

A heat transfer model was built using the COMSOL Multiphysics® software[18] to estimate the heating rate of a sample during CE fast pyrolysis in our microreactor reactor. In this model, the temperature gradient in the radial direction within the sample is assumed to be negligible. As a result, the system can be solved in the one-dimension domain. The average heating rate of a reaction time t can be calculated using the following equation:

$$\text{Average heating rate } (t) = \frac{T_i - T_0}{t}$$

where T_i and T_0 are the final and initial temperature, respectively. The thermal and physical parameters used in the model are summarized in **Table S6**.

Table S6. Parameters used in the heat transfer model.

	Cellulose	Copper	Glass
ρ[a] (kg m^{-3})	918	8,960	2,210
C_p[b] (J kg^{-1} K^{-1})	2,000	385	730
k[c] (W m^{-1} K^{-1})	$f(T)$[d]	400	1.4
Thickness (mm)	111.8	203.2	812.8
T_0 (K)	298.15	298.15	773.15

[a] ρ: density
[b] C_p: heat capacity.
[c] k: thermal conductivity.
[d] $f(T) = 1.81 \cdot 10^{-4} \cdot (T - 263.15) + 0.042$

The average temperature difference within the CE sample was found to be 0.3 K, with a deviation of 0.4 K. Thus, the heating rate was calculated based on the temperature at the center of the sample. As shown in **Figure S4**, the average heating rate decreases over time due to decreased temperature difference. The initial heating rate at 0.1 s was estimated as 2,322°C s^{-1}. The model predicted that the time needed to reach 499°C inside the sample is 3.3 seconds.

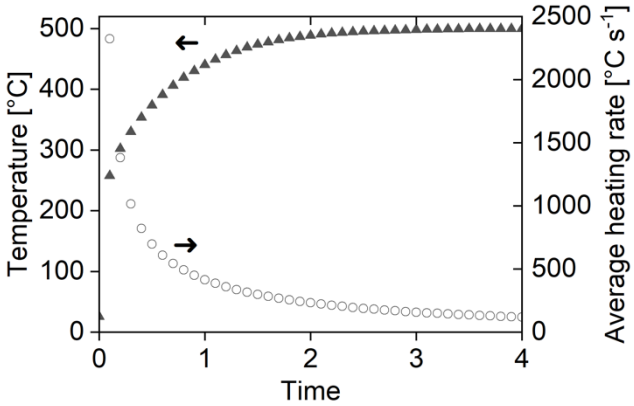

Figure S4. Estimated sample temperature and heating rate as a function of reaction time at the center of the CE sample.

S5. Supporting Computational Data

Table S7. Kinetic parameters and rate constant ratios for the elementary steps in **Scheme 1** of the main text.

Reaction	Index	A (s^{-1})	E_a (kcal mol^{-1})	k at 500°C (s^{-1})	k_{C3}/k_{neat} at 500°C
		Orange Path			
1 → **2** + **i1**	**TS1**$_{neat}$	2.3 x 10^{12}	48.3	5.1 x 10^{-2}	0.93
2 → **3** + **i2**	**TS2**$_{neat}$	2.5 x 10^{12}	52.1	4.6 x 10^{-3}	0.87
		Green Path			
1 → **4**	**TS3**$_{neat}$	2.2 x 10^{12}	48.0	6.0 x 10^{-2}	0.89
4 → **5** + **i3**	**TS4**$_{neat}$	3.5 x 10^{13}	36.3	1.9 x 10^{3}	1.24
5 → **6** + **i4**	**TS5**$_{neat}$	5.2 x 10^{12}	32.9	2.6 x 10^{3}	0.95
		Blue Path			
1 → **4**	**TS3**$_{neat}$	2.2 x 10^{12}	48.0	6.0 x 10^{-2}	0.89
4 → **7**	**TS6**$_{neat}$	1.1 x 10^{12}	32.4	7.9 x 10^{2}	0.87
7 → **8**	**TS7**$_{neat}$	6.2 x 10^{12}	36.5	3.0 x 10^{2}	1.07
8 → **9** + H_2O	**TS8**$_{neat}$	8.7 x 10^{13}	70.0	1.4 x 10^{-6}	1.24
9 → **10** + H_2O	**TS9**$_{neat}$	5.7 x 10^{12}	37.6	1.3 x 10^{2}	0.99
10 → **11** + **i5**	**TS10**$_{neat}$	6.8 x 10^{13}	53.4	5.4 x 10^{-2}	1.06

Table S8. Kinetic parameters and rate constant ratios in the presence of C3, Bz, DME, or Ace for the elementary steps in **Scheme 1** of the main text.

Reaction	A (s^{-1})	E_a (kcal mol^{-1})	k at 500°C (s^{-1})	R at 500°C	A (s^{-1})	E_a (kcal mol^{-1})	k at 500°C (s^{-1})	R at 500°C
Orange Path								
		In the presence of C3				In the presence of DME		
1 → **2** + **i1**	3.9×10^{12}	48.8	6.2×10^{-2}	1.00	4.7×10^{12}	51.9	9.7×10^{-3}	0.16
2 → **3** + **i2**	5.7×10^{12}	53.6	4.0×10^{-3}	1.00	7.0×10^{12}	54.6	2.6×10^{-3}	0.65
		In the presence of Bz				In the presence of Ace		
1 → **2** + **i1**	1.1×10^{13}	51.4	3.3×10^{-2}	0.53	2.8×10^{12}	50.9	1.1×10^{-2}	0.18
2 → **3** + **i2**	7.0×10^{12}	55.5	1.4×10^{-3}	0.35	8.9×10^{12}	52.9	1.0×10^{-2}	2.52
Green Path								
		In the presence of C3				In the presence of DME		
1 → **4**	2.0×10^{12}	48.0	5.4×10^{-2}	1.00	1.8×10^{13}	49.7	1.7×10^{-1}	3.11
4 → **5** + **i3**	1.1×10^{14}	37.8	2.4×10^{3}	1.00	2.0×10^{13}	31.5	2.5×10^{4}	10.5
5 → **6** + **i4**	5.1×10^{12}	33.0	2.4×10^{3}	1.00	5.3×10^{12}	35.6	4.5×10^{2}	0.19
		In the presence of Bz				In the presence of Ace		
1 → **4**	6.6×10^{12}	51.4	2.0×10^{-2}	0.37	8.6×10^{12}	51.7	2.1×10^{-2}	0.38
4 → **5** + **i3**	3.1×10^{13}	28.7	2.3×10^{5}	97.7	4.7×10^{13}	33.5	1.6×10^{4}	6.95
5 → **6** + **i4**	1.5×10^{13}	33.2	6.4×10^{3}	2.63	5.2×10^{12}	33.4	1.9×10^{3}	0.78
Blue Path								
		In the presence of C3				In the presence of DME		
1 → **4**	2.0×10^{12}	48.0	5.4×10^{-2}	1.00	1.8×10^{13}	49.7	1.7×10^{-1}	3.11
4 → **7**	1.5×10^{12}	33.0	6.9×10^{2}	1.00	2.4×10^{12}	35.6	2.1×10^{2}	0.31
7 → **8**	3.3×10^{12}	35.4	3.2×10^{2}	1.00	8.2×10^{12}	32.2	6.4×10^{3}	19.9
8 → **9** + H_2O	2.1×10^{14}	71.0	1.8×10^{-6}	1.00	7.5×10^{13}	66.9	9.4×10^{-6}	5.31
9 → **10** + H_2O	2.3×10^{12}	36.3	1.3×10^{2}	1.00	3.0×10^{12}	35.7	2.3×10^{2}	1.82
10 → **11** + **i5**	1.2×10^{14}	54.2	5.7×10^{-2}	1.00	1.5×10^{13}	48.9	2.2×10^{-1}	3.83
		In the presence of Bz				In the presence of Ace		
1 → **4**	6.6×10^{12}	51.4	2.0×10^{-2}	0.37	8.6×10^{12}	51.7	2.1×10^{-2}	0.38
4 → **7**	1.3×10^{12}	32.6	7.6×10^{2}	1.10	2.2×10^{13}	36.4	1.2×10^{3}	1.70
7 → **8**	2.0×10^{13}	35.4	1.9×10^{3}	6.08	7.5×10^{12}	33.8	2.1×10^{3}	6.49
8 → **9** + H_2O	2.6×10^{14}	69.8	4.9×10^{-6}	2.75	2.3×10^{14}	67.0	2.7×10^{-5}	15.2
9 → **10** + H_2O	1.2×10^{13}	38.2	1.9×10^{2}	1.45	1.6×10^{13}	38.0	2.8×10^{2}	2.18
10 → **11** + **i5**	5.8×10^{13}	49.4	6.3×10^{-1}	11.1	2.8×10^{13}	51.4	8.0×10^{-2}	1.41

Table S9. Energetic information of TSs for C−O cleavage **1** → **2** + **i1** in the absence of any surrogates and in the presence of C3, Bz, DME, or Ace at the M06-2X/6-31+G(2df,p) level of theory. The zero-point corrected energy, enthalpy, and Gibbs free energies are given relative to **1** in the absence of any surrogates or in the presence of C3, Bz, DME, or Ace, respectively.

Index	$\Delta^{\ddagger}E^0$ at 0 K (kcal mol^{-1})	$\Delta^{\ddagger}H^0$ at 773.15 K (kcal mol^{-1})	$\Delta^{\ddagger}G^0$ at 773.15 K (kcal mol^{-1})
TS1$_{neat}$	48.1	46.2	51.4
TS1$_{C3}$	48.6	46.7	51.5
TS1$_{Bz}$	50.8	49.5	52.0
TS1$_{DME}$	51.4	50.0	53.9
TS1$_{Ace}$	50.6	49.2	53.7

Table S10. Energetic information of TSs for C−O cleavage **2** → **3** + **i2** in the absence of any surrogates and in the presence of C3, Bz, DME, or Ace at the M06-2X/6-31+G(2df,p) level of theory. The zero-point corrected energy, enthalpy, and Gibbs free energies are given relative to **2** in the absence of any surrogates or in the presence of C3, Bz, DME, or Ace, respectively.

Index	$\Delta^{\ddagger}E^0$ at 0 K (kcal mol^{-1})	$\Delta^{\ddagger}H^0$ at 773.15 K (kcal mol^{-1})	$\Delta^{\ddagger}G^0$ at 773.15 K (kcal mol^{-1})
TS2$_{neat}$	51.9	50.0	55.1
TS2$_{C3}$	53.5	52.0	55.2
TS2$_{Bz}$	55.2	53.8	56.9
TS2$_{DME}$	55.9	54.6	55.7
TS2$_{Ace}$	52.6	51.2	53.8

Table S11. Energetic information of TSs for ring opening **1** → **4** in the absence of any surrogates or in the presence of C3, Bz, DME, or Ace at the M06-2X/6-31+G(2df,p) level of theory. The zero-point corrected energy, enthalpy, and Gibbs free energies are given relative to **1** in the absence of any surrogates or in the presence of C3, Bz, DME, or Ace, respectively.

Index	$\Delta^{\ddagger}E^0$ at 0 K (kcal mol^{-1})	$\Delta^{\ddagger}H^0$ at 773.15 K (kcal mol^{-1})	$\Delta^{\ddagger}G^0$ at 773.15 K (kcal mol^{-1})
TS3$_{neat}$	47.7	45.8	51.2
TS3$_{C3}$	47.8	45.8	51.3
TS3$_{Bz}$	51.0	49.3	52.9
TS3$_{DME}$	48.8	48.1	49.6
TS3$_{Ace}$	51.4	50.1	52.8

Table S12. Energetic information of TSs for retro-aldol **4** → **5** + **i3** in the absence of any surrogates or in the presence of C3, Bz, DME, or Ace at the M06-2X/6-31+G(2df,p) level of theory. The zero-point corrected energy, enthalpy, and Gibbs free energies are given relative to **4** in the absence of any surrogates or in the presence of C3, Bz, DME, or Ace, respectively.

Index	$\Delta^{\ddagger}E^0$ at 0 K (kcal mol^{-1})	$\Delta^{\ddagger}H^0$ at 773.15 K (kcal mol^{-1})	$\Delta^{\ddagger}G^0$ at 773.15 K (kcal mol^{-1})
TS4$_{neat}$	35.6	35.3	35.2
TS4$_{C3}$	37.1	37.1	34.8
TS4$_{Bz}$	28.3	27.7	27.8
TS4$_{DME}$	30.9	30.7	31.2
TS4$_{Ace}$	32.9	33.0	31.8

Table S13. Energetic information of TSs for retro-aldol **5** → **6** + **i4** in the absence of any surrogates or in the presence of C3, Bz, DME, or Ace at the M06-2X/6-31+G(2df,p) level of theory. The zero-point corrected energy, enthalpy, and Gibbs free energies are given relative to **5** in the absence of any surrogates or in the presence of C3, Bz, DME, or Ace, respectively.

Index	$\Delta^{\ddagger}E^0$ at 0 K (kcal mol^{-1})	$\Delta^{\ddagger}H^0$ at 773.15 K (kcal mol^{-1})	$\Delta^{\ddagger}G^0$ at 773.15 K (kcal mol^{-1})
TS5$_{neat}$	32.2	31.0	34.8
TS5$_{C3}$	32.5	31.2	34.9
TS5$_{Bz}$	32.4	31.1	33.4
TS5$_{DME}$	34.8	33.4	37.5
TS5$_{Ace}$	32.9	31.7	35.2

Table S14. Energetic information of TSs for isomerization **4** → **7** in the absence of any surrogates or in the presence of C3, Bz, DME, or Ace at the M06-2X/6-31+G(2df,p) level of theory. The zero-point corrected energy, enthalpy, and Gibbs free energies are given relative to **5** in the absence of any surrogates or in the presence of C3, Bz, DME, or Ace, respectively.

Index	$\Delta^{\ddagger}E^0$ at 0 K (kcal mol^{-1})	$\Delta^{\ddagger}H^0$ at 773.15 K (kcal mol^{-1})	$\Delta^{\ddagger}G^0$ at 773.15 K (kcal mol^{-1})
TS6$_{neat}$	32.5	30.4	36.5
TS6$_{C3}$	33.2	31.0	36.7
TS6$_{Bz}$	32.7	30.6	36.6
TS6$_{DME}$	35.5	33.9	38.5
TS6$_{Ace}$	35.9	35.0	35.9

Table S15. Energetic information of TSs for ring closing **7** → **8** in the absence of any surrogates or in the presence of C3, Bz, DME, or Ace at the M06-2X/6-31+G(2df,p) level of theory. The zero-point corrected energy, enthalpy, and Gibbs free energies are given relative to **7** in the absence of any surrogates or in the presence of C3, Bz, DME, or Ace, respectively.

Index	$\Delta^{\ddagger}E^0$ at 0 K (kcal mol^{-1})	$\Delta^{\ddagger}H^0$ at 773.15 K (kcal mol^{-1})	$\Delta^{\ddagger}G^0$ at 773.15 K (kcal mol^{-1})
TS7$_{neat}$	36.0	34.9	38.1
TS7$_{C3}$	34.8	33.5	38.0
TS7$_{Bz}$	34.7	33.6	35.2
TS7$_{DME}$	31.6	30.3	33.4
TS7$_{Ace}$	33.6	32.4	35.1

Table S16. Energetic information of TSs for dehydration **8** → **9** + H_2O in the absence of any surrogates or in the presence of C3, Bz, DME, or Ace at the M06-2X/6-31+G(2df,p) level of theory. The zero-point corrected energy, enthalpy, and Gibbs free energies are given relative to **8** in the absence of any surrogates or in the presence of C3, Bz, DME, or Ace, respectively.

Index	$\Delta^{\ddagger}E^0$ at 0 K (kcal mol^{-1})	$\Delta^{\ddagger}H^0$ at 773.15 K (kcal mol^{-1})	$\Delta^{\ddagger}G^0$ at 773.15 K (kcal mol^{-1})
TS8$_{neat}$	68.5	69.2	67.5
TS8$_{C3}$	69.2	69.9	67.2
TS8$_{Bz}$	68.1	68.8	65.6
TS8$_{DME}$	65.3	65.8	64.6
TS8$_{Ace}$	65.2	65.8	63.0

Table S17. Energetic information of TSs for dehydration **9** → **10** + H_2O in the absence of any surrogates or in the presence of C3, Bz, DME, or Ace at the M06-2X/6-31+G(2df,p) level of theory. The zero-point corrected energy, enthalpy, and Gibbs free energies are given relative to **9** in the absence of any surrogates or in the presence of C3, Bz, DME, or Ace, respectively.

Index	$\Delta^{\ddagger}E^0$ at 0 K (kcal mol^{-1})	$\Delta^{\ddagger}H^0$ at 773.15 K (kcal mol^{-1})	$\Delta^{\ddagger}G^0$ at 773.15 K (kcal mol^{-1})
TS9$_{neat}$	37.0	35.7	39.3
TS9$_{C3}$	35.8	34.5	39.3
TS9$_{Bz}$	37.5	36.3	38.8
TS9$_{DME}$	35.2	34.1	38.4
TS9$_{Ace}$	37.1	36.3	38.2

Table S18. Energetic information of TSs for C−O cleavage **10** → **11** + **i5** in the absence of any surrogates or in the presence of C3, Bz, DME, or Ace at the M06-2X/6-31+G(2df,p) level of theory. The zero-point corrected energy, enthalpy, and Gibbs free energies are given relative to **10** in the absence of any surrogates or in the presence of C3, Bz, DME, or Ace, respectively.

Index	$\Delta^{\ddagger}E^0$ at 0 K (kcal mol^{-1})	$\Delta^{\ddagger}H^0$ at 773.15 K (kcal mol^{-1})	$\Delta^{\ddagger}G^0$ at 773.15 K (kcal mol^{-1})
TS10$_{neat}$	52.0	52.6	51.3
TS10$_{C3}$	52.7	53.1	51.3
TS10$_{Bz}$	48.0	48.0	47.6
TS10$_{DME}$	47.6	47.1	49.3
TS10$_{Ace}$	50.0	49.7	50.8

S6. Cartesian Coordinates of All Stationary Points

In the Absence of Any Surrogates

The Cartesian coordinates for all stable structures in the absence of any surrogates reported in this work are listed below including computed absolute energies.

1 (Cellobiose) – E = -1297.616982 Hartree

Symbol	X	Y	Z
C	-4.2206250	-0.0245010	-0.1475430
C	-3.4261510	1.2782480	-0.0968460
C	-2.0611800	1.0762320	-0.7315460
C	-1.3954380	-0.1538070	-0.1282140
C	-2.3008200	-1.3823480	-0.1807520
C	-1.6909080	-2.5725350	0.5400300
O	-5.4024410	0.1942470	0.5440400
O	-4.1078330	2.2853880	-0.7975650
O	-1.2793760	2.2222990	-0.5140360
O	-0.2091390	-0.4263340	-0.8595400
O	-3.5241830	-1.0824940	0.4710390
O	-1.4152390	-2.2730170	1.8917400
H	-4.4178480	-0.2929290	-1.2012180
H	-3.2881280	1.5455090	0.9621590
H	-2.2033600	0.9035800	-1.8115850
H	-1.1522230	0.0623820	0.9201430
H	-2.4802930	-1.6516790	-1.2346820
H	-5.9743910	-0.5726620	0.4463480
H	-4.9686690	2.3999690	-0.3820960
H	-0.3533710	1.9677830	-0.6172410

H	2.4350720	3.1389490	-0.6670070
H	-2.2400970	-1.9896600	2.3008890
H	-2.3781430	-3.4245070	0.4566960
H	-0.7428160	-2.8396540	0.0650960
C	0.9503910	-0.4731160	-0.1173580
C	2.0051680	-1.2521130	-0.8882840
C	3.3367850	-1.1517070	-0.1600270
C	3.7038290	0.3013000	0.0795220
C	2.5663460	0.9744500	0.8524050
C	2.8142380	2.4499120	1.1099850
O	1.5793720	-2.5877960	-0.9799760
O	4.2917460	-1.8215840	-0.9502130
O	4.9193880	0.3124450	0.8010080
O	1.3791740	0.8659960	0.0823750
O	3.1811770	3.1471840	-0.0593360
H	0.7739080	-0.9478930	0.8645940
H	2.1028540	-0.7962770	-1.8851220
H	2.3245990	-3.1064220	-1.3031130
H	3.2380130	-1.6518720	0.8181640
H	5.1495550	-1.7151280	-0.5249230
H	3.8197780	0.8060910	-0.8876630
H	2.4359490	0.4650410	1.8216060
H	1.9180440	2.8823470	1.5726560
H	3.6443550	2.5564920	1.8135310
H	5.3662450	1.1497730	0.6482500

TS1$_{neat}$ – *E* = -1297.537918 Hartree

Symbol	X	Y	Z
C	4.1848290	0.1847180	0.1169190
C	3.4004240	-1.1063900	0.3301260
C	2.2108980	-1.1674430	-0.6150670
C	1.4196260	0.1396620	-0.5282150
C	2.3318220	1.3457000	-0.7282060
C	1.5935480	2.6610410	-0.5648300
O	5.1657450	0.2326900	1.0971450
O	4.2321540	-2.2134920	0.0950360
O	1.4226850	-2.2703540	-0.2468680
O	0.4028010	0.2098060	-1.4930160
O	3.3636290	1.3240530	0.2444080
O	0.9361750	2.7435630	0.6865100
H	4.6313150	0.1787810	-0.8937800
H	3.0236420	-1.1001910	1.3648260
H	2.5857010	-1.2812510	-1.6462550
H	1.0012510	0.1946260	0.4927330
H	2.7609340	1.3071790	-1.7434690
H	5.7508450	0.9758230	0.9239170
H	4.9712110	-2.1597170	0.7093950
H	0.5705680	-2.2275760	-0.7087680
H	-0.2517910	-0.5032540	-1.2808670
H	1.5934320	2.5761050	1.3713020
H	2.3036660	3.4885540	-0.6857240
H	0.8244190	2.7393960	-1.3362170

C	-1.6900720	0.8645940	0.2037070
C	-2.8347740	0.9411520	-0.7741330
C	-3.8754750	-0.1925800	-0.6673530
C	-3.8996390	-0.6793750	0.7907210
C	-2.5079790	-1.0053040	1.3225510
C	-1.6863810	-2.0485730	0.5154390
O	-3.3637710	2.2205370	-0.4699810
O	-3.6815480	-1.2141050	-1.5789650
O	-4.4584590	0.4014770	1.5295650
O	-1.6821920	0.1902530	1.2654750
O	-1.3462740	-1.5466430	-0.7067400
H	-0.9050650	1.6225750	0.1615620
H	-2.4260410	0.9738860	-1.7862850
H	-3.9229670	2.1269460	0.3139590
H	-4.8499460	0.2662560	-0.8661940
H	-2.7251540	-1.4979670	-1.4583990
H	-4.5182030	-1.5819540	0.8522620
H	-2.5417120	-1.2568440	2.3855460
H	-0.8084550	-2.3090700	1.1289650
H	-2.3279540	-2.9464620	0.4528390
H	-4.5482160	0.1686620	2.4581460

i1 (Glucose) – *E* = -687.009485 Hartree

Symbol	X	Y	Z
C	-0.9481460	-1.2693620	-0.4072300
C	-1.5317590	-0.0589770	0.3077600

C	-0.8040530	1.1853530	-0.1620490
C	0.6918480	1.0293550	0.0519530
C	1.1833290	-0.2549590	-0.6155260
C	2.6357960	-0.5595300	-0.2863490
O	-1.5828000	-2.3939260	0.0975480
O	-2.8980660	0.1125990	0.0124880
O	-1.2182860	2.3368130	0.5372410
O	1.3965460	2.1023210	-0.5256410
O	0.4313660	-1.3688560	-0.1499200
O	2.8152450	-0.7950730	1.0896990
H	-1.1096330	-1.1737410	-1.4963440
H	-1.3703120	-0.1967170	1.3872440
H	-0.9903670	1.3112790	-1.2418240
H	0.8926640	0.9627600	1.1311630
H	1.0720320	-0.1480040	-1.7070890
H	-1.2867170	-3.1709700	-0.3859730
H	-3.3708830	-0.6753480	0.2995500
H	-2.1761210	2.4033230	0.4612350
H	1.0166220	2.9178650	-0.1816590
H	2.1998020	-1.4903610	1.3458190
H	2.9582300	-1.4248960	-0.8813460
H	3.2505450	0.3025020	-0.5534390

2 (Cellobiosan) – *E* = -1221.195932 Hartree

Symbol	X	Y	Z
C	3.7952660	-0.1999340	0.8679930

C	2.7812680	0.9175670	1.1477900
C	1.9352100	1.1650320	-0.1157130
C	1.5211930	-0.1788790	-0.7621570
C	2.6712590	-1.1878650	-0.7569420
C	3.9630860	-0.6578250	-1.3783100
O	1.9912510	0.5673980	2.2540120
O	2.6004660	1.9821630	-1.0554590
O	3.0913330	-1.3836260	0.5901310
O	4.5390600	0.0981630	-0.3100830
H	4.4674780	-0.3778580	1.7093040
H	3.3053830	1.8435670	1.4044770
H	1.5065720	-0.2358470	2.0245170
H	1.0210050	1.6830080	0.1813690
H	3.5496030	1.8384110	-0.9710920
H	1.1826880	0.0187770	-1.7876480
H	2.3467170	-2.1485810	-1.1592840
H	4.6331070	-1.4799340	-1.6444110
H	3.8018750	-0.0109090	-2.2434540
O	0.4784100	-0.7851500	-0.0037570
C	-0.8107330	-0.5827130	-0.4676590
C	-1.7302250	-1.5183050	0.3056930
O	-1.1802950	0.7542650	-0.2499890
H	-0.8653320	-0.8087050	-1.5499910
C	-3.1586920	-1.2754880	-0.1432480
O	-1.4294610	-2.8702540	0.0528660
H	-1.6360490	-1.2794220	1.3753750

C	-2.4951010	1.0695560	-0.6939720
C	-3.5188090	0.1913230	0.0246650
O	-4.0829360	-2.0297230	0.6059970
H	-3.2363460	-1.5342020	-1.2126280
H	-0.5387730	-3.0481240	0.3717560
C	-2.6937680	2.5482980	-0.4021860
H	-2.5810910	0.8971440	-1.7792340
O	-4.7784630	0.4663960	-0.5389290
H	-3.5031930	0.4411290	1.0955060
H	-3.8281130	-2.9568670	0.5511000
O	-2.5314880	2.8337590	0.9661590
H	-1.9886780	3.1255480	-1.0154300
H	-3.7130510	2.8301140	-0.6742170
H	-1.6541270	2.5352230	1.2285340
H	-5.4124010	-0.1442120	-0.1478390

TS2$_{neat}$ – *E* = -1221.109694 Hartree

Symbol	X	Y	Z
C	4.3442450	0.1936680	0.4576530
C	3.5964670	1.0578610	-0.5676440
C	2.3772570	0.2779440	-1.0958770
C	1.6395040	-0.4152680	0.0771760
C	2.6220560	-1.0363650	1.0730980
C	3.6261630	-1.9893720	0.4236380
O	3.2270830	2.2704120	0.0323230
O	2.7240950	-0.6421610	-2.1123250

O	3.5025830	-0.0285030	1.5561800
O	4.6176540	-1.0965410	-0.0909760
H	5.2671810	0.6606230	0.8064770
H	4.2546360	1.2951590	-1.4098990
H	2.5861980	2.0636740	0.7272440
H	1.6833070	1.0012300	-1.5383270
H	3.6095500	-0.9752410	-1.9285780
H	1.0164320	-1.2191010	-0.3559520
H	2.0928550	-1.4619330	1.9279390
H	4.0825110	-2.6498540	1.1665730
H	3.2039150	-2.5800390	-0.3931010
O	0.8663400	0.5232300	0.7816960
H	0.2386690	0.9618630	0.0991130
O	-0.8492250	1.3721860	-0.8308820
C	-1.2993000	0.5148850	-1.7878730
C	-2.3010760	-0.5080220	-1.1879460
H	-0.4912600	-0.0749370	-2.2569170
H	-1.8449830	1.0195390	-2.6063250
C	-3.6210490	0.0548160	-0.6653080
O	-1.5810210	-1.1023970	-0.0628510
H	-2.4604660	-1.3463210	-1.8675370
C	-3.4169330	1.1670280	0.3775710
O	-4.3566530	-0.9479900	0.0173620
H	-4.1894650	0.4536730	-1.5164710
C	-1.5008140	-0.4486730	1.0071540
C	-2.4539670	0.6275530	1.4615600

O	-3.0308240	2.3744000	-0.1671110
H	-4.3815070	1.3076070	0.8775190
C	-4.8092940	-2.0252520	-0.7749860
H	-0.8431710	-0.8848760	1.7541760
O	-3.1244800	-0.0422440	2.5164400
H	-1.8765530	1.4512200	1.8869900
H	-2.0816770	2.2264230	-0.4794940
H	-4.0018420	-2.7295530	-1.0082360
H	-5.2521920	-1.6597590	-1.7100410
H	-5.5738180	-2.5478530	-0.1990700
H	-3.8222890	-0.5794950	2.1157890

3 (Levoglucosan) – *E* = -610.585923 Hartree

Symbol	X	Y	Z
C	0.6421680	-1.0477640	-0.7620070
C	-0.5959510	-1.2855400	0.1142760
C	-0.7522390	-0.1043570	1.0921370
C	-0.5239750	1.2393110	0.3596040
C	0.6489390	1.1556150	-0.6189240
C	1.9438590	0.6720300	0.0324960
O	-1.7229630	-1.4418710	-0.7072240
O	0.0860540	-0.2245810	2.2203240
O	-1.6488040	1.5747850	-0.4324750
O	0.4148780	0.0957740	-1.5417270
O	1.7732130	-0.7490580	0.0521240
H	0.8584690	-1.8904500	-1.4213790

H	-0.4812880	-2.2074750	0.6929900
H	-1.7943040	-0.6452720	-1.2511250
H	-1.7846460	-0.1176080	1.4619690
H	0.8966550	-0.6707610	1.9498560
H	-0.3155720	2.0124160	1.1121090
H	0.7470010	2.0841490	-1.1819610
H	2.8115780	0.9250890	-0.5827110
H	2.0872710	1.0384060	1.0515820
H	-2.4209980	1.6553430	0.1350020

TS3$_{neat}$ – *E* = -1297.536699 Hartree

Symbol	X	Y	Z
O	-4.1408710	0.7234470	-1.4264780
H	-4.6988520	0.1537530	0.1565830
C	-2.8138100	0.7081020	-1.4822880
C	-1.9594570	1.5006120	-0.4892990
C	-1.6632070	0.8360560	0.8817650
C	-1.4380860	-0.6815220	0.7482960
C	-2.5705990	-1.4392610	0.0560800
C	-3.9152450	-1.5386130	0.7831330
O	-0.7604210	1.8833760	-1.1333790
O	-2.5713740	1.1446440	1.8953570
O	-0.3001230	-0.9772120	-0.0623780
O	-2.7324250	-0.9203050	-1.2794380
O	-4.5979870	-0.3298340	1.0069610
H	-2.3682060	0.7673710	-2.4828950

H	-2.5234660	2.4170120	-0.2883620
H	-0.1178090	1.1675670	-1.0386830
H	-0.7155660	1.2753060	1.1962360
H	-3.4339920	0.7288300	1.7142000
H	-1.3024930	-1.0985440	1.7560400
H	-2.2177560	-2.4690660	-0.0752050
H	-4.5444450	-2.2295310	0.2040070
H	-3.7376940	-1.9969910	1.7612010
H	-3.8133980	-0.5690140	-1.4765780
H	1.3106300	2.8192840	-0.8159810
C	0.9650800	-0.7777310	0.4776080
C	1.9423360	-1.5962800	-0.3589580
C	3.3659590	-1.2644000	0.0498730
C	3.6134190	0.2319400	-0.0662440
C	2.5747310	0.9811380	0.7620770
C	2.6283520	2.4929640	0.5772560
O	1.7559980	-2.9794550	-0.1725550
O	4.3066640	-1.9173920	-0.7695640
O	4.8819040	0.5697650	0.4374580
O	1.2693750	0.5879270	0.3628880
O	2.2698960	2.8761000	-0.7262790
H	0.9947080	-1.0920270	1.5368910
H	1.7950830	-1.3122740	-1.4113610
H	0.9133230	-3.2300180	-0.5628850
H	3.5093010	-1.5595680	1.1030720
H	4.1232200	-2.8625390	-0.7437450

H	3.5096900	0.5347650	-1.1188760
H	2.7352590	0.7405670	1.8256550
H	1.9747970	2.9620540	1.3243110
H	3.6538910	2.8269000	0.7527020
H	5.5318420	0.0196510	-0.0128800

4 – *E* = -1297.593372 Hartree

Symbol	X	Y	Z
O	-4.2769530	1.4955880	-0.7294700
H	-4.7678800	-0.3978450	-0.0514930
C	-3.1740380	1.4728460	-1.2114130
C	-1.8877330	1.6536530	-0.4190750
C	-1.6933770	0.7496520	0.8290020
C	-1.4149870	-0.7612590	0.6096790
C	-2.4700030	-1.6417690	-0.0654390
C	-3.7634250	-1.9014240	0.7057500
O	-0.7837440	1.6448140	-1.2936100
O	-2.6920460	0.9427630	1.7841540
O	-0.2391310	-0.9797050	-0.1768350
O	-2.7438260	-1.0815040	-1.3390450
O	-4.6105930	-0.7876420	0.8193520
H	-3.0144530	1.3811240	-2.3037940
H	-1.9612820	2.6689280	-0.0068280
H	-0.4704480	0.7357260	-1.3807830
H	-0.7729120	1.1288360	1.2792740
H	-3.5412300	0.6032540	1.4578230

H	-1.2521170	-1.1704360	1.6181240
H	-1.9761790	-2.6179560	-0.1829330
H	-4.2880640	-2.7293090	0.2053760
H	-3.5251930	-2.2281100	1.7228680
H	-3.0787160	-1.7558360	-1.9360430
H	1.2424990	2.5148650	-0.8390750
C	1.0007240	-0.7855550	0.4282370
C	2.0248250	-1.5346980	-0.4171150
C	3.4239570	-1.1949280	0.0584210
C	3.6356490	0.3087290	-0.0021820
C	2.5608790	1.0128240	0.8205090
C	2.5428380	2.5222480	0.6026470
O	1.8615680	-2.9301520	-0.3126350
O	4.4085420	-1.7987820	-0.7480740
O	4.8823760	0.6636410	0.5441360
O	1.2676660	0.5861870	0.4220800
O	2.1424270	2.8460070	-0.7032700
H	0.9913120	-1.1794910	1.4617020
H	1.9091080	-1.1979200	-1.4581310
H	1.0209220	-3.1682130	-0.7148620
H	3.5351960	-1.5241720	1.1052990
H	4.2385020	-2.7464500	-0.7705160
H	3.5523480	0.6401830	-1.0479470
H	2.7332320	0.7891020	1.8855720
H	1.8746440	2.9743990	1.3489680
H	3.5506470	2.9169890	0.7511460

H	5.5579110	0.1507050	0.0878690

TS4$_{neat}$ – *E* = -1297.530616 Hartree

Symbol	X	Y	Z
C	3.5495190	2.0713670	1.3344380
C	3.1296060	0.7555890	1.3788280
C	2.0915180	0.9877230	-0.3826590
C	1.4679320	-0.4131500	-0.4859710
C	2.3465060	-1.6537270	-0.3142440
C	1.5943280	-2.9017140	-0.7754800
O	4.2748640	2.5201630	0.3691340
O	2.3364980	0.3511310	2.4316730
O	2.9423340	1.3661200	-1.2365590
O	0.4329500	-0.5238220	0.4867110
O	3.5116270	-1.4791980	-1.0930930
O	1.2343590	-2.8135630	-2.1321410
H	3.1515360	2.7898010	2.0576310
H	3.7630600	0.0060480	0.9094900
H	1.3317750	1.6973280	-0.0102070
H	1.0330710	-0.4333430	-1.4947780
H	2.5851310	-1.7603670	0.7546130
H	4.1437270	-2.1705320	-0.8737380
H	1.4751050	0.0768200	2.0910020
H	3.8646750	2.0431310	-0.5324910
H	-1.5497230	3.0747160	-0.1247370
H	2.0191680	-2.5477370	-2.6262710

H	2.2302130	-3.7811810	-0.5894890
H	0.6710520	-3.0302770	-0.2019350
C	-0.8618200	-0.5332400	-0.0216570
C	-1.8088190	-0.9403210	1.0978020
C	-3.2307600	-0.8820460	0.5685860
C	-3.5243730	0.4933490	-0.0090210
C	-2.4692900	0.8603370	-1.0517360
C	-2.6075960	2.2930540	-1.5394630
O	-1.5727550	-2.2622960	1.5263130
O	-4.1787190	-1.1293880	1.5801590
O	-4.7754800	0.5097360	-0.6509200
O	-1.1686210	0.7559610	-0.4796370
O	-2.4273320	3.2175140	-0.4933630
H	-0.9275260	-1.2541950	-0.8578200
H	-1.6970170	-0.2234800	1.9245440
H	-0.7299200	-2.2952440	1.9884300
H	-3.3308650	-1.6274210	-0.2378560
H	-3.9893780	-1.9908100	1.9667200
H	-3.4867050	1.2357500	0.8016680
H	-2.5618520	0.1734980	-1.9083540
H	-1.8846900	2.4619570	-2.3484980
H	-3.6167790	2.4375880	-1.9303490
H	-5.4323630	0.1957590	-0.0203170

5 – *E* = -1068.585388 Hartree

Symbol	X	Y	Z

C	-1.9720900	1.8952110	-0.6687750
C	-2.0496410	0.4932430	-0.0751940
C	-3.4342180	-0.1204380	-0.3113490
C	-3.5624760	-1.4734990	0.3809170
O	-1.2622540	2.1913480	-1.5869950
O	-1.1016130	-0.3674280	-0.6464280
O	-4.3728950	0.7911550	0.2417350
O	-3.3860780	-1.3514600	1.7704770
H	-2.6416740	2.6341800	-0.1893250
H	-1.9041160	0.5821920	1.0123580
H	-3.5813630	-0.2394490	-1.3937130
H	-5.2413770	0.6268420	-0.1353310
H	1.4679850	2.6677740	-0.7990840
H	-3.9891000	-0.6663990	2.0807740
H	-4.5483610	-1.9006840	0.1406770
H	-2.7940480	-2.1587010	0.0155100
C	0.0813120	-0.4831800	0.0747790
C	1.0153610	-1.3856140	-0.7174400
C	2.3488510	-1.4522290	0.0020190
C	2.9078090	-0.0515570	0.1885470
C	1.8851120	0.8308190	0.9030830
C	2.2904860	2.2976300	0.9116350
O	0.5181430	-2.7009350	-0.8154890
O	3.3000060	-2.1988980	-0.7214400
O	4.0698520	-0.0754290	0.9825880
O	0.6393590	0.7931340	0.2214710

O	2.3279360	2.8264710	-0.3902570
H	-0.1263640	-0.9176700	1.0722400
H	1.1544170	-0.9348380	-1.7102870
H	-0.2753960	-2.6858150	-1.3587690
H	2.1901890	-1.9023540	0.9963570
H	2.9205110	-3.0645380	-0.9065250
H	3.1147370	0.3829720	-0.8003260
H	1.7698850	0.4695160	1.9379510
H	1.5857730	2.8528670	1.5462820
H	3.2933390	2.3898940	1.3343070
H	4.6822730	-0.7017750	0.5822760

i3 (Ethene-diol) – *E* = -228.956313 Hartree

Symbol	X	Y	Z
C	0.5460320	-0.3744770	0.0313210
C	-0.5460320	0.3744780	-0.0313190
O	1.7902040	0.2001450	0.0522840
O	-1.7902040	-0.2001450	-0.0522860
H	0.4859860	-1.4563500	0.1079010
H	-0.4859860	1.4563500	-0.1079000
H	-2.4200960	0.3850160	0.3734790
H	2.4200950	-0.3850160	-0.3734830

TS5$_{neat}$ – *E* = -1068.529286 Hartree

Symbol	X	Y	Z
O	4.5814190	0.4948490	-0.5763810

O	2.6619160	-2.3417760	0.5301330
C	3.7439750	-0.1854200	0.0924170
C	3.3360160	-1.5643740	-0.4326810
H	4.1489530	1.7511140	-0.4764460
H	3.2751130	-2.6266370	1.2124210
H	3.7722920	-0.1537230	1.1971470
H	4.2663900	-2.0480660	-0.7572880
H	2.6821510	-1.4924250	-1.3042720
C	2.4658850	1.9403030	0.3866400
C	1.9633340	0.7860860	-0.1846100
O	3.4767070	2.5550790	-0.1207080
O	0.9949280	0.0712780	0.4750420
H	2.1124170	2.2495280	1.3746870
H	2.0315410	0.6417380	-1.2602600
H	-2.0990140	2.5267960	1.4487530
C	-0.2158300	-0.0814190	-0.1959080
C	-0.8978950	-1.3145560	0.3778130
C	-2.2755040	-1.4384330	-0.2454360
C	-3.0641370	-0.1557130	-0.0492580
C	-2.2680590	1.0291460	-0.5958510
C	-2.9251530	2.3644030	-0.2868990
O	-0.1864070	-2.4830520	0.0670830
O	-3.0171690	-2.4929960	0.3227140
O	-4.2834920	-0.2030610	-0.7506610
O	-0.9793800	1.0747560	0.0081650
O	-2.9934800	2.5984690	1.0994660

H	-0.0332370	-0.2270730	-1.2777090
H	-0.9963260	-1.1724200	1.4646940
H	0.7112030	-2.4303990	0.4303510
H	-2.1499170	-1.6064370	-1.3285960
H	-2.4851110	-3.2938970	0.2618260
H	-3.2345170	0.0014810	1.0258600
H	-2.1720910	0.9150160	-1.6879720
H	-2.3642320	3.1597430	-0.7960170
H	-3.9486440	2.3532850	-0.6670990
H	-4.7331020	-1.0161340	-0.4962720

6 (Glycolaldehyde) – *E* = -228.976128 Hartree

Symbol	X	Y	Z
C	-0.6695370	0.6459430	0.0001670
H	-0.9406080	1.2450780	-0.8826340
C	0.8279400	0.4840750	-0.0002310
H	1.4275380	1.4143710	-0.0005320
O	-1.3302810	-0.5780740	-0.0000280
H	-0.9399380	1.2446560	0.8835040
O	1.3496440	-0.5989540	-0.0000710
H	-0.6523170	-1.2679900	0.0008330

i4 – *E* = -839.569632 Hartree

Symbol	X	Y	Z
C	4.0479330	0.8740900	-0.3137600
C	2.7334230	1.0521470	-0.2566530

O	4.6423290	-0.2471710	0.1759630
O	1.9248280	0.1231760	0.3428870
H	4.6813200	1.6413630	-0.7433740
H	2.2598330	1.9527380	-0.6276220
H	-1.2295600	2.4645710	1.4730540
C	0.6859250	-0.0573420	-0.2586970
C	0.0646460	-1.2979710	0.3646500
C	-1.3232550	-1.4878770	-0.2148490
C	-2.1522820	-0.2316510	-0.0057660
C	-1.4152940	0.9824030	-0.5721560
C	-2.1101470	2.2916230	-0.2347590
O	0.8133990	-2.4529400	0.0735120
O	-2.0100720	-2.5589210	0.3917010
O	-3.3865920	-0.3264820	-0.6759480
O	-0.1118770	1.0719680	-0.0091520
O	-2.1366470	2.5202350	1.1537100
H	0.8072030	-0.1935060	-1.3489560
H	-0.0066550	-1.1293820	1.4494380
H	1.7121760	-2.3182450	0.3947330
H	-1.2266900	-1.6662400	-1.2989310
H	-1.4562930	-3.3441750	0.3250260
H	-2.3016730	-0.0788860	1.0730750
H	-1.3512530	0.8753360	-1.6673640
H	-1.5972590	3.1084440	-0.7608340
H	-3.1455560	2.2446140	-0.5784090
H	-3.8043400	-1.1490670	-0.3990710

H	5.5901230	-0.1990130	0.0397940

TS6$_{neat}$ – *E* = -1297.537889 Hartree

Symbol	X	Y	Z
O	-3.4299480	-3.0438970	-0.7352250
H	-4.6604030	1.4387670	-1.5219510
C	-3.8280150	-2.0676320	-0.1599750
C	-3.1187800	-0.7658170	-0.1982140
C	-1.9669890	-0.4587190	-0.7903500
C	-1.6376610	0.9728920	-0.4646040
C	-2.8622990	1.4044110	0.3726630
C	-3.6700370	2.5222080	-0.2576700
O	-0.4830990	1.1206690	0.3548760
O	-3.7152530	0.2488910	0.4895300
O	-4.0669240	2.1951180	-1.5676870
H	-4.7531090	-2.0790310	0.4474740
H	-1.3634130	-1.1274620	-1.3822150
H	-1.5202340	1.5942830	-1.3632290
H	-2.5305120	1.6815400	1.3787920
H	-4.5338840	2.7533000	0.3787240
H	-3.0453970	3.4182000	-0.3272600
H	1.1539160	-2.4072170	-0.7748840
C	0.7326190	1.1562960	-0.3085430
C	1.7991010	1.3810320	0.7560840
C	3.1714900	1.3027950	0.1189820
C	3.3294390	-0.0283480	-0.5945030

C	2.1968500	-0.2171370	-1.6019130
C	2.1916750	-1.6134450	-2.2054700
O	1.6769170	2.6491030	1.3556940
O	4.2003220	1.3979440	1.0768520
O	4.5403710	-0.0781420	-1.3085760
O	0.9357460	-0.0722230	-0.9614580
O	1.9847990	-2.6010270	-1.2240030
H	0.7455140	1.9757370	-1.0532240
H	1.6965880	0.5756880	1.4997190
H	0.8290950	2.6889820	1.8092990
H	3.2656890	2.1141520	-0.6221060
H	4.0636240	2.2049840	1.5844100
H	3.2743790	-0.8381760	0.1490230
H	2.3072510	0.5305740	-2.4039310
H	1.4181400	-1.6589080	-2.9843510
H	3.1643280	-1.8078770	-2.6618870
H	5.2497980	0.1383880	-0.6940560
C	1.3117500	-2.4063610	2.3721160
C	-0.0284130	-1.9559380	1.7936270
H	1.8928410	-2.9832700	1.6467460
H	1.9178170	-1.5436500	2.6732610
H	1.1660330	-3.0282200	3.2612570
C	-0.8354930	-1.1107730	2.7757610
H	0.1409280	-1.3653860	0.8870100
H	-0.6155680	-2.8324780	1.4934970
H	-1.7878690	-0.7884740	2.3419690

H	-1.0510380	-1.6695840	3.6922960
H	-0.2793970	-0.2091310	3.0576490

7 – *E* = -1297.60673 Hartree

Symbol	X	Y	Z
O	3.6977940	0.5027030	2.4265730
H	3.8181440	-0.5274960	-1.5025480
C	2.7328370	0.9919000	1.6016890
C	2.0711740	0.2626200	0.7109540
C	0.9911800	0.6941310	-0.2503690
C	0.4076520	-0.6739900	-0.6749510
C	1.5558520	-1.6617510	-0.4393820
C	2.4527550	-1.9060390	-1.6462640
O	1.4311750	1.4656780	-1.3396590
O	-0.6661290	-1.0679920	0.1640270
O	2.3350150	-1.0944300	0.6128690
O	3.0802640	-0.7196720	-2.0938470
H	2.5530870	2.0521420	1.7146650
H	3.7391620	-0.4544650	2.3118120
H	0.2170280	1.2776020	0.2452150
H	2.0877580	0.9476970	-1.8265050
H	0.0813890	-0.6405140	-1.7213940
H	1.1549310	-2.6176050	-0.0878460
H	3.2052460	-2.6586810	-1.3821990
H	1.8582920	-2.2944510	-2.4788260
H	-2.2391570	2.7118900	0.9702980

C	-1.9282320	-0.7192310	-0.2861510
C	-2.9473140	-1.3936150	0.6222610
C	-4.3388470	-0.9921560	0.1703540
C	-4.4676260	0.5219170	0.1402040
C	-3.3478030	1.1257370	-0.7065770
C	-3.3149200	2.6434650	-0.6326730
O	-2.8675180	-2.7977990	0.5476260
O	-5.3372590	-1.4880270	1.0322580
O	-5.6910230	0.9098450	-0.4369530
O	-2.0840180	0.6761330	-0.2323820
O	-3.0731240	3.0945400	0.6791220
H	-2.0656450	-1.0608620	-1.3306260
H	-2.7747630	-1.0367400	1.6479650
H	-2.0010890	-3.0676320	0.8677820
H	-4.4964270	-1.3755370	-0.8517260
H	-5.2271060	-2.4423740	1.0999540
H	-4.3763440	0.9074050	1.1660940
H	-3.4908150	0.8171740	-1.7550740
H	-2.5483440	3.0124170	-1.3269610
H	-4.2881080	3.0348420	-0.9359020
H	-6.3946820	0.4567820	0.0397430
C	6.8140560	-0.1356870	0.8266120
C	5.6885890	0.0932090	-0.1796700
H	7.0242120	-1.1996340	0.9656840
H	7.7363280	0.3489800	0.4914500
H	6.5434900	0.2913090	1.7972030

C	5.3929520	1.5777280	-0.3832110
H	5.9593920	-0.3697300	-1.1383580
H	4.7856860	-0.4141800	0.1881310
H	4.5507440	1.7486830	-1.0614770
H	5.1442500	2.0454760	0.5740970
H	6.2680990	2.0902520	-0.7946800

TS7$_{neat}$ – *E* = -1297.544456 Hartree

Symbol	X	Y	Z
O	3.6977940	0.5027030	2.4265730
H	3.8181440	-0.5274960	-1.5025480
C	2.7328370	0.9919000	1.6016890
C	2.0711740	0.2626200	0.7109540
C	0.9911800	0.6941310	-0.2503690
C	0.4076520	-0.6739900	-0.6749510
C	1.5558520	-1.6617510	-0.4393820
C	2.4527550	-1.9060390	-1.6462640
O	1.4311750	1.4656780	-1.3396590
O	-0.6661290	-1.0679920	0.1640270
O	2.3350150	-1.0944300	0.6128690
O	3.0802640	-0.7196720	-2.0938470
H	2.5530870	2.0521420	1.7146650
H	3.7391620	-0.4544650	2.3118120
H	0.2170280	1.2776020	0.2452150
H	2.0877580	0.9476970	-1.8265050
H	0.0813890	-0.6405140	-1.7213940

H	1.1549310	-2.6176050	-0.0878460
H	3.2052460	-2.6586810	-1.3821990
H	1.8582920	-2.2944510	-2.4788260
H	-2.2391570	2.7118900	0.9702980
C	-1.9282320	-0.7192310	-0.2861510
C	-2.9473140	-1.3936150	0.6222610
C	-4.3388470	-0.9921560	0.1703540
C	-4.4676260	0.5219170	0.1402040
C	-3.3478030	1.1257370	-0.7065770
C	-3.3149200	2.6434650	-0.6326730
O	-2.8675180	-2.7977990	0.5476260
O	-5.3372590	-1.4880270	1.0322580
O	-5.6910230	0.9098450	-0.4369530
O	-2.0840180	0.6761330	-0.2323820
O	-3.0731240	3.0945400	0.6791220
H	-2.0656450	-1.0608620	-1.3306260
H	-2.7747630	-1.0367400	1.6479650
H	-2.0010890	-3.0676320	0.8677820
H	-4.4964270	-1.3755370	-0.8517260
H	-5.2271060	-2.4423740	1.0999540
H	-4.3763440	0.9074050	1.1660940
H	-3.4908150	0.8171740	-1.7550740
H	-2.5483440	3.0124170	-1.3269610
H	-4.2881080	3.0348420	-0.9359020
H	-6.3946820	0.4567820	0.0397430
C	6.8140560	-0.1356870	0.8266120

C	5.6885890	0.0932090	-0.1796700
H	7.0242120	-1.1996340	0.9656840
H	7.7363280	0.3489800	0.4914500
H	6.5434900	0.2913090	1.7972030
C	5.3929520	1.5777280	-0.3832110
H	5.9593920	-0.3697300	-1.1383580
H	4.7856860	-0.4141800	0.1881310
H	4.5507440	1.7486830	-1.0614770
H	5.1442500	2.0454760	0.5740970
H	6.2680990	2.0902520	-0.7946800

8 – *E* = -1297.614904 Hartree

Symbol	X	Y	Z
O	3.6977940	0.5027030	2.4265730
H	3.8181440	-0.5274960	-1.5025480
C	2.7328370	0.9919000	1.6016890
C	2.0711740	0.2626200	0.7109540
C	0.9911800	0.6941310	-0.2503690
C	0.4076520	-0.6739900	-0.6749510
C	1.5558520	-1.6617510	-0.4393820
C	2.4527550	-1.9060390	-1.6462640
O	1.4311750	1.4656780	-1.3396590
O	-0.6661290	-1.0679920	0.1640270
O	2.3350150	-1.0944300	0.6128690
O	3.0802640	-0.7196720	-2.0938470
H	2.5530870	2.0521420	1.7146650

H	3.7391620	-0.4544650	2.3118120
H	0.2170280	1.2776020	0.2452150
H	2.0877580	0.9476970	-1.8265050
H	0.0813890	-0.6405140	-1.7213940
H	1.1549310	-2.6176050	-0.0878460
H	3.2052460	-2.6586810	-1.3821990
H	1.8582920	-2.2944510	-2.4788260
H	-2.2391570	2.7118900	0.9702980
C	-1.9282320	-0.7192310	-0.2861510
C	-2.9473140	-1.3936150	0.6222610
C	-4.3388470	-0.9921560	0.1703540
C	-4.4676260	0.5219170	0.1402040
C	-3.3478030	1.1257370	-0.7065770
C	-3.3149200	2.6434650	-0.6326730
O	-2.8675180	-2.7977990	0.5476260
O	-5.3372590	-1.4880270	1.0322580
O	-5.6910230	0.9098450	-0.4369530
O	-2.0840180	0.6761330	-0.2323820
O	-3.0731240	3.0945400	0.6791220
H	-2.0656450	-1.0608620	-1.3306260
H	-2.7747630	-1.0367400	1.6479650
H	-2.0010890	-3.0676320	0.8677820
H	-4.4964270	-1.3755370	-0.8517260
H	-5.2271060	-2.4423740	1.0999540
H	-4.3763440	0.9074050	1.1660940
H	-3.4908150	0.8171740	-1.7550740

H	-2.5483440	3.0124170	-1.3269610
H	-4.2881080	3.0348420	-0.9359020
H	-6.3946820	0.4567820	0.0397430
C	6.8140560	-0.1356870	0.8266120
C	5.6885890	0.0932090	-0.1796700
H	7.0242120	-1.1996340	0.9656840
H	7.7363280	0.3489800	0.4914500
H	6.5434900	0.2913090	1.7972030
C	5.3929520	1.5777280	-0.3832110
H	5.9593920	-0.3697300	-1.1383580
H	4.7856860	-0.4141800	0.1881310
H	4.5507440	1.7486830	-1.0614770
H	5.1442500	2.0454760	0.5740970
H	6.2680990	2.0902520	-0.7946800

TS8$_{neat}$ – *E* = -1297.49751 Hartree

Symbol	X	Y	Z
O	3.6977940	0.5027030	2.4265730
H	3.8181440	-0.5274960	-1.5025480
C	2.7328370	0.9919000	1.6016890
C	2.0711740	0.2626200	0.7109540
C	0.9911800	0.6941310	-0.2503690
C	0.4076520	-0.6739900	-0.6749510
C	1.5558520	-1.6617510	-0.4393820
C	2.4527550	-1.9060390	-1.6462640
O	1.4311750	1.4656780	-1.3396590

O	-0.6661290	-1.0679920	0.1640270
O	2.3350150	-1.0944300	0.6128690
O	3.0802640	-0.7196720	-2.0938470
H	2.5530870	2.0521420	1.7146650
H	3.7391620	-0.4544650	2.3118120
H	0.2170280	1.2776020	0.2452150
H	2.0877580	0.9476970	-1.8265050
H	0.0813890	-0.6405140	-1.7213940
H	1.1549310	-2.6176050	-0.0878460
H	3.2052460	-2.6586810	-1.3821990
H	1.8582920	-2.2944510	-2.4788260
H	-2.2391570	2.7118900	0.9702980
C	-1.9282320	-0.7192310	-0.2861510
C	-2.9473140	-1.3936150	0.6222610
C	-4.3388470	-0.9921560	0.1703540
C	-4.4676260	0.5219170	0.1402040
C	-3.3478030	1.1257370	-0.7065770
C	-3.3149200	2.6434650	-0.6326730
O	-2.8675180	-2.7977990	0.5476260
O	-5.3372590	-1.4880270	1.0322580
O	-5.6910230	0.9098450	-0.4369530
O	-2.0840180	0.6761330	-0.2323820
O	-3.0731240	3.0945400	0.6791220
H	-2.0656450	-1.0608620	-1.3306260
H	-2.7747630	-1.0367400	1.6479650
H	-2.0010890	-3.0676320	0.8677820

H	-4.4964270	-1.3755370	-0.8517260
H	-5.2271060	-2.4423740	1.0999540
H	-4.3763440	0.9074050	1.1660940
H	-3.4908150	0.8171740	-1.7550740
H	-2.5483440	3.0124170	-1.3269610
H	-4.2881080	3.0348420	-0.9359020
H	-6.3946820	0.4567820	0.0397430
C	6.8140560	-0.1356870	0.8266120
C	5.6885890	0.0932090	-0.1796700
H	7.0242120	-1.1996340	0.9656840
H	7.7363280	0.3489800	0.4914500
H	6.5434900	0.2913090	1.7972030
C	5.3929520	1.5777280	-0.3832110
H	5.9593920	-0.3697300	-1.1383580
H	4.7856860	-0.4141800	0.1881310
H	4.5507440	1.7486830	-1.0614770
H	5.1442500	2.0454760	0.5740970
H	6.2680990	2.0902520	-0.7946800

9 – *E* = -1221.175979 Hartree

Symbol	X	Y	Z
O	3.6977940	0.5027030	2.4265730
H	3.8181440	-0.5274960	-1.5025480
C	2.7328370	0.9919000	1.6016890
C	2.0711740	0.2626200	0.7109540
C	0.9911800	0.6941310	-0.2503690

C	0.4076520	-0.6739900	-0.6749510
C	1.5558520	-1.6617510	-0.4393820
C	2.4527550	-1.9060390	-1.6462640
O	1.4311750	1.4656780	-1.3396590
O	-0.6661290	-1.0679920	0.1640270
O	2.3350150	-1.0944300	0.6128690
O	3.0802640	-0.7196720	-2.0938470
H	2.5530870	2.0521420	1.7146650
H	3.7391620	-0.4544650	2.3118120
H	0.2170280	1.2776020	0.2452150
H	2.0877580	0.9476970	-1.8265050
H	0.0813890	-0.6405140	-1.7213940
H	1.1549310	-2.6176050	-0.0878460
H	3.2052460	-2.6586810	-1.3821990
H	1.8582920	-2.2944510	-2.4788260
H	-2.2391570	2.7118900	0.9702980
C	-1.9282320	-0.7192310	-0.2861510
C	-2.9473140	-1.3936150	0.6222610
C	-4.3388470	-0.9921560	0.1703540
C	-4.4676260	0.5219170	0.1402040
C	-3.3478030	1.1257370	-0.7065770
C	-3.3149200	2.6434650	-0.6326730
O	-2.8675180	-2.7977990	0.5476260
O	-5.3372590	-1.4880270	1.0322580
O	-5.6910230	0.9098450	-0.4369530
O	-2.0840180	0.6761330	-0.2323820

O	-3.0731240	3.0945400	0.6791220
H	-2.0656450	-1.0608620	-1.3306260
H	-2.7747630	-1.0367400	1.6479650
H	-2.0010890	-3.0676320	0.8677820
H	-4.4964270	-1.3755370	-0.8517260
H	-5.2271060	-2.4423740	1.0999540
H	-4.3763440	0.9074050	1.1660940
H	-3.4908150	0.8171740	-1.7550740
H	-2.5483440	3.0124170	-1.3269610
H	-4.2881080	3.0348420	-0.9359020
H	-6.3946820	0.4567820	0.0397430
C	6.8140560	-0.1356870	0.8266120
C	5.6885890	0.0932090	-0.1796700
H	7.0242120	-1.1996340	0.9656840
H	7.7363280	0.3489800	0.4914500
H	6.5434900	0.2913090	1.7972030
C	5.3929520	1.5777280	-0.3832110
H	5.9593920	-0.3697300	-1.1383580
H	4.7856860	-0.4141800	0.1881310
H	4.5507440	1.7486830	-1.0614770
H	5.1442500	2.0454760	0.5740970
H	6.2680990	2.0902520	-0.7946800

TS9$_{neat}$ – *E* = -1221.11262 Hartree

Symbol	X	Y	Z
O	-3.5393930	-2.6100730	-0.0646620

H	-4.8879490	0.6545350	-0.8620090
C	-3.7271320	-1.6381850	0.7302830
C	-2.9406790	-0.5042420	0.6049250
C	-1.9102740	-0.5058240	-0.3576050
C	-1.5079790	0.9447000	-0.5496230
C	-2.6630560	1.6999980	0.1401720
C	-3.7170900	2.1953350	-0.8434860
O	-2.6218580	-1.1373620	-1.8737340
O	-0.3072920	1.2343950	0.1384010
O	-3.2718020	0.7860150	1.0475970
O	-4.3503540	1.1172390	-1.5156810
H	-4.5397310	-1.6866300	1.4668640
H	-3.0471830	-1.9139950	-1.2948620
H	-1.1417870	-1.2678550	-0.3804870
H	-3.3297380	-0.5003100	-2.0785570
H	-1.4086630	1.2058860	-1.6117630
H	-2.2625190	2.5440770	0.7097870
H	-4.4618550	2.7918850	-0.3052160
H	-3.2571280	2.8259320	-1.6103420
H	1.2589380	-2.5584840	-0.0687320
C	0.8702760	1.0422000	-0.5724710
C	2.0050720	1.5103970	0.3290430
C	3.3288270	1.2295640	-0.3533520
C	3.4243370	-0.2464580	-0.6988480
C	2.2198180	-0.6687880	-1.5383990
C	2.1615520	-2.1748760	-1.7417780

O	1.9351330	2.8940060	0.5787600
O	4.4225210	1.5442340	0.4764710
O	4.5782710	-0.5137820	-1.4573740
O	1.0093840	-0.3211870	-0.8757980
O	2.0566120	-2.8608290	-0.5168320
H	0.8508170	1.6301370	-1.5107410
H	1.9474680	0.9314420	1.2629260
H	1.1418220	3.0696290	1.0946200
H	3.3785660	1.8151590	-1.2867700
H	4.3283780	2.4590020	0.7628630
H	3.4200830	-0.8292490	0.2348740
H	2.2748840	-0.1670690	-2.5179820
H	1.3166090	-2.4088070	-2.4032990
H	3.0872330	-2.5044670	-2.2177520
H	5.3342690	-0.1716760	-0.9683030
C	-0.2877300	-0.0281700	3.1814120
C	0.3332910	-1.2128260	2.4452640
H	-1.2586530	0.2442980	2.7574240
H	-0.4277780	-0.2589710	4.2425740
H	0.3647270	0.8515520	3.1207250
C	1.7046870	-1.5962060	2.9984680
H	-0.3449060	-2.0726990	2.5007490
H	0.4273340	-0.9570480	1.3840490
H	2.1503360	-2.4272530	2.4438990
H	2.3998480	-0.7496850	2.9437050
H	1.6332970	-1.8903090	4.0505330

10 – *E* = -1144.757178 Hartree

Symbol	X	Y	Z
O	-3.4299480	-3.0438970	-0.7352250
H	-4.6604030	1.4387670	-1.5219510
C	-3.8280150	-2.0676320	-0.1599750
C	-3.1187800	-0.7658170	-0.1982140
C	-1.9669890	-0.4587190	-0.7903500
C	-1.6376610	0.9728920	-0.4646040
C	-2.8622990	1.4044110	0.3726630
C	-3.6700370	2.5222080	-0.2576700
O	-0.4830990	1.1206690	0.3548760
O	-3.7152530	0.2488910	0.4895300
O	-4.0669240	2.1951180	-1.5676870
H	-4.7531090	-2.0790310	0.4474740
H	-1.3634130	-1.1274620	-1.3822150
H	-1.5202340	1.5942830	-1.3632290
H	-2.5305120	1.6815400	1.3787920
H	-4.5338840	2.7533000	0.3787240
H	-3.0453970	3.4182000	-0.3272600
H	1.1539160	-2.4072170	-0.7748840
C	0.7326190	1.1562960	-0.3085430
C	1.7991010	1.3810320	0.7560840
C	3.1714900	1.3027950	0.1189820
C	3.3294390	-0.0283480	-0.5945030
C	2.1968500	-0.2171370	-1.6019130

C	2.1916750	-1.6134450	-2.2054700
O	1.6769170	2.6491030	1.3556940
O	4.2003220	1.3979440	1.0768520
O	4.5403710	-0.0781420	-1.3085760
O	0.9357460	-0.0722230	-0.9614580
O	1.9847990	-2.6010270	-1.2240030
H	0.7455140	1.9757370	-1.0532240
H	1.6965880	0.5756880	1.4997190
H	0.8290950	2.6889820	1.8092990
H	3.2656890	2.1141520	-0.6221060
H	4.0636240	2.2049840	1.5844100
H	3.2743790	-0.8381760	0.1490230
H	2.3072510	0.5305740	-2.4039310
H	1.4181400	-1.6589080	-2.9843510
H	3.1643280	-1.8078770	-2.6618870
H	5.2497980	0.1383880	-0.6940560
C	1.3117500	-2.4063610	2.3721160
C	-0.0284130	-1.9559380	1.7936270
H	1.8928410	-2.9832700	1.6467460
H	1.9178170	-1.5436500	2.6732610
H	1.1660330	-3.0282200	3.2612570
C	-0.8354930	-1.1107730	2.7757610
H	0.1409280	-1.3653860	0.8870100
H	-0.6155680	-2.8324780	1.4934970
H	-1.7878690	-0.7884740	2.3419690
H	-1.0510380	-1.6695840	3.6922960

H	-0.2793970	-0.2091310	3.0576490

TS10$_{neat}$ – *E* = -1144.667034 Hartree

Symbol	X	Y	Z
O	-5.6851790	-1.8409150	-0.6811390
H	-3.5076450	3.1180110	-0.1752260
C	-5.3393210	-1.0026010	0.1015170
C	-3.9583150	-0.4392710	0.0741450
C	-2.8952620	-0.7826770	-0.7340740
C	-1.8415580	0.0268120	-0.3191630
C	-2.3068740	0.8392890	0.7996460
C	-2.0541120	2.3276860	0.8591300
O	-0.7148520	-1.0220480	1.4287230
O	-3.6941980	0.5157670	0.9353450
O	-2.5571900	3.0108050	-0.2644780
H	-6.0043820	-0.5911620	0.8810230
H	-2.9143560	-1.5374880	-1.5028410
H	-0.8629220	0.1240250	-0.7639230
H	-1.7044770	0.2426690	1.6066350
H	-2.4636780	2.7224830	1.7956540
H	-0.9700990	2.4645030	0.8759820
H	1.0293750	2.2255660	-0.6798030
C	0.5816130	-0.7370780	1.5300520
C	1.4400950	-1.6999840	0.6995690
C	2.9057260	-1.3504920	0.8393350
C	3.1434450	0.0988550	0.4518300

C	2.1916930	1.0143300	1.2243910
C	2.2893260	2.4612860	0.7699090
O	1.2560490	-3.0253850	1.1355680
O	3.7321460	-2.1480800	0.0133550
O	4.4620080	0.4935230	0.7568880
O	0.8482080	0.6058880	1.0357730
O	1.9011360	2.6219580	-0.5773210
H	0.9411300	-0.7621530	2.5824850
H	1.1317040	-1.5925130	-0.3540680
H	0.3078140	-3.1293480	1.2862380
H	3.1942030	-1.4800410	1.8953890
H	3.5355670	-3.0710200	0.2057950
H	2.9479260	0.2145060	-0.6245080
H	2.4583730	0.9639230	2.2935250
H	1.6693510	3.0820630	1.4327990
H	3.3265030	2.7939400	0.8464710
H	5.0535510	-0.1632570	0.3741460
C	2.2615620	0.5643740	-3.3388370
C	0.9109070	0.2118350	-2.7218450
H	2.6157280	1.5350940	-2.9828540
H	3.0102690	-0.1898820	-3.0722050
H	2.1949780	0.5944340	-4.4310790
C	0.4262690	-1.1761940	-3.1340160
H	1.0084630	0.2525240	-1.6295460
H	0.1664390	0.9684210	-3.0025900
H	-0.5280780	-1.4385970	-2.6642300

H	0.2907720	-1.2366880	-4.2183740
H	1.1573090	-1.9391230	-2.8461500

11 (5-Hydroxymethylfurfural) – *E* = -457.751131 Hartree

Symbol	X	Y	Z
C	2.4685550	-0.2977470	-0.0655630
C	1.1622000	0.3484730	-0.0231950
C	0.8059150	1.6556760	-0.1883010
C	-0.6120950	1.6999420	-0.0571670
C	-1.0051360	0.4171060	0.1831310
C	-2.3261700	-0.2374790	0.4116230
O	2.6561060	-1.4777970	0.0854930
O	0.0612640	-0.4056240	0.2081490
O	-2.6054260	-1.2318160	-0.5478750
H	3.3023930	0.4066080	-0.2547180
H	1.4795510	2.4752740	-0.3856310
H	-1.2588430	2.5585900	-0.1366680
H	-1.9114610	-1.8975710	-0.5113550
H	-2.3552870	-0.6530210	1.4284610
H	-3.1115290	0.5161880	0.3306020

H_2O – *E* = -76.402433 Hartree

Symbol	X	Y	Z
O	0.0000000	0.0000000	0.1162040
H	0.0000000	0.7639660	-0.4648180
H	0.0000000	-0.7639660	-0.4648180

C3 – *E* = Hartree

Symbol	X	Y	Z
C	1.2668270	-0.2606740	-0.0000210
C	0.0000000	0.5911300	-0.0000170
H	2.1693450	0.3564520	-0.0000680
H	1.3012420	-0.9068570	0.8831920
H	1.3011930	-0.9069190	-0.8831910
C	-1.2668260	-0.2606740	0.0000360
H	0.0000200	1.2480020	0.8768340
H	-0.0000200	1.2479520	-0.8769040
H	-2.1693450	0.3564510	0.0000450
H	-1.3012400	-0.9069080	-0.8831390
H	-1.3011950	-0.9068670	0.8832430

Bz – *E* = -232.163063 Hartree

Symbol	X	Y	Z
C	-0.3379690	-1.3498690	-0.0004120
C	0.9997080	-0.9678540	0.0002010
C	-1.3381450	-0.3819810	0.0003560
C	1.3381610	0.3824140	0.0000930
C	-1.0002410	0.9675590	-0.0000320
C	0.3383050	1.3496830	-0.0001660
H	1.7795750	-1.7215520	0.0002760
H	-2.3809440	-0.6799580	0.0005490
H	2.3809750	0.6800270	0.0001480

H	-1.7791480	1.7220730	-0.0002240
H	0.6013510	2.4018600	-0.0002660
H	-0.6007250	-2.4021610	-0.0007250

DME – *E* = -154.965347 Hartree

Symbol	X	Y	Z
O	0.0000000	0.5893480	-0.0000130
C	1.1623440	-0.1945340	0.0000200
C	-1.1623430	-0.1945350	-0.0000110
H	1.2099230	-0.8360630	0.8925400
H	2.0182660	0.4819760	0.0000190
H	1.2099490	-0.8360980	-0.8924740
H	-1.2099530	-0.8360520	0.8925150
H	-1.2099180	-0.8361080	-0.8924990
H	-2.0182660	0.4819760	-0.0000490

Ace – *E* = -193.083758 Hartree

Symbol	X	Y	Z
O	-0.0000020	1.3919910	0.0000210
C	0.0000000	0.1868530	-0.0001370
C	1.2860890	-0.6114360	-0.0000270
C	-1.2860880	-0.6114390	-0.0000280
H	1.3223660	-1.2597290	0.8809580
H	1.3213600	-1.2623500	-0.8790860
H	2.1422330	0.0621850	-0.0013810
H	-2.1422330	0.0621810	-0.0014000

H	-1.3223700	-1.2597170	0.8809690
H	-1.3213470	-1.2623690	-0.8790740

In the Presence of Propane (C3)

The Cartesian coordinates for all the stable structures in the presence of C3 reported in this work are listed below including computed absolute energies.

1$_{C3}$ – *E* = -1416.704909 Hartree

Symbol	X	Y	Z
C	4.3590810	-0.0151650	0.0060080
C	3.4683470	1.0832280	-0.5710830
C	2.0935130	1.0181460	0.0698770
C	1.5587570	-0.4050060	-0.0179560
C	2.5511240	-1.4176390	0.5482830
C	2.0770130	-2.8493230	0.3688930
O	5.5528890	0.0197700	-0.6983400
O	4.0304070	2.3432340	-0.3134120
O	1.2328110	1.9171820	-0.5810670
O	0.3524590	-0.4674470	0.7265560
O	3.7807120	-1.2918860	-0.1474550
O	1.8468920	-3.1535880	-0.9899870
H	4.5237480	0.1760370	1.0818540
H	3.3660600	0.8998600	-1.6516860
H	2.1950040	1.2848010	1.1361410
H	1.3665170	-0.6437990	-1.0717570
H	2.6933850	-1.2180300	1.6232990
H	6.1789450	-0.5875570	-0.2933230
H	4.9013960	2.3652320	-0.7229190

H	0.3275020	1.6239450	-0.4105110
H	-2.3098340	2.4256740	-1.1881500
H	2.6649970	-2.9831140	-1.4692930
H	2.8240950	-3.5255530	0.8043110
H	1.1303960	-2.9874790	0.8992690
C	-0.7423540	-0.9538510	0.0413310
C	-1.8046440	-1.3496390	1.0558350
C	-3.1108730	-1.6550930	0.3410990
C	-3.5127200	-0.4870270	-0.5399940
C	-2.3788350	-0.2109870	-1.5309410
C	-2.6598010	0.9733610	-2.4389950
O	-1.3318350	-2.4735190	1.7541830
O	-4.0697920	-1.9313790	1.3354780
O	-4.7143620	-0.8469220	-1.1916150
O	-1.2055450	0.0942040	-0.7949160
O	-3.0533960	2.1195460	-1.7192670
H	-0.4692380	-1.8231900	-0.5834660
H	-1.9587390	-0.4958690	1.7341930
H	-2.0648560	-2.8179490	2.2763340
H	-2.9634890	-2.5414170	-0.2989390
H	-4.9185180	-2.0536580	0.8963540
H	-3.6584400	0.4028970	0.0862080
H	-2.2152690	-1.1059470	-2.1540560
H	-1.7697070	1.1672720	-3.0506030
H	-3.4854120	0.7229030	-3.1108250
H	-5.1863300	-0.0474220	-1.4408530

C	-1.8199530	3.9152790	0.9534220
C	-1.6071840	2.5752470	1.6564060
H	-2.7753820	3.9529210	0.4202330
H	-1.8146590	4.7379520	1.6754970
H	-1.0118050	4.1101370	0.2381860
C	-0.3024900	2.5414330	2.4494190
H	-2.4535450	2.3682690	2.3221330
H	-1.5993570	1.7651310	0.9165430
H	-0.1120170	1.5478450	2.8656040
H	0.5420690	2.8080800	1.8051490
H	-0.3313310	3.2606730	3.2741990

TS1$_{C3}$ – *E* = -1416.624944 Hartree

Symbol	X	Y	Z
C	4.1533080	-0.7985250	-0.1425040
C	3.3590620	-0.1844540	-1.2914370
C	2.1682810	0.5971360	-0.7588510
C	1.3925600	-0.2660500	0.2378430
C	2.3144790	-0.8437150	1.3057890
C	1.5772740	-1.7706320	2.2547100
O	5.1362710	-1.5979400	-0.7077990
O	4.1814750	0.6810710	-2.0311270
O	1.3678510	0.9612830	-1.8550560
O	0.3887280	0.4585090	0.9016540
O	3.3404380	-1.5999880	0.6860490
O	0.8791210	-2.7898260	1.5630920

H	4.5972290	0.0084880	0.4680740
H	2.9826690	-1.0106830	-1.9144650
H	2.5411670	1.4918240	-0.2308960
H	0.9615180	-1.1073180	-0.3335510
H	2.7493160	-0.0150110	1.8903880
H	5.7241090	-1.9143050	-0.0157090
H	4.9202150	0.1647990	-2.3690990
H	0.5103740	1.2877010	-1.5370840
H	-0.2571050	0.7634720	0.2175410
H	1.5150570	-3.2547850	1.0080340
H	2.2945650	-2.2020700	2.9638980
H	0.8324680	-1.1962920	2.8094990
C	-1.7594130	-1.1828730	0.3560070
C	-2.8423930	-0.4369070	1.0928850
C	-3.8863890	0.2683690	0.2036500
C	-4.0235040	-0.5376560	-1.1004410
C	-2.6837850	-0.8384470	-1.7521390
C	-1.7984360	0.3907660	-2.0892930
O	-3.3913900	-1.4804380	1.8817190
O	-3.6203390	1.6090960	-0.0087460
O	-4.6096520	-1.8072630	-0.8126940
O	-1.8510080	-1.5957300	-0.8285820
O	-1.3666770	1.0000570	-0.9444370
H	-0.9561450	-1.6524560	0.9288570
H	-2.3773190	0.2870440	1.7652420
H	-3.9324140	-2.0310920	1.2985590

H	-4.8395180	0.1932320	0.7423220
H	-2.6773970	1.6361420	-0.3573220
H	-4.6215700	0.0341620	-1.8189290
H	-2.8191580	-1.5053020	-2.6037950
H	-0.9683310	0.0250010	-2.7151320
H	-2.4252970	1.0485950	-2.7174430
H	-5.5578000	-1.6954690	-0.6963710
C	1.6050020	3.5338860	1.6352150
C	0.4923780	3.7481460	0.6119490
H	2.5950260	3.6890870	1.1951040
H	1.4997390	4.2284320	2.4757230
H	1.5583380	2.5139060	2.0309830
C	-0.8925680	3.5311050	1.2144110
H	0.5599540	4.7608780	0.1989610
H	0.6335520	3.0650120	-0.2334090
H	-1.6853630	3.6735710	0.4758470
H	-0.9812840	2.5146630	1.6134890
H	-1.0702830	4.2272350	2.0413450

2$_{C3}$ – *E* = -1340.284902 Hartree

Symbol	X	Y	Z
C	-3.8333510	0.1042440	-0.9183440
C	-3.3782300	1.2693280	-0.0295310
C	-2.7671330	0.7099390	1.2716210
C	-1.8539810	-0.4950130	0.9644210
C	-2.4871800	-1.4348740	-0.0735970

C	-3.9125520	-1.8699770	0.2602420
O	-2.4847120	2.0888690	-0.7341380
O	-3.7498480	0.3648690	2.2217830
O	-2.7159310	-0.6802500	-1.2625860
O	-4.6937140	-0.7551370	-0.1791210
H	-4.3221660	0.4410390	-1.8340810
H	-4.2440240	1.8863470	0.2323470
H	-1.6414320	1.6232880	-0.8103510
H	-2.1384370	1.4889800	1.7131600
H	-4.5558480	0.1167700	1.7557330
H	-1.6378340	-1.0233930	1.9018140
H	-1.8257990	-2.2655800	-0.3258170
H	-4.1941150	-2.7576530	-0.3123120
H	-4.0795320	-2.0424870	1.3256680
O	-0.6681430	0.0530620	0.4065680
C	0.4474660	-0.7759150	0.3526160
C	1.0170670	-0.7179670	-1.0602030
O	1.3689860	-0.3055640	1.2966230
H	0.1711820	-1.8191570	0.5930970
C	2.3083980	-1.5082930	-1.1097170
O	0.1265580	-1.2935470	-1.9864600
H	1.2241860	0.3357620	-1.3003180
C	2.5956090	-1.0258950	1.3257960
C	3.2670370	-1.0011620	-0.0467900
O	2.9524550	-1.3914070	-2.3576980
H	2.0791300	-2.5668560	-0.8989520

H	-0.6916970	-0.7787120	-2.0159450
C	3.4469820	-0.3515790	2.3903020
H	2.4144610	-2.0753030	1.6116390
O	4.4102270	-1.8189410	0.0307970
H	3.5402850	0.0375750	-0.2815900
H	2.3244880	-1.6449570	-3.0426730
O	3.6489320	1.0116160	2.1014800
H	2.9614920	-0.4826840	3.3665560
H	4.4291480	-0.8279050	2.4151250
H	2.7824510	1.4263950	2.0225450
H	4.7870010	-1.8761200	-0.8537950
C	0.6424420	3.3039580	-1.1736020
C	1.7867050	2.9066570	-0.2439660
H	-0.2847320	3.4913270	-0.6257080
H	0.8911850	4.2118150	-1.7326560
H	0.4486920	2.5176420	-1.9149450
C	3.0985030	2.6882370	-0.9948480
H	1.9271070	3.6865930	0.5134270
H	1.5080410	1.9939400	0.2979390
H	3.9049040	2.3949100	-0.3164140
H	2.9932570	1.9055810	-1.7563880
H	3.4034290	3.6041450	-1.5114910

TS2$_{C3}$ – *E* = -1340.195729 Hartree

Symbol	X	Y	Z
C	3.5704580	-1.6581800	0.6121670

C	3.0679110	-0.2084540	0.6039740
C	1.9113140	-0.0790140	-0.4044890
C	0.9401830	-1.2782580	-0.2716930
C	1.6956690	-2.5946500	-0.0746250
C	2.7388390	-2.8626680	-1.1600310
O	2.6768430	0.1563360	1.9007780
O	2.3702260	0.0755680	-1.7333370
O	2.5371950	-2.4883790	1.0679780
O	3.8553900	-2.0847500	-0.7205780
H	4.4449660	-1.7968350	1.2505540
H	3.8746300	0.4681600	0.3015680
H	1.9244210	-0.4017090	2.1432250
H	1.3508270	0.8268720	-0.1479850
H	3.1920030	-0.4193090	-1.8284880
H	0.3653980	-1.3363040	-1.2144420
H	1.0015570	-3.4205800	0.0916240
H	3.0200190	-3.9193340	-1.1871360
H	2.4299510	-2.5319930	-2.1547770
O	0.1016180	-1.1046980	0.8421990
H	-0.3199670	-0.1740640	0.7638640
O	-1.1366500	1.0488450	0.5039440
C	-1.4028890	1.4439190	-0.7724400
C	-2.5777720	0.6219250	-1.3610250
H	-0.5449000	1.3116920	-1.4574280
H	-1.7089730	2.5038940	-0.8476580
C	-3.9406770	0.8155320	-0.7037730

O	-2.1683420	-0.7707940	-1.1816480
H	-2.6449250	0.7319180	-2.4464480
C	-3.9235350	0.5235140	0.8060850
O	-4.8707650	-0.1182670	-1.2431130
H	-4.2602880	1.8520520	-0.8587930
C	-2.3014660	-1.2962340	-0.0492180
C	-3.2764540	-0.8652930	1.0166260
O	-3.3479490	1.5291920	1.5547120
H	-4.9687860	0.4177340	1.1168320
H	-1.8563250	-2.2831930	0.0455080
O	-4.2095780	-1.9316940	0.9664740
H	-2.7727050	-0.8932710	1.9852770
H	-2.3657460	1.4972940	1.3234690
H	-4.8198830	-1.7505100	0.2380390
H	-5.0028430	0.0360240	-2.1829020
C	3.5843030	4.4306730	-0.2502210
C	2.6427650	3.2588700	0.0176020
H	4.6139030	4.0961810	-0.4060880
H	3.2728680	4.9841390	-1.1426280
H	3.5825110	5.1317240	0.5909160
C	1.1998230	3.7140070	0.2285830
H	2.6897330	2.5564950	-0.8238210
H	2.9757990	2.7083420	0.9053380
H	0.5425070	2.8794460	0.4931050
H	1.1425430	4.4468380	1.0406510
H	0.8069740	4.1932940	-0.6757930

TS3$_{C3}$ – *E* = -1416.624784 Hartree

Symbol	X	Y	Z
O	4.1915470	1.7974260	0.6197060
H	5.0329400	0.3642770	0.0086490
C	2.8771900	1.6303380	0.5252940
C	2.1963250	1.3393720	-0.8151520
C	2.1609000	-0.1373620	-1.2920350
C	1.9580540	-1.1166590	-0.1216620
C	2.9664200	-0.9733020	1.0174310
C	4.4219630	-1.3579930	0.7352370
O	0.8938500	1.8865370	-0.7823650
O	3.2221900	-0.5162610	-2.1157960
O	0.7003210	-0.9150800	0.5226570
O	2.8702140	0.3583550	1.5629250
O	5.0978180	-0.5881930	-0.2279550
H	2.2560500	2.3193400	1.1117510
H	2.7629570	1.9061970	-1.5604860
H	0.3147930	1.2703140	-0.3125360
H	1.2686960	-0.1958110	-1.9171560
H	4.0511210	-0.5450620	-1.6045300
H	2.0203920	-2.1404730	-0.5163910
H	2.6239880	-1.6380940	1.8192740
H	4.9572120	-1.3229810	1.6949630
H	4.4356360	-2.3963350	0.3889920
H	3.8895570	0.8981520	1.5593160

H	-1.1141900	1.9853870	-1.8670890
C	-0.4501940	-1.3563480	-0.1229140
C	-1.5262200	-1.5066880	0.9473990
C	-2.8762370	-1.7521240	0.3001480
C	-3.1875870	-0.6534260	-0.7039690
C	-2.0566880	-0.5721030	-1.7240070
C	-2.1958250	0.5959150	-2.6929700
O	-1.2582930	-2.5952580	1.8013140
O	-3.9117210	-1.7624970	1.2557820
O	-4.3749290	-0.9337770	-1.4022740
O	-0.8225410	-0.3727160	-1.0518340
O	-2.0519390	1.8349750	-2.0437450
H	-0.2683970	-2.3201650	-0.6330240
H	-1.5665510	-0.5626750	1.5077100
H	-0.5009370	-2.3733500	2.3509800
H	-2.8448500	-2.7151710	-0.2368530
H	-3.6953690	-2.4200040	1.9255910
H	-3.2563040	0.3094180	-0.1741270
H	-2.0331030	-1.5144770	-2.2956840
H	-1.4549720	0.4795970	-3.4944600
H	-3.1950340	0.5646030	-3.1339880
H	-5.0654220	-1.0987980	-0.7511420
C	-3.8914940	2.8328320	1.5012910
C	-2.8215030	1.9999980	2.2047420
H	-4.8724490	2.7061370	1.9666400
H	-3.6364060	3.8969070	1.5322350

H	-3.9726230	2.5496620	0.4460760
C	-1.4662800	2.1363020	1.5134360
H	-2.7386030	2.3086600	3.2525990
H	-3.1330030	0.9473370	2.2178840
H	-0.6859060	1.5386480	1.9991290
H	-1.5534890	1.8198310	0.4674620
H	-1.1308210	3.1783210	1.5072850

4$_{C3}$ – *E* = -1416.682103 Hartree

Symbol	X	Y	Z
O	4.4451490	1.6663290	-0.2779300
H	5.0378350	-0.1949430	0.3529500
C	3.3023860	1.8557970	0.0492630
C	2.0858370	1.4207550	-0.7555090
C	2.0483280	-0.0509710	-1.2500230
C	1.7874700	-1.1722530	-0.2096580
C	2.7519960	-1.3591230	0.9640060
C	4.1384700	-1.9131850	0.6439690
O	0.9131790	1.8211710	-0.0875260
O	3.1385860	-0.3617740	-2.0640800
O	0.5137900	-1.0292650	0.4251910
O	2.8397410	-0.1173010	1.6445810
O	4.9629380	-1.0490580	-0.0937070
H	3.0428970	2.4388080	0.9552920
H	2.1445790	2.0149850	-1.6775840
H	0.6472370	1.1201130	0.5229100

H	1.1719510	-0.0831490	-1.9023130
H	3.9524250	-0.3926220	-1.5361300
H	1.7951910	-2.1066560	-0.7908830
H	2.2614560	-2.1043950	1.6076070
H	4.6190530	-2.1791750	1.5975350
H	4.0356860	-2.8327270	0.0590930
H	3.0865650	-0.2552130	2.5627980
H	-1.1149330	2.1775680	-1.0179090
C	-0.6291080	-1.2932660	-0.3267330
C	-1.7350520	-1.6425920	0.6639900
C	-3.0710190	-1.7027260	-0.0499130
C	-3.3339860	-0.3916450	-0.7720560
C	-2.1840610	-0.0981350	-1.7301790
C	-2.2486400	1.3039370	-2.3282520
O	-1.5111960	-2.9007280	1.2603370
O	-4.1316140	-1.9126790	0.8547410
O	-4.5128490	-0.4673260	-1.5360830
O	-0.9457330	-0.1331450	-1.0406480
O	-2.0169150	2.2899610	-1.3541240
H	-0.4506610	-2.1403720	-1.0155010
H	-1.7690500	-0.8470900	1.4215310
H	-0.7406820	-2.8324950	1.8317620
H	-3.0418670	-2.5144540	-0.7963310
H	-3.9437780	-2.7135630	1.3555730
H	-3.3937440	0.4200790	-0.0316830
H	-2.2027100	-0.8482110	-2.5376920

H	-1.5149530	1.3713070	-3.1433570
H	-3.2462950	1.4701920	-2.7411620
H	-5.2211850	-0.7558050	-0.9505970
C	-1.2850150	3.3365750	1.8567470
C	-1.6234910	1.8539930	1.9922550
H	-0.2526030	3.4834900	1.5298030
H	-1.9417290	3.8051290	1.1169090
H	-1.4239880	3.8562460	2.8106240
C	-3.0650790	1.6345240	2.4466590
H	-1.4775740	1.3671210	1.0206480
H	-0.9323110	1.3732240	2.6980250
H	-3.3274910	0.5729210	2.5110230
H	-3.2355330	2.0826550	3.4309190
H	-3.7586010	2.1074420	1.7427450

TS4$_{C3}$ – *E* = -1416.61615 Hartree

Symbol	X	Y	Z
C	-2.6972880	2.3803590	-0.9942840
C	-2.3615180	1.0411450	-0.9857130
C	-1.1115790	1.3093370	0.6319380
C	-0.6360400	-0.1415230	0.8101980
C	-1.6622450	-1.2764860	0.8492650
C	-1.0237430	-2.5501730	1.4011290
O	-3.2899990	2.9282390	0.0109230
O	-1.7181190	0.5089970	-2.0807740
O	-1.8086650	1.8556590	1.5334820

O	0.2638540	-0.4651360	-0.2459710
O	-2.7349340	-0.8816860	1.6768470
O	-0.5732160	-2.3642270	2.7199450
H	-2.3424640	3.0260630	-1.8034260
H	-2.9826960	0.3756920	-0.3910280
H	-0.3360040	1.8913470	0.1049630
H	-0.0965960	-0.1278980	1.7675310
H	-1.9949560	-1.4675710	-0.1826670
H	-3.4955830	-1.4459110	1.5037940
H	-0.8765950	0.1275810	-1.7979190
H	-2.7748560	2.5112710	0.8952020
H	2.6049990	2.9644810	-0.3252130
H	-1.2962190	-1.9662180	3.2197880
H	-1.7625540	-3.3641200	1.3436570
H	-0.1570190	-2.8402010	0.7985780
C	1.6046490	-0.5426100	0.1151850
C	2.3715530	-1.1709490	-1.0393330
C	3.8466620	-1.1928460	-0.6806320
C	4.3243440	0.2048550	-0.3207370
C	3.4384990	0.7958740	0.7752820
C	3.7560320	2.2555580	1.0549690
O	1.9737670	-2.5038960	-1.2658750
O	4.6409310	-1.6514530	-1.7491870
O	5.6407070	0.1719030	0.1729630
O	2.0735620	0.7541300	0.3686330
O	3.5296170	3.0622360	-0.0762150

H	1.7087820	-1.1639860	1.0242840
H	2.2219880	-0.5488600	-1.9341180
H	1.0779150	-2.5073810	-1.6158880
H	3.9791910	-1.8439910	0.1994170
H	4.3329660	-2.5290320	-1.9988840
H	4.2527560	0.8462520	-1.2113840
H	3.5760280	0.2099040	1.6981960
H	3.1535130	2.5907370	1.9095200
H	4.8137720	2.3443990	1.3107360
H	6.1865170	-0.2809750	-0.4787710
C	-5.4258390	-0.5408240	-2.1479940
C	-5.3084800	-1.1176980	-0.7390830
H	-5.1189890	-1.2640640	-2.9077150
H	-6.4593220	-0.2468550	-2.3558910
H	-4.7981980	0.3491610	-2.2587880
C	-5.7267150	-0.1127520	0.3332290
H	-5.9237560	-2.0208970	-0.6594020
H	-4.2708530	-1.4433440	-0.5755100
H	-5.6734000	-0.5324570	1.3427580
H	-5.0979830	0.7839580	0.3119630
H	-6.7601820	0.2071760	0.1675250

5$_{C3}$ – *E* = -1187.673543 Hartree

Symbol	X	Y	Z
C	-1.8272580	-1.4809920	-1.0758280
C	-2.1908710	-0.0750590	-0.5807680

C	-3.5292300	-0.1587540	0.1474060
C	-4.0290380	1.2067000	0.5984720
O	-1.4883080	-2.3508560	-0.3242590
O	-1.2383780	0.4064960	0.3384670
O	-4.4384910	-0.7124370	-0.7966800
O	-4.2374720	2.0593540	-0.5003090
H	-1.9229590	-1.6604550	-2.1637860
H	-2.2822140	0.6092610	-1.4360550
H	-3.3941150	-0.8219700	1.0120630
H	-5.1182630	-1.2121010	-0.3378800
H	1.3855840	-2.2347480	-1.1806660
H	-4.8063380	1.5917830	-1.1223370
H	-4.9547120	1.0710190	1.1780660
H	-3.2877570	1.6824590	1.2448810
C	-0.1042730	0.9370720	-0.2641560
C	0.8525760	1.3556310	0.8431600
C	2.1641800	1.7956330	0.2233050
C	2.7228420	0.6818860	-0.6456860
C	1.6936370	0.2726190	-1.6971990
C	2.1139290	-0.9734610	-2.4626490
O	0.3455560	2.4417250	1.5834420
O	3.1301560	2.0940170	1.2047950
O	3.8754230	1.1078090	-1.3311440
O	0.4608440	-0.0624740	-1.0736130
O	2.2351690	-2.0887070	-1.6143390
H	-0.3770040	1.8099220	-0.8880220

H	1.0309380	0.4832140	1.4865590
H	-0.4373560	2.1491460	2.0600480
H	1.9799170	2.6797570	-0.4098740
H	2.7534120	2.7451820	1.8063110
H	2.9392520	-0.1898250	-0.0099860
H	1.5525080	1.1094460	-2.4002380
H	1.3829400	-1.1584340	-3.2621620
H	3.0929300	-0.7992210	-2.9140700
H	4.4881570	1.4604900	-0.6768850
C	-0.0224840	-1.9177130	2.7739640
C	0.9891440	-2.2558350	1.6828000
H	-1.0440890	-2.0310610	2.4021220
H	0.1068660	-2.5672410	3.6460910
H	0.1007860	-0.8832880	3.1182030
C	2.4354570	-2.0613900	2.1305190
H	0.8374430	-3.2909560	1.3569050
H	0.7799590	-1.6312240	0.8076720
H	3.1368170	-2.3129000	1.3292840
H	2.6233900	-1.0221050	2.4284270
H	2.6662510	-2.6935870	2.9943970

TS5$_{C3}$ – *E* = -1187.61695 Hartree

Symbol	X	Y	Z
O	4.7151370	0.3055980	-0.8670870
O	2.7161070	-2.2599530	0.6878460
C	3.8163880	-0.2254680	-0.1463840

C	3.5187490	-1.7153630	-0.3340660
H	4.2387950	1.5166860	-1.1679320
H	3.1893970	-2.2414480	1.5240450
H	3.6983230	0.0944970	0.9061210
H	4.4988630	-2.2088040	-0.3761450
H	3.0117380	-1.9112000	-1.2808910
C	2.4609960	1.8283590	-0.5800820
C	2.0577290	0.5382270	-0.8690770
O	3.5072050	2.3436220	-1.1250460
O	1.0554350	-0.0301110	-0.1263630
H	1.9867260	2.3639200	0.2489740
H	2.2460750	0.1140440	-1.8526770
H	-1.9551450	2.5574380	0.2490170
C	-0.1272980	-0.3416140	-0.7928680
C	-0.8181800	-1.4045360	0.0483820
C	-2.1966080	-1.6704780	-0.5194530
C	-2.9766980	-0.3706670	-0.6007420
C	-2.1969000	0.6552280	-1.4228780
C	-2.8428790	2.0314330	-1.3843490
O	-0.0992660	-2.6085710	0.0348670
O	-2.9306590	-2.5642360	0.2854810
O	-4.2161900	-0.5633860	-1.2383920
O	-0.8883450	0.8304910	-0.8902290
O	-2.8621630	2.5540540	-0.0765620
H	0.0932850	-0.7385610	-1.8015750
H	-0.9192420	-1.0031140	1.0684080

H	0.7859820	-2.4624830	0.4045570
H	-2.0866950	-2.0804500	-1.5377380
H	-2.3930120	-3.3529770	0.4165180
H	-3.1136540	0.0272370	0.4165120
H	-2.1410300	0.3038820	-2.4657910
H	-2.2998540	2.6966200	-2.0689380
H	-3.8793180	1.9480850	-1.7173550
H	-4.6597550	-1.2945880	-0.7950140
C	0.7546190	0.6116560	3.0587860
C	-0.4242570	1.4372970	2.5480970
H	1.7036890	0.9687060	2.6459490
H	0.8208950	0.6556840	4.1507250
H	0.6476260	-0.4402260	2.7702090
C	-1.7618540	0.9657910	3.1159670
H	-0.2719810	2.4917290	2.8073780
H	-0.4451970	1.3791540	1.4538830
H	-2.5980580	1.5393840	2.7056650
H	-1.9386300	-0.0914820	2.8862840
H	-1.7807490	1.0689920	4.2056830

TS6$_{C3}$ – *E* = -1416.625514 Hartree

Symbol	X	Y	Z
O	-3.4605090	1.0760240	-1.2652550
H	-3.9230360	-2.1635590	-0.6282500
C	-3.2268650	0.4951410	-0.1471750
C	-1.8300400	0.1561300	0.0029590

C	-1.3675970	-0.8189120	1.0971560
C	-0.7413930	-2.1283340	0.5547850
C	-1.5790220	-2.9652310	-0.4209120
C	-2.8653210	-3.5610240	0.1466920
O	-1.1737150	0.4214880	-1.0903360
O	-2.4053450	-1.0795420	2.0035400
O	0.4727770	-1.9283680	-0.1509490
O	-1.9599870	-2.2419120	-1.5685670
O	-3.8885390	-2.5825580	0.2427440
H	-4.0118940	0.3870910	0.5927460
H	-2.1125420	1.1836470	0.6771270
H	-2.4969960	0.9711090	-1.6830830
H	-0.5866250	-0.3233650	1.6730770
H	-3.1072870	-1.5667510	1.5387350
H	-0.5489820	-2.7404690	1.4508150
H	-0.9251910	-3.8053690	-0.7012620
H	-3.1953050	-4.3723820	-0.5116780
H	-2.7045250	-3.9684840	1.1482080
H	-1.3433360	-1.5061790	-1.7196010
H	0.4605240	1.6561000	-1.1012190
C	1.5037240	-1.2290250	0.4690380
C	2.7743750	-1.5515780	-0.3082900
C	3.8973580	-0.6425100	0.1499900
C	3.4894480	0.8070570	-0.0498600
C	2.1959010	1.0864960	0.7082660
C	1.5518590	2.4116310	0.3093310

O	3.1855280	-2.8832120	-0.0985390
O	5.0776630	-0.8615690	-0.5877740
O	4.4683220	1.6828630	0.4559520
O	1.2008110	0.1311450	0.3890220
O	1.1079020	2.3778130	-1.0197980
H	1.6097600	-1.5488930	1.5243790
H	2.5675260	-1.3613460	-1.3712110
H	2.5308990	-3.4681070	-0.4919240
H	4.0838660	-0.8137990	1.2238260
H	5.2823570	-1.8019930	-0.5495540
H	3.3160950	0.9836640	-1.1215320
H	2.4179720	1.0810400	1.7878730
H	0.7185050	2.6102470	1.0031770
H	2.2829250	3.2186790	0.4051250
H	5.3085210	1.4450210	0.0496170
C	-3.0205430	3.9197980	0.6829230
C	-1.8758020	3.8774990	-0.3272230
H	-3.8182240	3.2147820	0.4283110
H	-2.6629790	3.6868590	1.6926530
H	-3.4683050	4.9183930	0.7186060
C	-0.8052220	4.9248020	-0.0320740
H	-1.4047870	2.8854900	-0.3405020
H	-2.2710030	4.0321750	-1.3372300
H	0.0378930	4.8265580	-0.7197640
H	-1.2162000	5.9357730	-0.1209300
H	-0.4240510	4.8150570	0.9895210

7$_{C3}$ – *E* = -1416.693755 Hartree

Symbol	X	Y	Z
O	-0.6418940	3.1958920	1.2172570
H	-4.6316730	-0.1855300	-0.3817540
C	-1.1896090	2.0931650	1.8878460
C	-1.5784910	1.0046630	0.9084360
C	-1.7643820	-0.3939810	1.4936860
C	-1.6683840	-1.5400020	0.4635160
C	-2.7990760	-1.8078630	-0.5441470
C	-4.1861880	-1.9959130	0.0743500
O	-1.7666110	1.2989720	-0.2500870
O	-2.9033540	-0.4229720	2.3093230
O	-0.5086910	-1.3754450	-0.3393800
O	-2.9293090	-0.8339630	-1.5516050
O	-4.7602130	-0.7414670	0.4001650
H	-2.0890610	2.3609300	2.4621850
H	-0.4532060	1.7052370	2.5950130
H	-1.0709050	3.2412950	0.3509310
H	-0.9174100	-0.5390210	2.1733820
H	-3.6975700	-0.3475030	1.7456710
H	-1.5780270	-2.4623560	1.0599620
H	-2.5146730	-2.7581510	-1.0193200
H	-4.8221220	-2.5142930	-0.6517910
H	-4.1455910	-2.5884690	0.9921020
H	-2.3153170	-0.1042640	-1.3800540

H	1.2872320	2.7045540	0.7344190
C	0.7296480	-1.3471860	0.2851140
C	1.7575380	-1.7492580	-0.7671710
C	3.1464290	-1.6515130	-0.1729890
C	3.3752620	-0.2528520	0.3694960
C	2.2686810	0.1104390	1.3595390
C	2.3990570	1.5523740	1.8343290
O	1.5644470	-3.0800530	-1.1862070
O	4.1489090	-1.9112920	-1.1280210
O	4.5996630	-0.1809710	1.0604030
O	0.9893390	-0.0415450	0.7526660
O	2.2240260	2.4731370	0.7907340
H	0.7521480	-2.0617160	1.1315970
H	1.6676550	-1.0468660	-1.6076080
H	0.7272660	-3.1276620	-1.6585630
H	3.2246070	-2.3676400	0.6626090
H	3.9633300	-2.7660380	-1.5312270
H	3.3479320	0.4649940	-0.4630020
H	2.3540360	-0.5597710	2.2326090
H	1.6911900	1.7337900	2.6533270
H	3.4097210	1.6749430	2.2341970
H	5.2854300	-0.5107710	0.4698520
C	-1.1709370	2.6079210	-3.4266630
C	0.0982170	2.7859430	-2.5980410
H	-1.6671390	3.5626590	-3.6219120
H	-0.9406500	2.1453780	-4.3919790

H	-1.8820350	1.9570650	-2.9079280
C	0.8024510	1.4596870	-2.3274800
H	0.7833220	3.4713710	-3.1084840
H	-0.1506390	3.2640310	-1.6430010
H	1.6777530	1.5977830	-1.6859040
H	0.1266600	0.7632650	-1.8193960
H	1.1259440	0.9966730	-3.2668480

TS7$_{C3}$ – *E* = -1416.633738 Hartree

Symbol	X	Y	Z
O	-3.6949850	2.6313560	0.5566520
H	-4.9880110	-0.6661680	-0.3822720
C	-3.4374800	1.4311090	1.2179950
C	-2.2771300	0.6945970	0.5761060
C	-1.8942970	-0.6575690	1.1832880
C	-1.5100670	-1.5805380	0.0048750
C	-2.4627940	-1.2018460	-1.1447410
C	-3.7927800	-1.9432290	-1.2207110
O	-1.3331110	1.4705410	0.0806280
O	-2.9137640	-1.2265150	1.9584000
O	-0.2180390	-1.3830010	-0.5415370
O	-2.7406310	0.1897010	-0.9895150
O	-4.6819840	-1.5594540	-0.1880850
H	-4.3479430	0.8292210	1.2316690
H	-3.1403650	1.5843940	2.2686890
H	-2.8377290	2.9706560	0.2620260

H	-1.0437430	-0.4884480	1.8425220
H	-3.6723920	-1.4408890	1.3927240
H	-1.6265840	-2.6240530	0.3278600
H	-1.9235710	-1.3504210	-2.0854780
H	-4.2495070	-1.7528340	-2.1978800
H	-3.6293160	-3.0195790	-1.1211190
H	-1.8079160	0.8957150	-0.9915430
H	0.6346280	2.0899930	0.6265140
C	0.8836710	-1.3912410	0.3122830
C	2.1054790	-1.6159800	-0.5723690
C	3.3733990	-1.3618090	0.2180410
C	3.3432870	0.0410550	0.8001570
C	2.0977250	0.2103900	1.6617680
C	1.8502540	1.6616090	2.0684430
O	2.1585510	-2.9398240	-1.0550140
O	4.5183770	-1.4617380	-0.5981230
O	4.4615980	0.2684700	1.6237500
O	0.9359110	-0.1417510	0.9321650
O	1.4745990	2.4414790	0.9631270
H	0.7948290	-2.2020030	1.0605250
H	2.0488580	-0.8936990	-1.3994450
H	1.4367760	-3.0663810	-1.6776820
H	3.4331400	-2.0872590	1.0469840
H	4.5021750	-2.3217720	-1.0313310
H	3.3013880	0.7689660	-0.0231040
H	2.2062310	-0.4195950	2.5598480

H	1.0746670	1.6796020	2.8475420
H	2.7704220	2.0806850	2.4825020
H	5.2488100	0.0667220	1.1068160
C	2.5075710	1.9433240	-2.3864930
C	1.0090310	1.6561540	-2.3180630
H	3.1065620	1.0263220	-2.4080930
H	2.7518460	2.5176960	-3.2863870
H	2.8157750	2.5319570	-1.5159760
C	0.1946120	2.9484790	-2.3007120
H	0.7105420	1.0398540	-3.1764060
H	0.7806250	1.0740620	-1.4167530
H	-0.8821770	2.7573010	-2.2905220
H	0.4371260	3.5382010	-1.4104830
H	0.4198010	3.5605950	-3.1805210

8$_{C3}$ – *E* = -1416.704393 Hartree

Symbol	X	Y	Z
O	-3.7477620	2.8244840	-0.4948980
H	-5.0651710	-0.9973190	0.2191690
C	-3.3990210	1.9894030	0.5766900
C	-2.4402260	0.8927070	0.1424370
C	-1.9612330	-0.0272330	1.2825870
C	-1.5696880	-1.2907700	0.4973150
C	-2.5886420	-1.3080610	-0.6584320
C	-3.7815990	-2.2440740	-0.4968810
O	-1.3657600	1.5465330	-0.4821820

O	-2.9547950	-0.3059900	2.2291890
O	-0.2957360	-1.2071440	-0.1391030
O	-3.0938590	0.0178530	-0.7633200
O	-4.6525190	-1.8117280	0.5316010
H	-4.3159100	1.5433860	0.9645610
H	-2.9194580	2.5486960	1.3927050
H	-2.9377610	3.0417630	-0.9693980
H	-1.1216350	0.4227900	1.8098420
H	-3.6294350	-0.8830720	1.8363450
H	-1.6112280	-2.1804270	1.1375100
H	-2.0502680	-1.5793350	-1.5756640
H	-4.3213000	-2.2983470	-1.4490140
H	-3.4438260	-3.2505220	-0.2356340
H	-0.6662340	0.9076530	-0.6748020
H	1.0126720	2.6155620	0.1725070
C	0.8304050	-1.0552800	0.6642290
C	2.0106510	-1.6020350	-0.1325350
C	3.3128230	-1.2631100	0.5648220
C	3.4010170	0.2370510	0.7911180
C	2.1812940	0.7018930	1.5814970
C	2.1050330	2.2165470	1.7206610
O	1.9403990	-3.0031320	-0.2577850
O	4.4285260	-1.6452050	-0.2059180
O	4.5440980	0.5662390	1.5403760
O	0.9915070	0.3190630	0.9059110
O	1.8989880	2.8424550	0.4778980

H	0.7142060	-1.6054550	1.6156540
H	1.9986870	-1.1148410	-1.1183690
H	1.1915530	-3.2221830	-0.8207410
H	3.3363350	-1.7677810	1.5452750
H	4.3513290	-2.5851080	-0.4014330
H	3.4040030	0.7476110	-0.1846740
H	2.2173480	0.2453010	2.5841570
H	1.3038150	2.4673150	2.4285310
H	3.0537270	2.5814280	2.1202050
H	5.3046460	0.1686900	1.1027340
C	0.2019980	0.1137170	-3.2079460
C	1.1401630	1.1357620	-2.5685420
H	-0.8244600	0.2197450	-2.8415590
H	0.1815340	0.2384310	-4.2952590
H	0.5325960	-0.9107440	-2.9991350
C	2.5644840	1.0511060	-3.1115270
H	0.7442960	2.1449370	-2.7276530
H	1.1765650	0.9896710	-1.4815510
H	3.2115020	1.7973530	-2.6424050
H	3.0019440	0.0627480	-2.9259190
H	2.5804630	1.2188820	-4.1930820

TS8$_{C3}$ – *E* = -1416.585514 Hartree

Symbol	X	Y	Z
O	-2.9866170	2.2180010	0.9107960
H	-4.7721700	-3.3495540	0.8907570

C	-3.0880010	1.4991730	-0.2813910
C	-2.6535060	0.1327260	-0.1739250
C	-1.7733590	-0.4686860	0.8898750
C	-1.3545650	-1.8193860	0.2480410
C	-2.4155160	-2.0279070	-0.8475730
C	-3.4650250	-3.0743730	-0.5535640
O	-0.8177640	1.0304090	-1.3334450
O	-2.5479260	-0.6695570	2.0449570
O	-0.1119720	-1.8942950	-0.4027040
O	-3.0985490	-0.7533780	-0.9976580
O	-4.0089890	-2.7923520	0.7216570
H	-2.1638140	1.6841730	-1.0286440
H	-4.0471600	1.6115320	-0.7930860
H	-2.3457210	2.9250350	0.7884010
H	-0.9373800	0.1792920	1.1275910
H	-3.2292710	-1.3314580	1.8618100
H	-1.4181570	-2.5908850	1.0274990
H	-1.9206280	-2.2296610	-1.7993820
H	-4.2385950	-3.0375350	-1.3288140
H	-2.9846830	-4.0609540	-0.5723210
H	-0.5059230	0.7704580	-2.2059280
H	0.7444810	1.6560120	-0.8042190
C	1.0371960	-1.6317830	0.3517890
C	2.2054450	-2.1298070	-0.4902270
C	3.5085890	-1.6365410	0.1011950
C	3.4906530	-0.1191760	0.1305600

C	2.2988570	0.3769820	0.9435300
C	2.0115530	1.8571090	0.6919940
O	2.2496840	-3.5398350	-0.5284700
O	4.6149790	-2.0407400	-0.6734230
O	4.6513770	0.3877460	0.7467540
O	1.0920470	-0.2603060	0.5621960
O	1.6241140	2.0836570	-0.6288720
H	0.9973820	-2.1829790	1.3112350
H	2.0886730	-1.7089400	-1.4991970
H	1.4844630	-3.8533140	-1.0188060
H	3.6083560	-2.0149250	1.1325780
H	4.5609860	-2.9948500	-0.7927650
H	3.3947070	0.2545800	-0.8991250
H	2.5134620	0.2014690	2.0097300
H	1.2352340	2.1786190	1.4066410
H	2.9202160	2.4330840	0.8957110
H	5.4098120	0.0202360	0.2810680
C	0.6893550	5.0160560	0.5057800
C	-0.5632100	4.3183200	-0.0179690
H	0.7898840	4.9116270	1.5903300
H	1.5752190	4.5823480	0.0330490
H	0.6626040	6.0854470	0.2716790
C	-0.6935310	4.4298060	-1.5340110
H	-0.5088040	3.2531630	0.2448760
H	-1.4484710	4.7536550	0.4680800
H	-1.6005920	3.9416010	-1.9020930

H	-0.7183600	5.4800430	-1.8443250
H	0.1615780	3.9428170	-2.0112590

9$_{C3}$ – *E* = -1340.263271 Hartree

Symbol	X	Y	Z
O	3.6977940	0.5027030	2.4265730
H	3.8181440	-0.5274960	-1.5025480
C	2.7328370	0.9919000	1.6016890
C	2.0711740	0.2626200	0.7109540
C	0.9911800	0.6941310	-0.2503690
C	0.4076520	-0.6739900	-0.6749510
C	1.5558520	-1.6617510	-0.4393820
C	2.4527550	-1.9060390	-1.6462640
O	1.4311750	1.4656780	-1.3396590
O	-0.6661290	-1.0679920	0.1640270
O	2.3350150	-1.0944300	0.6128690
O	3.0802640	-0.7196720	-2.0938470
H	2.5530870	2.0521420	1.7146650
H	3.7391620	-0.4544650	2.3118120
H	0.2170280	1.2776020	0.2452150
H	2.0877580	0.9476970	-1.8265050
H	0.0813890	-0.6405140	-1.7213940
H	1.1549310	-2.6176050	-0.0878460
H	3.2052460	-2.6586810	-1.3821990
H	1.8582920	-2.2944510	-2.4788260
H	-2.2391570	2.7118900	0.9702980

C	-1.9282320	-0.7192310	-0.2861510
C	-2.9473140	-1.3936150	0.6222610
C	-4.3388470	-0.9921560	0.1703540
C	-4.4676260	0.5219170	0.1402040
C	-3.3478030	1.1257370	-0.7065770
C	-3.3149200	2.6434650	-0.6326730
O	-2.8675180	-2.7977990	0.5476260
O	-5.3372590	-1.4880270	1.0322580
O	-5.6910230	0.9098450	-0.4369530
O	-2.0840180	0.6761330	-0.2323820
O	-3.0731240	3.0945400	0.6791220
H	-2.0656450	-1.0608620	-1.3306260
H	-2.7747630	-1.0367400	1.6479650
H	-2.0010890	-3.0676320	0.8677820
H	-4.4964270	-1.3755370	-0.8517260
H	-5.2271060	-2.4423740	1.0999540
H	-4.3763440	0.9074050	1.1660940
H	-3.4908150	0.8171740	-1.7550740
H	-2.5483440	3.0124170	-1.3269610
H	-4.2881080	3.0348420	-0.9359020
H	-6.3946820	0.4567820	0.0397430
C	6.8140560	-0.1356870	0.8266120
C	5.6885890	0.0932090	-0.1796700
H	7.0242120	-1.1996340	0.9656840
H	7.7363280	0.3489800	0.4914500
H	6.5434900	0.2913090	1.7972030

C	5.3929520	1.5777280	-0.3832110
H	5.9593920	-0.3697300	-1.1383580
H	4.7856860	-0.4141800	0.1881310
H	4.5507440	1.7486830	-1.0614770
H	5.1442500	2.0454760	0.5740970
H	6.2680990	2.0902520	-0.7946800

TS9$_{C3}$ – *E* = -1340.201781 Hartree

Symbol	X	Y	Z
O	-3.5393930	-2.6100730	-0.0646620
H	-4.8879490	0.6545350	-0.8620090
C	-3.7271320	-1.6381850	0.7302830
C	-2.9406790	-0.5042420	0.6049250
C	-1.9102740	-0.5058240	-0.3576050
C	-1.5079790	0.9447000	-0.5496230
C	-2.6630560	1.6999980	0.1401720
C	-3.7170900	2.1953350	-0.8434860
O	-2.6218580	-1.1373620	-1.8737340
O	-0.3072920	1.2343950	0.1384010
O	-3.2718020	0.7860150	1.0475970
O	-4.3503540	1.1172390	-1.5156810
H	-4.5397310	-1.6866300	1.4668640
H	-3.0471830	-1.9139950	-1.2948620
H	-1.1417870	-1.2678550	-0.3804870
H	-3.3297380	-0.5003100	-2.0785570
H	-1.4086630	1.2058860	-1.6117630

H	-2.2625190	2.5440770	0.7097870
H	-4.4618550	2.7918850	-0.3052160
H	-3.2571280	2.8259320	-1.6103420
H	1.2589380	-2.5584840	-0.0687320
C	0.8702760	1.0422000	-0.5724710
C	2.0050720	1.5103970	0.3290430
C	3.3288270	1.2295640	-0.3533520
C	3.4243370	-0.2464580	-0.6988480
C	2.2198180	-0.6687880	-1.5383990
C	2.1615520	-2.1748760	-1.7417780
O	1.9351330	2.8940060	0.5787600
O	4.4225210	1.5442340	0.4764710
O	4.5782710	-0.5137820	-1.4573740
O	1.0093840	-0.3211870	-0.8757980
O	2.0566120	-2.8608290	-0.5168320
H	0.8508170	1.6301370	-1.5107410
H	1.9474680	0.9314420	1.2629260
H	1.1418220	3.0696290	1.0946200
H	3.3785660	1.8151590	-1.2867700
H	4.3283780	2.4590020	0.7628630
H	3.4200830	-0.8292490	0.2348740
H	2.2748840	-0.1670690	-2.5179820
H	1.3166090	-2.4088070	-2.4032990
H	3.0872330	-2.5044670	-2.2177520
H	5.3342690	-0.1716760	-0.9683030
C	-0.2877300	-0.0281700	3.1814120

C	0.3332910	-1.2128260	2.4452640
H	-1.2586530	0.2442980	2.7574240
H	-0.4277780	-0.2589710	4.2425740
H	0.3647270	0.8515520	3.1207250
C	1.7046870	-1.5962060	2.9984680
H	-0.3449060	-2.0726990	2.5007490
H	0.4273340	-0.9570480	1.3840490
H	2.1503360	-2.4272530	2.4438990
H	2.3998480	-0.7496850	2.9437050
H	1.6332970	-1.8903090	4.0505330

10$_{C3}$ – *E* = -1263.845867 Hartree

Symbol	X	Y	Z
O	-3.4299480	-3.0438970	-0.7352250
H	-4.6604030	1.4387670	-1.5219510
C	-3.8280150	-2.0676320	-0.1599750
C	-3.1187800	-0.7658170	-0.1982140
C	-1.9669890	-0.4587190	-0.7903500
C	-1.6376610	0.9728920	-0.4646040
C	-2.8622990	1.4044110	0.3726630
C	-3.6700370	2.5222080	-0.2576700
O	-0.4830990	1.1206690	0.3548760
O	-3.7152530	0.2488910	0.4895300
O	-4.0669240	2.1951180	-1.5676870
H	-4.7531090	-2.0790310	0.4474740
H	-1.3634130	-1.1274620	-1.3822150

H	-1.5202340	1.5942830	-1.3632290
H	-2.5305120	1.6815400	1.3787920
H	-4.5338840	2.7533000	0.3787240
H	-3.0453970	3.4182000	-0.3272600
H	1.1539160	-2.4072170	-0.7748840
C	0.7326190	1.1562960	-0.3085430
C	1.7991010	1.3810320	0.7560840
C	3.1714900	1.3027950	0.1189820
C	3.3294390	-0.0283480	-0.5945030
C	2.1968500	-0.2171370	-1.6019130
C	2.1916750	-1.6134450	-2.2054700
O	1.6769170	2.6491030	1.3556940
O	4.2003220	1.3979440	1.0768520
O	4.5403710	-0.0781420	-1.3085760
O	0.9357460	-0.0722230	-0.9614580
O	1.9847990	-2.6010270	-1.2240030
H	0.7455140	1.9757370	-1.0532240
H	1.6965880	0.5756880	1.4997190
H	0.8290950	2.6889820	1.8092990
H	3.2656890	2.1141520	-0.6221060
H	4.0636240	2.2049840	1.5844100
H	3.2743790	-0.8381760	0.1490230
H	2.3072510	0.5305740	-2.4039310
H	1.4181400	-1.6589080	-2.9843510
H	3.1643280	-1.8078770	-2.6618870
H	5.2497980	0.1383880	-0.6940560

C	1.3117500	-2.4063610	2.3721160
C	-0.0284130	-1.9559380	1.7936270
H	1.8928410	-2.9832700	1.6467460
H	1.9178170	-1.5436500	2.6732610
H	1.1660330	-3.0282200	3.2612570
C	-0.8354930	-1.1107730	2.7757610
H	0.1409280	-1.3653860	0.8870100
H	-0.6155680	-2.8324780	1.4934970
H	-1.7878690	-0.7884740	2.3419690
H	-1.0510380	-1.6695840	3.6922960
H	-0.2793970	-0.2091310	3.0576490

TS10$_{C3}$ – *E* = -1263.755124 Hartree

Symbol	X	Y	Z
O	-5.6851790	-1.8409150	-0.6811390
H	-3.5076450	3.1180110	-0.1752260
C	-5.3393210	-1.0026010	0.1015170
C	-3.9583150	-0.4392710	0.0741450
C	-2.8952620	-0.7826770	-0.7340740
C	-1.8415580	0.0268120	-0.3191630
C	-2.3068740	0.8392890	0.7996460
C	-2.0541120	2.3276860	0.8591300
O	-0.7148520	-1.0220480	1.4287230
O	-3.6941980	0.5157670	0.9353450
O	-2.5571900	3.0108050	-0.2644780
H	-6.0043820	-0.5911620	0.8810230

H	-2.9143560	-1.5374880	-1.5028410
H	-0.8629220	0.1240250	-0.7639230
H	-1.7044770	0.2426690	1.6066350
H	-2.4636780	2.7224830	1.7956540
H	-0.9700990	2.4645030	0.8759820
H	1.0293750	2.2255660	-0.6798030
C	0.5816130	-0.7370780	1.5300520
C	1.4400950	-1.6999840	0.6995690
C	2.9057260	-1.3504920	0.8393350
C	3.1434450	0.0988550	0.4518300
C	2.1916930	1.0143300	1.2243910
C	2.2893260	2.4612860	0.7699090
O	1.2560490	-3.0253850	1.1355680
O	3.7321460	-2.1480800	0.0133550
O	4.4620080	0.4935230	0.7568880
O	0.8482080	0.6058880	1.0357730
O	1.9011360	2.6219580	-0.5773210
H	0.9411300	-0.7621530	2.5824850
H	1.1317040	-1.5925130	-0.3540680
H	0.3078140	-3.1293480	1.2862380
H	3.1942030	-1.4800410	1.8953890
H	3.5355670	-3.0710200	0.2057950
H	2.9479260	0.2145060	-0.6245080
H	2.4583730	0.9639230	2.2935250
H	1.6693510	3.0820630	1.4327990
H	3.3265030	2.7939400	0.8464710

H	5.0535510	-0.1632570	0.3741460
C	2.2615620	0.5643740	-3.3388370
C	0.9109070	0.2118350	-2.7218450
H	2.6157280	1.5350940	-2.9828540
H	3.0102690	-0.1898820	-3.0722050
H	2.1949780	0.5944340	-4.4310790
C	0.4262690	-1.1761940	-3.1340160
H	1.0084630	0.2525240	-1.6295460
H	0.1664390	0.9684210	-3.0025900
H	-0.5280780	-1.4385970	-2.6642300
H	0.2907720	-1.2366880	-4.2183740
H	1.1573090	-1.9391230	-2.8461500

In the Presence of Benzene (Bz)

The Cartesian coordinates for all the stable structures in the presence of Bz reported in this work are listed below including computed absolute energies.

1$_{Bz}$ – *E* = -1529.795633 Hartree

Symbol	X	Y	Z
C	-1.0767110	1.0976700	0.4678650
C	-0.6941700	-0.3626670	0.6373170
C	-1.9168060	-1.2807580	0.4607770
C	-1.5871730	-2.6979950	0.9141390
O	-0.7063670	1.7982340	-0.4327740
O	0.2726370	-0.7662830	-0.2980740
O	-2.9857130	-0.8272260	1.2681940
O	-1.3396840	-2.7354150	2.2994930

H	-1.7587230	1.4785050	1.2537230
H	-0.3311220	-0.4909900	1.6695190
H	-2.1896420	-1.2886180	-0.6020940
H	-3.6432290	-0.3692220	0.7317860
H	1.8999210	2.8310600	-0.1417670
H	-2.1141070	-2.3629800	2.7363790
H	-2.4250610	-3.3545260	0.6432040
H	-0.6829310	-3.0556210	0.4147330
C	1.5846050	-0.6760800	0.1494240
C	2.4884110	-1.1084280	-0.9954990
C	3.9326720	-0.9198220	-0.5738990
C	4.1661590	0.5227580	-0.1574120
C	3.1710510	0.9203540	0.9318320
C	3.1989770	2.4132640	1.2271480
O	2.3118620	-2.4695940	-1.3159980
O	4.8291840	-1.2129260	-1.6211630
O	5.4594800	0.6901040	0.3724830
O	1.8424380	0.6528270	0.5080670
O	2.7691730	3.1618610	0.1174510
H	1.7311990	-1.3350150	1.0280580
H	2.2694410	-0.4624820	-1.8576980
H	1.4173110	-2.5887530	-1.6493940
H	4.1351810	-1.5724200	0.2918520
H	4.6371540	-2.1021320	-1.9374120
H	4.0099120	1.1746210	-1.0294100
H	3.4065730	0.3540480	1.8475550

H	2.5691350	2.6089790	2.1061430
H	4.2238180	2.7155910	1.4534100
H	6.0847740	0.3466320	-0.2745990
C	-5.1399030	1.7161570	0.2339730
C	-4.0358860	1.9385770	-0.5857680
C	-3.7169970	1.0254570	-1.5886350
C	-4.5054450	-0.1081690	-1.7730990
C	-5.6061710	-0.3347040	-0.9492380
C	-5.9235700	0.5780960	0.0544410
H	-5.3863500	2.4253460	1.0162360
H	-3.4125520	2.8148180	-0.4431690
H	-2.8470560	1.1971720	-2.2133740
H	-4.2594580	-0.8180150	-2.5557060
H	-6.2145550	-1.2214780	-1.0874140
H	-6.7779650	0.4005650	0.6978100

TS1$_{Bz}$ – *E* = -1529.71051 Hartree

Symbol	X	Y	Z
C	-1.0767110	1.0976700	0.4678650
C	-0.6941700	-0.3626670	0.6373170
C	-1.9168060	-1.2807580	0.4607770
C	-1.5871730	-2.6979950	0.9141390
O	-0.7063670	1.7982340	-0.4327740
O	0.2726370	-0.7662830	-0.2980740
O	-2.9857130	-0.8272260	1.2681940
O	-1.3396840	-2.7354150	2.2994930

H	-1.7587230	1.4785050	1.2537230
H	-0.3311220	-0.4909900	1.6695190
H	-2.1896420	-1.2886180	-0.6020940
H	-3.6432290	-0.3692220	0.7317860
H	1.8999210	2.8310600	-0.1417670
H	-2.1141070	-2.3629800	2.7363790
H	-2.4250610	-3.3545260	0.6432040
H	-0.6829310	-3.0556210	0.4147330
C	1.5846050	-0.6760800	0.1494240
C	2.4884110	-1.1084280	-0.9954990
C	3.9326720	-0.9198220	-0.5738990
C	4.1661590	0.5227580	-0.1574120
C	3.1710510	0.9203540	0.9318320
C	3.1989770	2.4132640	1.2271480
O	2.3118620	-2.4695940	-1.3159980
O	4.8291840	-1.2129260	-1.6211630
O	5.4594800	0.6901040	0.3724830
O	1.8424380	0.6528270	0.5080670
O	2.7691730	3.1618610	0.1174510
H	1.7311990	-1.3350150	1.0280580
H	2.2694410	-0.4624820	-1.8576980
H	1.4173110	-2.5887530	-1.6493940
H	4.1351810	-1.5724200	0.2918520
H	4.6371540	-2.1021320	-1.9374120
H	4.0099120	1.1746210	-1.0294100
H	3.4065730	0.3540480	1.8475550

H	2.5691350	2.6089790	2.1061430
H	4.2238180	2.7155910	1.4534100
H	6.0847740	0.3466320	-0.2745990
C	-5.1399030	1.7161570	0.2339730
C	-4.0358860	1.9385770	-0.5857680
C	-3.7169970	1.0254570	-1.5886350
C	-4.5054450	-0.1081690	-1.7730990
C	-5.6061710	-0.3347040	-0.9492380
C	-5.9235700	0.5780960	0.0544410
H	-5.3863500	2.4253460	1.0162360
H	-3.4125520	2.8148180	-0.4431690
H	-2.8470560	1.1971720	-2.2133740
H	-4.2594580	-0.8180150	-2.5557060
H	-6.2145550	-1.2214780	-1.0874140
H	-6.7779650	0.4005650	0.6978100

2$_{Bz}$ – *E* = -1453.375697 Hartree

Symbol	X	Y	Z
C	-1.0767110	1.0976700	0.4678650
C	-0.6941700	-0.3626670	0.6373170
C	-1.9168060	-1.2807580	0.4607770
C	-1.5871730	-2.6979950	0.9141390
O	-0.7063670	1.7982340	-0.4327740
O	0.2726370	-0.7662830	-0.2980740
O	-2.9857130	-0.8272260	1.2681940
O	-1.3396840	-2.7354150	2.2994930

H	-1.7587230	1.4785050	1.2537230
H	-0.3311220	-0.4909900	1.6695190
H	-2.1896420	-1.2886180	-0.6020940
H	-3.6432290	-0.3692220	0.7317860
H	1.8999210	2.8310600	-0.1417670
H	-2.1141070	-2.3629800	2.7363790
H	-2.4250610	-3.3545260	0.6432040
H	-0.6829310	-3.0556210	0.4147330
C	1.5846050	-0.6760800	0.1494240
C	2.4884110	-1.1084280	-0.9954990
C	3.9326720	-0.9198220	-0.5738990
C	4.1661590	0.5227580	-0.1574120
C	3.1710510	0.9203540	0.9318320
C	3.1989770	2.4132640	1.2271480
O	2.3118620	-2.4695940	-1.3159980
O	4.8291840	-1.2129260	-1.6211630
O	5.4594800	0.6901040	0.3724830
O	1.8424380	0.6528270	0.5080670
O	2.7691730	3.1618610	0.1174510
H	1.7311990	-1.3350150	1.0280580
H	2.2694410	-0.4624820	-1.8576980
H	1.4173110	-2.5887530	-1.6493940
H	4.1351810	-1.5724200	0.2918520
H	4.6371540	-2.1021320	-1.9374120
H	4.0099120	1.1746210	-1.0294100
H	3.4065730	0.3540480	1.8475550

H	2.5691350	2.6089790	2.1061430
H	4.2238180	2.7155910	1.4534100
H	6.0847740	0.3466320	-0.2745990
C	-5.1399030	1.7161570	0.2339730
C	-4.0358860	1.9385770	-0.5857680
C	-3.7169970	1.0254570	-1.5886350
C	-4.5054450	-0.1081690	-1.7730990
C	-5.6061710	-0.3347040	-0.9492380
C	-5.9235700	0.5780960	0.0544410
H	-5.3863500	2.4253460	1.0162360
H	-3.4125520	2.8148180	-0.4431690
H	-2.8470560	1.1971720	-2.2133740
H	-4.2594580	-0.8180150	-2.5557060
H	-6.2145550	-1.2214780	-1.0874140
H	-6.7779650	0.4005650	0.6978100

TS2$_{Bz}$ – *E* = -1453.282849 Hartree

Symbol	X	Y	Z
C	-1.0767110	1.0976700	0.4678650
C	-0.6941700	-0.3626670	0.6373170
C	-1.9168060	-1.2807580	0.4607770
C	-1.5871730	-2.6979950	0.9141390
O	-0.7063670	1.7982340	-0.4327740
O	0.2726370	-0.7662830	-0.2980740
O	-2.9857130	-0.8272260	1.2681940
O	-1.3396840	-2.7354150	2.2994930

H	-1.7587230	1.4785050	1.2537230
H	-0.3311220	-0.4909900	1.6695190
H	-2.1896420	-1.2886180	-0.6020940
H	-3.6432290	-0.3692220	0.7317860
H	1.8999210	2.8310600	-0.1417670
H	-2.1141070	-2.3629800	2.7363790
H	-2.4250610	-3.3545260	0.6432040
H	-0.6829310	-3.0556210	0.4147330
C	1.5846050	-0.6760800	0.1494240
C	2.4884110	-1.1084280	-0.9954990
C	3.9326720	-0.9198220	-0.5738990
C	4.1661590	0.5227580	-0.1574120
C	3.1710510	0.9203540	0.9318320
C	3.1989770	2.4132640	1.2271480
O	2.3118620	-2.4695940	-1.3159980
O	4.8291840	-1.2129260	-1.6211630
O	5.4594800	0.6901040	0.3724830
O	1.8424380	0.6528270	0.5080670
O	2.7691730	3.1618610	0.1174510
H	1.7311990	-1.3350150	1.0280580
H	2.2694410	-0.4624820	-1.8576980
H	1.4173110	-2.5887530	-1.6493940
H	4.1351810	-1.5724200	0.2918520
H	4.6371540	-2.1021320	-1.9374120
H	4.0099120	1.1746210	-1.0294100
H	3.4065730	0.3540480	1.8475550

H	2.5691350	2.6089790	2.1061430
H	4.2238180	2.7155910	1.4534100
H	6.0847740	0.3466320	-0.2745990
C	-5.1399030	1.7161570	0.2339730
C	-4.0358860	1.9385770	-0.5857680
C	-3.7169970	1.0254570	-1.5886350
C	-4.5054450	-0.1081690	-1.7730990
C	-5.6061710	-0.3347040	-0.9492380
C	-5.9235700	0.5780960	0.0544410
H	-5.3863500	2.4253460	1.0162360
H	-3.4125520	2.8148180	-0.4431690
H	-2.8470560	1.1971720	-2.2133740
H	-4.2594580	-0.8180150	-2.5557060
H	-6.2145550	-1.2214780	-1.0874140
H	-6.7779650	0.4005650	0.6978100

TS3$_{Bz}$ – *E* = -1529.709729 Hartree

Symbol	X	Y	Z
C	-1.0767110	1.0976700	0.4678650
C	-0.6941700	-0.3626670	0.6373170
C	-1.9168060	-1.2807580	0.4607770
C	-1.5871730	-2.6979950	0.9141390
O	-0.7063670	1.7982340	-0.4327740
O	0.2726370	-0.7662830	-0.2980740
O	-2.9857130	-0.8272260	1.2681940
O	-1.3396840	-2.7354150	2.2994930

H	-1.7587230	1.4785050	1.2537230
H	-0.3311220	-0.4909900	1.6695190
H	-2.1896420	-1.2886180	-0.6020940
H	-3.6432290	-0.3692220	0.7317860
H	1.8999210	2.8310600	-0.1417670
H	-2.1141070	-2.3629800	2.7363790
H	-2.4250610	-3.3545260	0.6432040
H	-0.6829310	-3.0556210	0.4147330
C	1.5846050	-0.6760800	0.1494240
C	2.4884110	-1.1084280	-0.9954990
C	3.9326720	-0.9198220	-0.5738990
C	4.1661590	0.5227580	-0.1574120
C	3.1710510	0.9203540	0.9318320
C	3.1989770	2.4132640	1.2271480
O	2.3118620	-2.4695940	-1.3159980
O	4.8291840	-1.2129260	-1.6211630
O	5.4594800	0.6901040	0.3724830
O	1.8424380	0.6528270	0.5080670
O	2.7691730	3.1618610	0.1174510
H	1.7311990	-1.3350150	1.0280580
H	2.2694410	-0.4624820	-1.8576980
H	1.4173110	-2.5887530	-1.6493940
H	4.1351810	-1.5724200	0.2918520
H	4.6371540	-2.1021320	-1.9374120
H	4.0099120	1.1746210	-1.0294100
H	3.4065730	0.3540480	1.8475550

H	2.5691350	2.6089790	2.1061430
H	4.2238180	2.7155910	1.4534100
H	6.0847740	0.3466320	-0.2745990
C	-5.1399030	1.7161570	0.2339730
C	-4.0358860	1.9385770	-0.5857680
C	-3.7169970	1.0254570	-1.5886350
C	-4.5054450	-0.1081690	-1.7730990
C	-5.6061710	-0.3347040	-0.9492380
C	-5.9235700	0.5780960	0.0544410
H	-5.3863500	2.4253460	1.0162360
H	-3.4125520	2.8148180	-0.4431690
H	-2.8470560	1.1971720	-2.2133740
H	-4.2594580	-0.8180150	-2.5557060
H	-6.2145550	-1.2214780	-1.0874140
H	-6.7779650	0.4005650	0.6978100

4$_{Bz}$ – *E* = -1529.768972 Hartree

Symbol	X	Y	Z
O	-3.7974860	-1.2525620	-0.3694400
H	-3.3140430	-3.1993910	-0.0009190
C	-2.8736370	-0.6891470	-0.8991780
C	-1.6861230	-0.0737150	-0.1780690
C	-1.0268250	-0.9022810	0.9569930
C	-0.1149200	-2.0954920	0.5619610
C	-0.7009620	-3.2500800	-0.2544410
C	-1.6805240	-4.1829830	0.4549470

O	-0.7664120	0.4109670	-1.1311690
O	-1.9405340	-1.2767380	1.9445420
O	1.0148160	-1.6822670	-0.2162920
O	-1.2799420	-2.6903600	-1.4235830
O	-2.9177110	-3.6077100	0.7808850
H	-2.8476550	-0.5173800	-1.9947220
H	-2.1063460	0.8037630	0.3315350
H	-0.1520470	-0.3008100	-1.3505310
H	-0.3505970	-0.1946000	1.4401320
H	-2.5752930	-1.9172660	1.5885040
H	0.2418570	-2.5129640	1.5155870
H	0.1689660	-3.8663040	-0.5268130
H	-1.8262340	-5.0624100	-0.1912580
H	-1.2336160	-4.5334990	1.3907530
H	-1.3409480	-3.3546800	-2.1151810
H	0.5347420	2.0575960	-0.6648820
C	2.0104890	-0.9333670	0.4066950
C	3.2536340	-1.0448020	-0.4696800
C	4.3112700	-0.0699740	0.0112120
C	3.7489220	1.3421980	0.0120270
C	2.4947150	1.3867630	0.8783600
C	1.7136210	2.6904220	0.7418730
O	3.8093630	-2.3387230	-0.4225740
O	5.4447400	-0.0793940	-0.8258110
O	4.6728050	2.2521390	0.5571760
O	1.5741260	0.3922590	0.4677330

O	1.1331400	2.8110560	-0.5306300
H	2.2134390	-1.3278930	1.4201820
H	2.9605160	-0.7757710	-1.4953880
H	3.1842570	-2.9519500	-0.8205880
H	4.5986300	-0.3342130	1.0428830
H	5.7624510	-0.9863500	-0.8894710
H	3.4780030	1.6210520	-1.0172910
H	2.7915610	1.2377520	1.9291970
H	0.9472490	2.7147750	1.5314180
H	2.3924480	3.5346100	0.8848400
H	5.5024480	2.1472570	0.0792560
C	-3.2756360	2.6339200	-1.5050020
C	-4.2897980	2.2830330	-0.6174080
C	-4.1410530	2.5332160	0.7444690
C	-2.9795840	3.1392020	1.2160780
C	-1.9645860	3.4895310	0.3272030
C	-2.1117940	3.2349970	-1.0329860
H	-3.3873280	2.4311090	-2.5649540
H	-5.1911630	1.8028840	-0.9831240
H	-4.9243860	2.2469040	1.4371430
H	-2.8626420	3.3314890	2.2770910
H	-1.0529340	3.9553800	0.6851740
H	-1.3098300	3.4929270	-1.7155930

TS4$_{Bz}$ – *E* = -1529.718973 Hartree

Symbol	X	Y	Z

C	-2.3907610	2.4293700	-0.9108940
C	-1.9538020	1.1185630	-0.9944720
C	-0.9903320	1.2932010	0.8123390
C	-0.2948100	-0.0667900	0.9177050
C	-1.2085640	-1.2801570	1.1094970
C	-0.3973510	-2.5492140	1.3398750
O	-3.1428450	2.8679630	0.0419810
O	-1.1671250	0.8081620	-2.0781790
O	-1.9250770	1.5470010	1.6446830
O	0.5411300	-0.2718810	-0.2128080
O	-2.0139190	-1.1236620	2.2541340
O	0.4230520	-2.4311560	2.4798120
H	-1.9967420	3.1665610	-1.6150660
H	-2.5892740	0.3324060	-0.5884390
H	-0.2725250	2.0847970	0.5436850
H	0.3283440	0.0293030	1.8190120
H	-1.8172390	-1.4215190	0.2017440
H	-2.3279900	-0.2053850	2.2755420
H	-0.3909150	0.3337240	-1.7540500
H	-2.8525650	2.3150330	0.9044900
H	3.0273870	3.0049770	-0.0460700
H	-0.1515780	-2.1743960	3.2108610
H	-1.1021990	-3.3849520	1.4444830
H	0.2578380	-2.7559190	0.4892420
C	1.8913960	-0.4562480	0.0762250
C	2.5775050	-0.9777250	-1.1780490

C	4.0641240	-1.1006390	-0.8937860
C	4.6207350	0.2266900	-0.4048110
C	3.8100890	0.7267790	0.7903180
C	4.2044690	2.1325000	1.2117040
O	2.1131530	-2.2590840	-1.5380440
O	4.7903420	-1.4682510	-2.0429630
O	5.9542840	0.0852480	0.0187480
O	2.4291670	0.7869390	0.4451110
O	3.9586470	3.0688140	0.1895540
H	2.0023840	-1.1758660	0.9065750
H	2.4198820	-0.2505710	-1.9888800
H	1.2075850	-2.1897180	-1.8546200
H	4.2025710	-1.8517700	-0.0985360
H	4.4307950	-2.2983050	-2.3733250
H	4.5408370	0.9660810	-1.2152850
H	3.9596380	0.0363080	1.6356240
H	3.6581210	2.3926230	2.1282740
H	5.2759110	2.1526250	1.4208710
H	6.4490930	-0.3174210	-0.7029320
C	-4.4852660	-1.5315720	0.1961390
C	-4.9477210	-0.3515370	0.7752050
C	-5.4107790	0.6844730	-0.0304660
C	-5.3999990	0.5461100	-1.4159390
C	-4.9319080	-0.6290410	-1.9956810
C	-4.4778500	-1.6703640	-1.1891160
H	-4.1207770	-2.3315470	0.8320750

H	-4.9479880	-0.2456140	1.8548850
H	-5.7661400	1.6051820	0.4181510
H	-5.7508270	1.3583720	-2.0432840
H	-4.9179190	-0.7338520	-3.0748980
H	-4.1172430	-2.5882830	-1.6411300

5$_{Bz}$ – E = -1300.76219 Hartree

Symbol	X	Y	Z
C	-1.0767110	1.0976700	0.4678650
C	-0.6941700	-0.3626670	0.6373170
C	-1.9168060	-1.2807580	0.4607770
C	-1.5871730	-2.6979950	0.9141390
O	-0.7063670	1.7982340	-0.4327740
O	0.2726370	-0.7662830	-0.2980740
O	-2.9857130	-0.8272260	1.2681940
O	-1.3396840	-2.7354150	2.2994930
H	-1.7587230	1.4785050	1.2537230
H	-0.3311220	-0.4909900	1.6695190
H	-2.1896420	-1.2886180	-0.6020940
H	-3.6432290	-0.3692220	0.7317860
H	1.8999210	2.8310600	-0.1417670
H	-2.1141070	-2.3629800	2.7363790
H	-2.4250610	-3.3545260	0.6432040
H	-0.6829310	-3.0556210	0.4147330
C	1.5846050	-0.6760800	0.1494240
C	2.4884110	-1.1084280	-0.9954990

C	3.9326720	-0.9198220	-0.5738990
C	4.1661590	0.5227580	-0.1574120
C	3.1710510	0.9203540	0.9318320
C	3.1989770	2.4132640	1.2271480
O	2.3118620	-2.4695940	-1.3159980
O	4.8291840	-1.2129260	-1.6211630
O	5.4594800	0.6901040	0.3724830
O	1.8424380	0.6528270	0.5080670
O	2.7691730	3.1618610	0.1174510
H	1.7311990	-1.3350150	1.0280580
H	2.2694410	-0.4624820	-1.8576980
H	1.4173110	-2.5887530	-1.6493940
H	4.1351810	-1.5724200	0.2918520
H	4.6371540	-2.1021320	-1.9374120
H	4.0099120	1.1746210	-1.0294100
H	3.4065730	0.3540480	1.8475550
H	2.5691350	2.6089790	2.1061430
H	4.2238180	2.7155910	1.4534100
H	6.0847740	0.3466320	-0.2745990
C	-5.1399030	1.7161570	0.2339730
C	-4.0358860	1.9385770	-0.5857680
C	-3.7169970	1.0254570	-1.5886350
C	-4.5054450	-0.1081690	-1.7730990
C	-5.6061710	-0.3347040	-0.9492380
C	-5.9235700	0.5780960	0.0544410
H	-5.3863500	2.4253460	1.0162360

H	-3.4125520	2.8148180	-0.4431690
H	-2.8470560	1.1971720	-2.2133740
H	-4.2594580	-0.8180150	-2.5557060
H	-6.2145550	-1.2214780	-1.0874140
H	-6.7779650	0.4005650	0.6978100

TS5$_{Bz}$ – *E* = -1300.705697 Hartree

Symbol	X	Y	Z
O	2.6490090	2.3034360	-1.1003150
O	1.9145960	-1.1204260	-0.3901070
C	2.1251880	1.3007830	-0.5175720
C	2.0091220	-0.0302310	-1.2720450
H	1.9113330	3.3249250	-0.7255750
H	2.7791810	-1.3064340	-0.0029530
H	2.3020150	1.1381130	0.5589630
H	2.9014490	-0.1006820	-1.9057290
H	1.1334640	-0.0654440	-1.9246340
C	0.3988430	2.8703370	0.3370280
C	0.1295640	1.7304380	-0.3937090
O	1.0886400	3.8350350	-0.1661160
O	-0.4345440	0.6417490	0.2212640
H	0.1788200	2.8869440	1.4089390
H	0.0361020	1.7903930	-1.4752840
H	-3.9497290	1.6862330	1.9509830
C	-1.6153960	0.1601890	-0.3358730
C	-1.7447790	-1.3020280	0.0676300

C	-3.0895780	-1.8180480	-0.4094510
C	-4.2135290	-0.9389940	0.1082440
C	-3.9585600	0.5122780	-0.2974850
C	-4.9587480	1.4752370	0.3210400
O	-0.7569360	-2.0930450	-0.5363960
O	-3.3310520	-3.1351320	0.0290630
O	-5.4487000	-1.3224770	-0.4476760
O	-2.6766360	0.9298770	0.1586590
O	-4.8644310	1.4865190	1.7255360
H	-1.5743740	0.2391660	-1.4390970
H	-1.6976120	-1.3546850	1.1658670
H	0.1269960	-1.8111400	-0.2503160
H	-3.1003590	-1.7806940	-1.5121490
H	-2.5741460	-3.6724940	-0.2295130
H	-4.2413640	-0.9973640	1.2061640
H	-4.0145440	0.5856720	-1.3959280
H	-4.7875760	2.4771210	-0.0953910
H	-5.9695620	1.1521410	0.0638820
H	-5.5489250	-2.2697880	-0.3044540
C	5.2922260	0.0553820	-0.4176490
C	4.9779040	0.4513680	0.8797570
C	4.6972280	-0.5048690	1.8524280
C	4.7314530	-1.8596040	1.5285980
C	5.0469290	-2.2569310	0.2303960
C	5.3275370	-1.2985420	-0.7422040
H	5.4942430	0.8052760	-1.1747740

H	4.9417360	1.5074870	1.1247360
H	4.4487190	-0.1958720	2.8617010
H	4.5107440	-2.6044900	2.2849120
H	5.0712280	-3.3107550	-0.0236020
H	5.5701700	-1.6085050	-1.7528510

TS6$_{Bz}$ – *E* = -1529.713676 Hartree

Symbol	X	Y	Z
O	-3.0149130	-0.6909280	0.8976610
H	-0.0151480	-5.8445170	0.9749300
C	-2.5864440	-1.3353160	-0.2588520
C	-1.2985260	-1.9477970	-0.1233860
C	-0.2674020	-1.6756190	0.9364300
C	1.0260040	-2.2481030	0.2963170
C	0.4793740	-3.2008260	-0.7844530
C	0.5990940	-4.6764370	-0.4840510
O	-0.6884450	-0.0286930	-1.3637430
O	-0.6290330	-2.4002470	2.0865820
O	1.8935040	-1.3678830	-0.3731420
O	-0.9349430	-2.8922960	-0.9228590
O	0.0488100	-4.9029570	0.7995210
H	-2.0921040	-0.5839040	-1.0508550
H	-3.3338220	-1.9707270	-0.7434370
H	-3.2477940	0.2186670	0.6728670
H	-0.2143000	-0.6230390	1.1829240
H	-0.5668860	-3.3479640	1.9018100

H	1.5723510	-2.7918270	1.0792190
H	0.9421810	-2.9605650	-1.7435680
H	0.0593710	-5.2451050	-1.2497280
H	1.6613290	-4.9505240	-0.5157340
H	-0.2004800	0.0661720	-2.1872250
H	-0.3031240	1.5182050	-0.6777900
C	2.4534900	-0.3136960	0.3569910
C	3.5214020	0.2891830	-0.5476960
C	3.9813220	1.6169120	0.0162500
C	2.7884040	2.5510310	0.1144750
C	1.7113830	1.9304220	0.9981590
C	0.3569010	2.6200670	0.8358410
O	4.6482020	-0.5539120	-0.6521790
O	4.9405690	2.2281220	-0.8168720
O	3.1538410	3.7766790	0.7043780
O	1.4365560	0.5896900	0.6347700
O	-0.1435280	2.4786530	-0.4586650
H	2.9129890	-0.6956620	1.2891620
H	3.0608440	0.4595880	-1.5314900
H	4.3861060	-1.3527820	-1.1185680
H	4.3990450	1.4605980	1.0252080
H	5.6437740	1.5899880	-0.9774610
H	2.3738200	2.7054880	-0.8922700
H	2.0493980	1.9906090	2.0450500
H	-0.3271050	2.1910880	1.5872600
H	0.4771690	3.6872620	1.0494480

H	3.8862660	4.1362230	0.1930460
C	-4.4687640	2.4764670	0.9522010
C	-3.3263810	2.6091740	0.1642610
C	-3.2720650	2.0099750	-1.0929030
C	-4.3638400	1.2808250	-1.5595810
C	-5.5041270	1.1456880	-0.7716870
C	-5.5566810	1.7427020	0.4852690
H	-4.5078250	2.9378430	1.9330310
H	-2.4646510	3.1651300	0.5160630
H	-2.3662630	2.0920540	-1.6812180
H	-4.3177960	0.8078360	-2.5350500
H	-6.3500390	0.5710410	-1.1333630
H	-6.4411460	1.6310750	1.1026190

7$_{Bz}$ – *E* = -1529.783708 Hartree

Symbol	X	Y	Z
O	-3.0149130	-0.6909280	0.8976610
H	-0.0151480	-5.8445170	0.9749300
C	-2.5864440	-1.3353160	-0.2588520
C	-1.2985260	-1.9477970	-0.1233860
C	-0.2674020	-1.6756190	0.9364300
C	1.0260040	-2.2481030	0.2963170
C	0.4793740	-3.2008260	-0.7844530
C	0.5990940	-4.6764370	-0.4840510
O	-0.6884450	-0.0286930	-1.3637430
O	-0.6290330	-2.4002470	2.0865820

O	1.8935040	-1.3678830	-0.3731420
O	-0.9349430	-2.8922960	-0.9228590
O	0.0488100	-4.9029570	0.7995210
H	-2.0921040	-0.5839040	-1.0508550
H	-3.3338220	-1.9707270	-0.7434370
H	-3.2477940	0.2186670	0.6728670
H	-0.2143000	-0.6230390	1.1829240
H	-0.5668860	-3.3479640	1.9018100
H	1.5723510	-2.7918270	1.0792190
H	0.9421810	-2.9605650	-1.7435680
H	0.0593710	-5.2451050	-1.2497280
H	1.6613290	-4.9505240	-0.5157340
H	-0.2004800	0.0661720	-2.1872250
H	-0.3031240	1.5182050	-0.6777900
C	2.4534900	-0.3136960	0.3569910
C	3.5214020	0.2891830	-0.5476960
C	3.9813220	1.6169120	0.0162500
C	2.7884040	2.5510310	0.1144750
C	1.7113830	1.9304220	0.9981590
C	0.3569010	2.6200670	0.8358410
O	4.6482020	-0.5539120	-0.6521790
O	4.9405690	2.2281220	-0.8168720
O	3.1538410	3.7766790	0.7043780
O	1.4365560	0.5896900	0.6347700
O	-0.1435280	2.4786530	-0.4586650
H	2.9129890	-0.6956620	1.2891620

H	3.0608440	0.4595880	-1.5314900
H	4.3861060	-1.3527820	-1.1185680
H	4.3990450	1.4605980	1.0252080
H	5.6437740	1.5899880	-0.9774610
H	2.3738200	2.7054880	-0.8922700
H	2.0493980	1.9906090	2.0450500
H	-0.3271050	2.1910880	1.5872600
H	0.4771690	3.6872620	1.0494480
H	3.8862660	4.1362230	0.1930460
C	-4.4687640	2.4764670	0.9522010
C	-3.3263810	2.6091740	0.1642610
C	-3.2720650	2.0099750	-1.0929030
C	-4.3638400	1.2808250	-1.5595810
C	-5.5041270	1.1456880	-0.7716870
C	-5.5566810	1.7427020	0.4852690
H	-4.5078250	2.9378430	1.9330310
H	-2.4646510	3.1651300	0.5160630
H	-2.3662630	2.0920540	-1.6812180
H	-4.3177960	0.8078360	-2.5350500
H	-6.3500390	0.5710410	-1.1333630
H	-6.4411460	1.6310750	1.1026190

TS7$_{Bz}$ – *E* = -1529.723703 Hartree

Symbol	X	Y	Z
O	-3.0149130	-0.6909280	0.8976610
H	-0.0151480	-5.8445170	0.9749300

C	-2.5864440	-1.3353160	-0.2588520
C	-1.2985260	-1.9477970	-0.1233860
C	-0.2674020	-1.6756190	0.9364300
C	1.0260040	-2.2481030	0.2963170
C	0.4793740	-3.2008260	-0.7844530
C	0.5990940	-4.6764370	-0.4840510
O	-0.6884450	-0.0286930	-1.3637430
O	-0.6290330	-2.4002470	2.0865820
O	1.8935040	-1.3678830	-0.3731420
O	-0.9349430	-2.8922960	-0.9228590
O	0.0488100	-4.9029570	0.7995210
H	-2.0921040	-0.5839040	-1.0508550
H	-3.3338220	-1.9707270	-0.7434370
H	-3.2477940	0.2186670	0.6728670
H	-0.2143000	-0.6230390	1.1829240
H	-0.5668860	-3.3479640	1.9018100
H	1.5723510	-2.7918270	1.0792190
H	0.9421810	-2.9605650	-1.7435680
H	0.0593710	-5.2451050	-1.2497280
H	1.6613290	-4.9505240	-0.5157340
H	-0.2004800	0.0661720	-2.1872250
H	-0.3031240	1.5182050	-0.6777900
C	2.4534900	-0.3136960	0.3569910
C	3.5214020	0.2891830	-0.5476960
C	3.9813220	1.6169120	0.0162500
C	2.7884040	2.5510310	0.1144750

C	1.7113830	1.9304220	0.9981590
C	0.3569010	2.6200670	0.8358410
O	4.6482020	-0.5539120	-0.6521790
O	4.9405690	2.2281220	-0.8168720
O	3.1538410	3.7766790	0.7043780
O	1.4365560	0.5896900	0.6347700
O	-0.1435280	2.4786530	-0.4586650
H	2.9129890	-0.6956620	1.2891620
H	3.0608440	0.4595880	-1.5314900
H	4.3861060	-1.3527820	-1.1185680
H	4.3990450	1.4605980	1.0252080
H	5.6437740	1.5899880	-0.9774610
H	2.3738200	2.7054880	-0.8922700
H	2.0493980	1.9906090	2.0450500
H	-0.3271050	2.1910880	1.5872600
H	0.4771690	3.6872620	1.0494480
H	3.8862660	4.1362230	0.1930460
C	-4.4687640	2.4764670	0.9522010
C	-3.3263810	2.6091740	0.1642610
C	-3.2720650	2.0099750	-1.0929030
C	-4.3638400	1.2808250	-1.5595810
C	-5.5041270	1.1456880	-0.7716870
C	-5.5566810	1.7427020	0.4852690
H	-4.5078250	2.9378430	1.9330310
H	-2.4646510	3.1651300	0.5160630
H	-2.3662630	2.0920540	-1.6812180

H	-4.3177960	0.8078360	-2.5350500
H	-6.3500390	0.5710410	-1.1333630
H	-6.4411460	1.6310750	1.1026190

8$_{Bz}$ – *E* = -1529.791942 Hartree

Symbol	X	Y	Z
O	-3.0149130	-0.6909280	0.8976610
H	-0.0151480	-5.8445170	0.9749300
C	-2.5864440	-1.3353160	-0.2588520
C	-1.2985260	-1.9477970	-0.1233860
C	-0.2674020	-1.6756190	0.9364300
C	1.0260040	-2.2481030	0.2963170
C	0.4793740	-3.2008260	-0.7844530
C	0.5990940	-4.6764370	-0.4840510
O	-0.6884450	-0.0286930	-1.3637430
O	-0.6290330	-2.4002470	2.0865820
O	1.8935040	-1.3678830	-0.3731420
O	-0.9349430	-2.8922960	-0.9228590
O	0.0488100	-4.9029570	0.7995210
H	-2.0921040	-0.5839040	-1.0508550
H	-3.3338220	-1.9707270	-0.7434370
H	-3.2477940	0.2186670	0.6728670
H	-0.2143000	-0.6230390	1.1829240
H	-0.5668860	-3.3479640	1.9018100
H	1.5723510	-2.7918270	1.0792190
H	0.9421810	-2.9605650	-1.7435680

H	0.0593710	-5.2451050	-1.2497280
H	1.6613290	-4.9505240	-0.5157340
H	-0.2004800	0.0661720	-2.1872250
H	-0.3031240	1.5182050	-0.6777900
C	2.4534900	-0.3136960	0.3569910
C	3.5214020	0.2891830	-0.5476960
C	3.9813220	1.6169120	0.0162500
C	2.7884040	2.5510310	0.1144750
C	1.7113830	1.9304220	0.9981590
C	0.3569010	2.6200670	0.8358410
O	4.6482020	-0.5539120	-0.6521790
O	4.9405690	2.2281220	-0.8168720
O	3.1538410	3.7766790	0.7043780
O	1.4365560	0.5896900	0.6347700
O	-0.1435280	2.4786530	-0.4586650
H	2.9129890	-0.6956620	1.2891620
H	3.0608440	0.4595880	-1.5314900
H	4.3861060	-1.3527820	-1.1185680
H	4.3990450	1.4605980	1.0252080
H	5.6437740	1.5899880	-0.9774610
H	2.3738200	2.7054880	-0.8922700
H	2.0493980	1.9906090	2.0450500
H	-0.3271050	2.1910880	1.5872600
H	0.4771690	3.6872620	1.0494480
H	3.8862660	4.1362230	0.1930460
C	-4.4687640	2.4764670	0.9522010

C	-3.3263810	2.6091740	0.1642610
C	-3.2720650	2.0099750	-1.0929030
C	-4.3638400	1.2808250	-1.5595810
C	-5.5041270	1.1456880	-0.7716870
C	-5.5566810	1.7427020	0.4852690
H	-4.5078250	2.9378430	1.9330310
H	-2.4646510	3.1651300	0.5160630
H	-2.3662630	2.0920540	-1.6812180
H	-4.3177960	0.8078360	-2.5350500
H	-6.3500390	0.5710410	-1.1333630
H	-6.4411460	1.6310750	1.1026190

TS8$_{C3}$ – *E* = -1529.674981 Hartree

Symbol	X	Y	Z
O	-3.0149130	-0.6909280	0.8976610
H	-0.0151480	-5.8445170	0.9749300
C	-2.5864440	-1.3353160	-0.2588520
C	-1.2985260	-1.9477970	-0.1233860
C	-0.2674020	-1.6756190	0.9364300
C	1.0260040	-2.2481030	0.2963170
C	0.4793740	-3.2008260	-0.7844530
C	0.5990940	-4.6764370	-0.4840510
O	-0.6884450	-0.0286930	-1.3637430
O	-0.6290330	-2.4002470	2.0865820
O	1.8935040	-1.3678830	-0.3731420
O	-0.9349430	-2.8922960	-0.9228590

O	0.0488100	-4.9029570	0.7995210
H	-2.0921040	-0.5839040	-1.0508550
H	-3.3338220	-1.9707270	-0.7434370
H	-3.2477940	0.2186670	0.6728670
H	-0.2143000	-0.6230390	1.1829240
H	-0.5668860	-3.3479640	1.9018100
H	1.5723510	-2.7918270	1.0792190
H	0.9421810	-2.9605650	-1.7435680
H	0.0593710	-5.2451050	-1.2497280
H	1.6613290	-4.9505240	-0.5157340
H	-0.2004800	0.0661720	-2.1872250
H	-0.3031240	1.5182050	-0.6777900
C	2.4534900	-0.3136960	0.3569910
C	3.5214020	0.2891830	-0.5476960
C	3.9813220	1.6169120	0.0162500
C	2.7884040	2.5510310	0.1144750
C	1.7113830	1.9304220	0.9981590
C	0.3569010	2.6200670	0.8358410
O	4.6482020	-0.5539120	-0.6521790
O	4.9405690	2.2281220	-0.8168720
O	3.1538410	3.7766790	0.7043780
O	1.4365560	0.5896900	0.6347700
O	-0.1435280	2.4786530	-0.4586650
H	2.9129890	-0.6956620	1.2891620
H	3.0608440	0.4595880	-1.5314900
H	4.3861060	-1.3527820	-1.1185680

H	4.3990450	1.4605980	1.0252080
H	5.6437740	1.5899880	-0.9774610
H	2.3738200	2.7054880	-0.8922700
H	2.0493980	1.9906090	2.0450500
H	-0.3271050	2.1910880	1.5872600
H	0.4771690	3.6872620	1.0494480
H	3.8862660	4.1362230	0.1930460
C	-4.4687640	2.4764670	0.9522010
C	-3.3263810	2.6091740	0.1642610
C	-3.2720650	2.0099750	-1.0929030
C	-4.3638400	1.2808250	-1.5595810
C	-5.5041270	1.1456880	-0.7716870
C	-5.5566810	1.7427020	0.4852690
H	-4.5078250	2.9378430	1.9330310
H	-2.4646510	3.1651300	0.5160630
H	-2.3662630	2.0920540	-1.6812180
H	-4.3177960	0.8078360	-2.5350500
H	-6.3500390	0.5710410	-1.1333630
H	-6.4411460	1.6310750	1.1026190

9$_{Bz}$ – E = -1453.353571 Hartree

Symbol	X	Y	Z
O	2.6103690	-0.1483030	3.4573620
H	3.6181220	-0.6066310	-1.2154920
C	1.8378170	0.5242800	2.5594600
C	1.5127760	0.0390130	1.3667980

C	0.6517790	0.6320720	0.2879210
C	0.1280910	-0.6531160	-0.3942530
C	1.2227040	-1.6976160	-0.1191560
C	2.1825810	-1.9289860	-1.2745470
O	1.3262010	1.4748470	-0.6141180
O	-1.0702120	-1.1199180	0.2045070
O	1.9598420	-1.2178080	1.0069170
O	2.7932670	-0.7303520	-1.7030600
H	1.5258390	1.5048120	2.8907210
H	2.7434950	-1.0429060	3.1197440
H	-0.1785050	1.2055880	0.6958370
H	1.9808050	0.9451840	-1.0946480
H	-0.0266620	-0.4788410	-1.4660160
H	0.7491070	-2.6474080	0.1540450
H	2.9394850	-2.6602190	-0.9674190
H	1.6294710	-2.3456930	-2.1232800
H	-2.7391840	2.5213760	1.3258440
C	-2.2403050	-0.6688390	-0.3815330
C	-3.3971660	-1.4412930	0.2378150
C	-4.6947220	-0.9347180	-0.3634480
C	-4.8097190	0.5694940	-0.1798680
C	-3.5639270	1.2607460	-0.7329110
C	-3.5351040	2.7475800	-0.4192800
O	-3.3137220	-2.8198440	-0.0385060
O	-5.8226490	-1.5255630	0.2402820
O	-5.9209730	1.0768040	-0.8785890

O	-2.3963020	0.7067540	-0.1383560
O	-3.5037850	2.9846290	0.9684990
H	-2.2086020	-0.8436040	-1.4745340
H	-3.3915900	-1.2491030	1.3205780
H	-2.5071010	-3.1585770	0.3623690
H	-4.6854770	-1.1540160	-1.4443400
H	-5.7289940	-2.4819850	0.1771890
H	-4.8850500	0.7922210	0.8944340
H	-3.5363870	1.1199880	-1.8257460
H	-2.6648050	3.1947940	-0.9178700
H	-4.4445970	3.2107500	-0.8072150
H	-6.6949450	0.5779560	-0.5961800
C	4.9564460	1.7196720	-1.1656500
C	4.5043110	1.5001510	0.1332920
C	4.8692640	0.3393240	0.8110870
C	5.6852740	-0.6027230	0.1871270
C	6.1381160	-0.3825690	-1.1131090
C	5.7737240	0.7797740	-1.7887710
H	4.6616430	2.6188950	-1.6952110
H	3.8478470	2.2193600	0.6093940
H	4.5094490	0.1715150	1.8204920
H	5.9691510	-1.5074740	0.7139510
H	6.7709510	-1.1169070	-1.5991410
H	6.1185960	0.9474710	-2.8028570

TS9$_{Bz}$ – *E* = -1453.28941 Hartree

Symbol	X	Y	Z
O	2.1871460	2.3968180	1.6982810
H	3.5497560	-0.8338630	-1.2873550
C	2.3192900	1.2165190	2.1540000
C	1.5311640	0.2003460	1.6488590
C	0.5335860	0.5261050	0.7059470
C	0.0940150	-0.7856850	0.0819060
C	1.1886310	-1.7627350	0.5648550
C	2.2023470	-2.0493910	-0.5324110
O	1.3221840	1.5519930	-0.5192660
O	-1.1649030	-1.1887900	0.5905330
O	1.8170410	-1.1674710	1.6906600
O	2.5922580	-0.8460170	-1.1753310
H	3.0958680	1.0072870	2.9026340
H	1.7428700	2.1034940	0.2672390
H	-0.2206630	1.2791890	0.8973440
H	2.0068240	0.9481990	-0.8655740
H	0.0524520	-0.7207740	-1.0126140
H	0.7325490	-2.7053120	0.8834030
H	3.0700690	-2.5435230	-0.0828450
H	1.7505810	-2.7272790	-1.2700140
H	-2.8315630	2.6439110	1.0796320
C	-2.2561520	-0.7948720	-0.1674800
C	-3.4939890	-1.4608480	0.4168100
C	-4.7048780	-1.0063040	-0.3768130
C	-4.7869270	0.5113460	-0.3928970

C	-3.4684760	1.1029240	-0.8902030
C	-3.4250920	2.6166770	-0.7617300
O	-3.4288460	-2.8643040	0.3205790
O	-5.9080060	-1.4926910	0.1716300
O	-5.8013750	0.9492370	-1.2643930
O	-2.3869900	0.6027870	-0.1121480
O	-3.5549860	3.0317310	0.5768280
H	-2.1172350	-1.1071440	-1.2209900
H	-3.5931440	-1.1345500	1.4621190
H	-2.6920210	-3.1711040	0.8582100
H	-4.5918620	-1.3599430	-1.4154330
H	-5.8403620	-2.4510680	0.2385730
H	-4.9657400	0.8693620	0.6312750
H	-3.3327340	0.8256450	-1.9484540
H	-2.4867130	2.9798360	-1.2020070
H	-4.2647850	3.0424170	-1.3148360
H	-6.6185080	0.5108190	-1.0042010
C	5.1805240	-0.0602690	0.7140520
C	4.9066740	1.1664640	0.1131710
C	5.1465670	1.3400610	-1.2479720
C	5.6613580	0.2915610	-2.0079280
C	5.9428750	-0.9330310	-1.4039320
C	5.7032230	-1.1071860	-0.0410290
H	4.9798150	-0.2061190	1.7695190
H	4.4923660	1.9801290	0.6997580
H	4.9296400	2.2933690	-1.7174360

H	5.8439750	0.4273530	-3.0680740
H	6.3491750	-1.7479140	-1.9930780
H	5.9227840	-2.0588580	0.4309850

10$_{Bz}$ – E = -1376.933682 Hartree

Symbol	X	Y	Z
O	-3.2593800	3.1820070	0.6946080
H	-5.1091310	-1.2348180	1.2221850
C	-3.8289480	2.2895240	0.1252120
C	-3.2870120	0.9128760	0.0448620
C	-2.1624020	0.4234390	0.5638970
C	-2.0542010	-1.0228430	0.1673070
C	-3.3283360	-1.2257110	-0.6816000
C	-4.2535700	-2.3018540	-0.1480180
O	-0.9222640	-1.3055570	-0.6463730
O	-4.0430080	0.0248950	-0.6625880
O	-4.6066040	-2.0551680	1.1917240
H	-4.7987660	2.4433300	-0.3844710
H	-1.4433280	0.9620260	1.1607060
H	-2.0414630	-1.6912850	1.0393590
H	-3.0408920	-1.4366270	-1.7171320
H	-5.1402380	-2.3758930	-0.7906160
H	-3.7321400	-3.2638510	-0.1703670
H	1.6349810	1.7109720	1.0679550
C	0.2251650	-1.6504040	0.0532040
C	1.2978300	-1.9894560	-0.9719750

C	2.5941450	-2.2955240	-0.2469570
C	2.9683140	-1.1468260	0.6747650
C	1.8029030	-0.8267800	1.6093310
C	2.0612250	0.4094410	2.4544770
O	0.9583870	-3.1263060	-1.7317510
O	3.6634680	-2.4877780	-1.1457120
O	4.0740840	-1.4879940	1.4753000
O	0.6308160	-0.5655850	0.8457840
O	2.3642350	1.5386170	1.6782610
H	0.0253990	-2.5256210	0.7025940
H	1.4372910	-1.1065130	-1.6125740
H	0.1557340	-2.9324360	-2.2255840
H	2.4463440	-3.2007530	0.3653050
H	3.4173840	-3.1892880	-1.7578170
H	3.1786890	-0.2534790	0.0678660
H	1.6329830	-1.6888970	2.2760900
H	1.1818620	0.5808600	3.0920810
H	2.9256170	0.2190970	3.0947130
H	4.7836310	-1.7675990	0.8873220
C	0.9695980	3.9597140	-0.2187620
C	2.2904310	3.9219460	-0.6550990
C	2.7337780	2.8598650	-1.4368870
C	1.8581660	1.8332000	-1.7774630
C	0.5388600	1.8627200	-1.3318730
C	0.0923500	2.9307340	-0.5551370
H	0.6217090	4.7850190	0.3924390

H	2.9760670	4.7147260	-0.3783300
H	3.7642140	2.8263850	-1.7726750
H	2.2108730	1.0076730	-2.3876720
H	-0.1394940	1.0503470	-1.5743330
H	-0.9349680	2.9652090	-0.2067610

TS10$_{Bz}$ – *E* = -1376.851139 Hartree

Symbol	X	Y	Z
O	-5.5921600	0.3204000	1.8747820
H	-0.7127600	-1.9200390	-1.7501620
C	-5.2873290	0.4591270	0.7248930
C	-3.8602490	0.3713490	0.2902710
C	-2.7235290	0.1837350	1.0631920
C	-1.6734980	0.2071650	0.1647030
C	-2.1995360	0.4541030	-1.1703560
C	-1.7874350	-0.4404570	-2.3363850
O	-0.8701580	2.5553970	-0.2956000
O	-3.6254780	0.4881020	-0.9835830
O	-1.6504890	-1.7848510	-1.9605580
H	-6.0181620	0.6513370	-0.0793650
H	-2.7111950	0.0678230	2.1346720
H	-0.6213280	0.0429820	0.3407230
H	-1.8230410	1.5419710	-1.2839890
H	-2.5660190	-0.3621920	-3.1010710
H	-0.8544190	-0.0347310	-2.7318570
H	1.6869200	-1.8512750	-0.8962090

C	0.4192090	2.3959980	-0.5457430
C	1.2228510	2.3226660	0.7665680
C	2.6793440	2.0075140	0.5159340
C	2.7716050	0.6965490	-0.2411220
C	1.9650950	0.8016630	-1.5357620
C	1.9508160	-0.5058630	-2.3160470
O	1.1333680	3.5408570	1.4628490
O	3.4141160	1.8532550	1.7172920
O	4.1044390	0.3656010	-0.5579700
O	0.6321790	1.1338690	-1.2525560
O	1.2050830	-1.5213820	-1.6640110
H	0.8670550	3.1895380	-1.1887710
H	0.7837980	1.5053580	1.3671720
H	0.2122370	3.8220030	1.3780070
H	3.1253400	2.8080270	-0.0960340
H	3.2529680	2.6339370	2.2582470
H	2.3216950	-0.0857600	0.3922660
H	2.4423660	1.5697970	-2.1700620
H	1.4576690	-0.3416350	-3.2780850
H	2.9801430	-0.8304610	-2.5024970
H	4.6386540	0.5593600	0.2206220
C	0.2482960	-3.7705520	0.4087830
C	1.6344640	-3.8826840	0.4949190
C	2.3550540	-3.0190350	1.3176940
C	1.6873020	-2.0515410	2.0668400
C	0.3017040	-1.9484710	1.9874580

C	-0.4178820	-2.8026190	1.1543330
H	-0.3117570	-4.4297610	-0.2451780
H	2.1540200	-4.6351950	-0.0879910
H	3.4350180	-3.0987950	1.3762230
H	2.2469740	-1.3738170	2.7028600
H	-0.2144100	-1.1966010	2.5769890
H	-1.4966420	-2.7137330	1.0772790

In the Presence of Dimethyl Ether (DME)

The Cartesian coordinates for all the stable structures in the presence of DME reported in this work are listed below including computed absolute energies.

1$_{DME}$ – E = -1452.602723 Hartree

Symbol	X	Y	Z
C	4.3343520	-0.0962920	0.1118240
C	3.4393430	1.0597430	-0.3219350
C	2.0473670	0.8948980	0.2646940
C	1.5313640	-0.5141600	-0.0026210
C	2.5432910	-1.5879170	0.3952450
C	2.0903460	-2.9753890	-0.0276640
O	5.5467150	0.0611840	-0.5432140
O	3.9731790	2.2800330	0.1248720
O	1.2115960	1.8690820	-0.3005610
O	0.3517400	-0.7237570	0.7587040
O	3.7797810	-1.3385780	-0.2523480
O	1.8975170	-3.0527500	-1.4234400
H	4.4668180	-0.0697930	1.2088010

H	3.3647770	1.0304860	-1.4197370
H	2.1196860	1.0297180	1.3586980
H	1.3150200	-0.6094080	-1.0744970
H	2.6712230	-1.5678890	1.4902060
H	6.1667180	-0.6026320	-0.2272260
H	4.8549770	2.3682030	-0.2513360
H	0.2842600	1.6058500	-0.1962050
H	-2.7592780	2.6106640	-0.2782470
H	2.7246730	-2.7975190	-1.8460860
H	2.8361430	-3.7072740	0.3091730
H	1.1329240	-3.2061160	0.4474980
C	-0.7837290	-1.0137990	0.0304900
C	-1.8010270	-1.6789860	0.9465830
C	-3.1333490	-1.8080310	0.2234520
C	-3.5656900	-0.4560750	-0.3096870
C	-2.4703690	0.0813030	-1.2317830
C	-2.8238380	1.4384520	-1.8245500
O	-1.2971380	-2.9373680	1.3166840
O	-4.0541420	-2.3416000	1.1479020
O	-4.7967390	-0.6291160	-0.9779740
O	-1.2838590	0.2141250	-0.4636280
O	-3.4389060	2.2973690	-0.8988660
H	-0.5495040	-1.6849160	-0.8161400
H	-1.9368560	-1.0335980	1.8282280
H	-2.0150020	-3.4218230	1.7394010
H	-3.0076150	-2.4999500	-0.6262060

H	-4.9230610	-2.3300900	0.7316370
H	-3.6780980	0.2399580	0.5315090
H	-2.3001620	-0.6315850	-2.0559870
H	-1.9093900	1.8776640	-2.2463020
H	-3.5328390	1.2854880	-2.6440280
O	-1.2628770	3.0679510	0.6651520
C	-0.9743620	2.4932730	1.9194590
C	-0.6114050	4.3076530	0.4753230
H	0.1096480	2.3712280	2.0455730
H	-1.4506420	1.5113200	1.9470130
H	-1.3633090	3.1199220	2.7330630
H	0.4756290	4.1701930	0.5039740
H	-0.9204520	5.0271550	1.2452190
H	-0.9046780	4.6816190	-0.5069740
H	-5.2203040	0.2324890	-1.0502720

TS1$_{DME}$ – E = -1452.516841 Hartree

Symbol	X	Y	Z
C	4.1963700	-0.7278490	-0.1579520
C	3.4308940	0.3104070	-0.9737740
C	2.2420860	0.8271590	-0.1790980
C	1.4258480	-0.3563730	0.3468510
C	2.3194560	-1.3171720	1.1264420
C	1.5791600	-2.5473580	1.6145400
O	5.1779860	-1.2580370	-0.9841160
O	4.2798450	1.3841930	-1.2889570

O	1.4495280	1.6360300	-1.0045990
O	0.3810260	0.0496640	1.1821550
O	3.3640010	-1.7770570	0.2815660
O	0.9710300	-3.2501200	0.5465170
H	4.6433300	-0.2347900	0.7244290
H	3.0574610	-0.1856010	-1.8835180
H	2.6208030	1.4062190	0.6797580
H	1.0428680	-0.8946390	-0.5393240
H	2.7381820	-0.7895260	2.0001750
H	5.7484420	-1.8343100	-0.4672510
H	5.0213750	1.0325570	-1.7918700
H	0.9918250	2.2757080	-0.4319840
H	-0.2678900	0.6276210	0.6650140
H	1.6505340	-3.4055480	-0.1193910
H	2.2774500	-3.1970360	2.1570790
H	0.7814450	-2.2400420	2.2948000
C	-1.6305460	-1.3870020	0.0684450
C	-2.8440370	-1.1463400	0.9292660
C	-3.9275110	-0.2316630	0.3158190
C	-3.8373430	-0.3523930	-1.2142640
C	-2.4216840	-0.1366940	-1.7394480
C	-1.7381990	1.2054600	-1.3605420
O	-3.2921680	-2.4708700	1.1595420
O	-3.8689020	1.0743870	0.7636170
O	-4.2630620	-1.6810650	-1.4998880
O	-1.5459540	-1.1473560	-1.1620760

O	-1.5157040	1.2568850	-0.0164080
H	-0.8401660	-2.0407700	0.4409510
H	-2.5105060	-0.7288780	1.8820040
H	-3.7859700	-2.7514770	0.3768590
H	-4.8913470	-0.6595770	0.6124030
H	-2.9115040	1.3566760	0.5817720
H	-4.4966240	0.3960380	-1.6686090
H	-2.3678510	-0.3261190	-2.8147810
H	-0.8071800	1.2719180	-1.9449520
H	-2.4228500	1.9966950	-1.7224450
O	0.4085530	3.5135970	0.7987870
C	-0.5495190	4.3129510	0.1451580
C	-0.0190070	3.1286320	2.0863250
H	-1.5059150	3.7796030	0.0718400
H	-0.1697620	4.5283110	-0.8561770
H	-0.6966530	5.2586610	0.6850040
H	-0.9683010	2.5816010	2.0280730
H	-0.1429700	4.0134410	2.7262050
H	0.7448310	2.4730430	2.5059920
H	-4.2583090	-1.8423750	-2.4477550

2$_{DME}$ – E = -1376.179048 Hartree

Symbol	X	Y	Z
C	-3.4345760	0.5523010	0.1632790
C	-2.4174060	0.5305380	1.3052630
C	-1.7601880	-0.8660290	1.3694930

C	-1.5265750	-1.5157280	-0.0247370
C	-2.6486330	-1.1576680	-0.9979770
C	-4.0390300	-1.5608700	-0.5106620
O	-1.5105270	1.5827810	1.1785820
O	-2.5432780	-1.7592970	2.1405780
O	-2.7839710	0.2586450	-1.0467210
O	-4.3904240	-0.4872800	0.3612710
H	-3.9339730	1.5195300	0.0707960
H	-2.9461810	0.6822710	2.2528660
H	-0.9281230	1.4438390	0.4133100
H	-0.8040730	-0.7510540	1.8868230
H	-3.4699220	-1.5139110	2.0408050
H	-1.5003160	-2.6018580	0.1426140
H	-2.4085310	-1.5141980	-2.0006990
H	-4.7479520	-1.6048630	-1.3423680
H	-4.0532190	-2.5038840	0.0410210
O	-0.3420380	-1.1170080	-0.7024570
C	0.8406620	-1.0967420	0.0206660
C	1.9844430	-1.5030700	-0.8996300
O	1.0248900	0.2162370	0.4727500
H	0.7976000	-1.8016590	0.8721260
C	3.2919920	-1.3540950	-0.1454920
O	1.8718970	-2.8501950	-1.2984110
H	1.9856880	-0.8328610	-1.7709390
C	2.2103790	0.4357830	1.2247210
C	3.4335250	0.0622250	0.3888370

O	4.4069100	-1.6139190	-0.9684950
H	3.2823640	-2.0503230	0.7098830
H	1.0778090	-2.9412370	-1.8338690
C	2.1967570	1.9078380	1.6134330
H	2.2015930	-0.1837480	2.1374790
O	4.5653470	0.1716860	1.2177390
H	3.4972600	0.7599280	-0.4594100
H	4.3028540	-2.4946380	-1.3436340
O	2.2008420	2.7477760	0.4883590
H	1.3169380	2.0873750	2.2457410
H	3.0993890	2.1230890	2.1905750
H	1.3415560	2.6892190	0.0451520
H	5.3250680	-0.1415200	0.7156040
O	-0.1992640	2.4919230	-1.1267850
C	0.1869450	1.7617100	-2.2694810
C	-1.3088690	3.3295070	-1.3711610
H	-0.5976010	1.0478640	-2.5510650
H	1.0975010	1.2203890	-2.0089920
H	0.3921670	2.4398690	-3.1084040
H	-2.1637840	2.7354730	-1.7208460
H	-1.0594280	4.0866390	-2.1261200
H	-1.5643290	3.8152830	-0.4290520

TS2$_{DME}$ – *E* = -1376.085624 Hartree

Symbol	X	Y	Z
C	4.7793720	0.4818540	0.6053300

C	3.6977930	1.5714240	0.6267190
C	2.5958130	1.2123260	-0.3884690
C	2.2389820	-0.2914150	-0.2770320
C	3.4896680	-1.1571110	-0.1079750
C	4.5404340	-0.9270640	-1.1948510
O	3.1935890	1.6959140	1.9295960
O	2.9429370	1.5719250	-1.7113960
O	4.2107210	-0.7232150	1.0395600
O	5.2157600	0.2464390	-0.7343150
H	5.6308760	0.7228840	1.2444320
H	4.1320190	2.5373170	0.3486460
H	2.7433530	0.8663490	2.1432040
H	1.6983830	1.7824990	-0.1240890
H	3.8963870	1.4725750	-1.8105130
H	1.7305810	-0.5798640	-1.2150080
H	3.2205740	-2.2050880	0.0371270
H	5.2490870	-1.7589030	-1.2423930
H	4.1140250	-0.7416130	-2.1838240
O	1.4245890	-0.5104810	0.8477020
H	0.6135490	0.0999160	0.7429930
O	-0.6870960	0.7904860	0.4158740
C	-1.0947370	0.9347360	-0.8777710
C	-1.7620800	-0.3675180	-1.3903400
H	-0.2647560	1.1656580	-1.5686070
H	-1.8586170	1.7223670	-1.0107670
C	-3.0747420	-0.7591630	-0.7228370

O	-0.7652990	-1.4067690	-1.1276840
H	-1.8584650	-0.3715200	-2.4785940
C	-2.9421710	-0.9192810	0.8009500
O	-3.4820360	-2.0449010	-1.1895050
H	-3.8121800	0.0213090	-0.9374120
C	-0.6639720	-1.8588620	0.0379740
C	-1.7515420	-1.8621220	1.0822040
O	-2.8602720	0.2824910	1.4784980
H	-3.8378500	-1.4518850	1.1415470
H	0.1905910	-2.5116750	0.1973440
O	-2.1058920	-3.2351100	1.0844200
H	-1.3097310	-1.6191150	2.0510010
H	-1.9549540	0.6675080	1.2106810
H	-2.7153750	-3.3781290	0.3465340
H	-3.7399380	-2.0009520	-2.1143280
O	-4.8821360	1.9859060	-0.5760230
C	-4.2026150	3.0556180	0.0393170
C	-5.7589610	1.3501460	0.3238920
H	-4.9146650	3.8031050	0.4176020
H	-3.5699460	3.5250820	-0.7165950
H	-3.5829390	2.6961010	0.8714150
H	-6.5484480	2.0405770	0.6536180
H	-5.2133700	0.9798580	1.2019970
H	-6.2245840	0.5127450	-0.2024920

TS3$_{DME}$ – *E* = -1452.518684 Hartree

Symbol	X	Y	Z
O	-3.3757650	1.2922590	-0.8942840
H	-4.4174970	-0.5576640	1.1035560
C	-2.1426910	1.0234170	-1.2253040
C	-1.0084420	1.6505520	-0.4344960
C	-0.7445020	0.9931780	0.9402680
C	-0.5495050	-0.5324950	0.8545840
C	-1.7554770	-1.3093490	0.3081190
C	-2.8432290	-1.6814140	1.3232840
O	0.1559050	1.7570660	-1.2241550
O	-1.7060830	1.3288360	1.8945220
O	0.5297060	-0.8802670	-0.0220380
O	-2.3660730	-0.6389930	-0.7837360
O	-3.6475120	-0.5929520	1.6998490
H	-1.8933990	0.8699820	-2.2839570
H	-1.3482190	2.6700750	-0.2239200
H	0.6360320	0.9218600	-1.1753480
H	0.1978160	1.4232380	1.2862770
H	-2.5452290	0.8654160	1.7320550
H	-0.3238760	-0.9036660	1.8641330
H	-1.3398560	-2.2543320	-0.0664900
H	-3.4622010	-2.4696280	0.8770950
H	-2.3681580	-2.0934460	2.2201090
H	-3.3142840	0.0517810	-0.6019240
H	2.2142610	2.6152230	-0.8371590
C	1.8263800	-0.7659190	0.4703930

C	2.7230090	-1.5913530	-0.4454600
C	4.1767100	-1.3417110	-0.0920510
C	4.4838230	0.1442390	-0.1841970
C	3.5284620	0.9230570	0.7149500
C	3.6102450	2.4309040	0.5037390
O	2.4776110	-2.9709090	-0.3064500
O	5.0482400	-2.0136900	-0.9711160
O	5.7916140	0.4149300	0.2572140
O	2.1825160	0.5868520	0.4139370
O	3.1619100	2.7992410	-0.7748580
H	1.8810850	-1.1410230	1.5088980
H	2.5437040	-1.2576480	-1.4786990
H	1.5926660	-3.1581290	-0.6342160
H	4.3526700	-1.6729580	0.9452590
H	4.8149650	-2.9481250	-0.9691670
H	4.3391470	0.4767120	-1.2229570
H	3.7600480	0.6816980	1.7648400
H	3.0255210	2.9268150	1.2905580
H	4.6531140	2.7440150	0.5934800
H	6.3915480	-0.1462520	-0.2456200
O	-5.6725830	-0.5161630	-0.1531800
C	-6.3074270	0.7485670	-0.0837860
C	-5.6277990	-1.0136490	-1.4733830
H	-5.7734520	1.4764040	-0.7039320
H	-6.2801040	1.0706620	0.9587240
H	-7.3518500	0.6640380	-0.4097700

H	-5.1051800	-0.3087550	-2.1325850
H	-6.6444380	-1.1819730	-1.8514980
H	-5.0880620	-1.9621250	-1.4533460

4$_{DME}$ – E = -1452.577749 Hartree

Symbol	X	Y	Z
O	-3.4110270	1.8820850	-0.2790920
H	-4.0485170	0.0929000	0.7355950
C	-2.3630220	1.6857850	-0.8391350
C	-0.9938470	1.8631880	-0.2019030
C	-0.7202020	1.0737160	1.1063090
C	-0.5887850	-0.4682050	1.0154250
C	-1.7912450	-1.3059540	0.5726820
C	-2.9929570	-1.3518480	1.5167660
O	0.0078910	1.6905730	-1.1768140
O	-1.5860940	1.4469950	2.1351870
O	0.4472640	-0.8584560	0.1072520
O	-2.1497180	-0.8982760	-0.7298670
O	-3.7315510	-0.1598150	1.6159330
H	-2.3130330	1.4265830	-1.9164020
H	-0.9640930	2.9166370	0.1054790
H	0.2366670	0.7527990	-1.2118010
H	0.2723430	1.4162210	1.4092440
H	-2.4871250	1.1359380	1.9438160
H	-0.3172180	-0.7976750	2.0299880
H	-1.4069400	-2.3397830	0.5431250

H	-3.6421230	-2.1726900	1.1734140
H	-2.6500520	-1.6028340	2.5252480
H	-3.0650530	-1.1585610	-0.9092970
H	2.1415830	2.4060630	-0.9892640
C	1.7676880	-0.7562380	0.5322400
C	2.5925780	-1.6448290	-0.3918600
C	4.0680660	-1.4273290	-0.1217670
C	4.4091750	0.0414730	-0.3086610
C	3.5264850	0.8962780	0.5963300
C	3.6175160	2.3839910	0.2727580
O	2.3099070	-3.0089010	-0.1851010
O	4.8754520	-2.1707740	-1.0053900
O	5.7465450	0.2972720	0.0466110
O	2.1565990	0.5812700	0.4059610
O	3.0744700	2.6667850	-0.9906530
H	1.8637980	-1.0943250	1.5810080
H	2.3697850	-1.3463300	-1.4272810
H	1.3970630	-3.1697430	-0.4442890
H	4.2864620	-1.7104750	0.9217600
H	4.6026450	-3.0931100	-0.9552930
H	4.2173310	0.3221270	-1.3549560
H	3.8245790	0.7200140	1.6423580
H	3.1009740	2.9452400	1.0640770
H	4.6679810	2.6839060	0.2596720
H	6.3018410	-0.3095570	-0.4544200
O	-4.9819020	-0.7878660	-0.9288800

C	-5.2289130	0.0659260	-2.0295490
C	-6.1688020	-1.1523410	-0.2567970
H	-5.8935850	-0.4256380	-2.7512370
H	-4.2689360	0.2752990	-2.5047500
H	-5.6724680	1.0099250	-1.6941560
H	-6.8343030	-1.7140070	-0.9243900
H	-6.6928000	-0.2607410	0.1104540
H	-5.8918910	-1.7769970	0.5941000

TS4$_{DME}$ – *E* = -1452.522573 Hartree

Symbol	X	Y	Z
C	-2.9676930	2.4119870	-0.7306870
C	-2.0386620	1.4366010	-1.0325430
C	-1.5194500	1.1948210	0.9573120
C	-0.7697160	-0.1426910	0.8961820
C	-1.6806580	-1.3776850	0.9386080
C	-0.8783370	-2.6701600	0.8671460
O	-3.9948940	2.1748870	0.0183470
O	-0.9576560	1.8291570	-1.7725420
O	-2.5802910	1.2237310	1.6722740
O	0.0827110	-0.1892790	-0.2411740
O	-2.3648460	-1.4349290	2.1742020
O	0.0189230	-2.7702180	1.9517850
H	-2.7658920	3.4490650	-1.0153900
H	-2.3705260	0.4019720	-1.0949180
H	-0.8427790	2.0624900	0.9558220

H	-0.1544750	-0.1506050	1.8076760
H	-2.3845420	-1.3469260	0.0929340
H	-2.7563160	-0.5627590	2.3282150
H	-0.2419840	1.2141610	-1.5700860
H	-3.5755630	1.6633040	0.8809470
H	2.6511680	2.9458050	0.4837520
H	-0.5015370	-2.6436870	2.7539700
H	-1.5873380	-3.5078980	0.8641830
H	-0.2842550	-2.7184540	-0.0487410
C	1.4221910	-0.4622210	0.0345790
C	2.1156650	-0.7846210	-1.2814560
C	3.5921200	-1.0023870	-1.0012130
C	4.1775680	0.2094230	-0.2936290
C	3.3584680	0.5370740	0.9543920
C	3.7825260	1.8463470	1.5989380
O	1.6177740	-1.9643350	-1.8678780
O	4.3287720	-1.1991530	-2.1851990
O	5.4975450	-0.0415990	0.1217970
O	1.9859700	0.6913790	0.6051630
O	3.5803920	2.9398230	0.7358400
H	1.5010200	-1.3095000	0.7362370
H	2.0015160	0.0772060	-1.9580290
H	0.7120250	-1.8129570	-2.1548980
H	3.6926720	-1.8778740	-0.3386970
H	3.9496250	-1.9499720	-2.6541830
H	4.1363980	1.0720360	-0.9750190

H	3.4743830	-0.2827560	1.6809520
H	3.2271330	1.9734010	2.5379580
H	4.8501900	1.8017660	1.8232400
H	5.9951010	-0.3373160	-0.6481130
O	-4.3585180	-0.7659650	-1.0211830
C	-5.1736540	-0.9582570	0.1111010
C	-5.0475530	-0.1122420	-2.0587630
H	-5.5320980	0.0049400	0.5001420
H	-4.5737020	-1.4603080	0.8736640
H	-6.0418610	-1.5857930	-0.1352280
H	-5.4178690	0.8662020	-1.7246530
H	-5.8962840	-0.7176100	-2.4071240
H	-4.3481440	0.0281330	-2.8858530

5$_{DME}$ – E = -1223.571794 Hartree

Symbol	X	Y	Z
C	2.4142710	2.0643690	-0.2467660
C	2.3546500	0.5496650	-0.1712500
C	3.6505990	-0.0783610	0.3514210
C	3.5432170	-1.5956170	0.3941090
O	3.4351020	2.6999620	-0.2872380
O	1.2630010	0.2154440	0.6633600
O	4.7152320	0.2140460	-0.5256040
O	3.2811700	-2.1206390	-0.8880230
H	1.4221110	2.5569710	-0.2601850
H	2.1826760	0.1880480	-1.1956700

H	3.8485960	0.3000750	1.3656920
H	4.8098540	1.1735180	-0.5738720
H	-2.0333790	1.8098620	-1.1753390
H	3.9817760	-1.8084700	-1.4720270
H	4.4796030	-1.9959000	0.8033170
H	2.7189050	-1.9052670	1.0422560
C	0.3038940	-0.5989680	0.0639020
C	-0.6504030	-1.0748980	1.1474640
C	-1.7335670	-1.9093520	0.4912130
C	-2.4244540	-1.0980930	-0.5917220
C	-1.3979720	-0.5470290	-1.5830720
C	-2.0142250	0.4412100	-2.5590290
O	0.0019810	-1.8888240	2.0967380
O	-2.7206000	-2.3114620	1.4146780
O	-3.3269860	-1.8954070	-1.3201480
O	-0.3791060	0.1676530	-0.8908570
O	-2.6126740	1.5277290	-1.8986000
H	0.7945850	-1.4611140	-0.4251010
H	-1.1080050	-0.1922940	1.6162870
H	0.6336660	-1.3462130	2.5784910
H	-1.2649400	-2.7934260	0.0279550
H	-2.2842080	-2.7901380	2.1272420
H	-2.9383380	-0.2509090	-0.1153130
H	-0.9569240	-1.3886440	-2.1413670
H	-1.2268500	0.7789090	-3.2478280
H	-2.7911410	-0.0667820	-3.1354110

H	-3.9138460	-2.3220390	-0.6868160
O	-2.1113540	2.1158940	0.8265350
C	-1.2686740	2.5079360	1.8789880
C	-3.4668870	2.4130290	1.0731410
H	-1.2749990	3.5994280	2.0071320
H	-0.2587850	2.1716230	1.6328860
H	-1.5812320	2.0438100	2.8264340
H	-3.6086250	3.4897390	1.2395080
H	-3.8295750	1.8658310	1.9545570
H	-4.0297460	2.1048580	0.1900540

TS5$_{DME}$ – *E* = -1223.511766 Hartree

Symbol	X	Y	Z
O	3.4693980	1.3685010	-0.9102150
O	2.1940070	-1.7930710	0.0390210
C	2.6916500	0.5608940	-0.3052960
C	2.3773460	-0.8037960	-0.9402450
H	2.9013300	2.5509860	-0.7707040
H	3.0288470	-1.8738820	0.5235490
H	2.7310020	0.4887120	0.7946430
H	3.2247240	-1.0313730	-1.5987980
H	1.4733970	-0.7942230	-1.5531120
C	1.2598060	2.5312170	0.1854180
C	0.8254510	1.3644030	-0.4098450
O	2.1453270	3.2737420	-0.3854940
O	0.0566920	0.4802570	0.3024700

H	0.9914280	2.7393800	1.2257720
H	0.7958940	1.2890310	-1.4941140
H	-3.3702060	2.2066160	1.6000310
C	-1.1428970	0.0827260	-0.2817110
C	-1.5000780	-1.2817090	0.2933100
C	-2.8755260	-1.6751570	-0.2133670
C	-3.8918680	-0.5923180	0.0998220
C	-3.4123560	0.7413130	-0.4713850
C	-4.3009460	1.9046460	-0.0622650
O	-0.6043760	-2.2726280	-0.1336080
O	-3.3250850	-2.8751250	0.3715860
O	-5.1350520	-0.8830610	-0.4929680
O	-2.1127500	1.0463130	0.0230100
O	-4.2888160	2.0990670	1.3318040
H	-1.0223050	0.0021460	-1.3789310
H	-1.5221380	-1.1919130	1.3897600
H	0.2883910	-2.1079640	0.2103490
H	-2.8176470	-1.7891570	-1.3093820
H	-2.6382330	-3.5386310	0.2424260
H	-3.9898650	-0.4929390	1.1907520
H	-3.3938410	0.6670650	-1.5710380
H	-3.9662100	2.8073180	-0.5910520
H	-5.3303490	1.6847780	-0.3525330
H	-5.3761540	-1.7794830	-0.2354920
O	4.8843540	-1.1589570	0.6931360
C	5.6922100	-1.2086210	-0.4632120

C	5.2671050	-0.1077660	1.5536170
H	5.5814370	-0.2872620	-1.0514130
H	5.3690570	-2.0673830	-1.0552300
H	6.7475910	-1.3412160	-0.1909010
H	5.1784350	0.8615460	1.0443250
H	6.3024850	-0.2455970	1.8916030
H	4.6039740	-0.1318470	2.4204950

TS6$_{DME}$ – *E* = -1452.516586 Hartree

Symbol	X	Y	Z
O	-3.4816870	0.9297450	-1.2045310
H	-3.6641830	-2.3441650	-0.6636360
C	-3.1914630	0.3326990	-0.1045830
C	-1.7797700	0.0960210	0.0238850
C	-1.2332530	-0.8617630	1.0917630
C	-0.5104120	-2.1088310	0.5235860
C	-1.2788870	-2.9814530	-0.4774660
C	-2.5162120	-3.6886240	0.0716850
O	-1.1537260	0.4360490	-1.0751520
O	-2.2430810	-1.2251710	1.9966950
O	0.6921820	-1.8076980	-0.1663220
O	-1.7109450	-2.2640310	-1.6103590
O	-3.6104630	-2.7935180	0.1914890
H	-3.9566640	0.1529990	0.6419330
H	-2.1180020	1.0952590	0.6895090
H	-2.5119720	0.9028090	-1.6284060

H	-0.4917490	-0.3188390	1.6772950
H	-2.9074990	-1.7518770	1.5201220
H	-0.2806670	-2.7266720	1.4069230
H	-0.5617250	-3.7619690	-0.7750620
H	-2.7833900	-4.5044520	-0.6094930
H	-2.3248570	-4.1100980	1.0620840
H	-1.1795500	-1.4566870	-1.7217570
H	0.3877960	1.7186070	-1.0828070
C	1.6607930	-1.0408960	0.4734780
C	2.9593000	-1.2635940	-0.2926340
C	4.0063910	-0.2756410	0.1792830
C	3.4930840	1.1380850	-0.0302100
C	2.1749830	1.3254730	0.7148080
C	1.4374280	2.5930120	0.2884810
O	3.4655530	-2.5625290	-0.0846670
O	5.2095060	-0.4072580	-0.5428460
O	4.4000820	2.0868090	0.4793260
O	1.2571180	0.2931860	0.4037010
O	0.9895550	2.4839350	-1.0380580
H	1.7790160	-1.3639230	1.5265200
H	2.7486470	-1.0846830	-1.3567630
H	2.8561270	-3.1913910	-0.4829460
H	4.1912070	-0.4314440	1.2557520
H	5.4777000	-1.3316910	-0.5073280
H	3.3175090	1.2966070	-1.1044370
H	2.3891530	1.3524960	1.7954720

H	0.5950270	2.7590050	0.9769710
H	2.1176030	3.4462130	0.3507630
H	5.2599150	1.9060470	0.0848290
O	-2.3176540	3.2048680	0.3974950
C	-3.6027650	3.4900180	0.8864810
C	-2.0465530	3.8901500	-0.8070160
H	-3.7144190	4.5617460	1.1020440
H	-3.7409720	2.9289720	1.8145800
H	-4.3748880	3.1943760	0.1605500
H	-2.1063790	4.9767700	-0.6521530
H	-2.7722190	3.6044570	-1.5822070
H	-1.0380760	3.6185060	-1.1217500

7$_{\mathbf{DME}}$ – *E* = -1452.585978 Hartree

Symbol	X	Y	Z
O	-0.0055870	3.1335860	0.6117390
H	4.9555510	-0.0382690	0.7569840
C	0.8459810	2.7293810	-0.4253180
C	1.6183440	1.4773850	-0.0659340
C	2.0453120	0.5595120	-1.2161580
C	2.0076890	-0.9353000	-0.8104590
C	3.1359780	-1.5601960	0.0317040
C	4.5493480	-1.3954230	-0.5414730
O	1.8891150	1.2500070	1.0919540
O	3.2456430	1.0079380	-1.7795580
O	0.8235860	-1.1896960	-0.0677970

O	3.1608450	-1.1379330	1.3737750
O	5.0889680	-0.1316740	-0.1961590
H	1.5806430	3.5189420	-0.6365240
H	0.2871080	2.5460620	-1.3497640
H	-0.0850290	2.4049440	1.2558290
H	1.2924400	0.6747990	-2.0000650
H	3.9836780	0.8457520	-1.1616330
H	1.9867060	-1.5074370	-1.7515140
H	2.9039290	-2.6343050	0.0304400
H	5.1840150	-2.1894410	-0.1323680
H	4.5581520	-1.4665210	-1.6322740
H	2.6718170	-0.2995510	1.4484990
H	-1.6695820	2.6929240	-0.2381090
C	-0.3983920	-1.1684050	-0.7193360
C	-1.3812560	-1.8707150	0.2106610
C	-2.7677560	-1.8302820	-0.3937530
C	-3.1524560	-0.3930840	-0.6915040
C	-2.0839150	0.2657240	-1.5623610
C	-2.3891990	1.7374000	-1.8025170
O	-1.0347200	-3.2212560	0.4062170
O	-3.7376610	-2.3601530	0.4824560
O	-4.3699720	-0.3344250	-1.3950690
O	-0.8075630	0.1633390	-0.9385510
O	-2.5342070	2.4724970	-0.6172860
H	-0.3287760	-1.6989180	-1.6892920
H	-1.3821530	-1.3105290	1.1561230

H	-0.1745320	-3.2482900	0.8383020
H	-2.7617150	-2.3972830	-1.3396920
H	-3.4615260	-3.2491200	0.7296400
H	-3.2136460	0.1632940	0.2549080
H	-2.0623020	-0.2478920	-2.5390780
H	-1.6113940	2.1594030	-2.4545720
H	-3.3412030	1.7899780	-2.3373790
H	-5.0191830	-0.8397990	-0.8943990
O	-0.9431410	0.9669250	2.1585300
C	-0.2705460	0.1495530	3.0888590
C	-2.1982970	1.4055420	2.6336440
H	0.0356810	0.7267370	3.9715010
H	0.6104010	-0.2599700	2.5924170
H	-0.9201280	-0.6751300	3.4166400
H	-2.0859600	1.9910880	3.5562970
H	-2.8523990	0.5454740	2.8370490
H	-2.6480390	2.0232990	1.8536690

TS7$_{DME}$ – *E* = -1452.531185 Hartree

Symbol	X	Y	Z
O	-3.0915780	2.3934260	-0.4774950
H	-4.1049690	-1.1390100	0.5538280
C	-2.6085700	1.6445940	0.6017170
C	-1.4233810	0.7987990	0.1774000
C	-0.7754190	-0.0571960	1.2717360
C	-0.4002270	-1.4014090	0.6067560

C	-1.5300280	-1.6896030	-0.3971370
C	-2.7432210	-2.4545480	0.1205560
O	-0.6613810	1.3329330	-0.7611280
O	-1.6016880	-0.2559480	2.3837510
O	0.7736840	-1.3872350	-0.1903690
O	-1.9627130	-0.4107990	-0.8699030
O	-3.4974250	-1.7192980	1.0543310
H	-3.4166230	1.0275860	0.9969240
H	-2.2445030	2.2851840	1.4201540
H	-2.3156020	2.6165140	-1.0132590
H	0.1120590	0.4718990	1.6153500
H	-2.3800020	-0.7753020	2.1135480
H	-0.3171380	-2.1696610	1.3872240
H	-1.1000500	-2.2437120	-1.2375230
H	-3.3704230	-2.7302400	-0.7360030
H	-2.4062320	-3.3784980	0.6024120
H	-1.1481980	0.2603580	-1.3530180
H	1.2993310	2.3081410	-0.7895640
C	1.9591180	-0.9212730	0.3722650
C	3.0871990	-1.4282300	-0.5197610
C	4.3922340	-0.7630060	-0.1287040
C	4.2448310	0.7478660	-0.2033930
C	3.0900500	1.1859450	0.6910000
C	2.6999140	2.6498430	0.5007270
O	3.2632890	-2.8216100	-0.3968790
O	5.4434740	-1.1365110	-0.9903510

O	5.4087060	1.3894250	0.2595340
O	1.9126250	0.4733080	0.3591140
O	2.0974110	2.8584550	-0.7480530
H	2.0804100	-1.3032320	1.4042350
H	2.8376260	-1.1483120	-1.5533980
H	2.4783030	-3.2582230	-0.7406720
H	4.6377270	-1.0399740	0.9104970
H	5.4881710	-2.0984280	-1.0063030
H	4.0177780	1.0371760	-1.2402580
H	3.3771840	1.0075600	1.7405260
H	2.0258760	2.9382120	1.3206950
H	3.5971200	3.2713980	0.5530260
H	6.1543480	1.0294580	-0.2324260
O	-5.1686990	-0.1740970	-0.4740940
C	-5.9490750	0.8571710	0.0951910
C	-4.9563070	0.0233740	-1.8579970
H	-5.4683540	1.8313950	-0.0573710
H	-6.0402920	0.6501270	1.1635420
H	-6.9509650	0.8688650	-0.3532420
H	-4.4136940	0.9595210	-2.0282940
H	-5.9182640	0.0435260	-2.3870160
H	-4.3589640	-0.8126860	-2.2234270

8$_{\mathbf{DME}}$ – *E* = -1452.596507 Hartree

Symbol	X	Y	Z
O	3.9269670	2.4171760	-0.9603280

H	4.8322340	-1.4707010	-0.1352180
C	3.4151820	1.2357990	-1.5179700
C	2.4080300	0.5709990	-0.5874350
C	1.7144510	-0.6615750	-1.1973820
C	1.3762060	-1.4982670	0.0490070
C	2.4948140	-1.1269830	1.0387230
C	3.6039490	-2.1626310	1.1772120
O	1.5032010	1.5711760	-0.2335480
O	2.5371300	-1.3835260	-2.0734620
O	0.1497290	-1.1581990	0.6888720
O	3.0899030	0.0676520	0.5539830
O	4.3358640	-2.2911660	-0.0282720
H	4.2554430	0.5640700	-1.6997180
H	2.9130560	1.4211480	-2.4778760
H	3.1772490	2.9190410	-0.6217500
H	0.8327840	-0.3525730	-1.7617230
H	3.2119230	-1.8564070	-1.5613760
H	1.3674650	-2.5641450	-0.2117230
H	2.0374360	-0.9526700	2.0212080
H	4.2708780	-1.8697840	1.9959200
H	3.1834360	-3.1449390	1.4088450
H	0.6601870	1.2265820	0.0995510
H	-1.6691530	2.7125590	0.1518740
C	-0.9800040	-1.1007770	-0.1174150
C	-2.1778860	-1.6220340	0.6640700
C	-3.4238800	-1.4405570	-0.1829000

C	-3.5721240	0.0127320	-0.6052250
C	-2.2962690	0.5011110	-1.2894140
C	-2.3142660	2.0006360	-1.5506890
O	-2.0499450	-2.9971590	0.9433730
O	-4.5930220	-1.8003240	0.5166200
O	-4.6263040	0.1602690	-1.5243800
O	-1.1718440	0.2488100	-0.4542970
O	-2.4829840	2.7425910	-0.3724770
H	-0.8448330	-1.7123310	-1.0281950
H	-2.2721840	-1.0361450	1.5891090
H	-1.3186120	-3.1177950	1.5565530
H	-3.3192950	-2.0581230	-1.0907150
H	-4.4980220	-2.7119200	0.8120230
H	-3.7424480	0.6291940	0.2898770
H	-2.1806430	-0.0339060	-2.2469830
H	-1.3845020	2.2718820	-2.0696370
H	-3.1593520	2.2243840	-2.2065000
H	-5.4174630	-0.2166460	-1.1249280
O	-0.4650550	2.4378280	1.6320820
C	0.6847330	3.0061730	2.2190870
C	-1.1302780	1.5492280	2.4970880
H	0.4171780	3.5532180	3.1327520
H	1.1190370	3.6921770	1.4923590
H	1.4247930	2.2303870	2.4569530
H	-1.3609150	2.0358500	3.4541160
H	-0.5186060	0.6541080	2.6820590

H	-2.0621280	1.2593430	2.0072680

TS8$_{DME}$ – *E* = -1452.483832 Hartree

Symbol	X	Y	Z
O	3.3326740	-1.8813100	0.6934380
H	3.5837570	4.2013500	1.2947150
C	3.4350780	-0.9667120	-0.3433480
C	2.7440900	0.2731700	-0.1316710
C	1.6303040	0.5287710	0.8475940
C	0.9247830	1.7613790	0.2407450
C	1.9725290	2.3166110	-0.7409750
C	2.6178140	3.6137210	-0.3156460
O	1.2597730	-0.7216200	-1.8196490
O	2.2415220	0.8075870	2.0827030
O	-0.2512170	1.5028640	-0.4655830
O	3.0303090	1.3152030	-0.8220530
O	3.0888690	3.4307190	1.0071260
H	2.6718220	-1.1744870	-1.2305510
H	4.4422550	-0.8468130	-0.7520520
H	2.7190110	-2.5839130	0.4150510
H	0.9674150	-0.3224640	0.9618620
H	2.6798620	1.6687130	2.0277090
H	0.7327010	2.4746790	1.0546600
H	1.5402970	2.3822280	-1.7412870
H	3.4414070	3.8559340	-0.9967890
H	1.8632300	4.4087770	-0.3656950

H	1.1444400	-0.4305480	-2.7288550
H	-0.1949620	-1.0625390	-1.4514970
C	-1.4084560	1.4188320	0.3349240
C	-2.6050920	1.3937960	-0.6077950
C	-3.7772930	0.8223540	0.1648720
C	-3.4905220	-0.6473410	0.4118790
C	-2.0681940	-0.8645270	0.9630630
C	-1.2573570	-1.7905500	0.0631000
O	-2.9416880	2.7046750	-1.0263100
O	-4.9839290	0.9098220	-0.5566590
O	-4.4119000	-1.2059320	1.3267700
O	-1.3784380	0.3629910	1.2415340
O	-1.1624300	-1.3076320	-1.2377960
H	-1.4657280	2.3312920	0.9504400
H	-2.3762410	0.7453020	-1.4613580
H	-2.3756130	2.9446960	-1.7636740
H	-3.8716300	1.3417300	1.1320360
H	-5.0487610	1.8070210	-0.9019410
H	-3.5724690	-1.1489400	-0.5626000
H	-2.1768800	-1.3302740	1.9470770
H	-0.2649470	-1.9572320	0.5098080
H	-1.7782610	-2.7647890	0.0754680
H	-5.2943360	-1.0662620	0.9669670
O	1.4441580	-3.7229990	-0.1071620
C	1.0006130	-4.6684810	0.8345030
C	0.8844650	-3.9240670	-1.3915730

H	-0.0900880	-4.6122950	0.9545060
H	1.4807380	-4.4407660	1.7882960
H	1.2719960	-5.6869850	0.5250370
H	-0.2113120	-3.9406010	-1.3321570
H	1.2410190	-4.8730030	-1.8146780
H	1.1830900	-3.0764850	-2.0093880

9$_{\mathbf{DME}}$ – E = -1376.159323 Hartree

Symbol	X	Y	Z
O	3.2239460	0.2434930	3.0716580
H	3.9150140	-0.6027690	-1.5437920
C	2.4325350	0.8132940	2.1221430
C	2.0986600	0.2161300	0.9829900
C	1.1672540	0.6771470	-0.1008190
C	0.5962520	-0.6827040	-0.5651250
C	1.7280350	-1.6812700	-0.2683330
C	2.5890660	-2.0420980	-1.4689820
O	1.7825730	1.3758470	-1.1560620
O	-0.5319240	-1.0729230	0.2002230
O	2.5566840	-1.0615150	0.7224630
O	3.1558400	-0.9077060	-2.0792290
H	2.1027770	1.8137210	2.3656090
H	3.3830530	-0.6728220	2.8124220
H	0.3725850	1.3118480	0.2869430
H	2.3020000	0.7410270	-1.6748850
H	0.3373330	-0.6470970	-1.6305290

H	1.2964620	-2.5922640	0.1613250
H	3.3702380	-2.7413220	-1.1443950
H	1.9692530	-2.5512910	-2.2146470
H	-2.1429180	2.6489250	1.0791430
C	-1.7602150	-0.6958610	-0.3148630
C	-2.8383450	-1.4023740	0.4959310
C	-4.1966280	-0.9727550	-0.0255440
C	-4.3182630	0.5416650	0.0057080
C	-3.1448270	1.1761270	-0.7401560
C	-3.1099460	2.6883250	-0.5919620
O	-2.7589480	-2.8022670	0.3641080
O	-5.2502730	-1.5012250	0.7466330
O	-5.5011520	0.9635180	-0.6291950
O	-1.9146140	0.6974300	-0.2094010
O	-2.9426540	3.0737580	0.7521500
H	-1.8315130	-0.9903780	-1.3798450
H	-2.7304190	-1.0924120	1.5455350
H	-1.9101350	-3.0897610	0.7148110
H	-4.2890390	-1.3081770	-1.0721670
H	-5.1474150	-2.4582820	0.7778430
H	-4.2912320	0.8792670	1.0520190
H	-3.2231630	0.9177300	-1.8087430
H	-2.3020610	3.0843960	-1.2216960
H	-4.0615870	3.1014900	-0.9323630
H	-6.2350300	0.4926910	-0.2200060
O	5.1265190	0.3565320	-0.6837010

C	5.6201180	0.0536920	0.6012950
C	5.0232230	1.7479810	-0.9040030
H	6.6611840	0.3893170	0.6994880
H	5.5767030	-1.0299870	0.7246040
H	5.0125200	0.5348320	1.3773560
H	6.0085660	2.2230220	-0.8101790
H	4.3208790	2.2001190	-0.1930020
H	4.6464540	1.8948340	-1.9177190

TS9$_{DME}$ – *E* = -1376.098576 Hartree

Symbol	X	Y	Z
O	-3.1495660	1.7366730	-2.5625450
H	-3.5046870	-1.2050470	1.5161450
C	-3.6471910	0.6313820	-2.1911710
C	-2.8471860	-0.2943210	-1.5445060
C	-1.4630430	-0.0618950	-1.3927090
C	-1.0169150	-1.0259990	-0.3118710
C	-2.1463910	-2.0679260	-0.3421590
C	-2.4194730	-2.6983640	1.0101260
O	-1.2760190	1.6819340	-0.9050590
O	0.2335640	-1.6303840	-0.5372760
O	-3.3041340	-1.3371550	-0.7248560
O	-2.8092030	-1.7178800	1.9468160
H	-4.7184520	0.4398650	-2.3366700
H	-2.0245400	1.9272940	-1.6071250
H	-0.8048940	0.1290240	-2.2339040

H	-1.6456310	1.7522660	-0.0004570
H	-1.0390040	-0.5147210	0.6573140
H	-1.9093320	-2.8343130	-1.0955060
H	-3.1931350	-3.4695500	0.9036860
H	-1.5071350	-3.1722340	1.3849560
H	0.7321900	2.4304190	-1.2560760
C	1.2874200	-1.0120910	0.1350480
C	2.5862600	-1.5284760	-0.4680010
C	3.7532330	-0.7615950	0.1269250
C	3.5528340	0.7361100	-0.0516030
C	2.2068960	1.1367390	0.5455080
C	1.8420440	2.5967170	0.3047920
O	2.7911630	-2.8947490	-0.1916960
O	4.9725570	-1.1079070	-0.4879680
O	4.5534900	1.4563460	0.6261150
O	1.1752530	0.3694620	-0.0536260
O	1.5765320	2.8518510	-1.0471990
H	1.2374200	-1.2463270	1.2175410
H	2.5446250	-1.3409530	-1.5505790
H	2.1082500	-3.4046070	-0.6382490
H	3.7998530	-0.9762890	1.2079080
H	5.0783280	-2.0632430	-0.4263880
H	3.5461450	0.9776820	-1.1246670
H	2.2440830	0.9469450	1.6331530
H	0.9741580	2.8508250	0.9314980
H	2.6841970	3.2224450	0.6104270

H	5.4061000	1.1221140	0.3276210
O	-2.1249460	1.4115410	1.6772340
C	-1.1439680	1.1159660	2.6494720
C	-3.4136510	1.5595630	2.2292940
H	-1.0846460	1.9172910	3.3971070
H	-0.1860160	1.0378070	2.1278270
H	-1.3756940	0.1625910	3.1409930
H	-3.4590140	2.4426940	2.8792950
H	-3.6831470	0.6729880	2.8182340
H	-4.1147600	1.6823240	1.4015190

10$_{\mathbf{DME}}$ – *E* = -1299.736329 Hartree

Symbol	X	Y	Z
O	-3.5923980	3.1799540	0.4414640
H	-4.7849010	-1.3849920	1.4212570
C	-4.0447050	2.1730620	-0.0320610
C	-3.3243560	0.8774420	-0.0133370
C	-2.1241030	0.5907810	0.4864570
C	-1.8354830	-0.8592490	0.2108810
C	-3.0993750	-1.3039130	-0.5574130
C	-3.8465010	-2.4464000	0.1024300
O	-0.7018020	-1.0602560	-0.6259730
O	-3.9796510	-0.1645700	-0.6026310
O	-4.1837300	-2.1366850	1.4329930
H	-5.0359160	2.1489730	-0.5242260
H	-1.4609740	1.2764210	0.9905600

H	-1.7028920	-1.4383290	1.1349830
H	-2.8235370	-1.5612860	-1.5857250
H	-4.7362100	-2.6944880	-0.4905760
H	-3.1974170	-3.3271080	0.1324780
H	1.6396300	2.1137270	0.7503180
C	0.4938850	-1.2421050	0.0561050
C	1.5888810	-1.4635190	-0.9775600
C	2.9100220	-1.6192170	-0.2488500
C	3.1620390	-0.4110810	0.6375220
C	1.9733150	-0.1879570	1.5728850
C	2.0845900	1.1075780	2.3586870
O	1.3767520	-2.6393030	-1.7254780
O	3.9952630	-1.7269450	-1.1420410
O	4.3010500	-0.6065560	1.4409660
O	0.7693590	-0.0968920	0.8171830
O	2.2165230	2.2266440	1.5218030
H	0.4156490	-2.1199690	0.7277000
H	1.6299900	-0.5727830	-1.6220030
H	0.5545930	-2.5425380	-2.2155200
H	2.8546380	-2.5179070	0.3882850
H	3.8125400	-2.4538480	-1.7466600
H	3.2740330	0.4753390	-0.0032380
H	1.9118730	-1.0346250	2.2765240
H	1.1956740	1.1921010	3.0009880
H	2.9719930	1.0585820	2.9947740
H	5.0316860	-0.8358830	0.8570070

O	1.4522580	2.1674320	-1.1842210
C	0.2227150	2.1295450	-1.8678980
C	2.2159800	3.3094260	-1.4993310
H	-0.4102140	2.9840460	-1.5890340
H	-0.2788630	1.2014160	-1.5863210
H	0.3818570	2.1471170	-2.9555500
H	1.6603930	4.2282600	-1.2670070
H	2.4861640	3.3151390	-2.5639360
H	3.1198100	3.2737010	-0.8887070

TS10$_{DME}$ – *E* = -1299.655448 Hartree

Symbol	X	Y	Z
O	-5.6049570	0.3552680	2.1264690
H	-0.8656060	-2.5705290	-1.1350890
C	-5.3511140	0.2456600	0.9613630
C	-3.9392840	0.0938330	0.4926250
C	-2.7680020	0.0926840	1.2393650
C	-1.7561700	-0.0615690	0.3141230
C	-2.3378790	-0.1142740	-1.0229790
C	-1.9647700	-1.2422120	-1.9844620
O	-0.9711100	2.1408640	-0.7128720
O	-3.7577120	-0.0571680	-0.7840870
O	-1.8098360	-2.4763640	-1.3412070
H	-6.1183480	0.2432930	0.1682350
H	-2.7114000	0.2042760	2.3094770
H	-0.6940970	-0.1676000	0.4754220

H	-1.9991430	0.9105280	-1.4095000
H	-2.7725950	-1.3221380	-2.7182990
H	-1.0508510	-0.9285380	-2.4921660
H	1.5641310	-2.3316310	-0.2360620
C	0.3030130	1.9082420	-0.9740680
C	1.1683610	2.1637860	0.2748570
C	2.6088140	1.7671140	0.0537450
C	2.6513860	0.3027750	-0.3334920
C	1.7964690	0.0743450	-1.5795400
C	1.7307880	-1.3988120	-1.9664480
O	1.1170840	3.5223500	0.6327590
O	3.3975010	1.9125860	1.2231050
O	3.9666410	-0.1369400	-0.5858070
O	0.4813040	0.5035610	-1.3474300
O	1.0158640	-2.1752210	-1.0217560
H	0.7209930	2.5063570	-1.8179900
H	0.7509000	1.5402080	1.0858760
H	0.1937040	3.7853630	0.5173900
H	3.0342640	2.3722680	-0.7626500
H	3.2656330	2.8080740	1.5530570
H	2.2084300	-0.2737120	0.4949220
H	2.2576330	0.6285720	-2.4162540
H	1.1960650	-1.4925240	-2.9162960
H	2.7478050	-1.7823370	-2.1042470
H	4.5390580	0.2900770	0.0619840
O	2.1652180	-2.4543750	1.5340460

C	3.4250550	-2.0862430	2.0539510
C	1.1025600	-2.0344500	2.3559210
H	3.4837760	-0.9984130	2.2032200
H	4.1796990	-2.3909780	1.3286670
H	3.6046020	-2.5893270	3.0129740
H	1.1047860	-0.9392420	2.4705010
H	1.1735190	-2.4918890	3.3513790
H	0.1716990	-2.3519070	1.8799280

In the Presence of Acetone (Ace)

The Cartesian coordinates for all the stable structures in the presence of Ace reported in this work are listed below including computed absolute energies.

1$_{Ace}$ – E = -1490.721073 Hartree

Symbol	X	Y	Z
C	4.4723610	-0.0807840	0.0800450
C	3.6671400	1.0682450	-0.5162170
C	2.2500110	1.0753340	0.0363330
C	1.6457240	-0.3224630	-0.0608550
C	2.5751610	-1.3817170	0.5348620
C	2.0538330	-2.7966200	0.3559990
O	5.6964660	-0.1009770	-0.5718510
O	4.2778190	2.2932010	-0.2009780
O	1.5157600	2.0149270	-0.6920720
O	0.4235560	-0.3292670	0.6626270
O	3.8321550	-1.3196120	-0.1182510
O	1.8310710	-3.1032310	-1.0038840

H	4.6011540	0.0855580	1.1651730
H	3.6149460	0.9117240	-1.6044420
H	2.3046500	1.3501160	1.1055930
H	1.4607730	-0.5480310	-1.1183050
H	2.6933300	-1.1816070	1.6133320
H	6.2672860	-0.7525800	-0.1543180
H	5.1611260	2.2868580	-0.5832350
H	0.5838880	2.0083160	-0.4281480
H	-2.5190140	2.3465200	-1.2604260
H	2.6581860	-2.9568150	-1.4755350
H	2.7765740	-3.4917700	0.8031310
H	1.0995770	-2.9062130	0.8778990
C	-0.6548160	-0.8950650	0.0060800
C	-1.6782040	-1.3283980	1.0460480
C	-2.9565450	-1.7632140	0.3500370
C	-3.4494920	-0.6658790	-0.5721150
C	-2.3397670	-0.3105440	-1.5645730
C	-2.7250390	0.8419130	-2.4796980
O	-1.1314840	-2.3745000	1.8075470
O	-3.8909830	-2.0743100	1.3602670
O	-4.6140660	-1.1499140	-1.2104110
O	-1.1972920	0.0983350	-0.8334170
O	-3.2392580	1.9405580	-1.7702460
H	-0.3398350	-1.7636030	-0.5994840
H	-1.8994130	-0.4545950	1.6810530
H	-1.8535220	-2.7776620	2.3028040

H	-2.7399700	-2.6604890	-0.2534740
H	-4.7282190	-2.2767890	0.9285620
H	-3.6775370	0.2260280	0.0255540
H	-2.1052680	-1.1960860	-2.1793040
H	-1.8450830	1.1184600	-3.0744740
H	-3.5048150	0.5038130	-3.1697350
O	-1.2307040	2.8797110	0.0424560
C	-1.4707510	2.6836060	1.2148160
C	-2.8862680	2.5592500	1.7182310
C	-0.3585360	2.5339420	2.2191040
H	-2.9922030	1.6633310	2.3385460
H	-3.1094470	3.4182540	2.3600140
H	-3.5891890	2.5326680	0.8846590
H	0.5456670	3.0195780	1.8478460
H	-0.1568100	1.4606190	2.3281540
H	-0.6405050	2.9310210	3.1965720
H	-5.1195070	-0.4016300	-1.5408920

TS1$_{Ace}$ – E = -1490.636406 Hartree

Symbol	X	Y	Z
O	-4.3831700	1.2226000	-1.1087640
H	-4.9412620	-0.4552230	0.0095730
C	-3.2239960	1.0590270	-1.3850780
C	-2.0638100	1.5689960	-0.5411080
C	-2.0015210	1.0962620	0.9400170
C	-1.6752780	-0.3854180	1.2507350

C	-2.5963880	-1.4927190	0.7228410
C	-3.9993530	-1.5831620	1.3063470
O	-0.8594590	1.3930880	-1.2503350
O	-3.1274920	1.5127800	1.6538550
O	-0.4061410	-0.7788650	0.7228930
O	-2.7051100	-1.4308720	-0.6829060
O	-4.8548240	-0.5185160	0.9695110
H	-2.9130130	0.5763120	-2.3329120
H	-2.2270280	2.6509730	-0.4643430
H	-0.6113230	0.4562790	-1.2292350
H	-1.1566940	1.6565360	1.3516530
H	-3.9113050	1.0265010	1.3447000
H	-1.6489170	-0.4552310	2.3492810
H	-2.0997970	-2.4308720	1.0200420
H	-4.4286500	-2.5370670	0.9746730
H	-3.9330990	-1.5991030	2.3984300
H	-1.8366150	-1.5882350	-1.0829000
H	0.9722840	2.3234210	-1.0057830
C	0.7602790	-0.3240560	1.3207850
C	1.8498960	-1.3020580	0.8914590
C	3.2195200	-0.7729500	1.2575280
C	3.4118580	0.6013100	0.6415500
C	2.2924090	1.5324750	1.0982460
C	2.2768140	2.8505230	0.3283670
O	1.6890730	-2.5604370	1.5009120
O	4.2443190	-1.6082590	0.7637950

O	4.6324400	1.1716240	1.0427440
O	1.0248480	0.9600650	0.8329030
O	1.8873060	2.6487700	-1.0074600
H	0.6573150	-0.3107800	2.4219900
H	1.7827740	-1.3883100	-0.2023420
H	0.8519690	-2.9317050	1.2032810
H	3.2951810	-0.6837910	2.3536920
H	4.0972760	-2.4961380	1.1071000
H	3.3636600	0.5068660	-0.4556260
H	2.4206790	1.7275570	2.1750770
H	1.5967150	3.5470520	0.8365740
H	3.2814410	3.2796530	0.3268020
H	5.3262520	0.5236180	0.8793530
O	-0.1049940	-1.3313610	-2.1272260
C	0.9461120	-1.1143730	-2.6973080
C	2.0010320	-2.1842410	-2.8193630
C	1.2750750	0.2378460	-3.2674260
H	2.1561960	-2.4213580	-3.8766270
H	2.9549430	-1.8091650	-2.4320660
H	1.7019190	-3.0820680	-2.2786700
H	1.8924020	0.7797400	-2.5366990
H	0.3670130	0.8174370	-3.4342130
H	1.8594210	0.1473960	-4.1857310

2$_{\mathbf{Ace}}$ – *E* = -1414.300347 Hartree

Symbol	X	Y	Z

O	-4.3831700	1.2226000	-1.1087640
H	-4.9412620	-0.4552230	0.0095730
C	-3.2239960	1.0590270	-1.3850780
C	-2.0638100	1.5689960	-0.5411080
C	-2.0015210	1.0962620	0.9400170
C	-1.6752780	-0.3854180	1.2507350
C	-2.5963880	-1.4927190	0.7228410
C	-3.9993530	-1.5831620	1.3063470
O	-0.8594590	1.3930880	-1.2503350
O	-3.1274920	1.5127800	1.6538550
O	-0.4061410	-0.7788650	0.7228930
O	-2.7051100	-1.4308720	-0.6829060
O	-4.8548240	-0.5185160	0.9695110
H	-2.9130130	0.5763120	-2.3329120
H	-2.2270280	2.6509730	-0.4643430
H	-0.6113230	0.4562790	-1.2292350
H	-1.1566940	1.6565360	1.3516530
H	-3.9113050	1.0265010	1.3447000
H	-1.6489170	-0.4552310	2.3492810
H	-2.0997970	-2.4308720	1.0200420
H	-4.4286500	-2.5370670	0.9746730
H	-3.9330990	-1.5991030	2.3984300
H	-1.8366150	-1.5882350	-1.0829000
H	0.9722840	2.3234210	-1.0057830
C	0.7602790	-0.3240560	1.3207850
C	1.8498960	-1.3020580	0.8914590

C	3.2195200	-0.7729500	1.2575280
C	3.4118580	0.6013100	0.6415500
C	2.2924090	1.5324750	1.0982460
C	2.2768140	2.8505230	0.3283670
O	1.6890730	-2.5604370	1.5009120
O	4.2443190	-1.6082590	0.7637950
O	4.6324400	1.1716240	1.0427440
O	1.0248480	0.9600650	0.8329030
O	1.8873060	2.6487700	-1.0074600
H	0.6573150	-0.3107800	2.4219900
H	1.7827740	-1.3883100	-0.2023420
H	0.8519690	-2.9317050	1.2032810
H	3.2951810	-0.6837910	2.3536920
H	4.0972760	-2.4961380	1.1071000
H	3.3636600	0.5068660	-0.4556260
H	2.4206790	1.7275570	2.1750770
H	1.5967150	3.5470520	0.8365740
H	3.2814410	3.2796530	0.3268020
H	5.3262520	0.5236180	0.8793530
O	-0.1049940	-1.3313610	-2.1272260
C	0.9461120	-1.1143730	-2.6973080
C	2.0010320	-2.1842410	-2.8193630
C	1.2750750	0.2378460	-3.2674260
H	2.1561960	-2.4213580	-3.8766270
H	2.9549430	-1.8091650	-2.4320660
H	1.7019190	-3.0820680	-2.2786700

H	1.8924020	0.7797400	-2.5366990
H	0.3670130	0.8174370	-3.4342130
H	1.8594210	0.1473960	-4.1857310

TS2$_{Ace}$ – E = -1414.211849 Hartree

Symbol	X	Y	Z
O	-4.3831700	1.2226000	-1.1087640
H	-4.9412620	-0.4552230	0.0095730
C	-3.2239960	1.0590270	-1.3850780
C	-2.0638100	1.5689960	-0.5411080
C	-2.0015210	1.0962620	0.9400170
C	-1.6752780	-0.3854180	1.2507350
C	-2.5963880	-1.4927190	0.7228410
C	-3.9993530	-1.5831620	1.3063470
O	-0.8594590	1.3930880	-1.2503350
O	-3.1274920	1.5127800	1.6538550
O	-0.4061410	-0.7788650	0.7228930
O	-2.7051100	-1.4308720	-0.6829060
O	-4.8548240	-0.5185160	0.9695110
H	-2.9130130	0.5763120	-2.3329120
H	-2.2270280	2.6509730	-0.4643430
H	-0.6113230	0.4562790	-1.2292350
H	-1.1566940	1.6565360	1.3516530
H	-3.9113050	1.0265010	1.3447000
H	-1.6489170	-0.4552310	2.3492810
H	-2.0997970	-2.4308720	1.0200420

H	-4.4286500	-2.5370670	0.9746730
H	-3.9330990	-1.5991030	2.3984300
H	-1.8366150	-1.5882350	-1.0829000
H	0.9722840	2.3234210	-1.0057830
C	0.7602790	-0.3240560	1.3207850
C	1.8498960	-1.3020580	0.8914590
C	3.2195200	-0.7729500	1.2575280
C	3.4118580	0.6013100	0.6415500
C	2.2924090	1.5324750	1.0982460
C	2.2768140	2.8505230	0.3283670
O	1.6890730	-2.5604370	1.5009120
O	4.2443190	-1.6082590	0.7637950
O	4.6324400	1.1716240	1.0427440
O	1.0248480	0.9600650	0.8329030
O	1.8873060	2.6487700	-1.0074600
H	0.6573150	-0.3107800	2.4219900
H	1.7827740	-1.3883100	-0.2023420
H	0.8519690	-2.9317050	1.2032810
H	3.2951810	-0.6837910	2.3536920
H	4.0972760	-2.4961380	1.1071000
H	3.3636600	0.5068660	-0.4556260
H	2.4206790	1.7275570	2.1750770
H	1.5967150	3.5470520	0.8365740
H	3.2814410	3.2796530	0.3268020
H	5.3262520	0.5236180	0.8793530
O	-0.1049940	-1.3313610	-2.1272260

C	0.9461120	-1.1143730	-2.6973080
C	2.0010320	-2.1842410	-2.8193630
C	1.2750750	0.2378460	-3.2674260
H	2.1561960	-2.4213580	-3.8766270
H	2.9549430	-1.8091650	-2.4320660
H	1.7019190	-3.0820680	-2.2786700
H	1.8924020	0.7797400	-2.5366990
H	0.3670130	0.8174370	-3.4342130
H	1.8594210	0.1473960	-4.1857310

TS3$_{Ace}$ – E = -1490.634469 Hartree

Symbol	X	Y	Z
O	3.0715520	-1.1937860	-1.0160310
H	3.5284980	-0.9021360	0.6877790
C	1.7740400	-0.9226010	-1.1556700
C	0.7210680	-1.7664460	-0.4233500
C	0.3434090	-1.3230470	1.0122320
C	0.3120300	0.2103670	1.1326740
C	1.6170170	0.8978100	0.7375920
C	2.8337700	0.6794320	1.6436080
O	-0.4326430	-1.8716110	-1.2368000
O	1.1005690	-1.9089910	2.0293350
O	-0.6551630	0.7871200	0.2527070
O	1.9122580	0.5815350	-0.6392020
O	3.3933890	-0.6146000	1.6182720
H	1.4319010	-0.7358110	-2.1818940

H	1.1510110	-2.7698800	-0.3530700
H	-0.9688780	-1.0786340	-1.1070420
H	-0.6753860	-1.6847360	1.1574000
H	2.0284970	-1.6132890	1.9753450
H	0.0792010	0.4754690	2.1733030
H	1.4148160	1.9750640	0.7474500
H	3.5876490	1.4207980	1.3615420
H	2.5232700	0.8774640	2.6749890
H	2.9835260	0.1483500	-0.8070110
H	-2.6070750	-2.5549830	-1.1979730
C	-1.9955540	0.7155470	0.6104600
C	-2.7330100	1.7580660	-0.2226450
C	-4.2295440	1.5974960	-0.0313290
C	-4.6533290	0.1778690	-0.3752040
C	-3.8464940	-0.8094770	0.4620890
C	-4.0643080	-2.2628520	0.0572600
O	-2.3903850	3.0688680	0.1603390
O	-4.9563360	2.4733620	-0.8610790
O	-6.0128300	-0.0248670	-0.0772830
O	-2.4582450	-0.5691790	0.2865970
O	-3.5719770	-2.5274290	-1.2315510
H	-2.1254500	0.9116220	1.6905780
H	-2.4837730	1.5739580	-1.2782820
H	-1.4703810	3.2242590	-0.0746460
H	-4.4736760	1.7872780	1.0275510
H	-4.6436540	3.3696220	-0.6978160

H	-4.4471220	-0.0122790	-1.4390500
H	-4.1251780	-0.6806500	1.5206800
H	-3.5895280	-2.9106270	0.8060700
H	-5.1380540	-2.4653800	0.0512980
H	-6.5160050	0.6627600	-0.5264260
O	4.8460920	1.2120170	-0.5744100
C	5.9603620	0.7433860	-0.6582500
C	6.1966770	-0.7425870	-0.7563750
C	7.1816700	1.6302490	-0.6458030
H	7.0770740	-0.9631090	-1.3644410
H	6.3954920	-1.1155920	0.2556080
H	5.3107650	-1.2432140	-1.1478410
H	6.9033210	2.6591390	-0.4209000
H	7.6636930	1.5850800	-1.6279230
H	7.9083560	1.2606560	0.0838230

4$_{\mathbf{Ace}}$ – E = -1490.702387 Hartree

Symbol	X	Y	Z
O	-4.3831700	1.2226000	-1.1087640
H	-4.9412620	-0.4552230	0.0095730
C	-3.2239960	1.0590270	-1.3850780
C	-2.0638100	1.5689960	-0.5411080
C	-2.0015210	1.0962620	0.9400170
C	-1.6752780	-0.3854180	1.2507350
C	-2.5963880	-1.4927190	0.7228410
C	-3.9993530	-1.5831620	1.3063470

O	-0.8594590	1.3930880	-1.2503350
O	-3.1274920	1.5127800	1.6538550
O	-0.4061410	-0.7788650	0.7228930
O	-2.7051100	-1.4308720	-0.6829060
O	-4.8548240	-0.5185160	0.9695110
H	-2.9130130	0.5763120	-2.3329120
H	-2.2270280	2.6509730	-0.4643430
H	-0.6113230	0.4562790	-1.2292350
H	-1.1566940	1.6565360	1.3516530
H	-3.9113050	1.0265010	1.3447000
H	-1.6489170	-0.4552310	2.3492810
H	-2.0997970	-2.4308720	1.0200420
H	-4.4286500	-2.5370670	0.9746730
H	-3.9330990	-1.5991030	2.3984300
H	-1.8366150	-1.5882350	-1.0829000
H	0.9722840	2.3234210	-1.0057830
C	0.7602790	-0.3240560	1.3207850
C	1.8498960	-1.3020580	0.8914590
C	3.2195200	-0.7729500	1.2575280
C	3.4118580	0.6013100	0.6415500
C	2.2924090	1.5324750	1.0982460
C	2.2768140	2.8505230	0.3283670
O	1.6890730	-2.5604370	1.5009120
O	4.2443190	-1.6082590	0.7637950
O	4.6324400	1.1716240	1.0427440
O	1.0248480	0.9600650	0.8329030

O	1.8873060	2.6487700	-1.0074600
H	0.6573150	-0.3107800	2.4219900
H	1.7827740	-1.3883100	-0.2023420
H	0.8519690	-2.9317050	1.2032810
H	3.2951810	-0.6837910	2.3536920
H	4.0972760	-2.4961380	1.1071000
H	3.3636600	0.5068660	-0.4556260
H	2.4206790	1.7275570	2.1750770
H	1.5967150	3.5470520	0.8365740
H	3.2814410	3.2796530	0.3268020
H	5.3262520	0.5236180	0.8793530
O	-0.1049940	-1.3313610	-2.1272260
C	0.9461120	-1.1143730	-2.6973080
C	2.0010320	-2.1842410	-2.8193630
C	1.2750750	0.2378460	-3.2674260
H	2.1561960	-2.4213580	-3.8766270
H	2.9549430	-1.8091650	-2.4320660
H	1.7019190	-3.0820680	-2.2786700
H	1.8924020	0.7797400	-2.5366990
H	0.3670130	0.8174370	-3.4342130
H	1.8594210	0.1473960	-4.1857310

TS4$_{Ace}$ – *E* = -1490.643589 Hartree

Symbol	X	Y	Z
C	2.8235850	2.3531680	0.6461010
C	1.8209820	1.4659030	0.9732680

C	1.3291950	1.1927610	-1.0303850
C	0.5651170	-0.1346920	-0.9420560
C	1.4716670	-1.3739020	-0.9832270
C	0.6715530	-2.6630620	-0.8581090
O	3.8474090	1.9881970	-0.0601090
O	0.7423870	1.9656290	1.6415860
O	2.3915170	1.1955210	-1.7471160
O	-0.2662820	-0.1559490	0.2112010
O	2.1159370	-1.4617470	-2.2400760
O	-0.2558670	-2.7885750	-1.9152740
H	2.6873970	3.4189850	0.8533890
H	2.0691740	0.4143060	1.0977530
H	0.6717000	2.0738230	-1.0366270
H	-0.0665530	-0.1495830	-1.8422840
H	2.2029610	-1.3270570	-0.1616920
H	2.5130970	-0.5990240	-2.4236210
H	0.0155220	1.3464600	1.5031610
H	3.3847510	1.5504920	-0.9602730
H	-2.8810400	2.9400170	-0.5077600
H	0.2424650	-2.6825050	-2.7341840
H	1.3800780	-3.5008980	-0.8545680
H	0.1035570	-2.6890220	0.0748260
C	-1.6080780	-0.4476740	-0.0292470
C	-2.2671700	-0.7534670	1.3084880
C	-3.7475060	-0.9905540	1.0668780
C	-4.3616990	0.2032250	0.3529910

C	-3.5755180	0.5174690	-0.9193910
C	-4.0281360	1.8109570	-1.5762730
O	-1.7438390	-1.9166260	1.9045620
O	-4.4541350	-1.1743800	2.2710300
O	-5.6885920	-0.0674360	-0.0267490
O	-2.1968970	0.6912650	-0.6055430
O	-3.8157550	2.9217620	-0.7380430
H	-1.6956350	-1.3072040	-0.7143470
H	-2.1467980	0.1217320	1.9667820
H	-0.8339980	-1.7510650	2.1708630
H	-3.8544400	-1.8782110	0.4217930
H	-4.0538530	-1.9111180	2.7448770
H	-4.3133020	1.0776640	1.0186980
H	-3.7001470	-0.3159820	-1.6288220
H	-3.4970130	1.9264500	-2.5307260
H	-5.1004620	1.7523830	-1.7734330
H	-6.1644470	-0.3560240	0.7594200
O	3.9081730	-0.8963490	1.4278990
C	4.9383150	-0.5169120	0.9175970
C	5.9738460	0.2505600	1.7017250
C	5.2601610	-0.7970110	-0.5308020
H	6.9558630	-0.2207610	1.5995470
H	6.0475000	1.2594750	1.2844830
H	5.6876030	0.3028190	2.7516980
H	4.4003710	-1.2349010	-1.0406010
H	6.1016790	-1.4964710	-0.5804280

H	5.5736440	0.1241080	-1.0302250

5$_{Ace}$ – E = -1261.690518 Hartree

Symbol	X	Y	Z
C	-1.6455490	-0.7568220	-1.0047710
C	-1.2246310	0.6685430	-0.7012470
C	-2.4235860	1.5599280	-0.3204460
C	-2.0159970	3.0272940	-0.3664390
O	-1.2823070	-1.7186510	-0.3815360
O	-0.3042620	0.7255900	0.3604590
O	-3.4827190	1.3994920	-1.2351270
O	-1.7100890	3.4205720	-1.6835480
H	-2.3371600	-0.8565100	-1.8626690
H	-0.7934520	1.0796470	-1.6284910
H	-2.7343560	1.2955180	0.6985800
H	-4.0832270	0.7269030	-0.8869880
H	1.3104880	-2.6615830	-0.8090890
H	-2.4826000	3.2213360	-2.2248590
H	-2.8358500	3.6294480	0.0467460
H	-1.1186220	3.1928340	0.2361760
C	1.0299360	0.7585390	-0.0264160
C	1.8698230	0.8118290	1.2408390
C	3.3352740	0.7333510	0.8598000
C	3.5906540	-0.5206970	0.0407550
C	2.6595120	-0.5525370	-1.1703900
C	2.7018980	-1.8872240	-1.9013590

O	1.6756720	2.0165620	1.9455640
O	4.1714080	0.6807080	1.9932130
O	4.9119370	-0.5448100	-0.4434200
O	1.3087970	-0.4016130	-0.7586830
O	2.1934860	-2.9238210	-1.0984320
H	1.2200690	1.6517260	-0.6535730
H	1.6040620	-0.0596680	1.8566570
H	0.7582490	2.0560470	2.2329170
H	3.5867130	1.6127130	0.2435930
H	3.9708030	1.4420320	2.5478750
H	3.3835480	-1.4020600	0.6654550
H	2.9480830	0.2593290	-1.8574460
H	2.1324200	-1.7943360	-2.8364410
H	3.7384860	-2.1325000	-2.1424980
H	5.4995330	-0.4180460	0.3091670
O	-4.3705200	-0.7845580	0.3046470
C	-3.8682160	-1.6059360	1.0437430
C	-3.9559620	-3.0803280	0.7617650
C	-3.0807340	-1.1891950	2.2597920
H	-2.9431720	-3.4938060	0.7307180
H	-4.4945320	-3.5785390	1.5740370
H	-4.4625430	-3.2556700	-0.1864810
H	-3.3729000	-0.1879410	2.5782520
H	-2.0218330	-1.1818670	1.9700370
H	-3.1979490	-1.9012350	3.0794720

TS5$_{Ace}$ – *E* = -1261.63339 Hartree

Symbol	X	Y	Z
O	3.2703960	1.1667560	-0.9381820
O	1.8280290	-1.8957180	0.1926020
C	2.5061450	0.3966750	-0.2651690
C	2.1594480	-0.9916170	-0.8262690
H	2.7246990	2.3842970	-0.7839810
H	2.6362040	-2.1025330	0.6813270
H	2.5958390	0.3722910	0.8347850
H	3.0483030	-1.3189860	-1.3807350
H	1.3202360	-0.9646900	-1.5255070
C	1.1097800	2.3877380	0.2068360
C	0.6566440	1.2228110	-0.3791830
O	2.0143770	3.1116680	-0.3616260
O	-0.1559690	0.3777450	0.3300090
H	0.8337970	2.6164580	1.2400820
H	0.6387050	1.1343160	-1.4628550
H	-3.5058470	2.3143630	1.5344020
C	-1.3669880	0.0361280	-0.2667090
C	-1.8077370	-1.2940890	0.3283580
C	-3.1944820	-1.6217700	-0.1944820
C	-4.1545240	-0.4783750	0.0791520
C	-3.5921820	0.8150640	-0.5091230
C	-4.4218540	2.0337780	-0.1397510
O	-0.9600620	-2.3394980	-0.0628960
O	-3.7192960	-2.7828640	0.4060120

O	-5.4018220	-0.7119670	-0.5302120
O	-2.2863430	1.0581430	0.0029230
O	-4.4240930	2.2560130	1.2502120
H	-1.2335450	-0.0729750	-1.3599920
H	-1.8427330	-1.1801970	1.4223550
H	-0.0602720	-2.1985920	0.2748340
H	-3.1248330	-1.7615500	-1.2868400
H	-3.0667620	-3.4848030	0.3048350
H	-4.2653830	-0.3515410	1.1659800
H	-3.5586110	0.7172150	-1.6065750
H	-4.0277390	2.9054590	-0.6796110
H	-5.4564690	1.8654410	-0.4454660
H	-5.6955180	-1.5891170	-0.2612090
O	4.5575700	-1.5132740	0.8294480
C	5.3221990	-0.6453500	0.4632210
C	5.6028580	0.5656500	1.3142420
C	5.9857380	-0.6998400	-0.8879430
H	6.6795460	0.6937000	1.4563220
H	5.2320120	1.4483560	0.7813240
H	5.1047550	0.4730300	2.2790970
H	5.8466190	-1.6824100	-1.3387390
H	7.0496290	-0.4607720	-0.8141000
H	5.5148140	0.0663980	-1.5151440

TS6$_{Ace}$ – *E* = -1490.639814 Hartree

Symbol	X	Y	Z

O	-3.5569800	2.9130230	0.2569240
H	-5.1907130	-0.7901660	-0.2156660
C	-3.2986480	1.7760140	1.0378610
C	-2.4206090	0.7766600	0.2993170
C	-2.0675330	-0.4753440	1.1251720
C	-1.7579020	-1.4914650	0.0130800
C	-2.7288000	-1.0726750	-1.1099790
C	-4.0033890	-1.8971240	-1.2521120
O	-1.2811350	1.4954170	-0.0983830
O	-3.1256740	-0.9194750	1.9318680
O	-0.4634700	-1.3616350	-0.5607690
O	-3.1165950	0.2680690	-0.8252500
O	-4.8804320	-1.7022370	-0.1583140
H	-4.2549410	1.3133070	1.2845760
H	-2.7917430	2.0347230	1.9788550
H	-2.7283320	3.1562570	-0.1704100
H	-1.2194520	-0.2803890	1.7764150
H	-3.8261020	-1.2973750	1.3765960
H	-1.9132210	-2.5176810	0.3700720
H	-2.1772980	-1.1088710	-2.0574270
H	-4.5031190	-1.6212730	-2.1877660
H	-3.7642530	-2.9631670	-1.2915380
H	-0.6994710	0.9727540	-0.6778150
H	0.8075140	1.9341200	0.8967630
C	0.6448110	-1.5279600	0.2619600
C	1.8216840	-1.8323820	-0.6606040

C	3.1206010	-1.7727810	0.1163390
C	3.2510910	-0.4166210	0.7848310
C	2.0464680	-0.1820300	1.6884600
C	1.9921360	1.2350250	2.2507390
O	1.7166170	-3.1265770	-1.2141700
O	4.2390250	-1.9414890	-0.7270520
O	4.4093560	-0.3496870	1.5811170
O	0.8472800	-0.3215690	0.9505560
O	1.6816970	2.1703190	1.2426540
H	0.4839950	-2.3572270	0.9762120
H	1.8299200	-1.0588530	-1.4392940
H	0.9847190	-3.1284270	-1.8380820
H	3.1148560	-2.5532230	0.8960950
H	4.1120150	-2.7550740	-1.2269730
H	3.2587350	0.3601110	0.0064050
H	2.0862550	-0.9067750	2.5181690
H	1.2464960	1.2710900	3.0559720
H	2.9684970	1.4980540	2.6633430
H	5.1446450	-0.6753550	1.0504310
O	1.0359110	1.1643940	-1.7416230
C	1.6454150	2.2119060	-1.6999280
C	0.9608500	3.5259680	-1.4220150
C	3.1365860	2.2643900	-1.9173450
H	1.4600060	4.0277490	-0.5882690
H	1.0501030	4.1710210	-2.3021110
H	-0.0908600	3.3618030	-1.1880030

H	3.5125800	1.2919600	-2.2376380
H	3.6064680	2.5514620	-0.9699730
H	3.3913290	3.0315250	-2.6540720

7$_{Ace}$ – E = -1490.711588 Hartree

Symbol	X	Y	Z
O	1.7660850	3.6378010	-0.3788990
H	4.8372720	-0.4313760	0.5308410
C	1.5264680	2.4924090	-1.1206600
C	2.0119250	1.2246100	-0.4586690
C	1.9388280	-0.0334780	-1.3287120
C	1.7295840	-1.3600400	-0.5674630
C	2.8059900	-1.9311350	0.3745280
C	4.1922150	-2.0801420	-0.2553330
O	2.4680280	1.2295410	0.6628880
O	3.0445940	-0.0507180	-2.1938890
O	0.5469020	-1.2858740	0.2208070
O	2.9269250	-1.2519120	1.5977410
O	4.8576090	-0.8324660	-0.3472600
H	2.0292760	2.5806940	-2.0909980
H	0.4545560	2.3274920	-1.3254380
H	1.3198770	3.5148800	0.4697900
H	1.0612880	0.0825600	-1.9749260
H	3.8542030	-0.1105530	-1.6554270
H	1.5950750	-2.1195330	-1.3541830
H	2.4491880	-2.9432540	0.6108140

H	4.7772850	-2.7674020	0.3660030
H	4.1336280	-2.4866240	-1.2689220
H	2.7489340	-0.3070730	1.4396230
H	-1.6956750	2.5506910	-0.1588290
C	-0.6622090	-1.2409030	-0.4512230
C	-1.7125690	-1.8686980	0.4557140
C	-3.0667840	-1.7889670	-0.2213230
C	-3.3774400	-0.3563350	-0.6234180
C	-2.2252870	0.2224550	-1.4431820
C	-2.4244950	1.6953270	-1.7659270
O	-1.4382850	-3.2246690	0.7089090
O	-4.1058020	-2.2270570	0.6247660
O	-4.5373290	-0.3003580	-1.4168030
O	-1.0070290	0.0993220	-0.7144330
O	-2.5471980	2.4905080	-0.6178660
H	-0.5969450	-1.8038500	-1.4021080
H	-1.7333900	-1.2868020	1.3896710
H	-0.5934410	-3.2789780	1.1681760
H	-3.0342700	-2.4065390	-1.1342930
H	-3.9078250	-3.1274970	0.9030670
H	-3.4928840	0.2512810	0.2857560
H	-2.1520330	-0.3378950	-2.3909270
H	-1.5942910	2.0292230	-2.4047140
H	-3.3528220	1.7946100	-2.3339140
H	-5.2427360	-0.7462340	-0.9359390
O	-0.3243570	2.5111120	1.2358870

C	-0.6432510	1.7597540	2.1365430
C	0.3826120	0.9773420	2.9092060
C	-2.0865410	1.5796360	2.5296740
H	1.3429030	1.4923980	2.8966490
H	0.0516260	0.7804700	3.9308730
H	0.5107470	0.0135320	2.3970430
H	-2.7534480	2.0042980	1.7792970
H	-2.2356110	2.0944150	3.4861050
H	-2.3159100	0.5242320	2.7035880

TS7$_{Ace}$ – E = -1490.653449 Hartree

Symbol	X	Y	Z
O	-3.5569800	2.9130230	0.2569240
H	-5.1907130	-0.7901660	-0.2156660
C	-3.2986480	1.7760140	1.0378610
C	-2.4206090	0.7766600	0.2993170
C	-2.0675330	-0.4753440	1.1251720
C	-1.7579020	-1.4914650	0.0130800
C	-2.7288000	-1.0726750	-1.1099790
C	-4.0033890	-1.8971240	-1.2521120
O	-1.2811350	1.4954170	-0.0983830
O	-3.1256740	-0.9194750	1.9318680
O	-0.4634700	-1.3616350	-0.5607690
O	-3.1165950	0.2680690	-0.8252500
O	-4.8804320	-1.7022370	-0.1583140
H	-4.2549410	1.3133070	1.2845760

H	-2.7917430	2.0347230	1.9788550
H	-2.7283320	3.1562570	-0.1704100
H	-1.2194520	-0.2803890	1.7764150
H	-3.8261020	-1.2973750	1.3765960
H	-1.9132210	-2.5176810	0.3700720
H	-2.1772980	-1.1088710	-2.0574270
H	-4.5031190	-1.6212730	-2.1877660
H	-3.7642530	-2.9631670	-1.2915380
H	-0.6994710	0.9727540	-0.6778150
H	0.8075140	1.9341200	0.8967630
C	0.6448110	-1.5279600	0.2619600
C	1.8216840	-1.8323820	-0.6606040
C	3.1206010	-1.7727810	0.1163390
C	3.2510910	-0.4166210	0.7848310
C	2.0464680	-0.1820300	1.6884600
C	1.9921360	1.2350250	2.2507390
O	1.7166170	-3.1265770	-1.2141700
O	4.2390250	-1.9414890	-0.7270520
O	4.4093560	-0.3496870	1.5811170
O	0.8472800	-0.3215690	0.9505560
O	1.6816970	2.1703190	1.2426540
H	0.4839950	-2.3572270	0.9762120
H	1.8299200	-1.0588530	-1.4392940
H	0.9847190	-3.1284270	-1.8380820
H	3.1148560	-2.5532230	0.8960950
H	4.1120150	-2.7550740	-1.2269730

H	3.2587350	0.3601110	0.0064050
H	2.0862550	-0.9067750	2.5181690
H	1.2464960	1.2710900	3.0559720
H	2.9684970	1.4980540	2.6633430
H	5.1446450	-0.6753550	1.0504310
O	1.0359110	1.1643940	-1.7416230
C	1.6454150	2.2119060	-1.6999280
C	0.9608500	3.5259680	-1.4220150
C	3.1365860	2.2643900	-1.9173450
H	1.4600060	4.0277490	-0.5882690
H	1.0501030	4.1710210	-2.3021110
H	-0.0908600	3.3618030	-1.1880030
H	3.5125800	1.2919600	-2.2376380
H	3.6064680	2.5514620	-0.9699730
H	3.3913290	3.0315250	-2.6540720

8$_{\mathbf{Ace}}$ – E = -1490.719012 Hartree

Symbol	X	Y	Z
O	-3.5569800	2.9130230	0.2569240
H	-5.1907130	-0.7901660	-0.2156660
C	-3.2986480	1.7760140	1.0378610
C	-2.4206090	0.7766600	0.2993170
C	-2.0675330	-0.4753440	1.1251720
C	-1.7579020	-1.4914650	0.0130800
C	-2.7288000	-1.0726750	-1.1099790
C	-4.0033890	-1.8971240	-1.2521120

O	-1.2811350	1.4954170	-0.0983830
O	-3.1256740	-0.9194750	1.9318680
O	-0.4634700	-1.3616350	-0.5607690
O	-3.1165950	0.2680690	-0.8252500
O	-4.8804320	-1.7022370	-0.1583140
H	-4.2549410	1.3133070	1.2845760
H	-2.7917430	2.0347230	1.9788550
H	-2.7283320	3.1562570	-0.1704100
H	-1.2194520	-0.2803890	1.7764150
H	-3.8261020	-1.2973750	1.3765960
H	-1.9132210	-2.5176810	0.3700720
H	-2.1772980	-1.1088710	-2.0574270
H	-4.5031190	-1.6212730	-2.1877660
H	-3.7642530	-2.9631670	-1.2915380
H	-0.6994710	0.9727540	-0.6778150
H	0.8075140	1.9341200	0.8967630
C	0.6448110	-1.5279600	0.2619600
C	1.8216840	-1.8323820	-0.6606040
C	3.1206010	-1.7727810	0.1163390
C	3.2510910	-0.4166210	0.7848310
C	2.0464680	-0.1820300	1.6884600
C	1.9921360	1.2350250	2.2507390
O	1.7166170	-3.1265770	-1.2141700
O	4.2390250	-1.9414890	-0.7270520
O	4.4093560	-0.3496870	1.5811170
O	0.8472800	-0.3215690	0.9505560

O	1.6816970	2.1703190	1.2426540
H	0.4839950	-2.3572270	0.9762120
H	1.8299200	-1.0588530	-1.4392940
H	0.9847190	-3.1284270	-1.8380820
H	3.1148560	-2.5532230	0.8960950
H	4.1120150	-2.7550740	-1.2269730
H	3.2587350	0.3601110	0.0064050
H	2.0862550	-0.9067750	2.5181690
H	1.2464960	1.2710900	3.0559720
H	2.9684970	1.4980540	2.6633430
H	5.1446450	-0.6753550	1.0504310
O	1.0359110	1.1643940	-1.7416230
C	1.6454150	2.2119060	-1.6999280
C	0.9608500	3.5259680	-1.4220150
C	3.1365860	2.2643900	-1.9173450
H	1.4600060	4.0277490	-0.5882690
H	1.0501030	4.1710210	-2.3021110
H	-0.0908600	3.3618030	-1.1880030
H	3.5125800	1.2919600	-2.2376380
H	3.6064680	2.5514620	-0.9699730
H	3.3913290	3.0315250	-2.6540720

TS8$_{Ace}$ – *E* = -1490.605955 Hartree

Symbol	X	Y	Z
O	-2.7735750	2.4829230	0.7308350
H	-5.1746510	-2.7996510	0.9215580

C	-2.8889980	1.7141070	-0.4142490
C	-2.6509840	0.3054740	-0.2334360
C	-1.8441600	-0.3465240	0.8587070
C	-1.5702250	-1.7607140	0.2732440
C	-2.6368280	-1.8934680	-0.8272680
C	-3.8164460	-2.7796950	-0.5014570
O	-0.5935370	0.9631380	-1.4373690
O	-2.6279100	-0.4132310	2.0216360
O	-0.3418520	-1.9974180	-0.3651940
O	-3.1486490	-0.5492780	-1.0535510
O	-4.3380020	-2.3630950	0.7455600
H	-1.9372350	1.7530690	-1.1230050
H	-3.7912860	1.9179030	-0.9986100
H	-1.9115980	2.9447770	0.7370780
H	-0.9431630	0.2208880	1.0666350
H	-3.3901710	-0.9860440	1.8604400
H	-1.7239080	-2.4891510	1.0811940
H	-2.1630790	-2.2034280	-1.7601110
H	-4.5676500	-2.6862820	-1.2938050
H	-3.4661830	-3.8189250	-0.4599100
H	-0.3149130	0.6208210	-2.2918380
H	0.8497910	1.4140590	-0.8152020
C	0.8310460	-1.8502050	0.3854390
C	1.9391580	-2.4506910	-0.4711960
C	3.2890840	-2.0796840	0.1037590
C	3.4092060	-0.5671390	0.1313680

C	2.2824880	0.0333830	0.9661060
C	2.1218710	1.5334100	0.7250310
O	1.8542780	-3.8589560	-0.5134120
O	4.3439270	-2.5836450	-0.6849290
O	4.6234950	-0.1678230	0.7237870
O	1.0163730	-0.4938560	0.6086890
O	1.7555780	1.8068880	-0.5935080
H	0.7439980	-2.4049590	1.3397450
H	1.8483150	-2.0174390	-1.4775890
H	1.0537590	-4.0995260	-0.9883570
H	3.3673310	-2.4661080	1.1339830
H	4.2001250	-3.5284990	-0.8033190
H	3.3279780	-0.1855130	-0.8967060
H	2.5001640	-0.1629750	2.0279930
H	1.3754050	1.9152980	1.4399390
H	3.0812340	2.0212080	0.9333640
H	5.3343590	-0.6149310	0.2526860
O	-0.3371160	3.7146690	0.8189280
C	0.3089350	4.1792630	-0.0997550
C	-0.2374230	4.2200560	-1.5009520
C	1.6823970	4.7498480	0.1249260
H	0.2092950	5.0232780	-2.0901180
H	0.0014700	3.2523460	-1.9576350
H	-1.3247090	4.3223320	-1.4751270
H	2.0207270	4.5315110	1.1378300
H	1.6442910	5.8344350	-0.0258520

H	2.3714980	4.3244520	-0.6086310

9$_{Ace}$ – E = -1414.282746 Hartree

Symbol	X	Y	Z
O	3.6903870	0.4426690	2.2570720
H	3.6834600	-0.7584570	-1.4832330
C	2.6789930	0.9288130	1.4779930
C	1.9321850	0.1698400	0.6858210
C	0.8546690	0.5952560	-0.2836880
C	0.2292690	-0.7710940	-0.6506380
C	1.3486890	-1.7796130	-0.3707630
C	2.2564180	-2.0759390	-1.5587930
O	1.3270470	1.3005740	-1.4044910
O	-0.8578830	-1.0953640	0.2027710
O	2.1182490	-1.1954190	0.6796060
O	2.8964710	-0.9163890	-2.0406090
H	2.5460780	1.9998990	1.5408010
H	3.7335520	-0.5124060	2.1145100
H	0.1020680	1.2253960	0.1876250
H	1.9474260	0.7146590	-1.8676470
H	-0.0957200	-0.7733400	-1.6979470
H	0.9227110	-2.7145950	0.0060060
H	3.0000720	-2.8205870	-1.2505810
H	1.6617910	-2.5026630	-2.3742160
H	-2.3104180	2.7272910	0.9280410
C	-2.1065220	-0.7172090	-0.2568940

C	-3.1472650	-1.3393910	0.6642330
C	-4.5252530	-0.9056070	0.2014720
C	-4.6078680	0.6106200	0.1410940
C	-3.4695660	1.1620640	-0.7167810
C	-3.3885600	2.6791930	-0.6729130
O	-3.1100870	-2.7465500	0.6211220
O	-5.5401530	-1.3541800	1.0704740
O	-5.8191600	1.0244150	-0.4440970
O	-2.2205910	0.6840630	-0.2326830
O	-3.1236730	3.1469150	0.6288050
H	-2.2543670	-1.0755600	-1.2942380
H	-2.9644400	-0.9654750	1.6821560
H	-2.2451820	-3.0332950	0.9311370
H	-4.6925920	-1.3043630	-0.8131540
H	-5.4547260	-2.3091540	1.1613960
H	-4.5049360	1.0134570	1.1592270
H	-3.6223690	0.8371650	-1.7589170
H	-2.6143600	3.0096830	-1.3781120
H	-4.3503680	3.0961610	-0.9783920
H	-6.5355530	0.5970040	0.0373360
O	5.0603550	-0.6250880	-0.3575310
C	5.5712070	0.4088450	0.0220940
C	5.1251820	1.7541830	-0.4861750
C	6.6969170	0.3984360	1.0218500
H	5.0290270	2.4571810	0.3458270
H	5.8977480	2.1456630	-1.1573400

H	4.1765970	1.6782260	-1.0186520
H	7.0471130	-0.6199380	1.1873030
H	6.3201710	0.8183110	1.9599060
H	7.5185600	1.0341690	0.6801740

TS9$_{Ace}$ – E = -1414.219409 Hartree

Symbol	X	Y	Z
O	-3.0917540	1.3434630	-1.3850480
H	-3.5001630	-1.5536620	1.2293980
C	-3.0309550	0.1112200	-1.7035190
C	-2.0031350	-0.6749350	-1.2288820
C	-0.9847210	-0.0848730	-0.4458920
C	-0.2365400	-1.2303860	0.2099290
C	-1.1493890	-2.4401930	-0.0846080
C	-1.9799020	-2.8142030	1.1356140
O	-1.7925140	0.9001020	0.7880620
O	1.0288960	-1.4209250	-0.3972750
O	-2.0031580	-2.0702070	-1.1601320
O	-2.6547240	-1.6970840	1.6762060
H	-3.8370170	-0.3380800	-2.3011000
H	-2.3947090	1.2970880	0.0513320
H	-0.4099960	0.7662570	-0.7901040
H	-2.3461440	0.2666200	1.2866930
H	-0.1135520	-1.0646430	1.2878200
H	-0.5460430	-3.2974490	-0.3999930
H	-2.6855670	-3.6057690	0.8611560

H	-1.3154330	-3.2015660	1.9168700
H	1.8262760	2.5851950	-1.3311630
C	2.0780230	-0.7520130	0.2125900
C	3.3700750	-1.2105300	-0.4487460
C	4.5266920	-0.4542120	0.1780480
C	4.2956820	1.0444810	0.0748830
C	2.9335180	1.4068470	0.6655210
C	2.5668940	2.8633950	0.4339950
O	3.6041070	-2.5839140	-0.2448820
O	5.7508900	-0.7412920	-0.4573680
O	5.2717700	1.7536780	0.7989620
O	1.9131120	0.6335750	0.0440740
O	2.4822250	3.1694220	-0.9373400
H	2.0991060	-0.9876890	1.2944540
H	3.3073320	-0.9688170	-1.5195940
H	2.8992370	-3.0788320	-0.6743070
H	4.5812060	-0.7258270	1.2456390
H	5.8770570	-1.6960560	-0.4464660
H	4.3047170	1.3337370	-0.9860170
H	2.9528080	1.2064940	1.7492680
H	1.6187080	3.0724770	0.9475500
H	3.3481120	3.4969080	0.8589740
H	6.1351740	1.4598410	0.4893280
O	-4.6213720	0.0651260	0.9943990
C	-5.1759650	0.9916150	0.4393580
C	-4.9269400	2.4187290	0.8513700

C	-6.1426710	0.7735850	-0.6937300
H	-4.1850420	2.4598630	1.6495330
H	-4.5777900	2.9803570	-0.0197790
H	-5.8613740	2.8739350	1.1944750
H	-6.2793380	-0.2920380	-0.8768320
H	-5.7367670	1.2629580	-1.5848540
H	-7.1046010	1.2419970	-0.4651450

10$_{Ace}$ – E = -1337.856552 Hartree

Symbol	X	Y	Z
O	3.2587210	1.7990600	1.7565250
H	3.5467490	-1.4599940	-1.1642200
C	3.2304780	0.5980840	1.8523500
C	2.2411430	-0.2394530	1.1374060
C	1.1721860	0.1433010	0.4399250
C	0.5012190	-1.0919050	-0.0915450
C	1.4772260	-2.2037710	0.3482870
C	2.2070790	-2.8421360	-0.8221420
O	-0.7804360	-1.3375590	0.4841120
O	2.4603640	-1.5764980	1.1934080
O	2.8098080	-1.8779840	-1.6425100
H	3.9569590	0.0414150	2.4718840
H	0.8347180	1.1568180	0.2940950
H	0.3980460	-1.0723550	-1.1851380
H	0.9498700	-2.9558080	0.9426490
H	2.9394940	-3.5635200	-0.4365710

H	1.4790850	-3.3877110	-1.4333140
H	-1.7932380	2.5650690	1.2681630
C	-1.8377050	-0.7495500	-0.1829610
C	-3.1271720	-1.2551000	0.4499620
C	-4.3020790	-0.5780520	-0.2297470
C	-4.1534890	0.9321200	-0.1542370
C	-2.7966640	1.3517950	-0.7184820
C	-2.5112740	2.8295750	-0.5054970
O	-3.2835000	-2.6440300	0.2779880
O	-5.5291440	-0.9164840	0.3748690
O	-5.1456380	1.5738390	-0.9186970
O	-1.7521640	0.6504210	-0.0557330
O	-2.4401590	3.1522890	0.8624110
H	-1.8106290	-1.0174490	-1.2573720
H	-3.1103450	-0.9831470	1.5154050
H	-2.5497660	-3.0866360	0.7161430
H	-4.3085060	-0.8753720	-1.2917910
H	-5.6025550	-1.8767470	0.3849020
H	-4.2063650	1.2427070	0.8994700
H	-2.7801410	1.1293910	-1.7980260
H	-1.5756430	3.0851720	-1.0223580
H	-3.3245380	3.4163720	-0.9374350
H	-5.9998370	1.2349430	-0.6301300
O	4.8496910	-0.2782250	-0.4677260
C	4.8125880	0.9001320	-0.7600690
C	5.8472310	1.8644250	-0.2432370

C	3.7070580	1.4749740	-1.6058310
H	6.3362690	2.3732120	-1.0790910
H	5.3464330	2.6272710	0.3619300
H	6.5858010	1.3371770	0.3597040
H	3.0858170	0.6815860	-2.0231310
H	4.1173880	2.1049070	-2.3997730
H	3.0976490	2.1174310	-0.9582580

TS10$_{Ace}$ – *E* = -1337.777658 Hartree

Symbol	X	Y	Z
O	-6.0055900	-0.0876660	2.3097980
H	-0.9887450	-2.7720940	-0.5420930
C	-5.7398910	-0.3290650	1.1675630
C	-4.3220790	-0.3341530	0.6906180
C	-3.1615010	-0.0583930	1.4023900
C	-2.1396870	-0.1941380	0.4859070
C	-2.7120590	-0.5213120	-0.8186480
C	-2.1886540	-1.7203030	-1.6085550
O	-1.6677630	1.9355290	-0.8744970
O	-4.1261220	-0.6342620	-0.5567530
O	-1.9217740	-2.8323070	-0.8021090
H	-6.4992330	-0.5641720	0.4020830
H	-3.1175820	0.2049750	2.4460670
H	-1.0733060	-0.1285040	0.6396530
H	-2.5327740	0.4580850	-1.3710510
H	-2.9589140	-1.9888350	-2.3378710

H	-1.2991770	-1.3741240	-2.1387490
H	1.4180540	-2.1083380	0.2721410
C	-0.3778610	1.8436870	-1.1338570
C	0.4594990	2.4452640	0.0102230
C	1.9355360	2.2263470	-0.2164010
C	2.1953560	0.7356540	-0.3037370
C	1.3607620	0.1452250	-1.4421020
C	1.4814240	-1.3733420	-1.5432810
O	0.2143200	3.8267210	0.1129650
O	2.7395930	2.7347830	0.8343950
O	3.5671440	0.4742110	-0.5439700
O	0.0021540	0.4321670	-1.2550720
O	0.8198500	-2.0468800	-0.4897330
H	-0.0601720	2.3285210	-2.0880380
H	0.1568290	1.9323470	0.9391360
H	-0.7399160	3.9274710	-0.0078610
H	2.2276920	2.6998970	-1.1680540
H	2.4586530	3.6414450	0.9999770
H	1.8891050	0.2730110	0.6480780
H	1.7366910	0.5781300	-2.3870300
H	1.0100450	-1.7006110	-2.4753980
H	2.5425670	-1.6492970	-1.5860700
H	4.0606840	1.1649190	-0.0849750
O	2.7704020	-1.8137350	1.4821010
C	3.9533310	-1.6597550	1.2622690
C	4.6780680	-2.4502140	0.2057290

C	4.7661030	-0.6839310	2.0751080
H	4.9602150	-1.7613680	-0.5969970
H	5.5972750	-2.8788290	0.6163300
H	4.0376630	-3.2401590	-0.1882210
H	5.1835250	-1.2188410	2.9356690
H	4.1233970	0.1186820	2.4403910
H	5.5996290	-0.2802310	1.4965220

S7. References

(1) Paulsen, A. D.; Mettler, M. S.; Dauenhauer, P. J. *Energy Fuels* **2013**, *27*, 2126-2134.

(2) Nallar, M.; Wong, H.-W. *ACS Sustainable Chem. Eng.* **2019**, *7*, 9480-9488.

(3) Nallar, M.; Wong, H.-W. *Ind. Eng. Chem. Res.* **2019**, *58*, 10776-10784.

(4) Zhao, Y.; Truhlar, D. G. *Theor. Chem. Acc.* **2008**, *120*, 215-241.

(5) Frisch, M. J.; Trucks, G. W.; Schlegel, H. B.; Scuseria, G. E.; Robb, M. A.; Cheeseman, J. R.; Scalmani, G.; Barone, V.; Petersson, G. A.; Nakatsuji, H.; et al. *Gaussian 16*, Rev. C.01; Gaussian, Inc.: Wallingford, CT, 2016.

(6) Zhao, Y.; Truhlar, D. G. *J. Chem. Theory Comput.* **2008**, *4*, 1849-1868.

(7) Grimme, S.; Antony, J.; Ehrlich, S.; Krieg, H. *J. Chem. Phys.* **2010**, *132*, 154104.

(8) Goerigk, L.; Hansen, A.; Bauer, C.; Ehrlich, S.; Najibi, A.; Grimme, S. *Phys. Chem. Chem. Phys.* **2017**, *19*, 32184-32215.

(9) Breneman, C. M.; Wiberg, K. B. *J. Comput. Chem.* **1990**, *11*, 361-373.

(10) Schlegel, H. B. *J. Comput. Chem.* **1982**, *3*, 214-218.

(11) Hratchian, H. P.; Schlegel, H. B. *J. Chem. Phys.* **2004**, *120*, 9918-9924.

(12) Hratchian, H. P.; Schlegel, H. B. Chapter 10 - Finding minima, transition states, and following reaction pathways on ab initio potential energy surfaces. In *Theory and Applications of Computational Chemistry*, Dykstra, C. E., Frenking, G., Kim, K. S., Scuseria, G. E. Eds.; Elsevier, Amsterdam, 2005; pp 195-249.

(13) Hratchian, H. P.; Schlegel, H. B. *J. Chem. Theory Comput.* **2005**, *1*, 61-69.

(14) Grimme, S. *Chem.Eur. J.* **2012**, *18*, 9955-9964.

(15) Chai, J.-D.; Head-Gordon, M. *Phys. Chem. Chem. Phys.* **2008**, *10*, 6615-6620.

(16) Eyring, H. *J. Chem. Phys.* **1935**, *3*, 107-115.

(17) Evans, M. G.; Polanyi, M. *Trans. Faraday Soc.* **1935**, *31*, 875-894.

(18) *COMSOL Multiphysics® v. 6.0*, www.comsol.com: Stockholm, Sweden.