Supporting Information

Computational Insights into Selective Glucose to 5-Hydroxymethylfurfural (HMF) Conversion by Reducing Humins Formation in Aqueous Media Under Brønsted Acid-Catalyzed Conditions

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1. Different possible orientations of water and hydronium ions around glucose, fructose, and HMF

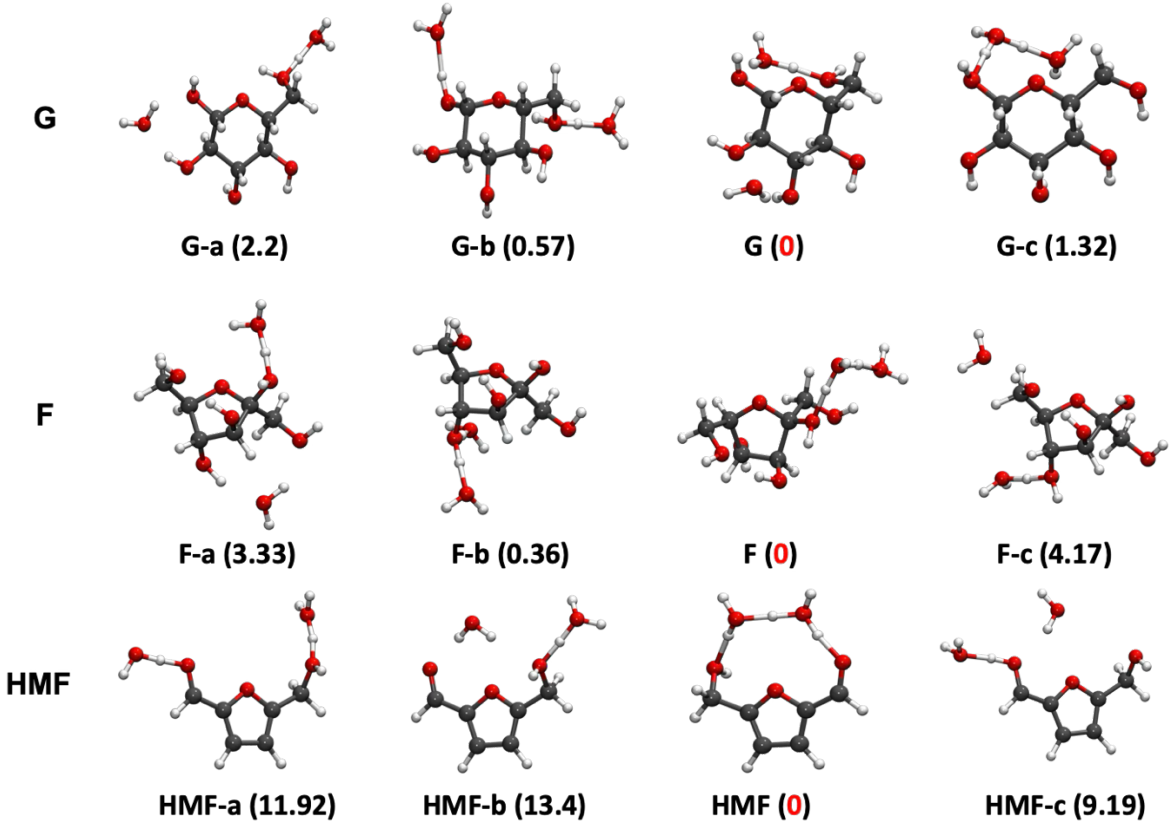


Figure S1: Different possible orientations of water and hydronium ions around glucose, fructose, and HMF. Relative (with respect to the lowest energy configuration) Gibbs free energies in kcal mol^{-1} of each configuration are given in parenthesis. Atom color codes: C (gray), O (red), H (white).

2. Effect of Implicit Solvent Model on the Free Energy Barriers

The free energy barriers computed using the PCM solvent model[1] were benchmarked by comparing them with that obtained using the SMD solvent model[2] for the condensation reactions between **G** and **F** (**G**+**F**→**I1**) and the addition reaction between **F** and **HMF** (**F**+**H**→**I3**). Since we noted that condensation reactions involving glucose and addition reactions involving **HMF** contribute majorly to polymerization, we selected these two reactions for the benchmark studies. We noted that the addition reaction has a lower free energy barrier, $\Delta\mathbf{G}^{\ddagger}$, as compared to the condensation reaction irrespective of the solvent model considered. In addition, $\Delta\mathbf{G}^{\ddagger}$ was found to be comparable in both PCM and SMD (Table S1, Table S2, and Figures S2, S3, S7, S12). We noted in passing that the level of theory used in this work (PCM-M06-2X/6-31+G(d,p)) was reported to have an accuracy of MP2 level of theory for the studies on the reactions involving carbohydrates.[3]

Table S1: Free energies, G (in a. u.) of the transition state (TS) and the free energy barriers ($\Delta G^{\ddagger}$) for the condensation reaction between glucose and fructose using PCM and SMD solvent models.

Solvent Model	G (au) of TS	$\Delta G^{\ddagger}$ (kcal mol^{-1})
PCM	-1526.764509	35.3
SMD	-1526.821658	36.58

Table S2: Free energies, G (in a. u.) of the transition state (TS) and free energy barrier ($\Delta G^{\ddagger}$) for the addition reaction between fructose and HMF using PCM and SMD solvent models.

Solvent Model	G (au) of TS	$\Delta G^{\ddagger}$ (kcal mol^{-1})
PCM	-1297.637211	19.81
SMD	-1297.675129	22.01

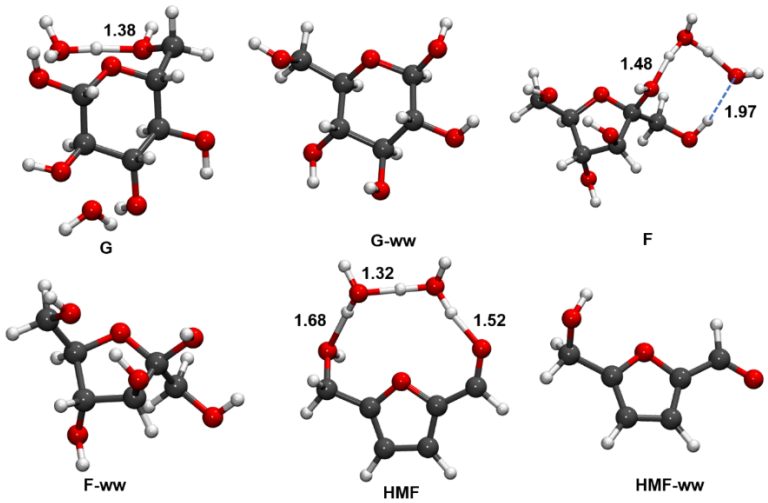


Figure S2: Optimized structures of **G**, **F,** and **HMF** in smd solvent model. "ww" represents the optimized structure without extra water molecules. Crucial distances are shown in Å. Atom color codes: C-grey, O-red, H-white.

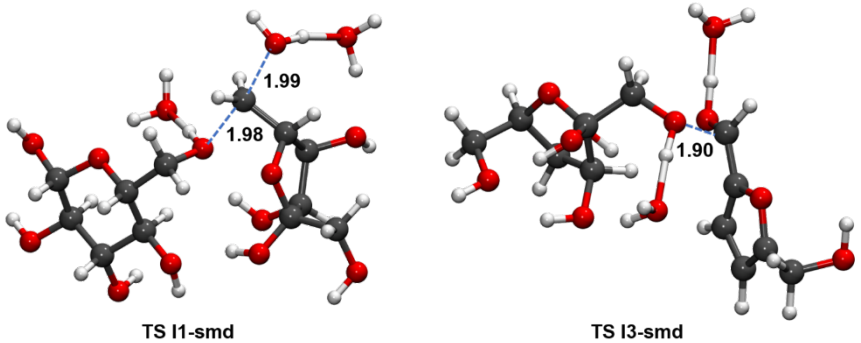


Figure S3: Optimized structures of the transition states for condensation reaction between **G** and **F** (**TS I1**) and addition reaction between **F** and **HMF** (**TS I3**) obtained in the presence of SMD

implicit solvent model. Crucial distances are shown in Å. Atom color codes are the same as those in Figure S2.

3. Free Energy Profile and Optimized Structures for G → FH3

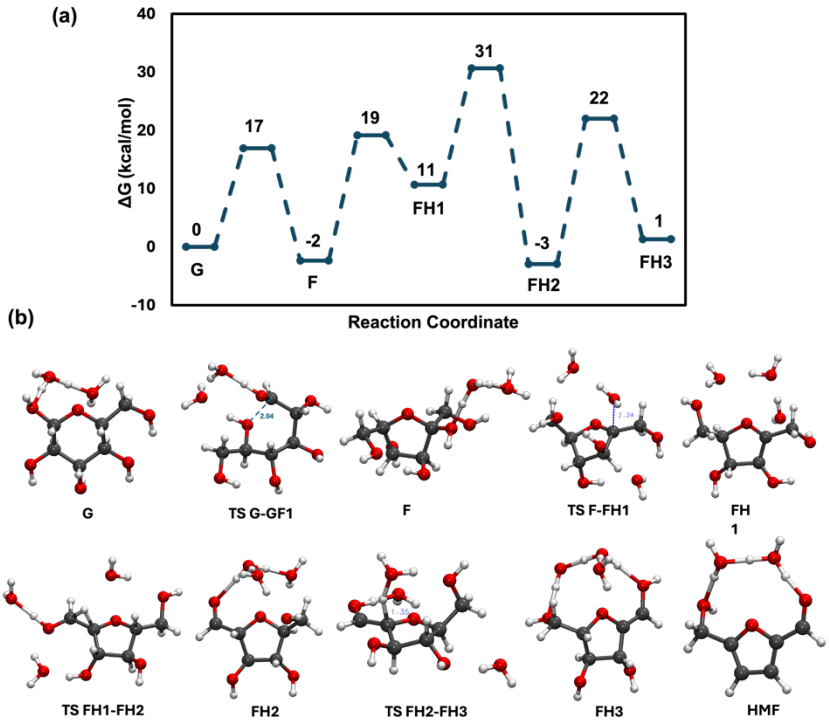


Figure S4: (a) Free energy profile for the **G → FH3** conversion, which is a crucial step in the Brønsted acid-catalyzed **G** to **HMF** conversion. Note that the free energy barrier shown for **G → F** corresponds to the effective free energy barrier for **GF1** formation from glucose; (b) Optimized structures of the minima and transition states involved in the acid-catalyzed **G** to **HMF** conversion. The name of the transition state structures begins with "TS". Crucial distances are shown in Å. Atom color codes: C-grey, O-red, H-white.

4. Microkinetic analysis of glucose to HMF conversion at 298 K.

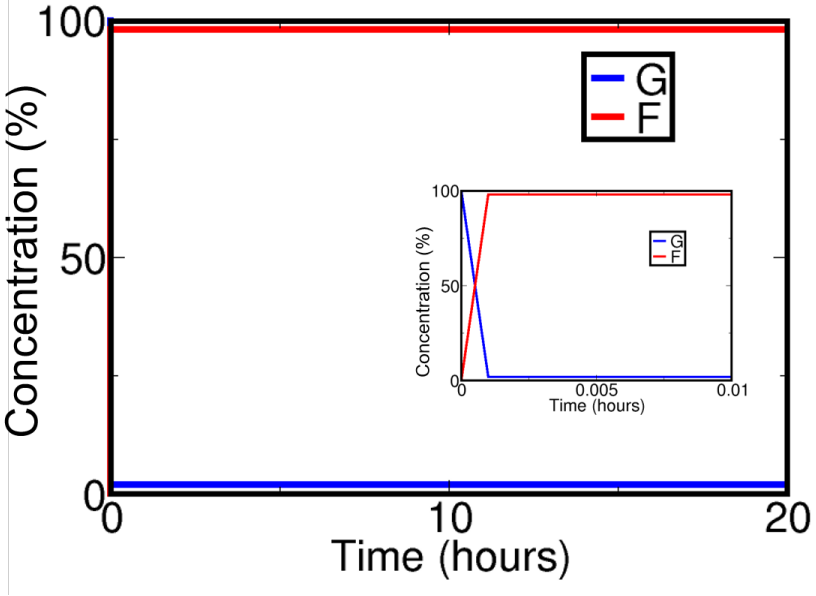


Figure S5: Kinetic profiles for glucose (**G**) and fructose (**F**) obtained from microkinetic analysis performed for the conversion of glucose to **HMF** at 298 K for the coupled reaction pathways in Figure 2 of the manuscript. **HMF** formation was found to be negligible (<1%) under this condition.

5. Free Energy Data

Table S3: Free energies, G (in a.u.) computed at 298.15 K for all the minima and transition states (TS) involved in the elementary reactions considered. "-c" in the name of the transition state represents condensation reaction and the name of the transition states without "-c" indicates the addition reaction. "smd" represent that the calculation is performed using SMD solvent model. "ww" represent the calculations without explicit water molecules in the structure. The transition state structures are indicated by "TS" at the beginning of the name.

	Free Energy (a.u.)
G	-840.006731
F	-840.008396
HMF	-610.843875
G-ww	-686.809974
F-ww	-686.814046
HMF-ww	-457.647912
DHH	-687.223683
THA	-1526.134384
DHE	-1068.494805
GD2.1	-763.621363
GD1.1b	-687.218612
I4	-1526.823134
TS I4	-1526.758612
I5	-1526.808603

	Free Energy (a.u.)
I3'	-1297.643657
TS I3'	-1297.634120
I3''	-1297.641616
TS I3''	-1297.632733
TS R1.2	-2900.386255
G-smd	-840.046013
F-smd	-840.045937
HMF-smd	-610.876586
G-ww-smd	-686.834016
F-ww-smd	-686.833638
HMF-ww-smd	-457.652774
TS I2-smd	-1297.644489
TS I3-smd	-1297.675129

TS I5	-1526.758898
I1	-1526.820623
TS I1	-1526.764509
I2	-1297.647674
TS I2	-1297.644489
I2'	-1297.644252
TS I2'	-1297.642145
GH-c	-1297.657772
TS GH	-1297.605125
I3	-1297.65062
TS I3	-1297.637211
FH-c	-1297.665426
TS FH-c	-1297.59918

G-ht	-840.032754
F-ht	-840.033817
HMF-ht	-610.875984
G-ww-ht	-686.83041
F-ww-ht	-686.83432
HMF-ww-ht	-457.663687
TS I1-ht	-1526.821658
TS I3-ht	-1297.671158
R1.1	-2060.427328
R2.1	-1831.255719
R3.1	-1831.252934
TS R2.2	-2442.090760
TS R3.2	-2442.074337

Table S4: Effective free energy barriers $\Delta G^{\ddagger}_{\text{eff}}$ (kcal mol^{-1}) for both forward and reverse reactions for the formation of different intermediates involved in the glucose to HMF conversion. Some of the barriers were taken from our previous study[6] performed at the same level of theory and the implicit solvent model.

Reaction	**$\Delta G^{\ddagger}_{\text{eff}}$**		**Reference**
	Forward	**Reverse**	
G → DHH	28	38	6
G → GD2.1	41	50	6
G → GD1.1b	28	35	6
GD2.1 → DHH	21	22	6
GD1.1b → DHH	18	21	6
F → DHH	32	41	6
F → GD2.1	42	50	6
F → GD1.1b	51	57	6
GD1.1b → GD2.1	19	21	6
HMF → GD1.1b	36	13	6
GD2.1 → HMF	21	42	6
HMF → DHE	38	33	6
HMF → THA	26	19	6
DHH → HMF	21	40	6
G → F	17	19	Current Study
F → HMF	33	52	Current Study

Table S5: Free energy barriers, $\Delta G^{\ddagger}$ (kcal mol^{-1}), and corresponding rate constants (hour^{-1}) for all the propagation routes (**PR1**-**PR15**) considered. Here the rate constants k_p, k_p', and k_p'' computed at 408 K correspond to free energy barrier $\Delta G^{\ddagger}_1$, $\Delta G^{\ddagger}_2$, and $\Delta G^{\ddagger}_3$, respectively.

Propagation route	**Free Energy barrier**			**Rate Constants**		
	$\Delta G^{\ddagger}_1$	$\Delta G^{\ddagger}_2$	$\Delta G^{\ddagger}_3$	k_p	k_p'	k_p''
PR1	35.3	35.3	-	3.77×10^{-03}	3.77×10^{-03}	-
PR2	31.07	12.68	-	6.95×10^{-01}	4.94×10^{09}	-

PR3	35.84	19.81	-	1.94×10^{-03}	7.48×10^{05}	-
PR4	36.48	-	-	8.79×10^{-04}	-	-
PR5	39.87	-	-	1.34×10^{-05}	-	-
PR6	22.8	-	-	1.87×10^{04}	-	-
PR7	31.07	35.3	19.81	6.95×10^{-01}	3.77×10^{-03}	7.48×10^{05}
PR8	35.3	31.07	19.81	3.77×10^{-03}	6.95×10^{-01}	7.48×10^{05}
PR9	31.07	12.68	36.48	6.95×10^{-01}	4.94×10^{09}	8.79×10^{-04}
PR10	35.84	19.81	39.87	1.94×10^{-03}	7.48×10^{05}	1.34×10^{-05}
PR11	31.07	22.8	12.68	6.95×10^{-01}	1.87×10^{04}	4.94×10^{09}
PR12	35.84	22.8	19.81	1.94×10^{-03}	1.87×10^{04}	7.48×10^{05}
PR13	35.84	31.07	-	1.94×10^{-03}	6.95×10^{-01}	-
PR14	38	12.68	-	1.35×10^{-04}	4.94×10^{09}	-
PR15	38	19.81	-	1.35×10^{-04}	7.48×10^{05}	-

Table S6: Free energy barriers, $\Delta G^{\ddagger}$ (kcal mol^{-1}), and corresponding rate constants (hour^{-1}) for all the termination reactions considered for polymerization under **T1** termination condition. Here the rate constants k_t, k_t', and k_t'' correspond to free energy barriers $\Delta G^{\ddagger}_1$, $\Delta G^{\ddagger}_2$, and $\Delta G^{\ddagger}_3$, respectively. Note that the termination steps are considered to be the last propagation steps. Therefore, the free energy barriers and corresponding rate constants given here are the same as that in Table S5.

Propagation route	**Free Energy barrier**			**Rate Constants**		
	$\Delta G^{\ddagger}_1$	$\Delta G^{\ddagger}_2$	$\Delta G^{\ddagger}_3$	k_t	k_t'	k_t''
PR1	35.3	35.3	-	3.77×10^{-03}	3.77×10^{-03}	-
PR2	31.07	12.68	-	6.95×10^{-01}	4.94×10^{09}	-
PR3	35.84	19.81	-	1.94×10^{-03}	7.48×10^{05}	-
PR4	36.48	-	-	8.79×10^{-04}	-	-
PR5	39.87	-	-	1.34×10^{-05}	-	-
PR6	22.8	-	-	1.87×10^{04}	-	-
PR7	31.07	35.3	19.81	6.95×10^{-01}	3.77×10^{-03}	7.48×10^{05}
PR8	35.3	31.07	19.81	3.77×10^{-03}	6.95×10^{-01}	7.48×10^{05}
PR9	31.07	12.68	36.48	6.95×10^{-01}	4.94×10^{09}	8.79×10^{-04}
PR10	35.84	19.81	39.87	1.94×10^{-03}	7.48×10^{05}	1.34×10^{-05}
PR11	31.07	22.8	12.68	6.95×10^{-01}	1.87×10^{04}	4.94×10^{09}
PR12	35.84	22.8	19.81	1.94×10^{-03}	1.87×10^{04}	7.48×10^{05}
PR13	35.84	31.07	-	1.94×10^{-03}	6.95×10^{-01}	-
PR14	38	12.68	-	1.35×10^{-04}	4.94×10^{09}	-
PR15	38	19.81	-	1.35×10^{-04}	7.48×10^{05}	-

Table S7: Free energy barriers, $\Delta G^{\ddagger}$ (kcal mol^{-1}), and the corresponding rate constants (hour^{-1}) for all the termination processes considered for polymerization under the **T2** termination condition. Here the rate constants k_t, k_t', and k_t'' correspond to free energy barrier $\Delta G^{\ddagger}_1$, $\Delta G^{\ddagger}_2$, and $\Delta G^{\ddagger}_3$, respectively.

Propagation route	**Free Energy barrier**			**Rate Constants**		
	$\Delta G^{\ddagger}_1$	$\Delta G^{\ddagger}_2$	$\Delta G^{\ddagger}_3$	k_t	k_t'	k_t''
PR1	35.3	35.3	-	2.88×10^{-10}	2.88×10^{-10}	-
PR2	31.07	12.68	-	3.65×10^{-07}	1.12×10^{07}	-

PR3	35.84	19.81	-	1.16×10^{-10}	6.61×10^{01}	-
PR4	36.48	-	-	3.93×10^{-11}	-	-
PR5	39.87	-	-	1.28×10^{-13}	-	-
PR6	22.8	-	-	4.24×10^{-01}	-	-
PR7	31.07	35.3	19.81	3.65×10^{-07}	2.88×10^{-10}	6.61×10^{01}
PR8	35.3	31.07	19.81	2.88×10^{-10}	3.65×10^{-07}	6.61×10^{01}
PR9	31.07	12.68	36.48	3.65×10^{-07}	1.12×10^{07}	3.93×10^{-11}
PR10	35.84	19.81	39.87	1.16×10^{-10}	6.61×10^{01}	1.28×10^{-13}
PR11	31.07	22.8	12.68	3.65×10^{-07}	4.24×10^{-01}	1.12×10^{07}
PR12	35.84	22.8	19.81	1.16×10^{-10}	4.24×10^{-01}	6.61×10^{01}
PR13	35.84	31.07	-	1.16×10^{-10}	3.65×10^{-07}	-
PR14	38	12.68	-	3.02×10^{-12}	1.12×10^{07}	-
PR15	38	19.81	-	3.02×10^{-12}	6.61×10^{01}	-

Table S8: The free energies of the transition state (TS) and free energy barriers $\Delta G^{\ddagger}$ at 298.15 and 408 K. Rate constants (in $hour^{-1}$) computed at 408 K using these barriers by employing Eyring equation are also given.

Reaction	**AT 298.15 K**			**AT 408 K**		
	G (au) of TS	$\Delta G^{\ddagger}$ (kcal mol^{-1})	k (at 408 K)	G (au) of TS	$\Delta G^{\ddagger}$ (kcal mol^{-1})	k' (at 408 K)
G + H → I2	-1297.644489	12.68	4.9×10^{9}	-1297.67535	19.48	1.1×10^{6}
F + H → I3	-1297.637211	19.81	7.4×10^{5}	-1297.671158	24.56	2.1×10^{3}
H + H → I6	-1068.480844	22.8	1.8×10^{4}	-1068.498497	25.83	4.4×10^{2}
G+F → I1	-1526.764509	35.3	3.7×10^{-3}	-1526.802169	38.94	4.2×10^{-5}
G + G → I4	-1526.75646	37.8	1.7×10^{-4}	-1526.797341	41.3	2.3×10^{-6}
F + F → I5	-1526.758898	39.87	1.3×10^{-5}	-1526.797465	44.34	5.4×10^{-8}

6. Mechanism of some of the crucial propagation pathways

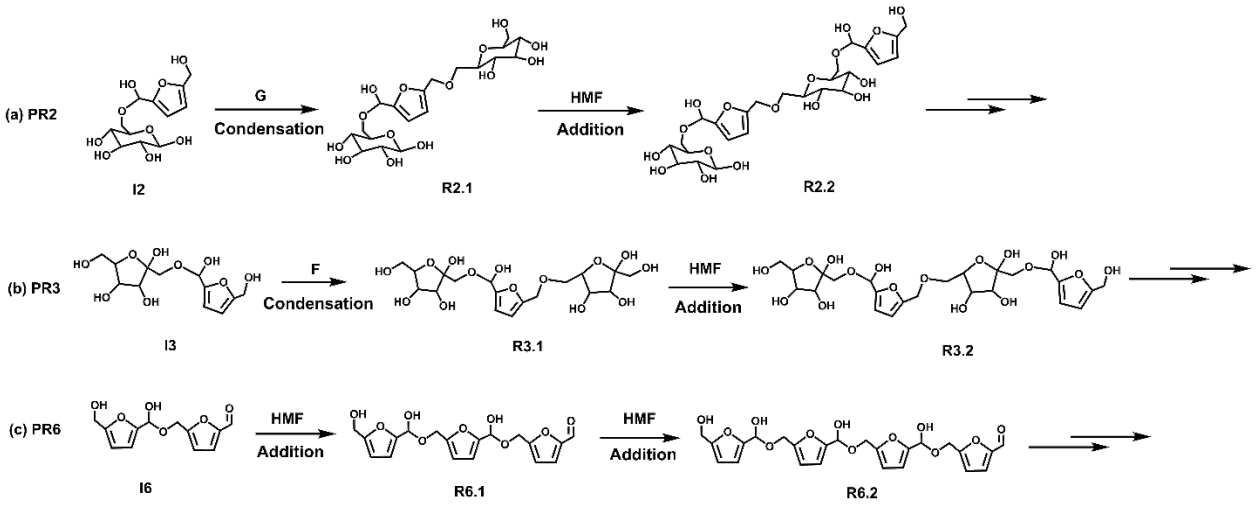


Figure S6: Propagation pathways (a) **PR2**, (b) **PR3**, and (c) **PR6** initiated by **I2**, **I3** and **I6**, respectively. Two solid arrows at the end of the mechanism indicate the continuation of the reaction in the same manner as the preceding steps.

7. Optimized Structures

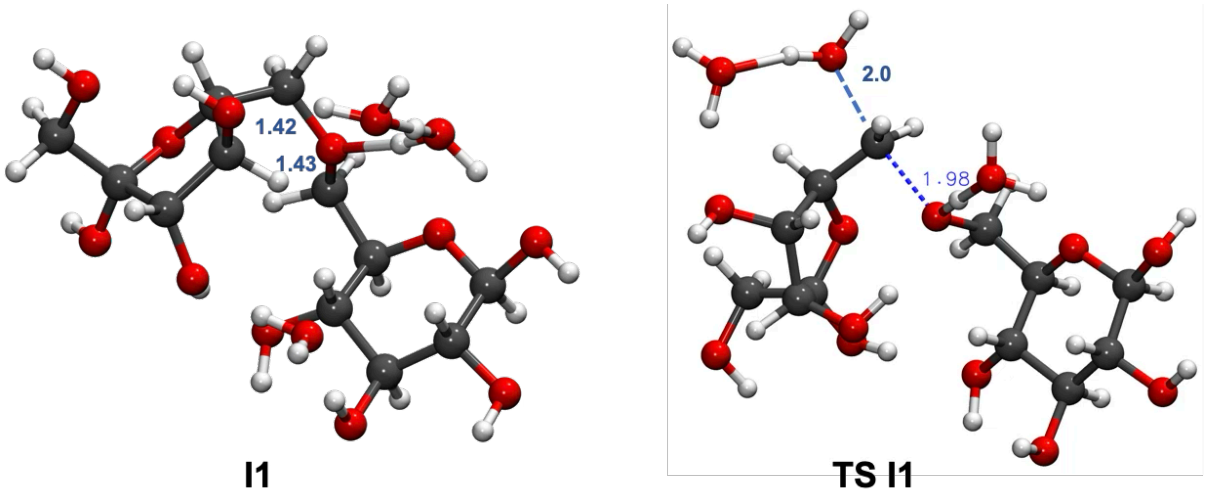


Figure S7: Optimized structures of minima and transition state of **G** and **F** condensation reaction. Crucial distances are shown in Å. The name of the transition state structures starts "TS". Atom color codes: C-grey, O-red, H-white.

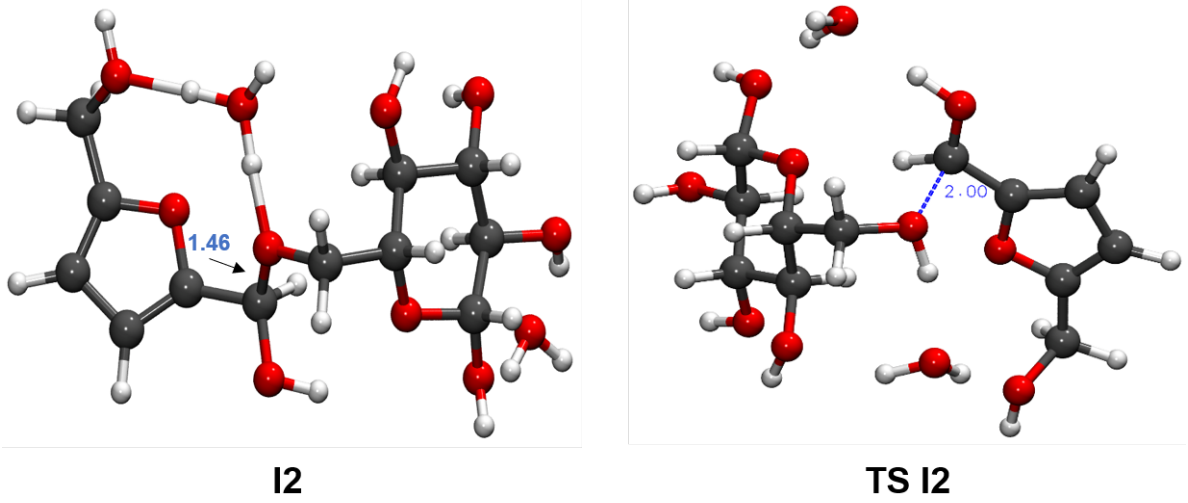


Figure S8: Optimized structures of minima and transition state of **G** and **HMF** addition reaction to form **I2**. The hydroxy methyl group bonded to C1 atom of **G** ring attack on carbonyl group of **HMF.** Crucial distances are shown in Å. All the descriptions and atom color codes are the same as those in Figure S7.

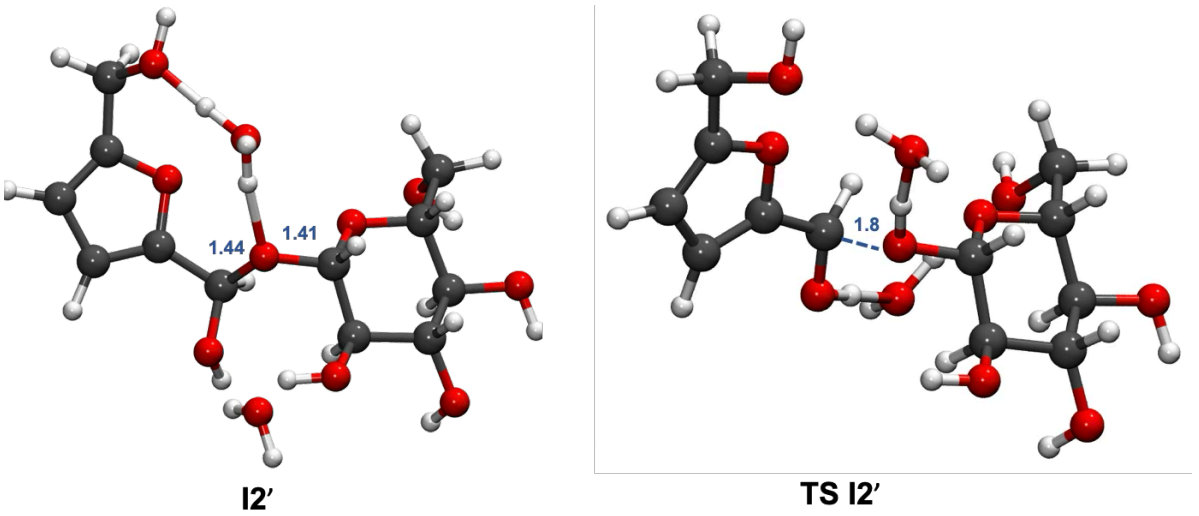


Figure S9: Optimized structures of minima and transition state for the addition reaction between **G** and **HMF**. The hydroxy group bonded to C5 atom of the **G** ring attacks on the carbonyl group of **HMF**. Crucial distances are shown in Å. All the descriptions and atom color codes are the same as those in Figure S7.

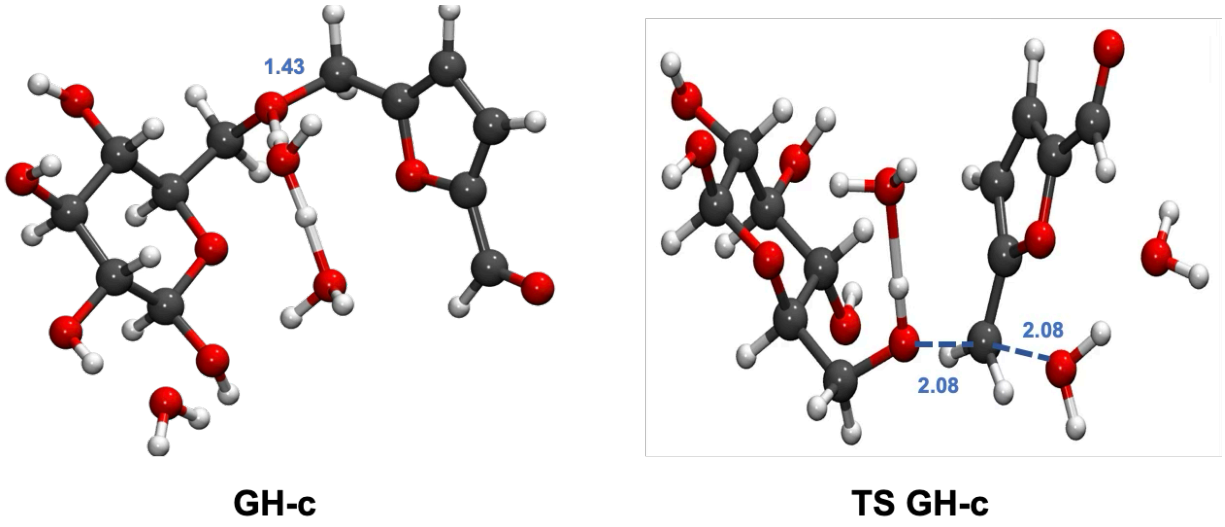


Figure S10: Optimized structures of the minima and transition state of **G** and **HMF** condensation reaction. The "c" in the name of minima and transition state represents the condensation reaction. Crucial distances are shown in Å. All the descriptions and atom color codes are the same as those in Figure S7.

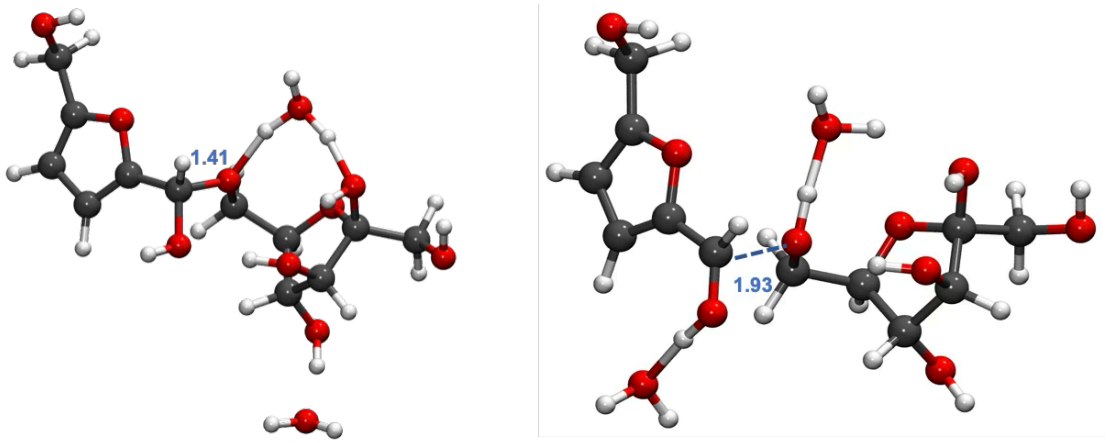


Figure S11: Optimized structures of the minima and transition state of **F** and **HMF** addition reaction. The hydroxy methyl group bonded to the C4 atom of the **F** ring attacks the carbonyl group of **HMF**. Crucial distances are shown in Å. All the descriptions and atom color codes are the same as those in Figure S7.

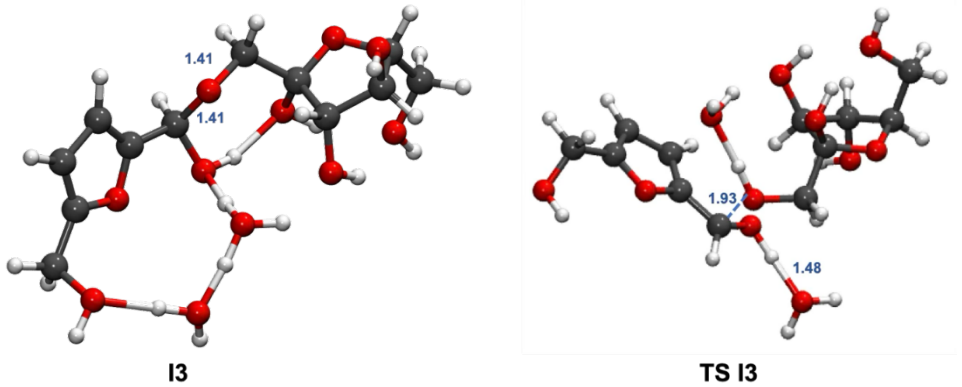


Figure S12: Optimized structures of minima and transition state of **F** and **HMF** addition reaction. The hydroxy methyl group bonded to the C1 atom of the **F** ring attack on the carbonyl group of **HMF**. Crucial distances are shown in Å. All the descriptions and atom color codes are the same as those in Figure S7.

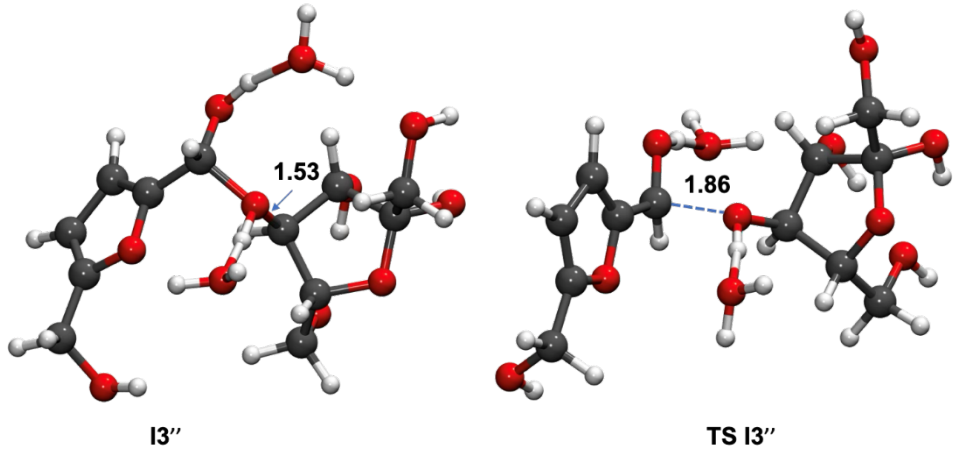


Figure S13: Optimized structures of minima and transition state of **F** and **HMF** addition reaction. The hydroxy group bonded to the C3 atom of the **F** ring attack on the carbonyl carbon of **HMF**. Crucial distances are shown in Å. All the descriptions and atom color codes are the same as those in Figure S7.

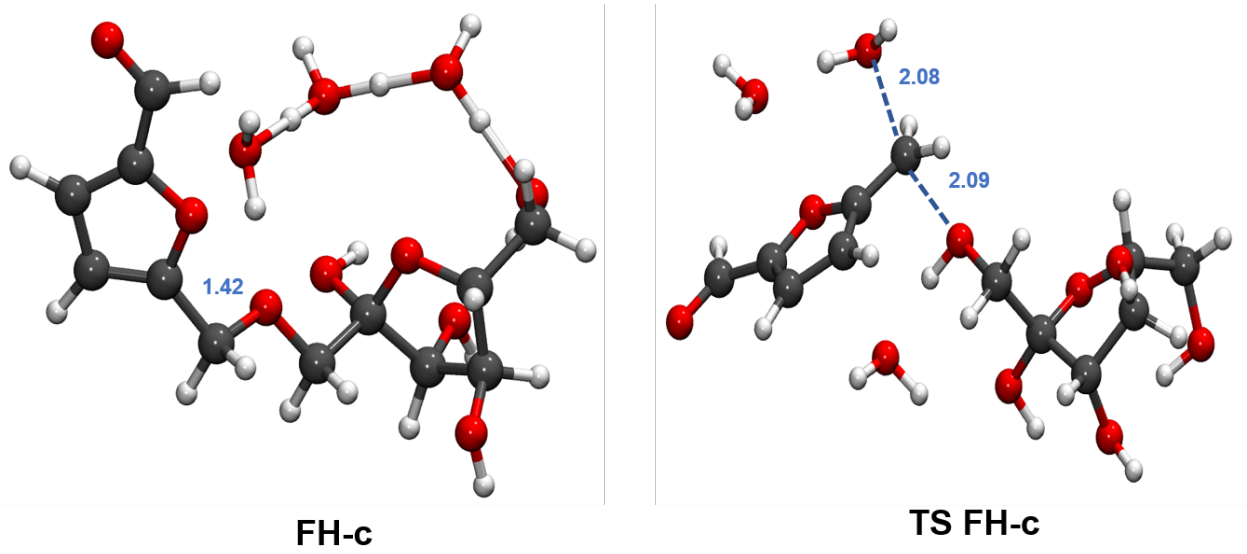


Figure S14: Optimized structures of minima and transition state of **F** and **HMF** condensation reaction. The "c" in the name of minima and transition state represents the condensation reaction. Crucial distances are shown in Å. All the descriptions and atom color codes are the same as those in Figure S7.

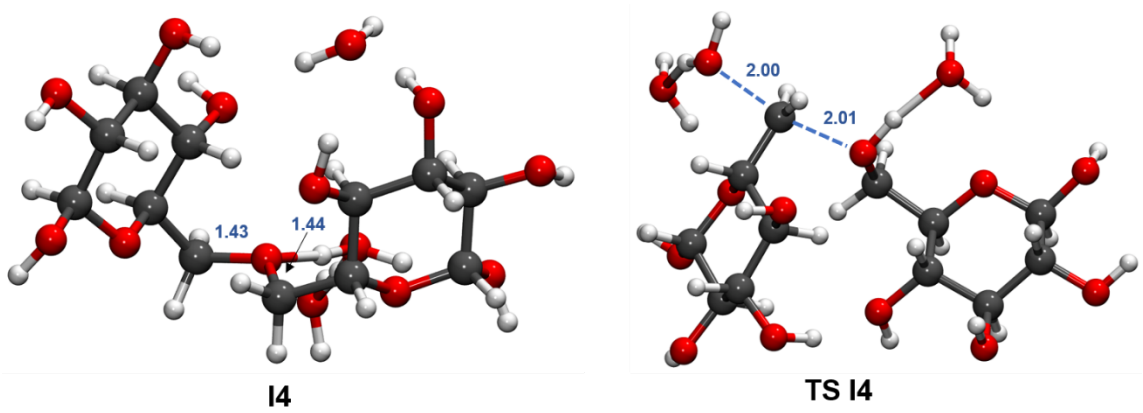


Figure S15: Optimized structure of **I4** and transition state for the condensation reaction between glucose molecules to form **I4**. Crucial distances are shown in Å. All the descriptions and atom color codes are the same as those in Figure S7.

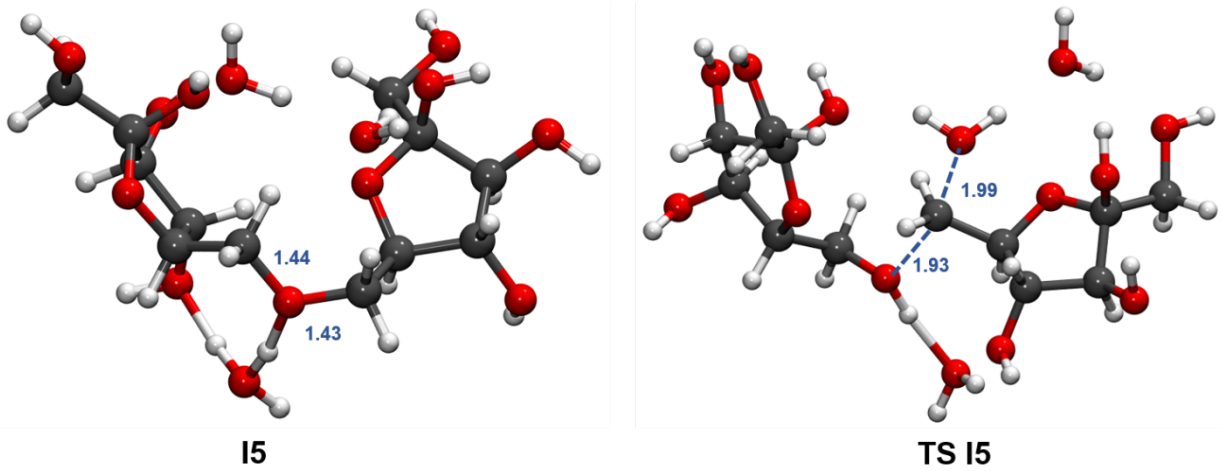


Figure S16: Optimized structures of **I5** and transition state for the condensation reaction between fructose molecules to form **I5**. Crucial distances are shown in Å. All the descriptions and atom color codes are the same as those in Figure S7.

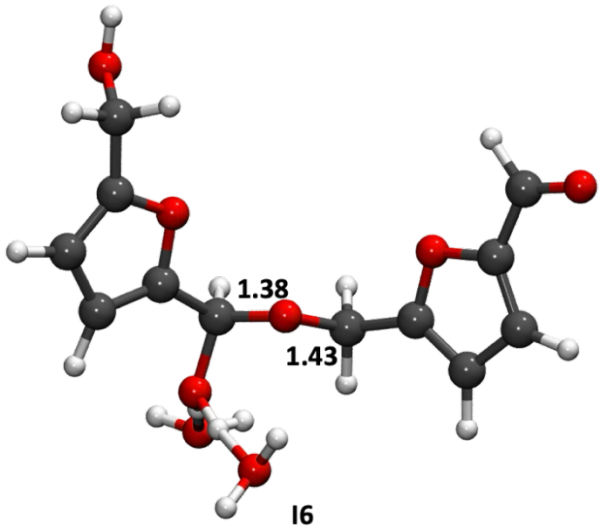


Figure S17: Optimized structure **I6** formed by the addition reaction between **HMF** molecules. Crucial distances are shown in Å. All the descriptions and atom color codes are the same as those in Figure S7.

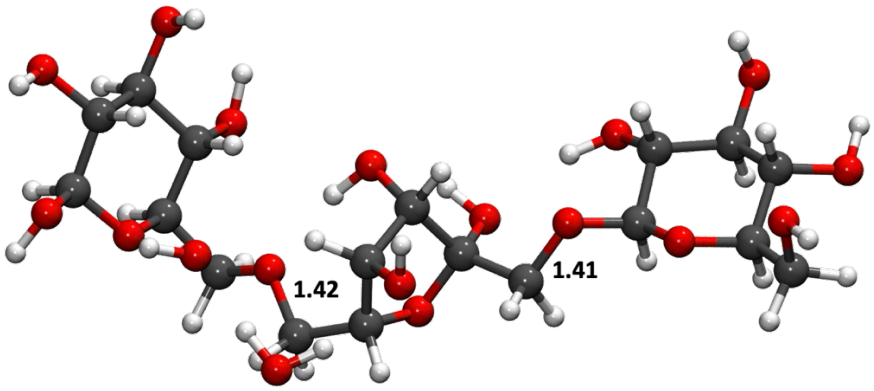


Figure S18: Optimized structure of **R1.1**. The condensation reaction of **I1** with **G** leads to **R1.1**. Crucial distances are shown in Å. All the descriptions and atom color codes are the same as those in Figure S7.

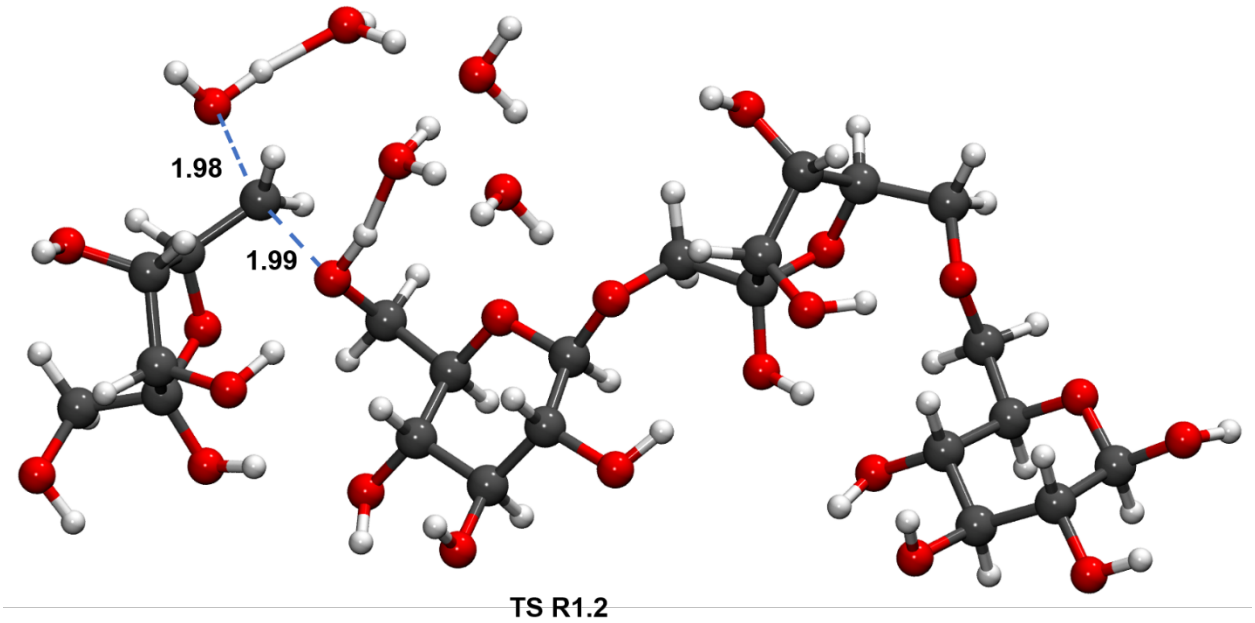


Figure S19: Optimized structures of the transition state for the condensation reaction of **G** moiety of **R1.1** with **F**. Crucial distances are shown in Å. All the descriptions and atom color codes are the same as those in Figure S7.

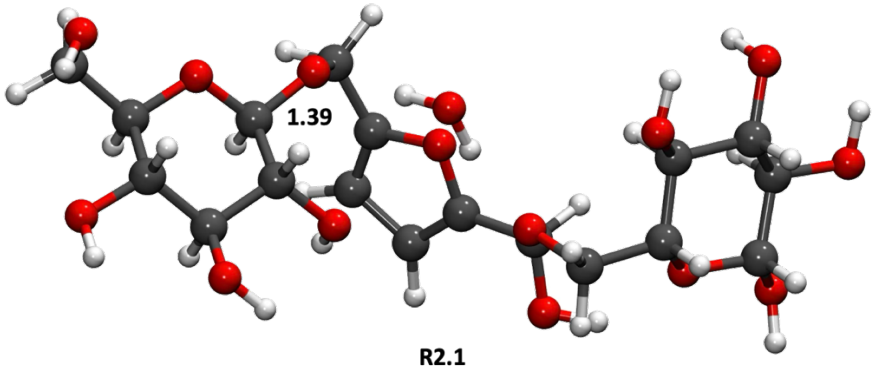


Figure S20: Optimized structure of **R2.1**. The condensation reaction of **I2** with **G** leads to **R2.1**. Crucial distances are shown in Å. All the descriptions and atom color codes are the same as those in Figure S7.

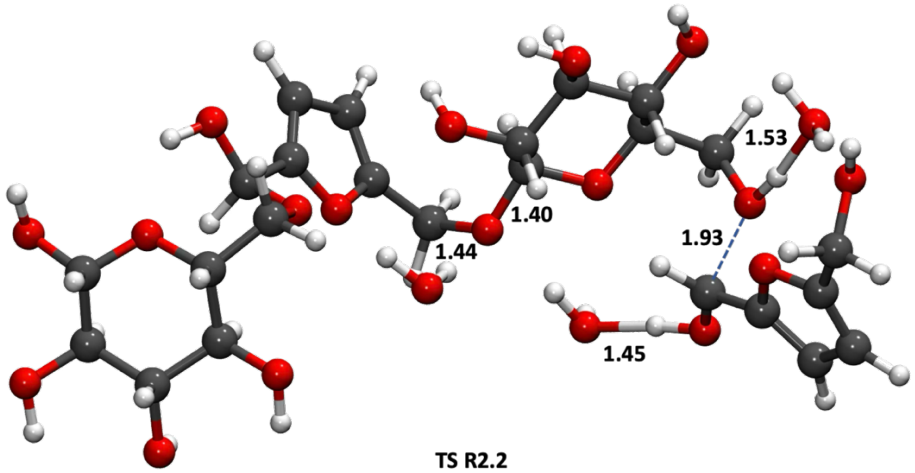


Figure S21: Optimized structure of the transition state for the addition reaction of **R2.1** with **HMF** that leads to **R2.2**. Crucial distances are shown in Å. All the descriptions and atom color codes are the same as those in Figure S7.

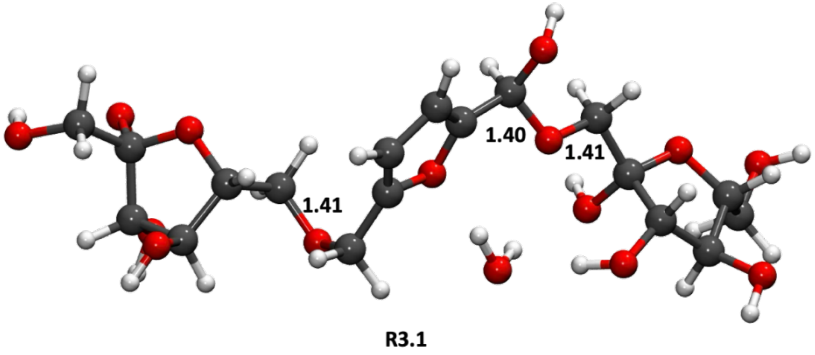


Figure S22: Optimized structure of **R3.1**. The condensation reaction of **I3** with **F** leads to **R3.1**. Crucial distances are shown in Å. All the descriptions and atom color codes are the same as those in Figure S7.

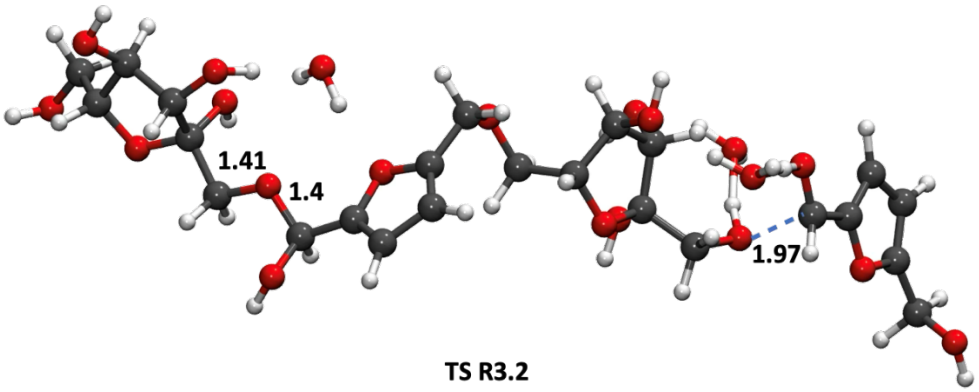


Figure S23: Optimized structure of the transition state for the addition reaction of **R3.1** with **HMF** that leads to **R3.2**. Crucial distances are shown in Å. All the descriptions and atom color codes are the same as those in Figure S7.

8. Chemical structures of P1, P5 and P8

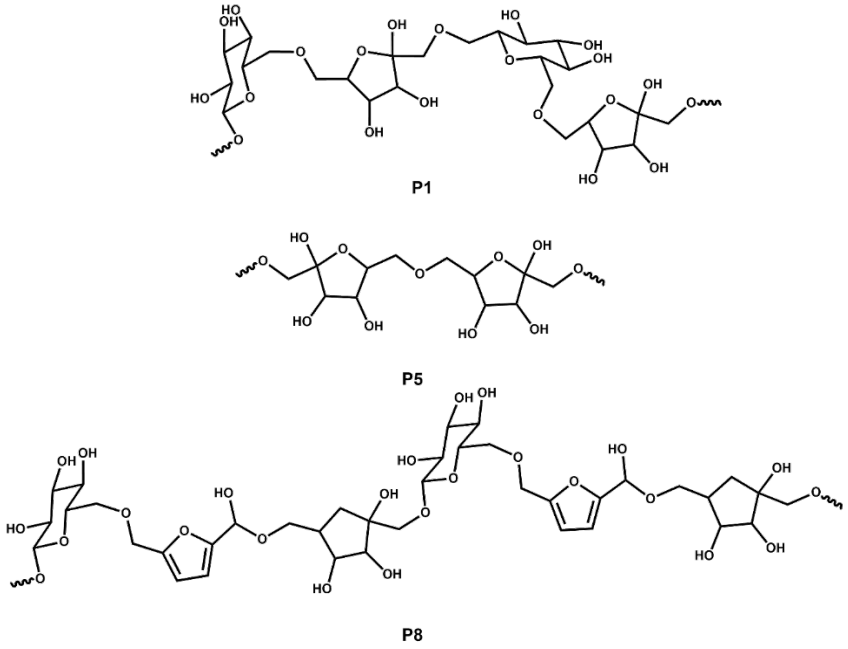


Figure S24: Chemical Structures of **P1**, **P5** and **P8**.

9. Derivation of Rate Expressions

9.1. Rate expression for the rate of homo-polymerization with classical polymerization equation

Consider the polymerization reaction:

$$\mathbf{M} + \mathbf{M} \xrightarrow{k_i} \mathbf{R1} \qquad \textbf{Initiation} \tag{S1}$$

$$\mathbf{R1} + \mathbf{M} \xrightarrow{k_p} \mathbf{R1} \qquad \textbf{Propagation} \tag{S2}$$

$$\cdot \qquad \cdot$$

$$\cdot \qquad \cdot$$

$$\mathbf{R1} + \mathbf{M} \xrightarrow{k_t} \mathbf{P} \qquad \textbf{Termination} \tag{S3}$$

In the above equation, Equation (S1) represents the initiation process, where **R1** is the initiator formed from two monomers of "**M**" with an initiation rate constant k_i. Equations (S2) represent propagation steps with rate constants k_p. The termination step is shown by Equations (S3) with rate constant k_t. Here, all the reactions involved in the polymerization lead to chains **R1** with end-group **M**.

The kinetics of polymerization can then be derived from these equations.

The assumptions employed to derive the rate expression are as follows:

(a) Steady-state approximation

(b) The rate constant of the reaction at the growing chain depends on the monomer unit at the growing end and is independent of the chain length.

(c) Termination by the complete consumption of monomers, i.e. the termination step is the last propagation step.[4]

The rate of polymerization can be written as the rate of monomer disappearance and is given by,

$$-\frac{\boldsymbol{d}[\mathbf{M}]}{\boldsymbol{dt}} = \mathbf{R_i} + \mathbf{R_p} \tag{S4}$$

Where, R_i and R_p are the rate of initiation and rate of propagation, respectively.

As the number of monomers in the initiation process is much less than the propagation steps, R_i can be neglected in comparison to R_p.

$$-\frac{\boldsymbol{d}[\mathbf{M}]}{\boldsymbol{dt}} = \mathbf{R_p} \tag{S5}$$

$$-\frac{\boldsymbol{d}[\mathbf{M}]}{\boldsymbol{dt}} = \boldsymbol{k_p}[\mathbf{M}][\mathbf{R1}] \tag{S6}$$

Applying steady-state approximation for **R1** and sum over all the equations

$$\boldsymbol{k_i}[\mathbf{M}]^{\mathbf{2}} = \boldsymbol{k_t}[\mathbf{R1}][\mathbf{M}] \tag{S7}$$

$$[\mathbf{R1}] = \left(\frac{\boldsymbol{k_i}}{\boldsymbol{k_t}}\right)[\mathbf{M}] \tag{S8}$$

By solving Equations S7 and S8 and substituting in Equation S6, the rate of polymerization becomes

$$-\frac{\boldsymbol{d}[\mathbf{M}]}{\boldsymbol{dt}} = \left(\frac{\boldsymbol{k_i}}{\boldsymbol{k_t}}\right)\boldsymbol{k_p}[\mathbf{M}]^{\mathbf{2}} \tag{S9}$$

Equation (S9) is the final rate expression for the homo-polymerization.

9.2. Walling's rate expression[5] for the rate of polymerization with two different monomers

$$\mathbf{A} + \mathbf{B} \xrightarrow{k_i} \mathbf{R1} \qquad \textbf{Initiation} \tag{S10}$$

$$\mathbf{R1} + \mathbf{A} \xrightarrow{k_p} \mathbf{R2} \qquad \textbf{Propagation} \tag{S11}$$

$$\mathbf{R2} + \mathbf{B} \xrightarrow{k_p'} \mathbf{R1} \qquad \textbf{Propagation}$$

$$\cdot \qquad \cdot \tag{S12}$$

$$\cdot \qquad \cdot$$

$$\mathbf{R1} + \mathbf{A} \xrightarrow{k_t} \mathbf{R2} \qquad \textbf{Termination} \tag{S13}$$

$$\mathbf{R2} + \mathbf{B} \xrightarrow{k_t'} \mathbf{R1} \qquad \textbf{Termination} \tag{S14}$$

In the above equation, Equation (S10) represents the initiation process, where **R1** in the intermediate formed from the monomers, **A** and **B** with an initiation rate constant k_i. Equations (S11) and (S12) represent propagation steps with k_p and k_p' rate constants, respectively. The termination steps are shown by Equations (S13) and (S14) with rate constants k_t and k_t', respectively. The kinetics of polymerization can then be derived from these equations. Here, all the reactions involved in the polymerization lead to chains, **R1** and **R2** with end-groups **A** and **B** respectively.

The assumptions employed to derive the rate expression are the following:
(a) Steady-state approximation
(b) The rate constant of the reaction at the growing chain depends on the monomer unit at the growing end and is independent of the chain length
(c) Termination by the complete consumption of monomers, i.e. the termination step is the last propagation step.

By assumption (b), the rate of polymerization is given by;

$$\frac{-\boldsymbol{d}([\mathbf{A}] + [\mathbf{B}])}{\boldsymbol{dt}} = \boldsymbol{k_p}[\mathbf{R1}][\mathbf{A}] + \boldsymbol{k_p'}[\mathbf{R2}][\mathbf{B}] \tag{S15}$$

By assumptions (a) and (c), the two steady-state equations can be written as;

$$\boldsymbol{k_p}[\mathbf{A}][\mathbf{R1}] = \boldsymbol{k_p'}[\mathbf{B}][\mathbf{R2}] \tag{S16}$$

$$\boldsymbol{k_i}[\mathbf{A}][\mathbf{B}] = \boldsymbol{k_t}[\mathbf{R1}][\mathbf{A}] + \boldsymbol{k_t'}[\mathbf{R2}][\mathbf{B}] \tag{S17}$$

Solving equation (S16) and (S17) for **R1** and **R2** and substitute these in equation (S6), the expression for the rate of polymerization becomes

$$\frac{-\boldsymbol{d}([\mathbf{A}]+[\mathbf{B}])}{\boldsymbol{dt}} = \mathbf{2}\,\frac{\boldsymbol{k_i k_p k_p'}[\mathbf{A}][\mathbf{B}]}{\boldsymbol{k_t k_p' + k_t' k_p}} \tag{S18}$$

Equation (S18) is the final rate expression for the formation of a polymer chain from two different monomers.

9.3. Walling's rate expression for the rate of polymerization with three different monomers

$$\mathbf{A} + \mathbf{B} + \mathbf{C} \xrightarrow{k_i} \mathbf{R1} \qquad \textbf{Initiation} \tag{S19}$$

$$\mathbf{R1} + \mathbf{A} \xrightarrow{k_p} \mathbf{R2} \qquad \textbf{Propagation} \tag{S20}$$

$$\mathbf{R2} + \mathbf{B} \xrightarrow{k_p'} \mathbf{R3} \qquad \textbf{Propagation} \tag{S21}$$

$$\mathbf{R3} + \mathbf{C} \xrightarrow{k_p''} \mathbf{R1} \qquad \textbf{Propagation} \tag{S22}$$

$$\begin{array}{ll} \cdot & \cdot \\ \cdot & \cdot \end{array}$$

$$\mathbf{R1} + \mathbf{A} \xrightarrow{k_t} \mathbf{R2} \qquad \textbf{Termination} \tag{S23}$$

$$\mathbf{R2} + \mathbf{B} \xrightarrow{k_t'} \mathbf{R3} \qquad \textbf{Termination} \tag{S24}$$

$$\mathbf{R3} + \mathbf{C} \xrightarrow{k_t''} \mathbf{R1} \qquad \textbf{Termination} \tag{S25}$$

In the above equation, Equation (S19) represents the initiation process, where **R1** in the intermediate is formed from three monomers, **A**, **B,** and **C** with an initiation rate constant k_i. Equations (S20), (S21) and (S22) represent propagation steps with k_p, k_p' and k_p'' rate constants, respectively. The termination steps are shown by Equations (S23), (S24), and (S25) with rate constants k_t, k_t' and k_t'', respectively. The kinetics of polymerization can then be derived from these equations. Here, all the reactions involved in the polymerization lead to chains, **R1**, **R2,** and **R3** with end-groups **A**, **B**, and **C** respectively.

Similar assumptions used in Section 9.2 were taken here. The rate expression can be written as

$$\frac{-\boldsymbol{d}([\mathbf{A}]+[\mathbf{B}]+[\mathbf{C}])}{\boldsymbol{dt}} = \boldsymbol{k_p}[\mathbf{R1}][\mathbf{A}] + \boldsymbol{k_p'}[\mathbf{R2}][\mathbf{B}] + \boldsymbol{k_p''}[\mathbf{R3}][\mathbf{C}] \tag{S26}$$

By assumptions (a) and (c), the two steady-state equations can be written as;

$$\boldsymbol{k_p}[\mathbf{A}][\mathbf{R1}] = \boldsymbol{k_p'}[\mathbf{B}][\mathbf{R2}] = \boldsymbol{k_p''}[\mathbf{C}][\mathbf{R3}] \tag{S27}$$

$$\boldsymbol{k_i}[\mathbf{A}][\mathbf{B}][\mathbf{C}] = \boldsymbol{k_t}[\mathbf{R1}][\mathbf{A}] + \boldsymbol{k_t'}[\mathbf{R2}][\mathbf{B}] + \boldsymbol{k_t''}[\mathbf{R3}][\mathbf{C}] \tag{S28}$$

Solving equation (S27) and (S28) for **R1**, **R2**, and **R3**, and substituting them in equation (S26), the expression for the rate of polymerization becomes

$$\frac{-\boldsymbol{d}([\mathbf{A}]+[\mathbf{B}]+[\mathbf{C}])}{\boldsymbol{dt}} = \frac{\boldsymbol{k_i k_p k_p' k_p''}([\mathbf{A}][\mathbf{B}]+[\mathbf{A}][\mathbf{C}]+[\mathbf{B}][\mathbf{C}])}{\boldsymbol{k_t k_p' k_p'' + k_t' k_p k_p'' + k_t'' k_p k_p'}} \tag{S29}$$

Equation (S29) is the final rate expression for the formation of a polymer from three different monomers.

9.4. Derivation of walling's rate expression for the rate of polymerization with two initiation steps

$$\mathbf{A}+\mathbf{B} \xrightarrow{k_i} \mathbf{R1} \quad \textbf{Initiation} \tag{S30}$$

$$\mathbf{A}+\mathbf{C} \xrightarrow{k_i'} \mathbf{R2} \quad \textbf{Initiation} \tag{S31}$$

$$\mathbf{R1}+\mathbf{R2} \xrightarrow{k_p} \mathbf{R2} \quad \textbf{Propagation} \tag{S32}$$

$$\mathbf{R2}+\mathbf{R1} \xrightarrow{k_p'} \mathbf{R1} \quad \textbf{Propagation} \tag{S33}$$

$$\cdot \qquad \cdot$$
$$\cdot \qquad \cdot$$

$$\mathbf{R1}+\mathbf{R2} \xrightarrow{k_t} \mathbf{R2} \quad \textbf{Termination} \tag{S34}$$

$$\mathbf{R2}+\mathbf{R1} \xrightarrow{k_t'} \mathbf{R1} \quad \textbf{Termination} \tag{S35}$$

In the above equation, Equation (S30) and (S31) represents the initiation process, where **R1 and R2** are the intermediate formed from Equations (S30) and (S31) with initiation rate constant k_i and k_i', respectively. Equations (S32) and (S33) represent propagation steps with k_p, and k_p' rate constants, respectively. The termination steps are shown by Equation (S35), and (S36) with rate constants k_t,and k_t' respectively. Here, all the reactions involved in the polymerization lead to chains, **R1** and **R2** with end-groups **B** and **C**.

The kinetics of polymerization can then be derived from these equations.
Similar assumptions as in the case of two monomers were used here. The rate expression can be written as

$$\frac{-\boldsymbol{d}([\mathbf{A}]+[\mathbf{B}]+[\mathbf{C}])}{\boldsymbol{dt}} = \boldsymbol{k_p}[\mathbf{R1}][\mathbf{R2}] + \boldsymbol{k_p'}[\mathbf{R2}][\mathbf{R1}] \tag{S36}$$

By assumptions (a) and (c), the two steady-state equations can be written as

$$\boldsymbol{k_p}[\mathbf{R1}][\mathbf{R2}] = \boldsymbol{k_p'}[\mathbf{R2}][\mathbf{R1}] \tag{S37}$$

$$\boldsymbol{k_i}[\mathbf{A}][\mathbf{B}] + \boldsymbol{k_i'}[\mathbf{A}][\mathbf{C}] = \boldsymbol{k_t}[\mathbf{R1}][\mathbf{R2}] + \boldsymbol{k_t'}[\mathbf{R2}][\mathbf{R1}] \tag{S38}$$

Solving equation (S37) and (S38) for **R1** and **R2** and substitute in equation (S36), we will get

$$\frac{-d([\mathbf{A}]+[\mathbf{B}]+[\mathbf{C}])}{dt} = \frac{(k_p + k_p')}{(k_t + k_t')}(k_i[\mathbf{A}][\mathbf{B}] + k_i'[\mathbf{A}][\mathbf{C}]) \quad \text{(S39)}$$

Equation (S39) is the final rate expression for the formation of a polymer chain from three different monomers, where the initiation occurs in two steps.

10. Validation of the Long-Chain Approximation, Steady State Approximation, and the Comparison of Reactivity of Hydroxyl Groups of Glucose and Fructose

The validity of the long-chain approximation was analyzed by comparing the free energy barriers for some of the crucial addition and condensation reactions. For this, the free energy barriers for the reaction between the monomers (**G**, **F**, **H**) were compared with the free energy barrier for the reaction between oligomers (**R1.1**, **R2.1**, **R3.1**) of higher chain length and one of the monomers. We noted a comparable barrier (within 4 kcal mol^{-1}), indicating the validity of the assumption (Table S9 and Figures S7, S8, S12, S18-S23).

Table S9: The free energy barrier ($\Delta G^{\ddagger}$) and the free energies of the transition state (TS) of the reactions considered to validate the long chain approximation.

Reactions		**$\Delta G^{\ddagger}$ (kcal mol^{-1})**	***G* (au) of TS**
R + F	Monomer (**R=G**)	35.3	-1526.764509
	Oligomer (**R=R1.1**)	31.04	-2900.386255
R' + HMF	Monomer (**R'=G**)	12.68	-1297.644489
	Oligomer (**R'=R2.1**)	12.54	-2442.090769
	Monomer (**R'=F**)	19.81	-1297.637211
	Oligomer (**R'=R3.1**)	20.91	-2442.074337

The application of steady-state approximation in deriving rate equations for polymerization reactions is well-accepted and used in deriving kinetics for different polymerization reactions.[5,7] This can be ascribed to the irreversible nature of the propagation step due to the high enthalpic preference of the oligomer as compared to the monomer. Thus, the oligomer formed at any point in time is expected to be reactive and react with available monomer to form an oligomer with a higher chain length.

To confirm the validity of the steady-state assumption in this work, we have analyzed the irreversible nature of the propagation step by comparing the forward and reverse barriers for some of the critical propagation steps considered (Table S10). This analysis indicates that the product of the propagation steps is more stable as compared to the reactants, indicating a high reverse barrier and irreversibility of the reaction. Moreover, the polymerization reactions are mostly driven by the lowering of enthalpy (more negative H of products as compared to reactants) during product formation. The comparison of enthalpy values for the reactants and product indicates that the reaction considered here is exothermic, suggesting that the product-to-reactant conversion (depolymerization) is thermodynamically less favorable (Table S11).

Table S10: The free energy barriers ($\Delta G^{\ddagger}$) for the forward and reverse reactions considered to validate the steady-state approximation.

Reactions	**$\Delta G^{\ddagger}$ (kcal mol^{-1})**

	Forward	Reverse
G + F → I1	35.3	37.54
G + G → I4	36.48	40.48

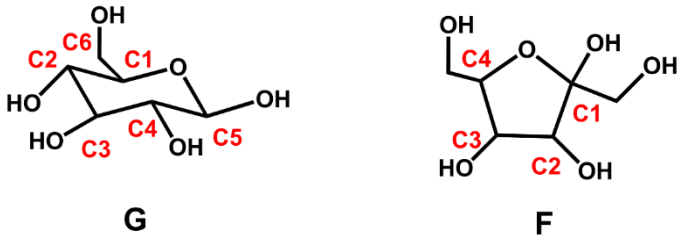
Table S11: Enthalpies, H, of the reactant (sum of the enthalpies of the reactants) and products and the enthalpy change, ΔH for reactions leading to **I1-I4**. Here, $\Delta H = H_{\text{product}} - H_{\text{reactant}}$.

Reactions	***H* (au)**		**ΔH (kcal mol^{-1})**
	Reactant	**Product**	
G + F → I1	-1526.70508	-1526.72942	-15.27
G + HMF → I2	-1297.55983	-1297.56705	-4.528
F + HMF → I3	-1297.56431	-1297.56715	-1.78
G + G → I4	-1526.7006	-1526.72805	-17.22

The assumption of similar reactivity of all the hydroxyl groups in glucose/fructose was analyzed by comparing the free energy barrier for the addition of different hydroxyl groups of fructose at the carbonyl carbon of HMF. We noted a comparable barrier (within 2 kcal mol^{-1}) for the addition of different hydroxyl groups (Table S12 and Figure S8, S9, S11, S12, and S13).

Table S12: Free energy (***G***) of the transition state (TS) and the free energy barrier, $\Delta G^{\ddagger}$ for addition reaction between different hydroxyl groups of fructose and glucose at the carbonyl carbon of **HMF**. Here, **I3, I3'**, and **I3''** are formed by the reaction of the hydroxyl group bonded to C1, C4, and C3 of **F** with the carbonyl carbon of **HMF** along the TSs **TS I3**, **TS I3'**, and **TS I3''**, respectively. The reaction of the hydroxyl group bonded to C6 and C5 atoms of glucose with the carbonyl carbon of **HMF** along TSs **TS I2'**and **TS I2''** leads to **I2** and **I2'** respectively. See Figure S25 for the atom labels.

Reactions	***G* (au) of TS**	**$\Delta G^{\ddagger}$ (kcal mol^{-1})**
F + HMF → I3	-1297.637211	19.81
F + HMF → I3'	-1297.63412	21.75
F + HMF → I3''	-1297.632733	22.62
G + HMF → I2	-1297.644489	12.68
G + HMF → I2'	-1297.642145	14.15



G **F**

Figure S25: Chemical Structures of **G** and **F** with atom numbers labeled.

11. Computed and experimental IR and NMR spectral values

Table S13: Comparison of the experimental and computed ^{13}C NMR and IR Spectral values. The computational part of the table has splitted into three parts: **I2**, **I3**, and **I6** as these model compounds were used for the calculations. The IR frequencies are obtained from the normal mode analysis and the NMR shielding tensors and degeneracy data are obtained from GIAO (NMR-GIAO) calculations as implemented in the Gaussian 16 package.

^{13}C NMR (ppm)				**IR (cm^{-1})**			
Experiment	**Computed**			**Experiment**	**Computed**		
	I2	**I3**	**I6**		**I2**	**I3**	**I6**
164-140	160.3 160.6	167.2 162.8	167.6 166.1 166.1 159.2	2950-2800	3020, 3026	3058, 3068	3037, 3062
				1710-1685	1649, 1654, 1710	1644, 1703	1673, 1695, 1707,
140-103	120.2 117.8 102.7	119.9 119.7 107	127.3 125.2 121.3 129.8	1610-1560	1598	1508, 1606	1598, 1605
				1440-1415	1425, 1434, 1438	1411, 1419	1423, 1441
80-65	79.2 77.4 77.3 74.2	81 74.8 67.3	96.2 66	1610-1360	1434, 1488, 1499, 1598	1361, 1411, 1484, 1493	1379, 1423,
				1200-1000	1106, 1152	1093, 1133	1059, 1158

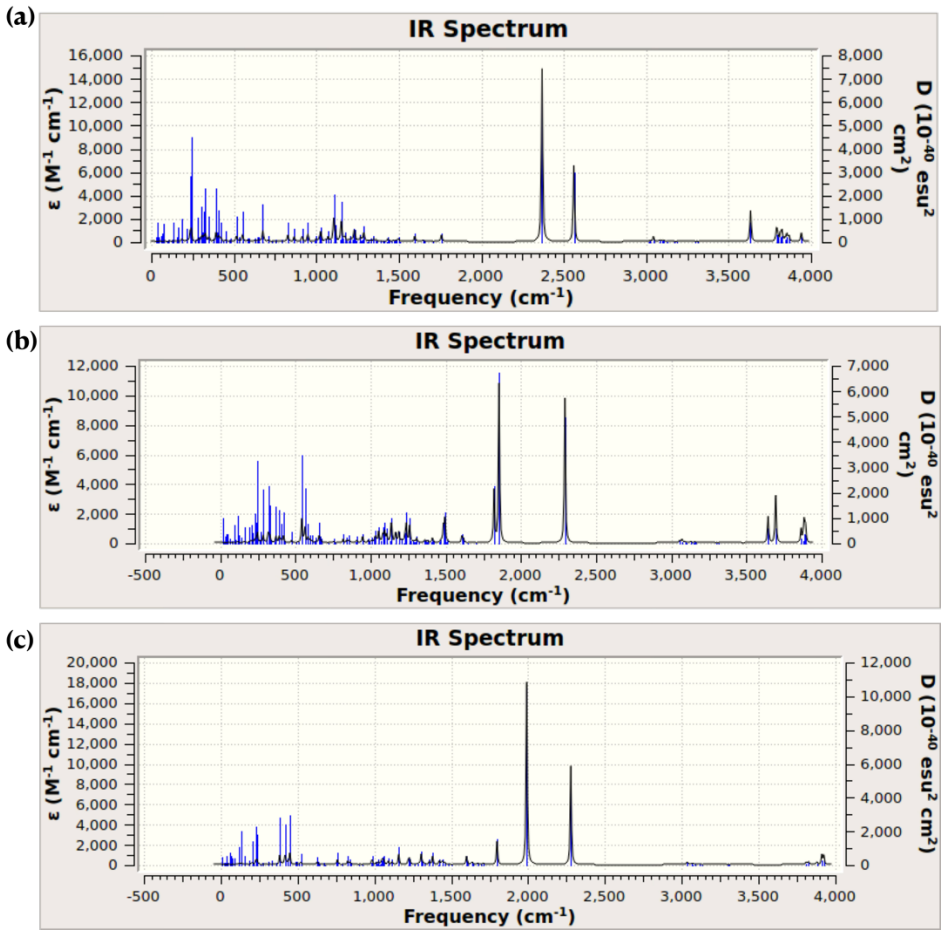


Figure S26: Computed Infrared (IR) spectra of (a) **I2**, (b) **I3**, and (c) **I6**. The optimized structures of **I2**, **I3**, and **I6** can be found in Figures S8, S12, and S17 respectively.

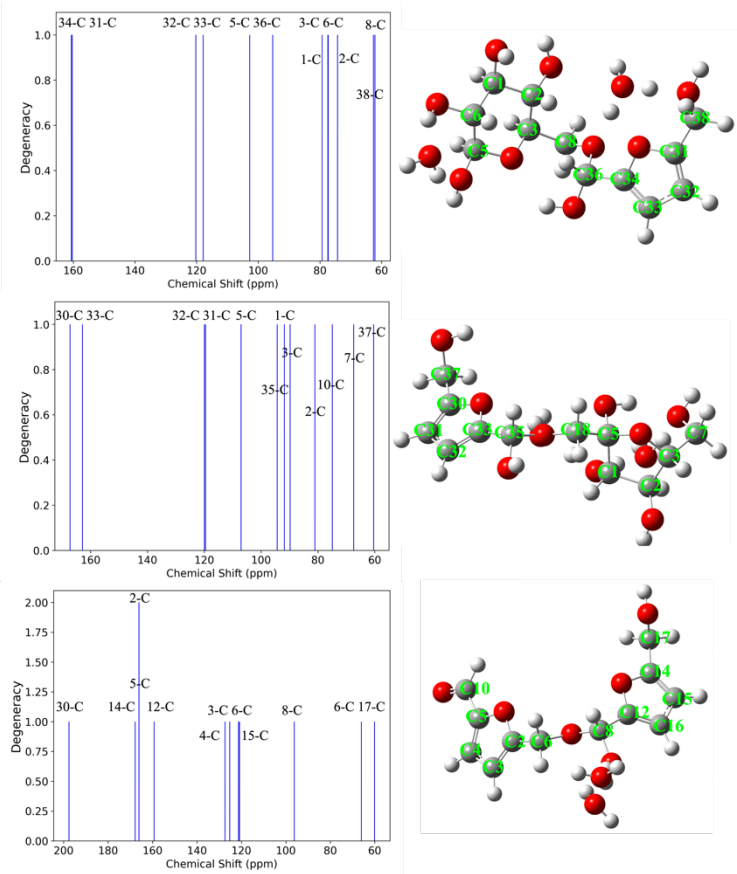


Figure S27: Computed NMR spectra of (a) **I2**, **(b) I3**, and (c) **I6**. The optimized structures of **I2**, **I3**, and **I6** with atom numbers labeled are also shown. Here, the line plots were generated using the Matplotlib library available in Python Program package using the NMR shielding tensors and degeneracy data obtained from GIAO (NMR-GIAO) calculations as implemented in Gaussian 16 package.

12. Cartesian Coordinates of the Optimized structures

Table S14: Optimized coordinates of all the chemical species considered in this work, where geometry optimization is carried out M06-2X/6-31+G(d,p) level of theory with PCM/SMD solvent model. The name of the chemical species ends with "smd" indicate that the calculation is performed with the SMD solvent model. "ww" represents optimization is carried out without explicit water molecules. The imaginary frequency is given in the parenthesis along with the name of the transition state (TS). The name of all the TSs begins with "TS".

1. **G**

C	-0.794471	-2.08263	0.366613
C	-1.789084	-0.950489	0.617468
C	-1.431398	0.271799	-0.223557
O	-0.072269	0.639901	-0.03695
C	0.932744	-0.347816	-0.10524
C	0.599527	-1.586345	0.72526
O	-3.096677	-1.339305	0.256365
C	-2.200642	1.512739	0.183005

2. **G-ww**

C	1.444166	-0.405347	-0.643629
C	0.24703	-1.272208	-0.258077
C	-1.031128	-0.71851	-0.887915
O	-1.202862	0.632267	-0.473034
C	-0.157672	1.470789	-0.921096
C	1.172502	1.050226	-0.297554
O	0.429416	-2.596829	-0.71589
C	-2.268002	-1.500829	-0.500701

O	-1.758386	1.862806	1.513835
O	2.058368	0.257423	0.482658
O	1.540487	-2.601869	0.464746
O	-1.182638	-3.233493	1.08227
O	-0.74303	-2.319831	3.679349
O	0.597284	1.973173	2.175392
H	2.58359	0.716838	-0.187298
H	-1.638786	0.050197	-1.280113
H	0.613696	-1.298929	1.788275
H	2.397683	-2.324217	0.814234
H	1.133941	-0.628196	-1.14744
H	-0.821973	-2.359111	-0.69649
H	-1.054282	-3.057165	2.035711
H	-1.746491	-0.682306	1.685389
H	-3.238113	-2.227208	0.616845
H	-1.982983	2.337749	-0.498647
H	-3.272183	1.308042	0.207978
H	-2.30776	2.568035	1.88497
H	1.195145	1.473775	1.562095
H	0.941413	2.867104	2.33203
H	-0.439073	1.95942	1.814685
H	-1.496212	-2.283198	4.282236
H	-0.018753	-2.701854	4.19083

O	-2.351653	-1.559268	0.914139
O	-0.410698	2.770226	-0.500702
O	2.226452	1.843955	-0.794685
O	2.630872	-0.911759	-0.057682
H	-1.093684	3.166933	-1.056709
H	-0.934805	-0.763337	-1.985439
H	1.074436	1.163107	0.794737
H	2.012077	2.768356	-0.607276
H	-0.089085	1.414037	-2.020601
H	1.60207	-0.486103	-1.727206
H	2.615523	-0.74122	0.894556
H	0.125614	-1.255706	0.835645
H	1.318647	-2.873624	-0.452527
H	-3.144259	-0.998189	-0.927261
H	-2.187839	-2.504775	-0.932922
H	-3.143745	-2.051609	1.157783

3. **F**

C	-2.288073	0.30973	1.80715
C	-0.989336	-0.507526	1.83619
C	-0.288799	-0.121315	0.519918
O	-0.912053	1.091489	0.066245
C	-1.875128	1.551062	0.990213
O	-0.144321	-0.102459	2.897296
C	-0.383783	-1.171371	-0.567027
O	-1.756535	-1.505233	-0.747416
O	-2.995556	2.039375	0.282507
C	-1.292858	2.705043	1.801335
O	-2.211424	3.216733	2.738711
O	-3.34718	-0.354675	1.148974
H	-0.424211	2.325887	2.345323
H	-2.629027	0.585368	2.807292
H	-1.204825	-1.580778	1.886213
H	0.767784	0.078046	0.727528
H	-2.972572	-0.918413	0.441539
H	-1.844619	-2.254076	-1.348871
H	0.035719	-0.77202	-1.496099
H	0.193576	-2.050289	-0.2594
H	-0.946958	3.475063	1.097866
H	-0.509808	-0.418201	3.733874
H	-3.612282	1.29595	0.131233
H	-2.76803	3.876095	2.300107
H	-2.89505	3.124134	-0.597807

4. **F-ww**

C	0.773655	0.715612	1.001817
C	1.970037	1.017848	0.091642
C	1.846485	-0.038988	-1.024309
O	0.528092	-0.587965	-0.932624
C	-0.260004	0.118641	0.024104
O	1.868992	2.295184	-0.514433
C	2.858083	-1.161555	-0.915729
O	2.762184	-1.720265	0.391302
O	-1.129576	-0.760955	0.656782
C	-1.124316	1.145896	-0.698061
O	-1.964341	1.835532	0.206273
O	1.081231	-0.231023	2.006481
H	-0.488123	1.886026	-1.187499
H	0.390001	1.613071	1.492831
H	2.912346	0.919069	0.642934
H	1.972376	0.457484	-1.993645
H	1.715184	-0.877646	1.638982
H	3.474511	-2.35358	0.537483
H	2.640488	-1.923507	-1.671688
H	3.86032	-0.754992	-1.092238
H	-1.704386	0.608974	-1.460528
H	2.032578	2.974667	0.152296
H	-0.657364	-1.131798	1.421089
H	-2.458653	1.167608	0.701481

O	-2.782261	4.074549	-1.052793
H	-3.361667	4.192582	-1.821709
H	-2.971269	4.773327	-0.312096
O	-3.127559	5.46257	0.983619
H	-2.493537	6.175698	1.150805
H	-4.008483	5.831533	1.145385

5. **HMF**

C	-0.600661	-1.094098	0.431839
C	0.013696	-0.722576	1.598103
C	1.305562	-0.2676	1.232705
C	1.388795	-0.409034	-0.130413
O	0.220612	-0.913804	-0.62364
C	2.47159	-0.1271	-1.02489
C	-1.980196	-1.589681	0.147802
O	0.87199	-1.638042	-3.65478
H	2.086273	0.108078	1.879178
H	-2.470867	-1.835631	1.092187
H	1.458284	-1.071607	-3.013666
H	-0.417474	-0.771874	2.5867
H	-0.207082	-1.683651	-3.419621
H	1.029857	-1.365892	-4.57077
O	-1.482893	-1.756005	-3.125245
H	-1.675153	-2.233185	-2.273371
H	-2.037197	-2.133994	-3.821085
O	2.462283	-0.345637	-2.239082
H	3.360592	0.318828	-0.56253
O	-1.986493	-2.70217	-0.739843
H	-2.560718	-0.809606	-0.352482
H	-1.544233	-3.463661	-0.339516

6. **HMF-ww**

C	-0.510582	-1.121265	0.330034
C	0.013693	-0.820505	1.557909
C	1.333489	-0.343908	1.323529
C	1.517101	-0.383747	-0.032468
O	0.392421	-0.862305	-0.639723
C	2.629036	-0.031122	-0.901142
O	3.69076	0.400345	-0.486187
C	-1.83616	-1.64049	-0.119844
O	-2.558129	-0.683937	-0.881442
H	2.059775	-0.009344	2.049932
H	2.449102	-0.181598	-1.979947
H	-2.130494	-0.580854	-1.740835
H	-1.697224	-2.566542	-0.690173
H	-2.436857	-1.865541	0.76234
H	-0.49206	-0.927927	2.506164

7. **I1**

C	2.746046	-1.697314	0.045487
C	1.415402	-1.250664	-0.54801
C	1.685025	-0.386378	-1.779499
O	2.495686	0.727621	-1.419015
C	3.680147	0.501726	-0.701441
C	3.484016	-0.440572	0.483121
O	0.600801	-2.350406	-0.912938
C	0.419973	0.229191	-2.348304
O	-0.027783	1.191985	-1.390036
O	4.002277	1.800343	-0.252537
O	4.775547	-0.707031	0.983385
O	2.573224	-2.607186	1.108881
O	0.873922	-1.102507	2.650275
O	1.390194	2.796051	-0.010974
H	4.738947	1.746236	0.374624
H	2.17224	-0.996121	-2.55349

8. **TS I1** (-601.960 cm^{-1})

C	3.641342	-1.321088	0.0908
C	2.170593	-0.971381	-0.134442
C	2.060511	0.17846	-1.134424
O	2.785317	1.292755	-0.627431
C	4.174029	1.04661	-0.450746
C	4.395659	-0.083593	0.554243
O	1.470851	-2.088973	-0.643112
C	0.643752	0.637922	-1.420352
O	-0.066753	1.019303	-0.22704
O	4.739013	2.193334	0.084874
O	5.764671	-0.394454	0.64894
O	3.750015	-2.421177	0.971778
O	-3.340611	3.057218	-1.148446
O	1.24557	2.807112	1.07235
H	4.929373	2.828845	-0.617674
H	2.487422	-0.145072	-2.096979

H	2.872966	0.077494	1.240042
H	4.69635	-1.344983	1.706151
H	4.469271	0.113663	-1.362633
H	3.333184	-2.22686	-0.717489
H	2.019019	-2.172101	1.794429
H	0.885858	-0.636658	0.196639
H	0.914037	-3.126634	-0.422111
H	0.629414	0.734129	-3.297128
H	-0.346	-0.539188	-2.490287
H	2.33882	2.545328	0.094039
H	0.848509	2.902175	0.891879
H	0.941677	2.11417	-0.630872
H	-0.000136	-1.286846	2.251987
H	0.777363	-1.209833	3.603925
C	-2.402948	-0.71441	0.929826
C	-1.927472	0.736758	0.688658
C	-2.375424	1.075702	-0.751074
O	-2.724449	-0.17681	-1.334002
C	-3.252864	-1.028828	-0.320404
O	-2.375288	1.681514	1.638721
C	-1.32024	1.759453	-1.595961
O	-3.055221	-2.343877	-0.717308
C	-4.733574	-0.754208	-0.068232
O	-1.322586	-1.613668	1.061714
H	-2.991086	-0.774339	1.848542
H	-0.836078	0.73307	0.76269
H	-3.253747	1.730706	-0.712455
H	-1.033996	-1.947735	0.190891
H	-1.587831	1.718213	-2.6565
H	-1.25372	2.81002	-1.295767
H	-5.267998	-0.754909	-1.025749
H	-3.345138	1.715756	1.604767
H	-3.501711	-2.492134	-1.563188
O	0.014449	3.023358	2.035552
H	0.019522	3.898964	2.444244
H	-0.92037	2.730331	1.97696
H	-5.123011	-1.553263	0.571611
C	2.746046	-1.697314	0.045487
C	1.415402	-1.250664	-0.54801

H	3.996586	0.256553	1.524248
H	6.231772	0.396262	0.952355
H	4.621853	0.786148	-1.421565
H	4.071936	-1.667517	-0.857897
H	3.553351	-2.13893	1.876461
H	1.742947	-0.654699	0.830457
H	1.78819	-2.868584	-0.159843
H	0.687784	1.490675	-2.106208
H	0.070787	-0.170217	-1.876892
H	2.128772	2.722968	0.676511
H	1.00151	3.740865	1.039855
H	0.440581	1.749259	0.266383
H	-3.04494	3.964652	-1.309086
H	-3.98281	3.077623	-0.383593
C	-2.062506	-1.237049	1.032533
C	-2.652188	0.178417	1.10938
C	-2.649965	0.66168	-0.362069
O	-2.18932	-0.408216	-1.164356
C	-2.289391	-1.645659	-0.439264
O	-4.005692	0.192932	1.542876
C	-1.800576	1.883432	-0.645415
O	-1.350132	-2.527375	-0.926545
C	-3.660441	-2.264013	-0.692695
O	-3.782049	-3.508464	-0.037056
O	-0.690259	-1.250047	1.352498
H	-4.444828	-1.611644	-0.299547
H	-2.569817	-1.926018	1.711862
H	-2.037124	0.810431	1.759982
H	-3.682956	0.904188	-0.635676
H	-0.281809	-0.468638	0.94178
H	-1.445058	2.053016	-1.651828
H	-1.581258	2.603807	0.129428
H	-3.786424	-2.35883	-1.778793
H	-4.050757	-0.083181	2.468979
H	-0.462314	-2.301633	-0.584248
H	-3.055507	-4.068889	-0.343013
O	-4.896127	2.77435	0.94649
H	-5.84428	2.92527	0.850191
H	-4.783846	1.864477	1.282475

9. **I2**

C	1.079569	-0.574754	0.318821
C	-0.208633	-1.384473	0.218918
C	-0.998916	-0.926303	-1.004349
O	-1.308516	0.455463	-0.846269
C	-0.150071	1.282745	-0.819777
C	0.757625	0.917943	0.3627
O	0.050524	-2.768891	0.098487
C	-2.29394	-1.687861	-1.189497
O	-3.06597	-1.778321	0.014391

10. **TS I2** (-205.670 cm^{-1})

C	-2.242393	-1.969631	-0.118971
C	-1.131248	-1.417566	0.76376
C	-1.612428	-0.132306	1.441225
O	-1.980704	0.800436	0.429586
C	-3.053197	0.376028	-0.374567
C	-2.67976	-0.905373	-1.120183
O	-0.76258	-2.3569	1.757724
C	-0.570244	0.557648	2.300244
O	0.625599	0.869482	1.579413

O	-0.577589	2.593816	-0.656376
O	1.959277	1.6411	0.307918
O	1.852535	-1.016544	1.417309
O	0.808306	3.880898	1.435271
O	-2.243416	-3.497028	1.658478
H	-0.927023	2.933891	-1.49084
H	-0.391836	-1.074881	-1.911245
H	0.19762	1.147209	1.284981
H	1.794924	2.518181	0.703959
H	0.398695	1.15636	-1.765727
H	1.695963	-0.77728	-0.567006
H	1.456611	-0.702728	2.242556
H	-0.810641	-1.193712	1.123357
H	0.787946	-2.977124	0.692684
H	-2.899434	-1.227657	-1.973545
H	-2.075485	-2.719292	-1.470266
H	-2.975422	-3.929962	2.253423
H	-1.627998	-4.115871	1.232975
H	-2.611443	-2.796627	0.978702
H	1.132817	4.788227	1.463918
H	0.120468	3.850072	0.752029
C	-5.28074	-2.475604	3.004686
C	-6.42702	-1.897937	2.559099
C	-6.035795	-0.936171	1.559044
C	-4.684315	-1.017265	1.47892
O	-4.213674	-1.922789	2.370617
C	-3.616026	-0.533308	0.558202
O	-4.145045	0.259831	-0.427217
C	-4.904224	-3.586076	3.916415
O	-4.057913	-4.472361	3.148315
H	-6.678269	-0.305914	0.962913
H	-2.804349	-0.029071	1.094007
H	-3.764622	-5.207339	3.705841
H	-4.345578	-3.220686	4.783198
H	-5.795648	-4.119884	4.24874
H	-7.430735	-2.137955	2.877427
H	-3.432865	0.822049	-0.773361

O	-3.253251	1.446691	-1.252749
O	-3.739585	-1.335765	-1.948551
O	-1.720927	-3.122515	-0.746773
O	-2.109234	3.793504	-0.081705
O	1.977768	-1.568993	1.835299
H	-3.934738	1.211721	-1.899
H	-2.478694	-0.361607	2.080853
H	-1.84504	-0.67646	-1.792982
H	-4.494268	-1.610163	-1.407511
H	-3.947315	0.215755	0.252872
H	-3.094294	-2.243306	0.525597
H	-2.428741	-3.578292	-1.221044
H	-0.262276	-1.187981	0.124164
H	-0.835208	-3.241112	1.365095
H	-0.980017	1.500971	2.667249
H	-0.311715	-0.075473	3.154329
H	2.478361	-1.892926	1.064408
H	1.183605	-2.123495	1.914579
H	1.221383	0.075713	1.589306
H	-2.537937	3.926959	0.772662
H	-2.575864	3.046105	-0.497702
C	3.565002	-0.0767	-0.998746
C	4.275152	1.065665	-0.743325
C	3.323777	2.055231	-0.377488
C	2.102898	1.439331	-0.445736
O	2.244903	0.139531	-0.825981
C	0.765013	1.858866	-0.153123
O	0.585916	3.085706	0.192484
C	3.962828	-1.451113	-1.408154
O	3.570611	-2.343628	-0.369523
H	3.504003	3.083498	-0.09957
H	-0.076554	1.293812	-0.54618
H	3.654175	-3.254733	-0.678081
H	3.465325	-1.713867	-2.34788
H	5.045778	-1.470248	-1.55809
H	5.347457	1.173921	-0.806844
H	-0.383328	3.342909	0.157975

11. **I2'**

C	0.980297	-1.542037	-0.964771
C	1.618242	-2.135417	0.291164
C	0.741479	-3.245506	0.864733
O	-0.553766	-2.711711	1.141822
C	-1.190829	-2.249071	-0.020639
C	-0.429645	-1.066688	-0.633113
O	2.887176	-2.683829	0.008356
C	1.298308	-3.845349	2.145825
O	1.599144	-2.870326	3.128522
O	-2.524108	-1.928103	0.314406
O	-1.069792	-0.611314	-1.798524

12. **TS I2'** (-216.770 cm^{-1})

C	3.101208	1.170902	0.690878
C	3.513727	0.099747	-0.319457
C	2.496411	0.016328	-1.458938
O	1.196973	-0.216749	-0.911239
C	0.780944	0.825909	-0.070121
C	1.674848	0.923535	1.167421
O	4.76768	0.407543	-0.888039
C	2.780858	-1.098951	-2.439332
O	2.829872	-2.326634	-1.717581
O	-0.553831	0.566809	0.319336
O	1.27273	1.998842	1.980282

O	1.802702	-0.524282	-1.502515
O	-0.752125	1.794775	1.276029
O	-3.816678	-4.213505	0.600488
H	0.650953	-4.053836	0.120941
H	-0.352358	-0.266714	0.118825
H	-1.896724	-0.186027	-1.520407
H	-1.275655	-3.055058	-0.764452
H	0.931925	-2.315493	-1.742345
H	1.782347	0.250427	-0.922671
H	1.70088	-1.33727	1.047234
H	3.382325	-2.027364	-0.50263
H	0.540307	-4.507916	2.571461
H	2.181443	-4.441779	1.895988
H	-4.523299	-4.353385	1.400857
H	-4.198162	-4.444851	-0.261824
H	-3.396527	-3.297179	0.56282
H	-0.852745	2.210358	2.142009
H	-0.339637	2.45959	0.70956
C	-5.398198	-2.328148	2.907249
C	-6.098978	-1.197162	2.634465
C	-5.198896	-0.323982	1.929718
C	-4.029095	-1.003349	1.82599
O	-4.124679	-2.211078	2.435852
C	-2.731745	-0.75596	1.129091
O	-2.827314	0.368283	0.326052
C	-5.70968	-3.667562	3.458116
O	-5.470409	-4.613762	2.384837
H	-5.403331	0.658226	1.53176
H	-1.895019	-0.678417	1.835337
H	-5.45379	-5.520315	2.72574
H	-5.059776	-3.918369	4.300052
H	-6.755818	-3.722942	3.759662
H	-7.13507	-1.014647	2.879098
H	2.48238	-2.518734	2.963423
H	-2.150983	1.020526	0.618532

O	4.042721	1.240214	1.743465
O	1.759582	-2.667368	0.752005
O	-1.980906	2.057728	-1.066341
H	2.499416	0.96706	-2.013491
H	1.623648	-0.032154	1.710611
H	0.405581	1.79492	2.355854
H	0.783097	1.78681	-0.609374
H	3.142117	2.153491	0.202168
H	3.973794	0.446567	2.292966
H	3.549815	-0.872497	0.195246
H	5.37578	0.61063	-0.162891
H	1.984733	-1.124798	-3.189698
H	3.740151	-0.90377	-2.928045
H	-1.893155	2.993422	-0.842
H	-2.941685	1.871538	-1.153786
H	-1.214759	1.152772	-0.251899
H	2.045109	-2.567289	-0.185441
H	1.875679	-3.595323	0.993448
C	-4.451128	-0.186421	0.127213
C	-4.570534	-0.569311	1.429984
C	-3.283507	-1.050214	1.828533
C	-2.487543	-0.922165	0.73152
O	-3.188159	-0.410497	-0.31243
C	-1.068827	-1.150983	0.481131
O	-0.393925	-1.646106	1.47132
C	-5.358154	0.449264	-0.864009
O	-4.736264	1.671728	-1.267243
H	-2.984195	-1.429897	2.794169
H	-0.782432	-1.434402	-0.531603
H	-5.185267	2.021082	-2.047806
H	-5.496195	-0.207051	-1.729743
H	-6.327676	0.636894	-0.395512
H	-5.463515	-0.503492	2.033549
H	2.90124	-3.06704	-2.332072
H	0.492446	-2.079712	1.155492

13. **I3’**

C	1.269198	1.067891	0.499695
C	2.074899	0.344649	-0.591595
C	1.21132	-0.861383	-0.986285
O	-0.128814	-0.540038	-0.589049
C	-0.188283	0.599699	0.233512
O	2.186812	1.155434	-1.74021
C	1.59667	-2.214397	-0.412981
O	1.305196	-2.24531	0.999623
O	-0.804697	0.245832	1.474265
C	-1.071383	1.638061	-0.441276
O	-1.247112	2.770654	0.379386
O	1.644643	0.756648	1.826132
H	-0.576391	1.96655	-1.358992

14. **TS I3’** (-192.690 cm^{-1})

C	2.671195	0.36991	0.803225
C	2.289171	-1.057248	0.386517
C	1.13826	-0.860437	-0.613301
O	1.221658	0.491068	-1.07176
C	2.260837	1.217455	-0.424841
O	3.338352	-1.688307	-0.322953
C	-0.25457	-1.0919	-0.052842
O	-0.50737	-0.17833	1.021798
O	1.765164	2.471469	-0.043034
C	3.383436	1.447064	-1.428903
O	4.407178	2.245407	-0.874887
O	2.001287	0.813344	1.966467
H	3.823991	0.48547	-1.703225

H	1.341409	2.151148	0.375223
H	3.060698	0.041397	-0.215858
H	1.231414	-0.948872	-2.076995
H	2.251075	-0.007242	1.853316
H	1.003342	-3.00251	-0.882877
H	2.657205	-2.414698	-0.58194
H	-2.025749	1.164202	-0.702047
H	2.770379	1.903939	-1.510273
H	-0.104758	0.35261	2.158676
H	-1.742797	2.501673	1.164218
H	-0.160898	-2.407494	1.342569
O	-1.154377	-2.196127	1.48673
H	-1.482853	-2.586438	2.312936
H	-1.162209	-1.136589	1.508884
O	3.878163	3.086635	-0.688315
H	3.537219	3.908323	-0.315185
H	4.557957	2.77862	-0.076829
C	2.96394	-6.087142	1.321393
C	4.193761	-5.676885	0.908883
C	4.210869	-4.247875	1.036519
C	2.989803	-3.906871	1.525435
O	2.219541	-5.010459	1.70176
C	2.352866	-2.603836	1.883466
O	3.28074	-1.549783	1.808491
C	2.307298	-7.419917	1.450558
O	2.053096	-7.773082	2.803875
H	5.017928	-3.570536	0.797466
H	1.876097	-2.65352	2.868079
H	1.341482	-7.215533	3.142553
H	1.378653	-7.437502	0.867786
H	2.981205	-8.17641	1.045759
H	4.991453	-6.314741	0.557578
H	3.978173	-1.659997	2.471449

H	3.742708	0.461124	0.9945
H	1.985714	-1.649468	1.258809
H	1.287325	-1.539481	-1.459484
H	1.101274	0.445242	1.976772
H	-1.002888	-0.94529	-0.837969
H	-0.337614	-2.110232	0.339704
H	2.944184	1.907787	-2.323087
H	4.0592	-1.892212	0.287106
H	1.672472	2.464601	0.927227
H	4.008848	3.085346	-0.60823
H	-0.784892	0.72472	0.602324
O	-1.074305	1.971043	-0.162435
H	-1.57889	2.656229	0.295428
H	-0.202492	2.345593	-0.388922
O	-1.821126	-4.166055	1.84569
H	-2.305223	-4.728253	2.466523
H	-1.030288	-4.66088	1.590329
C	-4.475275	0.108493	0.00807
C	-4.628873	-1.237879	-0.173462
C	-3.660375	-1.871529	0.655569
C	-2.999384	-0.858545	1.296195
O	-3.487405	0.34956	0.897867
C	-1.876301	-0.783824	2.204565
O	-1.353389	-1.832593	2.746314
C	-5.169329	1.30888	-0.5478
O	-5.860925	2.03698	0.453275
H	-3.474331	-2.930276	0.766051
H	-1.768796	0.129914	2.783211
H	-5.220448	2.513593	0.996056
H	-4.441905	1.945758	-1.06498
H	-5.910886	0.972383	-1.273338
H	-5.349377	-1.713961	-0.821573
H	-1.584615	-2.740365	2.343214

15. **I3**

C	-2.015239	0.31941	0.843994
C	-3.43152	0.339986	1.456069
C	-4.342932	-0.025064	0.285378
O	-3.543533	-0.888924	-0.534494
C	-2.181792	-0.540908	-0.458713
O	-3.585683	-0.689805	2.415442
C	-4.860774	1.163116	-0.50124
O	-3.741301	1.961073	-0.90557
O	-1.792849	0.141579	-1.631085
C	-1.377943	-1.840939	-0.401843
O	0.790569	0.197946	-1.219922
O	-1.455827	1.595269	0.624846
H	-1.816453	-2.472528	0.372683
H	-1.329858	-0.192166	1.524248
H	-3.659598	1.324547	1.881187

16. **TS I3** (-203.150 cm^{-1})

C	1.464244	-0.445074	0.588288
C	2.72905	0.064918	1.301
C	3.816081	-0.029962	0.231233
O	3.127491	0.221671	-0.997844
C	1.781675	-0.215073	-0.933729
O	2.60381	1.443618	1.606323
C	4.558536	-1.351578	0.181895
O	3.605292	-2.404095	0.003725
O	1.586717	-1.349653	-1.720243
C	0.933408	0.896935	-1.540287
O	-0.464853	0.653118	-1.408632
O	1.101762	-1.769973	0.907963
H	1.169801	1.828656	-1.019237
H	0.612644	0.171676	0.88573
H	2.950594	-0.53006	2.194946

H	-5.195929	-0.610224	0.637385
H	2.104439	1.966093	0.966158
H	-5.402993	0.80794	-1.382354
H	-5.534171	1.75141	0.130192
H	-1.441557	-2.350516	-1.371232
H	-3.034747	-0.494937	3.184581
H	-2.367534	0.924766	-1.730118
H	0.365627	1.863026	1.109187
O	1.200249	1.382913	0.935114
H	-2.102004	2.150229	0.15707
H	1.065693	0.913709	0.017923
O	3.32021	2.58175	1.00175
H	4.086997	1.957728	0.912045
H	3.433267	3.28378	0.347625
C	4.346914	-1.008511	-0.112301
C	4.151938	-2.268216	0.363425
C	2.778166	-2.588892	0.112578
C	2.248572	-1.497434	-0.499365
O	3.186852	-0.529084	-0.644629
C	0.866631	-1.200343	-1.004923
O	-0.024438	-1.63804	-0.017948
C	5.527126	-0.110113	-0.151107
H	2.253261	-3.50031	0.357009
H	0.647298	-1.708531	-1.953474
H	6.422155	-0.705646	0.042654
H	4.897636	-2.8893	0.83816
H	-4.049184	2.734605	-1.395593
O	5.39038	0.900148	0.86201
H	6.218842	1.395637	0.92301
H	5.613187	0.362276	-1.134949
H	-0.124086	0.398109	-1.540985

H	4.546365	0.771683	0.370585
H	1.883383	-2.338749	0.794662
H	5.257977	-1.338574	-0.659183
H	5.113703	-1.493708	1.115151
H	1.180136	1.004883	-2.600342
H	1.863511	1.570574	2.214252
H	2.202947	-2.034543	-1.408987
H	-0.373813	-2.042049	-0.187378
O	-1.113376	-1.764576	-0.766695
H	-0.69153	-0.324161	-1.233433
H	-1.07599	-2.352075	-1.532891
O	0.398945	4.336631	-0.483607
H	-0.133413	5.141287	-0.419816
H	1.305077	4.585968	-0.255549
C	-3.83254	-0.756133	0.484291
C	-3.253315	-0.827819	1.721024
C	-2.201192	0.129949	1.72607
C	-2.234281	0.722067	0.493761
O	-3.225403	0.188194	-0.265909
C	-1.417073	1.737548	-0.122938
O	-0.508202	2.272497	0.624245
C	-4.951483	-1.495714	-0.171502
O	-5.998289	-0.633155	-0.584745
H	-1.519916	0.368832	2.530493
H	-1.830177	2.31103	-0.95007
H	-5.699268	-0.119496	-1.345593
H	-4.559135	-2.069969	-1.019935
H	-5.374376	-2.195608	0.55035
H	-3.549141	-1.486023	2.524169
H	-0.134915	3.140755	0.223361
H	4.059904	-3.255085	-0.03845

17. **FH-c**

C	2.050972	1.132468	0.94874
C	2.458678	1.728755	-0.40061
C	1.772473	0.783233	-1.412315
O	0.809279	0.019581	-0.68032
C	0.669169	0.516212	0.652047
O	1.928546	3.024928	-0.594976
C	2.706846	-0.1794	-2.129266
O	3.270959	-1.159058	-1.25778
O	0.058079	-3.292245	0.5538
O	2.89969	0.032605	1.257024
H	2.028871	1.863793	1.760388
H	3.549405	1.729142	-0.509396
H	1.270616	1.403856	-2.164477
H	3.622934	0.317958	1.829799
H	2.148391	-0.730788	-2.890126
H	3.501435	0.388839	-2.624671
H	2.429584	3.657737	-0.064285

18. **TS FH-c** (493.880 cm^{-1})

C	-3.244206	0.487568	1.129875
C	-3.963641	-0.808128	0.72607
C	-3.73199	-0.882878	-0.799953
O	-2.827539	0.180993	-1.128382
C	-2.159108	0.62551	0.044013
O	-3.367544	-1.95022	1.314689
C	-4.982742	-0.690425	-1.637028
O	-5.707598	0.465844	-1.259648
O	2.924901	-3.093852	-0.808227
O	-4.073336	1.620381	0.939408
H	-2.83641	0.445971	2.14518
H	-5.030172	-0.747505	0.967912
H	-3.271694	-1.850094	-1.038079
H	-4.712012	1.693342	1.659726
H	-4.691597	-0.642471	-2.69411
H	-5.645223	-1.549744	-1.499063
H	-3.641284	-2.011305	2.238797

H	-0.201088	-4.206685	0.737921
H	2.296665	-2.393305	-1.223018
O	1.625035	-3.141605	-1.290876
H	2.098691	-3.956631	-1.501908
H	0.772192	-3.243624	-0.27802
O	-1.941914	-1.887569	0.240886
H	-1.73532	-0.940075	0.402928
H	-2.335262	-1.939741	-0.640503
C	-3.994102	0.797325	0.126687
C	-5.103244	0.471256	0.856255
C	-5.871701	-0.407344	0.042247
C	-5.169744	-0.556914	-1.122676
O	-4.021262	0.179243	-1.074458
C	-5.412051	-1.310783	-2.345744
O	-6.4025	-1.998092	-2.51708
C	-2.815182	1.657773	0.410611
H	-6.816904	-0.875132	0.275819
H	-4.630098	-1.218011	-3.119418
H	-2.701332	2.427196	-0.364197
H	-2.956622	2.146633	1.381255
H	-5.331929	0.820641	1.85226
H	3.386741	-0.794963	-0.358881
H	-0.802242	-2.686014	0.405853
C	-0.468038	1.525953	0.738652
H	-0.520056	1.934451	1.756403
H	-0.301331	2.341146	0.025562
O	-1.661251	0.828813	0.42979
O	0.342903	-0.537652	1.487707
H	1.135253	-1.087124	1.599028

H	3.789189	-2.8197	-0.414477
H	5.40785	-2.234358	1.13733
O	5.174404	-2.039279	0.221025
H	5.993202	-2.120476	-0.283991
H	2.633772	-3.884891	-0.334236
O	1.012687	2.282286	-0.245125
H	0.440676	0.726168	-0.706982
H	1.552507	2.417625	0.544195
C	2.453508	-0.645178	0.180701
C	2.594843	-0.438996	1.533522
C	3.584319	0.563085	1.67455
C	3.97401	0.885443	0.397167
O	3.289542	0.163327	-0.511262
C	4.970772	1.828727	-0.127745
O	5.640998	2.529319	0.601301
C	1.595022	-1.500667	-0.579632
H	3.973921	0.993663	2.584882
H	5.068787	1.855496	-1.225485
H	1.608747	-1.474302	-1.657323
H	0.918749	-2.167964	-0.066668
H	2.051274	-0.953312	2.313556
H	-5.077919	1.163163	-1.021006
H	0.128718	2.624835	-0.033511
C	-0.920269	-0.220743	0.335151
H	-0.449601	0.1343	1.261009
H	-1.220036	-1.263598	0.462846
O	-0.004235	-0.157151	-0.749685
O	-1.747744	1.9384	-0.15151
H	-2.53089	2.507528	-0.0743

19. **GH-c**

C	-2.918124	1.103223	-0.344232
C	-1.709981	1.561832	-1.160087
C	-0.979966	0.345414	-1.728064
O	-0.61196	-0.518064	-0.656166
C	-1.737271	-1.045466	0.021753
C	-2.516398	0.076233	0.713732
O	-2.11262	2.369487	-2.243737
C	0.278479	0.676045	-2.495902
O	1.191981	1.351902	-1.624307
O	-1.248627	-1.934812	0.991454
O	-3.676342	-0.418534	1.325169
O	-3.597409	2.221792	0.191212
O	-2.421669	-1.416885	3.558259
O	0.993931	1.342325	0.895464
H	-1.120284	-2.809803	0.597408
H	-1.655014	-0.178566	-2.422702
H	-1.840678	0.543523	1.451017
H	-3.420664	-0.802995	2.186328
H	-2.38775	-1.579759	-0.685524

20. **TS GH-c** (-501.730 cm^{-1})

C	2.78164	-0.887176	1.147481
C	1.64663	-1.21126	0.17996
C	2.116161	-1.013389	-1.258309
O	2.509656	0.349639	-1.409537
C	3.611432	0.705598	-0.586358
C	3.264611	0.533373	0.893776
O	1.202613	-2.542256	0.33554
C	1.043974	-1.313962	-2.288963
O	-0.193694	-0.662139	-2.026307
O	3.874245	2.05287	-0.783646
O	4.394571	0.783817	1.69472
O	2.371512	-1.115072	2.482459
O	-4.889679	-1.027354	0.745994
O	0.150883	1.815503	-1.118279
H	4.366921	2.17761	-1.605473
H	2.973052	-1.67438	-1.462557
H	2.451834	1.243705	1.122977
H	4.682083	1.692784	1.531657
H	4.476647	0.077902	-0.850169

H	-3.63731	0.630719	-1.026745
H	-3.081312	2.59887	0.917519
H	-1.029139	2.118674	-0.498198
H	-2.715368	3.043562	-1.898154
H	0.737511	-0.253972	-2.846277
H	0.039533	1.319957	-3.347393
H	1.079148	0.336861	1.35235
H	1.633136	1.975434	1.258466
H	1.056248	1.316222	-0.131354
H	-2.811381	-1.860123	4.32111
H	-1.895092	-2.080042	3.091703
C	3.434963	0.996917	-0.95963
C	4.374413	1.643479	-0.206435
C	4.79649	0.711185	0.786332
C	4.073842	-0.42914	0.567031
O	3.245339	-0.260374	-0.500964
C	4.020339	-1.728203	1.231714
O	4.697237	-1.999424	2.205794
C	2.553362	1.413089	-2.083737
O	1.121094	-0.880134	1.83858
H	5.529427	0.857172	1.566138
H	3.318393	-2.454318	0.788597
H	1.194684	-0.918919	2.803296
H	2.672167	0.740361	-2.938391
H	2.789522	2.433399	-2.391548
H	4.711027	2.660203	-0.346312
H	0.300503	-1.361614	1.578084

H	3.610101	-1.586395	0.9752
H	1.781926	-0.403193	2.769135
H	0.820484	-0.504088	0.36457
H	1.155814	-2.72583	1.28616
H	1.407696	-1.018585	-3.278831
H	0.843069	-2.388073	-2.295982
H	1.112306	1.888257	-1.231531
H	-0.243366	2.584123	-1.549426
H	-0.07324	0.291165	-1.772042
H	-5.756724	-0.991562	0.323093
H	-5.053262	-0.936887	1.693164
C	-1.999813	-0.435507	-0.094026
C	-1.73061	-0.078266	1.206237
C	-2.366628	1.168334	1.410543
C	-2.969716	1.478192	0.216976
O	-2.755525	0.510304	-0.696778
C	-3.774097	2.625055	-0.218369
O	-4.038128	3.549983	0.522275
C	-1.650172	-1.593661	-0.863071
O	-3.059046	-2.86255	0.010069
H	-2.386295	1.769638	2.307081
H	-4.124832	2.59058	-1.26333
H	-3.822113	-2.293605	0.273786
H	-2.111166	-1.76364	-1.822804
H	-0.908279	-2.279523	-0.474012
H	-1.164026	-0.660971	1.919219
H	-3.395199	-3.536794	-0.596524

21. **I5**

C	-2.798766	0.294899	1.549462
C	-1.764469	1.286908	0.996781
C	-2.13415	1.41955	-0.498192
O	-3.174112	0.470271	-0.735533
C	-3.145221	-0.508892	0.289876
O	-1.758915	2.539208	1.701971
C	-0.979721	1.107116	-1.444345
O	-2.091209	-1.406611	0.122578
C	-4.492164	-1.203648	0.3398
O	-4.608291	-2.002067	-0.821971
O	-2.34858	-0.490039	2.616844
H	-4.518407	-1.815098	1.250121
H	-3.688702	0.838397	1.889553
H	-0.754573	0.881781	1.120801
H	-2.54185	2.415936	-0.708594
H	-1.779313	-1.179968	2.241548
H	-5.282875	-0.4459	0.39018
H	-2.663509	2.856567	1.850461
H	-5.401786	-2.544938	-0.751889
H	-0.9676	3.496987	0.974869
O	0.930877	-1.452704	-2.646543

22. **TS I5** (-604.110 cm^{-1})

C	-2.798766	0.294899	1.549462
C	-1.764469	1.286908	0.996781
C	-2.13415	1.41955	-0.498192
O	-3.174112	0.470271	-0.735533
C	-3.145221	-0.508892	0.289876
O	-1.758915	2.539208	1.701971
C	-0.979721	1.107116	-1.444345
O	-2.091209	-1.406611	0.122578
C	-4.492164	-1.203648	0.3398
O	-4.608291	-2.002067	-0.821971
O	-2.34858	-0.490039	2.616844
H	-4.518407	-1.815098	1.250121
H	-3.688702	0.838397	1.889553
H	-0.754573	0.881781	1.120801
H	-2.54185	2.415936	-0.708594
H	-1.779313	-1.179968	2.241548
H	-5.282875	-0.4459	0.39018
H	-2.663509	2.856567	1.850461
H	-5.401786	-2.544938	-0.751889
H	-0.9676	3.496987	0.974869
O	0.930877	-1.452704	-2.646543

H	1.436469	-1.82224	-3.380492
H	1.412297	-1.698666	-1.832049
O	-0.42871	3.992079	0.220817
O	4.458639	1.7109	-0.593119
H	4.467513	2.178951	0.25375
O	2.261886	-2.117489	-0.265081
H	3.58033	0.163078	-1.524892
C	3.505089	0.680669	-0.560029
C	2.062805	1.130154	-0.322972
O	2.767168	-2.35493	2.507767
H	2.462148	-2.670578	3.366251
H	3.890271	0.166624	1.508653
C	3.69115	-0.346513	0.556839
H	5.501506	-0.885043	0.052398
O	1.388369	-0.047398	0.134154
O	4.671355	-1.319188	0.290404
C	1.832186	-1.427367	1.996945
C	2.30251	-1.015491	0.613565
H	0.83394	-1.870083	1.891319
H	1.764912	-0.529775	2.624596
O	0.047161	2.10337	-1.274844
H	-1.325694	1.131613	-2.481906
H	-0.56665	0.124124	-1.20991
C	1.385526	1.667924	-1.563918
H	1.34045	0.899118	-2.340982
H	1.931861	2.540403	-1.930508
H	3.165117	-2.465254	-0.357312
H	-2.122343	-1.813583	-0.777401
H	0.333096	4.479171	0.572562
H	-0.144613	3.239896	-0.473228
H	2.034942	1.888131	0.475519
O	-1.691925	-2.236371	-2.404723
H	-1.830882	-3.150055	-2.678262
H	-0.7444	-2.033685	-2.55981

H	1.436469	-1.82224	-3.380492
H	1.412297	-1.698666	-1.832049
O	-0.42871	3.992079	0.220817
O	4.458639	1.7109	-0.593119
H	4.467513	2.178951	0.25375
O	2.261886	-2.117489	-0.265081
H	3.58033	0.163078	-1.524892
C	3.505089	0.680669	-0.560029
C	2.062805	1.130154	-0.322972
O	2.767168	-2.35493	2.507767
H	2.462148	-2.670578	3.366251
H	3.890271	0.166624	1.508653
C	3.69115	-0.346513	0.556839
H	5.501506	-0.885043	0.052398
O	1.388369	-0.047398	0.134154
O	4.671355	-1.319188	0.290404
C	1.832186	-1.427367	1.996945
C	2.30251	-1.015491	0.613565
H	0.83394	-1.870083	1.891319
H	1.764912	-0.529775	2.624596
O	0.047161	2.10337	-1.274844
H	-1.325694	1.131613	-2.481906
H	-0.56665	0.124124	-1.20991
C	1.385526	1.667924	-1.563918
H	1.34045	0.899118	-2.340982
H	1.931861	2.540403	-1.930508
H	3.165117	-2.465254	-0.357312
H	-2.122343	-1.813583	-0.777401
H	0.333096	4.479171	0.572562
H	-0.144613	3.239896	-0.473228
H	2.034942	1.888131	0.475519
O	-1.691925	-2.236371	-2.404723
H	-1.830882	-3.150055	-2.678262
H	-0.7444	-2.033685	-2.55981

23. **I4**

C	2.145447	-2.197578	-0.58675
C	0.97972	-1.23905	-0.796515
C	1.334288	-0.097154	-1.743827
O	2.525128	0.548048	-1.311995
C	3.651789	-0.250836	-1.015811
C	3.325392	-1.396805	-0.056782
O	-0.149462	-1.904168	-1.322638
C	0.27473	0.989779	-1.717102
O	0.270357	1.52032	-0.383947
O	4.535157	0.602568	-0.337205
O	4.443501	-2.242398	0.074101
O	1.744877	-3.238474	0.278558
O	0.766702	-1.808525	2.502568
O	2.395069	2.101778	0.893632

24. **TS I4** (595.470 cm^{-1})

C	3.250341	-1.486294	-0.083431
C	1.840228	-0.890355	-0.127206
C	1.765119	0.2943	-1.104257
O	2.768668	1.248729	-0.777871
C	4.088387	0.735664	-0.859827
C	4.276087	-0.383037	0.160098
O	0.862697	-1.867189	-0.448568
C	0.42725	1.015448	-1.061188
O	0.134856	1.466756	0.264348
O	4.966045	1.756043	-0.525445
O	5.565012	-0.938198	0.046022
O	3.347248	-2.530924	0.858697
O	-4.484213	2.524969	-1.03997
O	1.839482	3.383742	0.750713

H	5.080005	1.094093	-0.967394
H	1.442576	-0.483639	-2.767023
H	3.047396	-0.956	0.914838
H	5.154872	-1.74547	0.500042
H	4.102562	-0.641575	-1.938414
H	2.422107	-2.672922	-1.537264
H	1.44757	-2.835003	1.119344
H	0.746652	-0.803151	0.187447
H	-0.199518	-2.769563	-0.889084
H	3.203209	1.734532	0.468873
H	1.578734	1.864331	0.310001
H	0.120416	-1.078995	2.45293
H	1.339354	-1.612888	3.25316
H	-0.706832	0.568598	-1.952231
H	0.51719	1.790068	-2.424446
O	-1.042078	0.348684	2.095266
C	-0.845403	2.334483	-0.027392
H	-1.587151	0.66745	2.828527
H	-1.227982	-0.413516	0.237786
C	-1.828994	0.189121	0.927782
C	-2.112069	1.534362	0.247268
H	-2.425989	-2.390258	1.174503
H	-2.753931	2.154217	0.896369
O	-2.903891	-1.818681	1.791651
C	-3.1346	-0.563396	1.189703
O	-2.787492	1.285054	-0.980619
H	-3.351294	-1.312432	-0.821066
H	-3.747128	-0.004342	1.911075
C	-3.914007	-0.67607	-0.11748
C	-4.060288	0.697956	-0.769558
O	-4.672439	0.501254	-1.998103
O	-5.181247	-1.224869	0.160323
H	-4.659337	1.36057	-0.123431
H	-5.029608	1.336759	-2.325745
H	-5.668841	-1.279842	-0.673221
H	-0.547473	2.85349	0.885307
H	-1.041354	3.073541	-0.812283
H	2.479353	3.128274	1.09063
O	2.502888	4.523678	1.394391
H	2.913982	4.767863	2.234913

H	5.132717	2.3164	-1.294554
H	1.917106	-0.071091	-2.133603
H	4.119032	0.054798	1.15969
H	6.20696	-0.228467	0.186612
H	4.270511	0.361373	-1.879193
H	3.477625	-1.950034	-1.053866
H	3.181104	-2.182995	1.745918
H	1.581698	-0.525077	0.875347
H	1.126407	-2.358748	-1.239705
H	2.568637	2.998942	0.237045
H	0.715221	2.254057	0.48107
H	-3.838861	1.878334	-1.368939
H	-4.58138	3.203444	-1.719098
H	-0.368982	0.330588	-1.359878
H	0.444871	1.863151	-1.75407
O	-1.292737	-0.286597	2.632628
C	-1.739202	1.970939	0.791226
H	-2.096686	-0.455221	3.143557
H	-0.555861	-0.510128	0.787221
C	-1.53131	-0.52448	1.264894
C	-2.387206	0.614273	0.679813
H	-0.411954	-2.773477	0.817952
H	-3.316783	0.663097	1.268152
O	-1.226324	-2.917532	1.331505
C	-2.140548	-1.901706	0.982676
O	-2.692595	0.390088	-0.690083
H	-1.668024	-1.98504	-1.119756
H	-3.030185	-2.061531	1.60798
C	-2.5656	-2.006016	-0.480676
C	-3.432652	-0.8178	-0.879842
O	-3.722249	-0.937874	-2.227389
O	-3.283835	-3.206008	-0.647092
H	-4.348179	-0.775493	-0.26919
H	-4.558775	-0.503508	-2.437817
H	-3.543123	-3.270631	-1.576631
H	-1.30683	2.264844	1.736362
H	-1.713018	2.633602	-0.060511
H	1.699546	4.279262	0.419056
O	-3.411666	2.918845	1.345989
H	-3.220455	3.831749	1.605

25. **TS R1.2** (-614.200 cm^{-1})

C	-1.2756	-2.616386	-0.389575
C	-2.666648	-1.985895	-0.398939
C	-2.606039	-0.647982	-1.134935
O	-1.693698	0.201228	-0.44846
C	-0.371691	-0.295273	-0.455521
C	-0.269542	-1.657526	0.231874
O	-3.583138	-2.836657	-1.059778
C	-3.929499	0.082577	-1.24482

26. **TS R2.2** (-207.17 cm^{-1})

C	2.248355	-1.874918	-1.637216
C	3.654808	-1.60368	-1.127687
C	3.791301	-2.147822	0.295771
O	2.789104	-1.539354	1.108956
C	1.46631	-1.841856	0.718648
C	1.210423	-1.28628	-0.683528
O	4.622054	-2.226348	-1.95676
C	5.128374	-1.863187	0.956934

O	-4.505362	0.372217	0.034422
O	0.410266	0.595757	0.276382
O	1.027427	-2.18115	0.079746
O	-1.31278	-3.883667	0.238999
O	-3.349884	2.174666	1.301536
H	-2.258223	-0.82697	-2.165515
H	-0.513853	-1.507638	1.297515
H	1.664657	-1.444953	0.040636
H	-0.002137	-0.370329	-1.491178
H	-0.975268	-2.818605	-1.425853
H	-1.422216	-3.770936	1.194126
H	-2.98325	-1.81311	0.641899
H	-3.381183	-3.744498	-0.782964
H	-3.761476	1.0179	-1.792164
H	-4.649656	-0.530064	-1.791218
H	-2.500513	1.951061	1.754023
H	-3.164591	2.922028	0.700493
H	-3.909908	1.049367	0.555736
C	-6.797266	-1.688399	1.049155
C	-7.147856	-0.231854	1.387735
C	-7.137693	0.479135	0.013283
O	-6.92895	-0.507938	-0.981764
C	-7.182538	-1.81453	-0.44059
O	-8.453974	-0.083226	1.909328
C	-6.095255	1.56123	-0.153766
O	-6.434951	-2.741962	-1.135087
C	-8.649648	-2.168291	-0.661531
O	-8.931864	-3.472711	-0.198397
O	-5.427272	-1.962413	1.238211
H	-9.288156	-1.478564	-0.103347
H	-7.367478	-2.392262	1.659929
H	-6.402501	0.185726	2.075352
H	-8.119546	0.944582	-0.121596
H	-4.926434	-1.182723	0.936239
H	-5.741321	1.796724	-1.1481
H	-5.711865	2.106885	0.697221
H	-8.858707	-2.06237	-1.733923
H	-8.4782	-0.435643	2.80838
H	-5.502701	-2.714482	-0.840179
H	-8.312164	-4.073016	-0.635794
O	-3.018057	4.208843	-0.619233
H	-2.523936	3.856054	-1.372089
H	-2.521266	4.982926	-0.320702
C	7.421078	-2.340269	0.16011
C	6.516011	-1.128376	-0.050309
C	7.12279	-0.20667	-1.107398
O	8.408911	0.201232	-0.663541
C	9.30877	-0.886224	-0.548122
C	8.826104	-1.876289	0.512989
O	5.235573	-1.546036	-0.486223
C	6.297783	1.024719	-1.411735

O	5.521638	-0.494614	0.886288
O	0.648906	-1.220657	1.675915
O	-0.10035	-1.525037	-1.14192
O	2.166252	-1.307989	-2.927074
O	2.431031	-0.260263	3.722253
O	6.648355	-0.375531	-1.389832
H	3.649737	-3.239465	0.281961
H	1.323148	-0.195749	-0.646517
H	-0.314195	-2.469558	-1.088675
H	1.312246	-2.933865	0.739315
H	2.102342	-2.967132	-1.695272
H	1.289858	-1.491902	-3.292229
H	3.815938	-0.513016	-1.119189
H	4.302198	-2.175356	-2.871221
H	5.066241	-2.138967	2.012549
H	5.908404	-2.466504	0.48137
H	6.658194	0.460097	-1.897442
H	6.13784	-1.030251	-1.898802
H	5.971622	-0.320006	-0.013636
H	2.588108	-1.014139	4.306631
H	1.862238	-0.583765	2.996515
C	6.178011	3.072373	-0.693973
C	6.74841	3.609016	0.424707
C	6.183661	2.915812	1.536178
C	5.309311	2.014358	1.002734
O	5.292668	2.107249	-0.352867
C	4.47462	0.977704	1.570943
O	4.490922	0.841387	2.846735
C	6.353606	3.305948	-2.151927
O	-8.800004	1.840363	0.835202
H	6.393489	3.056302	2.586293
H	3.590392	0.661274	1.019104
H	5.395899	3.582915	-2.605053
H	7.068225	4.120894	-2.295141
H	7.487316	4.396087	0.446218
H	3.66114	0.3266	3.206291
C	-6.482639	2.463487	0.554136
C	-5.122631	1.979085	0.069552
C	-5.282418	1.339696	-1.309581
O	-6.262692	0.304591	-1.246514
C	-7.566531	0.750134	-0.885709
C	-7.519783	1.344501	0.516117
O	-4.214175	3.051137	-0.06163
C	-3.992082	0.740139	-1.843237
O	-3.31788	-0.120312	-0.931865
O	-8.403674	-0.350083	-0.879091
O	-6.408675	3.051637	1.842845
O	-0.959648	1.033051	0.405016
H	-8.621728	-0.594968	-1.787915
H	-5.608475	2.114599	-2.021843
H	-7.227654	0.536836	1.207655

O	6.078542	1.777738	-0.220802
O	10.53928	-0.406008	-0.124502
O	9.67669	-2.997971	0.566267
O	6.851283	-3.21793	1.112834
O	-7.35784	3.072311	-0.440642
O	-5.672553	4.88801	-1.247672
H	11.004406	0.003505	-0.865395
H	7.208707	-0.7694	-2.052067
H	8.812117	-1.343683	1.478019
H	10.570134	-2.682597	0.760989
H	9.391597	-1.394516	-1.522895
H	7.461383	-2.915859	-0.773909
H	6.932021	-2.834641	1.997675
H	6.438952	-0.581249	0.902004
H	4.978312	-2.303331	0.063004
H	6.8505	1.638557	-2.132415
H	5.341664	0.727433	-1.858077
H	-4.735668	4.673306	-1.07081
H	-5.72897	5.157323	-2.172235
H	-7.791698	3.361069	0.375401
H	-6.7712	3.825169	-0.746218
C	3.164568	1.427118	1.197008
C	3.584664	2.900488	1.218705
C	4.050445	3.156114	-0.22391
O	3.403229	2.169683	-1.035785
C	2.660463	1.236484	-0.254294
O	2.484751	3.76195	1.458053
C	5.555533	3.084318	-0.4516
O	2.857296	-0.052942	-0.731824
C	1.181233	1.558497	-0.43945
O	4.246968	0.569245	1.47361
H	0.963807	2.552171	-0.041007
H	2.376081	1.209754	1.922753
H	4.384059	3.067479	1.950095
H	3.706402	4.152483	-0.524545
H	5.034264	0.914914	1.007825
H	5.779082	3.391012	-1.478441
H	6.061589	3.772117	0.232726
H	0.943868	1.53054	-1.507411
H	2.198157	3.662089	2.37534
H	3.735657	-0.391225	-0.457727
O	-0.984429	1.632782	2.462797
H	-0.968253	1.052498	3.233103
H	-7.896286	1.510679	-1.611243
H	-6.817737	3.273374	-0.107253
H	-6.112774	2.389421	2.484786
H	-4.728223	1.225766	0.770527
H	-4.210566	3.545767	0.769662
H	-4.202907	0.21107	-2.778558
H	-3.288203	1.548947	-2.046642
H	-1.667509	0.544155	-0.046407
H	-0.45257	0.340645	0.852412
C	-1.335369	-2.570578	1.468769
C	-1.599571	-3.751672	0.844323
C	-2.699375	-3.499226	-0.0452
C	-3.004631	-2.183689	0.111327
O	-2.199393	-1.613599	1.03606
C	-4.025083	-1.283116	-0.507207
O	-4.627924	-1.966315	-1.55392
C	-0.260699	-2.100716	2.377449
H	-3.191612	-4.19294	-0.70949
H	-4.778267	-0.983821	0.233613
H	-0.661785	-1.494145	3.191488
H	0.288325	-2.951218	2.79208
H	-1.069853	-4.682169	0.992053
H	-5.498638	-1.562382	-1.696938
O	6.839497	2.091327	-2.723106
H	6.799373	2.149395	-3.686247

27. **TS G-GF1** (-200.480 cm^{-1})

C	1.90166	-0.4701	0.322855
C	-0.325326	-1.612529	-0.283153
C	0.062065	1.202402	0.607776
C	-0.88242	2.1463	-0.131896
C	1.281191	0.817788	-0.242378

28. **TS F-FH1** (-174.540 cm^{-1})

C	0.556782	1.476116	-0.780768
O	0.023987	0.161481	-1.231291
C	-0.611656	-0.448429	-0.315204
C	-0.682666	0.37099	0.992795
C	-0.280311	1.774524	0.469908

O	-0.584074	-0.022275	0.97263
O	1.459945	-2.849097	0.563411
H	2.420357	-2.965937	0.589356
O	2.198146	1.889214	-0.317388
O	3.27827	-0.59348	0.057573
H	3.469158	-0.29762	-0.844135
O	-0.27506	3.402987	-0.351222
H	0.623975	3.26509	-0.685586
C	1.180015	-1.717807	-0.222592
H	1.506391	-1.860184	-1.26371
H	0.421136	1.68852	1.525755
H	1.806271	-0.484129	1.414405
H	0.96875	0.648225	-1.281863
H	-1.773044	2.331044	0.476055
H	2.635642	2.01335	0.537639
O	-0.843198	-1.214666	-1.363662
H	-3.810552	0.891571	1.456385
H	-0.910946	-2.193173	0.432656
H	-1.199375	1.677727	-1.075502
O	-3.328642	0.061799	1.33343
H	-3.623637	-0.522097	2.04671
H	-1.527222	0.111741	1.217096
O	-3.26772	-1.22004	-1.091655
H	-3.814604	-0.921448	-1.830767
H	-1.919669	-1.223171	-1.320961
H	-3.511027	-0.702405	-0.294127

H	0.311955	2.152044	-1.600661
C	2.05734	1.394814	-0.597966
H	2.446162	2.415449	-0.598377
O	0.874835	-2.020687	0.269655
H	0.87038	-2.209851	1.216697
C	-1.538585	-1.552353	-0.736933
H	-0.94955	-2.361783	-1.167264
H	-2.165805	-1.123784	-1.528679
O	-2.288877	-2.033204	0.339469
H	-3.052084	-1.446042	0.449254
H	0.31063	2.295061	1.226242
H	-1.716055	0.374346	1.341695
O	0.101757	-0.113597	2.036699
H	1.034905	-0.005603	1.777698
O	-1.39361	2.576104	0.165826
H	-2.137915	2.028967	-0.143413
H	2.500105	0.851628	-1.438069
O	2.397421	0.725704	0.618256
H	2.900837	1.321689	1.188648
O	3.405988	-1.557411	-0.555347
H	4.119579	-2.196735	-0.445351
H	1.815983	-1.919136	-0.00778
O	-3.467301	0.634516	-0.247321
H	-3.930343	0.661533	-1.096225
H	-4.127621	0.90561	0.406331
H	3.607908	-0.800249	0.015003

29. **FH1**

C	1.381792	-0.010296	0.004281
O	0.348677	0.157861	-1.05366
C	-0.675222	-0.533878	-0.802946
C	-0.565294	-1.34264	0.463835
C	0.948302	-1.29029	0.72734
H	1.282476	0.870318	0.645903
H	-1.090768	-0.791844	1.256449
H	1.409216	-2.167948	0.254652
C	-1.797417	-0.626419	-1.77428
H	-1.905893	0.3362	-2.28769
H	-1.496757	-1.381475	-2.513238
O	-2.95755	-1.071328	-1.125169
H	-3.252469	-0.333811	-0.562005
O	-1.020016	-2.651878	0.297575
H	-1.983384	-2.633515	0.181178
O	1.30475	-1.173916	2.074219
H	1.345788	-2.050936	2.476045
C	2.730129	-0.081669	-0.660502
H	3.453642	-0.366046	0.113506
H	2.716611	-0.854741	-1.437686
O	3.02307	1.190154	-1.206076
H	3.869879	1.16851	-1.668693
O	1.095571	3.098458	-0.647066

30. **TS FH1-FH2** (-716.860 cm^{-1})

C	1.402126	-1.578187	-0.474144
C	1.990857	-0.201235	-0.19069
O	1.011503	0.684524	-0.796404
C	-0.178871	0.182177	-0.476588
C	-0.109989	-1.334948	-0.255882
C	3.339363	0.162601	-0.740406
O	3.609364	1.460897	-0.227214
C	-1.309416	1.004746	-0.505043
O	-2.512959	0.50129	-0.372388
O	-0.882848	-2.034209	-1.181231
O	1.969603	-2.514683	0.4003
O	-4.239613	2.304098	-0.051937
O	1.020077	2.319818	1.292286
O	-3.085337	-2.251649	0.360159
H	1.9825	-0.01933	0.893539
H	-0.371901	-1.586553	0.779244
H	1.554802	-1.851036	-1.526704
H	-0.571974	0.85183	0.620492
H	-1.172552	2.065946	-0.722186
H	-3.206973	1.242969	-0.241039
H	-1.7504	-2.23051	-0.766165
H	1.784571	-3.407185	0.082334
H	4.075398	-0.570835	-0.392588

H	1.899025	2.634007	-0.941194
H	1.359153	3.995099	-0.410535
O	-2.246443	1.196154	0.217905
H	-2.374161	1.601601	1.083223
H	-2.024635	1.910965	-0.421447
O	-1.294634	2.607761	-1.834097
H	-0.401078	2.879822	-1.530436
H	-1.693345	3.370833	-2.267414

H	3.313053	0.161751	-1.836115
H	4.431538	1.797631	-0.602789
H	1.872526	2.327886	0.828486
H	-4.155288	2.871553	0.7257
H	-4.423215	2.883503	-0.803269
H	-3.443187	-1.355223	0.305904
H	1.170331	2.757128	2.137962
H	-3.827031	-2.855113	0.23296

31. **FH2**

C	-0.217281	-0.903683	-0.885966
O	0.63494	0.106272	-0.318236
C	-0.134435	1.000104	0.454151
C	-1.551894	0.928932	-0.121708
C	-1.637417	-0.570661	-0.41851
H	-0.172911	-0.832042	-1.979074
C	0.290301	-2.261142	-0.45156
H	-0.40782	-3.034783	-0.787618
O	3.326597	0.572355	-0.326241
H	3.100468	0.083149	-1.194999
H	2.688557	1.336742	-0.263584
O	2.751749	-1.003173	1.487627
H	2.845487	-0.69052	2.39634
H	3.084607	-0.084134	0.472644
H	1.84938	-1.393238	1.387172
H	-0.184595	0.687692	1.513989
C	0.476363	2.369777	0.437045
H	-0.148052	3.184836	0.835504
O	1.602396	2.593534	0.032869
H	-1.616848	1.487866	-1.065117
O	-2.467893	1.409292	0.829512
H	-3.283815	1.676495	0.389175
H	-1.861831	-1.090633	0.522739
O	-2.550906	-0.92745	-1.429574
H	-3.430351	-1.031817	-1.046759
H	1.275689	-2.444315	-0.894133
O	0.386042	-2.242628	0.97479
H	0.402438	-3.147475	1.311318
O	2.66787	-0.681795	-2.443726
H	3.372618	-1.148831	-2.912631
H	2.221698	-0.133722	-3.103768

32. **TS FH2-FH3** (-934.650 cm^{-1})

C	-0.939718	-0.553581	-0.319232
O	0.498048	-0.691234	-0.427515
C	1.090532	0.559499	-0.319953
C	0.041103	1.633198	-0.541328
C	-1.194371	0.921659	0.020824
H	-1.381442	-0.784288	-1.294994
C	-1.461491	-1.541456	0.699161
H	-2.554343	-1.476548	0.71424
O	1.191407	0.386433	2.297327
H	0.49155	-0.315474	2.325706
H	1.984674	0.050889	2.741104
O	2.478625	-2.551929	-0.907369
H	1.516456	-2.481454	-0.997449
H	2.967255	-1.156903	-0.76239
H	2.80628	-3.05483	-1.664529
H	1.38935	0.65039	0.990072
C	2.44765	0.72872	-0.537564
H	2.829075	1.747737	-0.486223
O	3.336469	-0.199309	-0.643668
H	-0.104822	1.808025	-1.614884
O	0.413657	2.808208	0.129444
H	0.025717	3.572829	-0.31311
H	-1.218215	1.070919	1.107857
O	-2.412329	1.324774	-0.567581
H	-2.749045	2.110545	-0.118435
H	-1.166642	-2.555228	0.408824
O	-0.916917	-1.211505	1.975996
H	-1.271206	-1.802991	2.651076
O	-4.032191	-0.927528	-1.188253
H	-3.672423	-0.033834	-1.066494
H	-4.74469	-0.845127	-1.831421

33. **FH3**

C	-0.636114	-1.173247	-0.608617
O	0.184567	0.016684	-0.600648
C	-0.631289	1.125752	-0.496755
C	-2.076598	0.712082	-0.538053
C	-1.973292	-0.727357	-0.022868

34. **I6**

O	-1.411918	0.005305	0.331971
C	-1.747121	-0.184688	1.624551
C	-0.680139	-0.666682	2.330829
C	0.390708	-0.782501	1.401115
C	-0.105574	-0.357917	0.19836

H	-0.788962	-1.495565	-1.647799
C	0.068645	-2.278693	0.14111
H	-0.529658	-3.189255	0.048986
O	3.038746	0.739569	0.031247
H	2.920485	0.177193	-0.819666
H	2.372415	1.476526	-0.03299
O	2.499749	-0.649879	1.980361
H	2.504306	-0.200531	2.835302
H	2.814222	0.151129	0.89202
H	1.622365	-1.10236	1.875026
C	-0.158204	2.356852	-0.346602
H	-0.823846	3.204809	-0.25618
O	1.199865	2.602353	-0.323881
H	-2.438729	0.676618	-1.575875
O	-2.869706	1.578009	0.237624
H	-3.78325	1.531383	-0.069992
H	-1.913478	-0.706173	1.072633
O	-2.98456	-1.595723	-0.474134
H	-3.743187	-1.542349	0.119418
H	1.055151	-2.456281	-0.302341
O	0.212215	-1.909242	1.513383
H	0.100461	-2.685587	2.076057
O	2.500256	-0.590353	-2.043818
H	2.962003	-0.42593	-2.876369
H	1.57203	-0.336772	-2.16693
H	1.377648	3.522362	-0.091376

C	-3.135072	0.161636	2.019249
O	-3.260545	1.59127	1.962009
C	-4.534667	2.072804	2.217833
O	-4.789993	2.057693	3.63769
C	0.475421	-0.229239	-1.13217
O	1.629307	-0.525328	-1.383587
C	-4.612975	3.49395	1.771603
O	-4.381046	3.717373	0.457263
C	-4.51284	5.057998	0.24939
C	-4.822602	5.679398	1.419167
C	-4.889461	4.654345	2.420937
C	-4.311817	5.541908	-1.14121
O	-5.382643	5.062125	-1.947488
O	-2.620303	2.259438	4.752103
H	-0.67255	-0.904959	3.384341
H	1.397118	-1.1294	1.584095
H	-0.20574	0.159433	-1.908739
H	-3.861641	-0.293586	1.336158
H	-3.350804	5.177682	-1.523575
H	-3.311087	-0.202393	3.036656
H	-5.305756	1.443912	1.755
H	-5.117787	4.762733	3.470635
H	-4.986457	6.738866	1.551136
H	-3.875701	2.172029	4.187206
H	-1.943094	2.463789	4.089376
H	-2.509874	2.88398	5.48313
H	-4.288441	6.636626	-1.119959
H	-5.197459	5.286396	-2.867751
H	-5.4611	1.304479	3.977553
O	-6.370145	0.372107	4.447928
H	-6.264622	-0.541334	4.146483
H	-7.302941	0.605095	4.338739

35. **I3’’**

C	-2.995559	-0.496415	-0.101405
C	-1.598465	0.103973	0.070588
C	-1.306741	0.768273	-1.2945
O	-2.549194	0.810026	-1.996096
C	-3.637057	0.434879	-1.151398
O	-1.634671	1.117366	1.114936
C	-0.293159	-0.01554	-2.106868
O	-0.739672	-1.363437	-2.176374
O	-4.613106	-0.21152	-1.888307
C	-4.285769	1.690217	-0.576996
O	-5.336525	1.357508	0.315633
O	-2.943229	-1.814291	-0.591838
H	-3.562324	2.280187	-0.010857
H	-3.561087	-0.508739	0.82985
H	-0.85411	-0.647503	0.349714
H	-0.92326	1.786708	-1.164359
H	-2.199019	-1.892506	-1.221548

36. **TS I3’’** (-195.020 cm^{-1})

C	-1.694301	0.725978	-1.509955
C	-1.844468	-0.014912	-0.177522
C	-3.364077	-0.027679	0.073402
C	-3.898472	1.164486	-0.796139
O	-2.771034	1.657343	-1.516676
O	-1.237418	0.730953	0.885295
O	-3.965775	-1.273798	-0.199445
O	-4.927146	0.810814	-1.658431
C	-4.385559	2.317044	0.06729
O	-5.483506	1.861101	0.832102
C	-1.724433	-0.180103	-2.728786
O	-2.93161	-0.94485	-2.702098
C	-0.64953	-0.263445	2.346816
O	-1.740444	-0.570751	2.970511
C	0.218756	0.704232	2.980987
O	1.471095	0.824181	2.463924
C	2.100586	1.788563	3.172012

H	-0.223259	0.420594	-3.108189
H	0.683224	0.049144	-1.613315
H	-4.652782	2.292213	-1.415834
H	-4.382017	-1.155176	-1.922277
H	-0.819189	3.985487	0.950254
O	-0.349294	3.149634	0.809912
H	-1.06102	2.045216	0.935124
H	0.446987	3.150295	1.364287
O	-4.436587	1.03555	2.913782
H	-5.125958	0.923412	3.579124
H	-4.882211	1.125505	2.046277
C	2.194814	0.283038	2.114075
C	2.00679	-0.929738	2.699705
C	0.605365	-1.037883	2.988513
C	0.052028	0.12325	2.558224
O	1.000176	0.942459	2.026903
C	-1.339066	0.64388	2.54201
O	-2.212014	-0.317339	2.887532
C	3.383691	0.978403	1.541584
O	3.367311	1.005387	0.12012
H	0.078965	-1.860258	3.449353
H	2.732131	1.667987	-0.178317
H	3.456378	1.993434	1.948432
H	4.27608	0.424512	1.836797
H	2.774904	-1.663314	2.89558
H	-0.069626	-1.920389	-2.590381
H	-5.958384	0.776517	-0.146281
H	-3.108786	0.10324	3.015409
H	-1.464156	1.592029	3.07689

C	1.268788	2.289067	4.134889
C	0.03696	1.585917	4.007565
C	3.514878	2.074805	2.787543
O	4.363648	0.957065	2.993788
O	-2.678457	-2.560636	1.782346
O	0.446211	2.590445	0.369719
H	-3.552707	2.633714	0.707345
H	-3.565313	0.181945	1.126425
H	-1.421812	-1.027063	-0.202261
H	-0.76125	1.295656	-1.549888
H	-3.72925	-1.541008	-1.105728
H	-1.696459	0.442022	-3.628008
H	-0.85173	-0.841108	-2.714581
H	-4.665711	3.144678	-0.595554
H	-4.583752	0.147104	-2.278993
H	1.277501	2.422191	-0.09346
H	0.086306	3.410434	0.005889
H	-0.547017	1.413422	0.594397
H	-3.302857	-2.316824	1.062399
H	-3.066024	-3.282454	2.293176
H	-0.86279	1.703013	4.593825
H	4.176065	0.291893	2.319731
H	3.555433	2.407556	1.743545
H	3.886133	2.882473	3.419674
H	1.515851	3.061119	4.848219
H	-2.970058	-1.524744	-3.473766
H	-5.749811	2.55714	1.443937
H	-2.178115	-1.407515	2.554643
H	-0.175691	-1.019606	1.717503

37. **TS I1-smd** (-622.900 cm^{-1})

C	3.626957	-1.293642	0.185149
C	2.16335	-0.94136	-0.063698
C	2.054461	0.135685	-1.139591
O	2.801761	1.278296	-0.720319
C	4.192956	1.009481	-0.580231
C	4.415551	-0.03301	0.51184
O	1.437889	-2.077086	-0.502482
C	0.632371	0.567969	-1.440052
O	-0.133452	0.873284	-0.265093
O	4.814513	2.19257	-0.183413
O	5.784222	-0.377867	0.600372
O	3.736762	-2.275571	1.201938
O	-3.241973	3.136592	-1.204557
O	1.258667	2.348711	1.366393
H	4.978188	2.744295	-0.961739
H	2.476008	-0.250185	-2.080413
H	4.055826	0.390194	1.462807
H	6.271259	0.387002	0.938402
H	4.588519	0.653055	-1.542207

38. **TS I3-smd** (-225.560 cm^{-1})

C	1.498575	-0.440697	0.658946
C	2.749999	0.014955	1.431376
C	3.859558	0.000073	0.384579
O	3.189876	0.330571	-0.843685
C	1.854037	-0.149163	-0.842471
O	2.611021	1.363882	1.85645
C	4.606326	-1.312847	0.274844
O	3.662304	-2.364281	0.055777
O	1.731207	-1.266588	-1.678707
C	1.003152	0.96067	-1.446852
O	-0.397236	0.685785	-1.395196
O	1.112639	-1.776582	0.910949
H	1.194963	1.876748	-0.882609
H	0.647537	0.174679	0.961921
H	2.955439	-0.649961	2.277646
H	4.585311	0.792935	0.582772
H	1.894738	-2.346756	0.798663
H	5.309545	-1.260614	-0.562091
H	5.160463	-1.485607	1.203635

H	4.042991	-1.752668	-0.720379
H	3.423748	-1.895842	2.037842
H	1.746107	-0.552815	0.878957
H	1.603342	-2.796563	0.127277
H	0.669069	1.443741	-2.097258
H	0.104984	-0.241174	-1.947806
H	2.092941	2.257973	0.871955
H	1.045253	3.292302	1.360336
H	0.370657	1.501078	0.342023
H	-2.818611	3.995925	-1.354271
H	-3.778486	3.228352	-0.370314
C	-2.172333	-1.215762	0.994551
C	-2.692476	0.228326	1.052164
C	-2.703996	0.699568	-0.416295
O	-2.323485	-0.400141	-1.229877
C	-2.356801	-1.625371	-0.486858
O	-4.027578	0.318437	1.53346
C	-1.787503	1.867231	-0.707852
O	-1.36232	-2.468795	-0.968456
C	-3.693969	-2.306705	-0.755076
O	-3.789728	-3.55409	-0.091628
O	-0.826087	-1.315621	1.411529
H	-4.50606	-1.67608	-0.383055
H	-2.759701	-1.866285	1.646526
H	-2.026582	0.839066	1.672132
H	-3.727697	0.996275	-0.667278
H	-0.329381	-0.598942	0.977739
H	-1.41042	2.00663	-1.711807
H	-1.521592	2.569067	0.070375
H	-3.801805	-2.421148	-1.840554
H	-4.034286	0.072783	2.470486
H	-0.483155	-2.181151	-0.647054
H	-3.090283	-4.128046	-0.43596
O	-4.537805	3.072068	1.12184
H	-5.475847	3.297471	1.059769
H	-4.507483	2.124938	1.361509

H	1.293431	1.112772	-2.490603
H	1.841301	1.428369	2.44033
H	2.321997	-1.961276	-1.334172
H	-0.341139	-2.037197	-0.260152
O	-1.066622	-1.762461	-0.857899
H	-0.619774	-0.295797	-1.236671
H	-0.963761	-2.306636	-1.651825
O	0.28025	4.415338	-0.515648
H	0.721593	4.191391	-1.348612
H	-0.423515	5.039222	-0.747132
C	-3.844446	-0.768527	0.44213
C	-3.242186	-0.848583	1.665298
C	-2.185893	0.108806	1.660889
C	-2.23257	0.707271	0.435233
O	-3.238986	0.180416	-0.317751
C	-1.425005	1.735704	-0.188663
O	-0.569796	2.335527	0.574786
C	-4.989473	-1.490276	-0.181714
O	-6.10736	-0.638299	-0.409081
H	-1.487008	0.335253	2.454331
H	-1.85254	2.283829	-1.026275
H	-5.898423	-0.046937	-1.145385
H	-4.664862	-1.955065	-1.119617
H	-5.314717	-2.274074	0.503727
H	-3.527167	-1.512755	2.468414
H	-0.227311	3.21351	0.139314
H	4.129303	-3.207153	-0.024335

39. **G-smd**

C	1.431517	-0.382895	-0.688204
C	0.254289	-1.283641	-0.32759
C	-1.01319	-0.827125	-1.048099
O	-1.250359	0.560154	-0.844052
C	-0.191322	1.47912	-1.029174
C	1.080665	1.04702	-0.306909
O	0.498489	-2.621923	-0.722543
C	-2.263007	-1.497819	-0.518704
O	-2.417667	-1.100509	0.85929
O	-0.634095	2.6664	-0.422379
O	2.153252	1.896234	-0.666213
O	2.614999	-0.83471	-0.058399

40. **G-ww-smd**

C	1.376835	-0.323339	-0.745537
C	0.20812	-1.226206	-0.361496
C	-1.098919	-0.648111	-0.904271
O	-1.265069	0.670718	-0.385078
C	-0.251145	1.558685	-0.828575
C	1.108267	1.10735	-0.301921
O	0.376362	-2.523241	-0.907436
C	-2.318697	-1.460094	-0.531281
O	-2.374815	-1.597108	0.883882
O	-0.5185	2.8231	-0.299956
O	2.140594	1.93069	-0.81163
O	2.59586	-0.828047	-0.222811

O	2.198252	-0.531837	2.672987
O	-2.175759	1.240516	1.597488
H	-1.200364	3.153037	-1.039626
H	-0.911392	-1.051891	-2.119327
H	0.891092	1.098176	0.776145
H	1.997485	2.768935	-0.278
H	0.003235	1.628646	-2.099354
H	1.612862	-0.439415	-1.769842
H	2.507525	-0.738815	0.913218
H	0.0978	-1.230254	0.760284
H	1.351674	-2.884826	-0.345978
H	-3.133196	-1.170257	-1.092826
H	-2.169075	-2.584426	-0.56811
H	-3.222693	-1.497637	1.225197
H	-1.752454	1.802661	0.905122
H	-3.029942	1.635551	1.843409
H	-2.311099	0.235711	1.215314
H	2.383771	-1.350845	3.152416
H	2.799454	0.122758	3.053973
H	-1.190536	3.259294	-0.842728
H	-1.042077	-0.608719	-2.003447
H	1.078699	1.154015	0.797369
H	2.027627	2.820545	-0.448369
H	-0.245997	1.584262	-1.928771
H	1.492412	-0.340397	-1.836907
H	2.556902	-0.7914	0.745347
H	0.147666	-1.278062	0.735437
H	1.253508	-2.84096	-0.646427
H	-3.209992	-0.943908	-0.905721
H	-2.250472	-2.439996	-1.016042
H	-3.176223	-2.087269	1.10912

41. **F-smd**

C	0.841013	0.719843	1.009411
C	2.010355	1.033401	0.067792
C	1.886462	-0.023761	-1.040686
O	0.547539	-0.547247	-0.958908
C	-0.204469	0.092367	0.062764
O	1.876945	2.312815	-0.531011
C	2.874483	-1.164159	-0.926457
O	2.72357	-1.774655	0.353952
O	-0.974379	-0.869456	0.738635
C	-1.167713	1.077845	-0.592077
O	-1.994707	1.730673	0.352041
O	1.200618	-0.197517	2.025618
H	-0.578267	1.83016	-1.122452
H	0.454458	1.619885	1.492412
H	2.963554	0.953311	0.601849
H	2.020287	0.456998	-2.015385
H	1.820777	-0.853508	1.645953
H	3.480042	-2.350386	0.527453
H	2.679894	-1.896521	-1.717287
H	3.886836	-0.76506	-1.049418
H	-1.765745	0.52225	-1.325582
H	1.978027	2.985754	0.157694
H	-0.424094	-1.311138	1.41086
H	-2.823332	1.228899	0.422449
H	-2.081644	-1.557419	0.026672
O	-2.93592	-1.849674	-0.471509
H	-3.280843	-2.66356	-0.067138
H	-3.62671	-1.066335	-0.346722
O	-4.377614	0.136509	-0.133386

42. **F-ww-smd**

C	0.79169	0.737096	0.983419
C	1.990813	1.030155	0.074323
C	1.877504	-0.024816	-1.038355
O	0.534939	-0.535788	-0.985534
C	-0.243102	0.125241	0.014666
O	1.896713	2.312677	-0.527045
C	2.851452	-1.174821	-0.899994
O	2.664812	-1.778416	0.379137
O	-1.073699	-0.80555	0.643708
C	-1.149181	1.138347	-0.673781
O	-1.965378	1.834335	0.252024
O	1.110201	-0.180439	2.013778
H	-0.539728	1.879682	-1.194136
H	0.409966	1.645282	1.455027
H	2.929028	0.934032	0.632256
H	2.041906	0.455405	-2.009134
H	1.710153	-0.861119	1.646167
H	3.393245	-2.387818	0.557229
H	2.666489	-1.908112	-1.692372
H	3.870863	-0.787249	-1.001129
H	-1.755253	0.5953	-1.409929
H	1.979113	2.982001	0.167226
H	-0.572734	-1.196768	1.379922
H	-2.520009	1.184681	0.70727

H	-4.803423	0.469482	-0.938173
H	-5.082147	0.032647	0.524408

43. **HMF-smd**

C	-0.050981	1.567107	-0.108727
C	1.074837	2.340142	-0.004185
C	2.168696	1.43946	0.032259
C	1.630376	0.178889	-0.038685
O	0.266887	0.253263	-0.127189
C	2.283102	-1.094735	-0.017033
C	-1.490624	1.929473	-0.251718
O	-0.736303	-2.736629	0.355138
H	3.222585	1.669898	0.110952
H	-1.599108	3.000539	-0.062712
H	0.21818	-2.43526	0.146541
H	1.098891	3.419307	0.039494
H	-1.504279	-2.062539	-0.057411
H	-0.856489	-3.632238	-0.000701
O	-2.431263	-1.244362	-0.531782
H	-2.45142	-0.397362	-0.018584
H	-3.314608	-1.63694	-0.469389
O	1.709196	-2.18951	-0.031164
H	3.379594	-1.051632	0.011426
O	-2.335546	1.167229	0.603272
H	-1.825442	1.717271	-1.271441
H	-2.088434	1.314077	1.528735

44. **HMF-ww-smd**

C	-1.044199	0.377668	0.187984
C	-0.461345	1.588398	-0.071991
C	0.936729	1.349994	-0.167419
C	1.111114	0.007153	0.03544
O	-0.102103	-0.591869	0.258048
C	2.275412	-0.853195	0.05535
O	3.415304	-0.438258	-0.120499
C	-2.458475	-0.046941	0.396118
O	-2.899432	-0.953542	-0.608134
H	1.721901	2.066489	-0.364659
H	2.077507	-1.921113	0.240821
H	-2.491641	-1.815026	-0.444013
H	-2.568517	-0.494482	1.390248
H	-3.094231	0.837623	0.33867
H	-0.981907	2.528852	-0.181953

45. **G-a**

C	1.466122	-0.418089	-0.791763
C	0.301174	-1.289375	-0.328894
C	-0.998883	-0.776496	-0.942906
O	-1.184226	0.58404	-0.581236
C	-0.159896	1.450657	-1.058318
C	1.202281	1.05227	-0.479673
O	0.47231	-2.626709	-0.741145
C	-2.226738	-1.495906	-0.427554
O	-2.378666	-1.127469	0.974742
O	-0.46668	2.733208	-0.626027
O	2.227516	1.825731	-1.046374
O	2.678042	-0.898943	-0.243577
O	1.739529	3.9742	0.619373
O	-4.245894	-2.074683	2.160545
H	-1.185197	3.099136	-1.159073
H	-0.960983	-0.897695	-2.035504
H	1.150288	1.19706	0.612273
H	2.26105	2.673846	-0.563876
H	-0.13178	1.395164	-2.157323
H	1.576036	-0.53021	-1.878718

46. **G-b**

C	-1.766218	1.164606	0.066993
C	-0.254923	1.364735	-0.031032
C	0.341514	0.408073	-1.062275
O	-0.032286	-0.929068	-0.770546
C	-1.417997	-1.191416	-0.653337
C	-2.065219	-0.29008	0.397136
O	0.057188	2.676608	-0.443133
C	1.855253	0.400803	-1.052441
O	2.297364	-0.072441	0.244733
O	-1.527016	-2.502925	-0.197752
O	-3.459264	-0.483147	0.410774
O	-2.319934	2.079439	0.992814
O	-1.385795	-3.87308	-2.284072
O	4.694966	0.390807	0.668024
H	-1.50876	-3.117877	-0.943153
H	0.002337	0.702254	-2.066672
H	-1.620002	-0.548313	1.372521
H	-3.634419	-1.402362	0.654854
H	-1.910482	-1.056052	-1.627389
H	-2.224558	1.417043	-0.898078

H	2.717252	-0.678784	0.6978
H	0.224557	-1.228672	0.76883
H	1.372774	-2.892924	-0.505491
H	-3.124022	-1.190044	-0.966783
H	-2.098759	-2.576994	-0.451849
H	-3.263594	-1.566436	1.506001
H	-4.069828	-2.9366	2.56626
H	-5.085738	-2.136531	1.681527
H	-2.310331	-0.156623	1.06553
H	0.808203	3.942845	0.350112
H	2.028293	4.888245	0.516532

H	-2.087832	1.811396	1.893206
H	0.193295	1.151309	0.952276
H	-0.453125	3.285889	0.109624
H	2.24325	-0.263989	-1.82661
H	2.249312	1.40947	-1.177967
H	3.311417	0.114585	0.412798
H	4.904576	1.28204	0.979136
H	5.320619	0.182223	-0.039121
H	2.01142	-1.07371	0.476561
H	-1.040983	-3.78567	-3.189945
H	-1.774816	-4.753206	-2.192619

47. **G-c**

C	-1.266709	-1.213118	0.347821
C	0.708257	-0.954828	-1.142091
C	-0.701135	0.921889	-0.800886
C	-0.622375	2.443743	-0.732384
C	-1.307099	0.304302	0.460153
O	0.630518	0.438241	-0.949209
O	0.195349	-3.07051	-0.193584
H	-0.34171	-3.518705	0.475359
O	-2.636124	0.777209	0.579939
O	-1.809002	-1.852983	1.489336
H	-1.292917	-1.615367	2.273878
O	-1.895781	3.040622	-0.879845
H	-2.487547	2.64352	-0.223416
C	0.158177	-1.690175	0.073685
H	0.799489	-1.438202	0.935759
H	-1.306362	0.635995	-1.675934
H	-1.910973	-1.522483	-0.485281
H	-0.702802	0.62863	1.322583
H	-0.00034	2.798878	-1.557342
H	-3.056951	0.337736	1.331981
O	2.080064	-1.254789	-1.262141
H	2.364174	-1.181681	-2.185609
H	0.176511	-1.257742	-2.053954
H	-0.147497	2.737678	0.213387
O	3.3322	0.360415	0.241777
H	2.666261	0.859063	0.913521
H	2.862833	-0.315211	-0.375085
O	1.800173	1.524924	1.767258
H	1.768274	1.175626	2.66998
H	1.973168	2.474821	1.84092
H	4.068888	-0.056765	0.71521

48. **F-a**

C	0.415814	0.879783	0.981386
C	1.61307	1.116318	0.053559
C	1.50165	-0.013807	-0.983491
O	0.101493	-0.388368	-0.993384
C	-0.619602	0.29467	-0.006743
O	1.462088	2.3327	-0.648567
C	2.366002	-1.231443	-0.740667
O	2.085344	-1.747065	0.556295
O	-1.415888	-0.671094	0.721206
C	-1.572471	1.288012	-0.657555
O	-2.223829	2.09908	0.296888
O	0.650366	-0.043705	2.021504
H	-0.972675	1.950521	-1.28518
H	0.057892	1.802344	1.438308
H	2.559272	1.07917	0.607274
H	1.743587	0.389139	-1.97097
H	1.289881	-0.721777	1.70933
H	2.693713	-2.464428	0.771948
H	2.149751	-1.986731	-1.502828
H	3.416165	-0.930667	-0.822816
H	-2.281966	0.744117	-1.290918
H	1.054766	3.013251	-0.07753
H	-0.910898	-0.867408	1.550856
H	-2.893889	1.595581	0.777343
H	-1.589363	-1.627124	0.05811
O	-1.705772	-2.537643	-0.755699
H	-0.907622	-2.580571	-1.307954
H	-1.879076	-3.415254	-0.380143
O	-0.239373	4.005799	0.822234
H	-1.137043	3.636314	0.751069
H	-0.312187	4.956806	0.68333

49. **F-b**

C	0.922193	0.787441	0.87966
C	2.19599	0.906114	0.028258

50. **F-c**

C	-0.156596	0.516424	0.970694
C	-0.036702	-0.856986	0.30876

C	2.052181	-0.184764	-1.037755
O	0.649476	-0.37219	-1.194447
C	-0.102406	0.124583	-0.09121
O	2.271632	2.194186	-0.627273
C	2.755786	-1.481542	-0.682389
O	2.30371	-1.906347	0.597879
O	-0.827969	-0.887513	0.525461
C	-1.122986	1.107634	-0.654787
O	-1.966058	1.600403	0.362026
O	1.125852	0.033846	2.048393
H	-0.608672	1.964076	-1.09716
H	0.559039	1.768937	1.194445
H	3.101378	0.814444	0.630536
H	2.459248	0.153935	-1.996482
H	1.705221	-0.722216	1.832089
H	2.74697	-2.725275	0.851422
H	2.509251	-2.230299	-1.441254
H	3.838356	-1.311778	-0.678995
H	-1.686151	0.594869	-1.445241
H	2.165951	3.019271	0.025391
H	-0.343431	-1.185007	1.311863
H	-2.357942	0.834132	0.804334
H	0.666408	3.158249	-3.009089
O	1.260177	2.407768	-2.86226
H	1.903872	2.418641	-3.585544
H	1.81893	2.300688	-1.578811
O	2.018291	4.026905	0.991371
H	1.325004	4.681205	0.825047
H	2.82235	4.514365	1.219555

C	-0.990641	-0.779953	-0.897345
O	-1.281168	0.602854	-1.0943
C	-0.530447	1.438377	-0.213594
O	1.316797	-1.037	-0.200475
C	-2.280502	-1.542384	-0.658367
O	-2.838923	-1.103274	0.567197
O	-1.30355	2.512365	0.196625
C	0.660083	2.020286	-0.968578
O	1.424748	2.868112	-0.137956
O	-1.171091	0.530665	1.94463
H	1.317534	1.219804	-1.314382
H	0.772559	0.840424	1.446449
H	-0.266121	-1.674522	0.994764
H	-0.506317	-1.180293	-1.796183
H	-1.911367	-0.03408	1.63241
H	-3.597225	-1.675514	0.809012
H	-2.965117	-1.346875	-1.491185
H	-2.055325	-2.616008	-0.627966
H	0.263801	2.552114	-1.843196
H	1.977343	-0.995725	0.512951
H	-1.788817	2.241593	0.993944
H	0.831171	3.552096	0.20183
H	-5.668676	-2.753808	0.536874
O	-4.924544	-2.752769	1.151238
H	-4.723237	-3.679973	1.32658
H	1.479218	-2.000802	-0.889809
O	1.554046	-2.946193	-1.625319
H	2.143095	-2.818347	-2.386003
H	1.787225	-3.782341	-1.191251

51. **HMF-a**

C	-0.042258	1.566602	-0.113592
C	1.079539	2.345344	-0.009834
C	2.176226	1.448366	0.036471
C	1.640067	0.186074	-0.028151
O	0.2803	0.256291	-0.122075
C	2.282254	-1.094022	0.003
C	-1.485855	1.916272	-0.265764
O	3.118687	-3.937538	-0.109554
H	3.227615	1.686386	0.117082
H	-1.613451	2.985788	-0.084197
H	2.509394	-3.113989	0.052143
H	1.102674	3.424174	0.025581
H	-3.110117	0.447355	0.263551
H	4.044162	-3.656474	-0.159803
O	-3.735702	-0.301383	-0.265284
H	-4.073427	-0.974671	0.385085
H	-4.013894	-0.564829	-1.152711
O	1.697143	-2.18016	-0.004516
H	3.378379	-1.070509	0.033164

52. **HMF-b**

C	0.054623	-1.231646	0.28719
C	0.894975	-2.300239	0.159257
C	2.204822	-1.75203	0.034906
C	2.054353	-0.392616	0.082966
O	0.742803	-0.071691	0.245115
C	3.000815	0.701504	-0.046944
C	-1.41165	-1.107287	0.486376
O	-0.121506	2.596445	-0.681235
H	3.136591	-2.285286	-0.087966
H	-1.894654	-2.082308	0.425454
H	-0.595185	1.757286	-0.630052
H	0.608877	-3.341394	0.155
H	-3.076518	0.307496	-0.253195
H	0.784517	2.377979	-0.408068
O	-4.082604	0.820289	-0.047708
H	-4.00908	1.659875	0.435616
H	-4.737718	0.256292	0.395071
O	2.664642	1.875496	-0.066896
H	4.05646	0.402917	-0.133326

O	-2.324937	1.146196	0.587764
H	-1.817585	1.694737	-1.283941
H	-2.13684	1.336532	1.517342

O	-1.964247	-0.208747	-0.514413
H	-1.642097	-0.636495	1.44366
H	-1.930278	-0.601792	-1.403234

53. **HMF-c**

C	-0.876688	-1.303253	0.264111
C	-0.534739	-2.606732	-0.047279
C	0.822751	-2.581951	-0.396116
C	1.226916	-1.257659	-0.278348
O	0.173072	-0.488495	0.128705
C	2.461357	-0.650306	-0.490288
C	-2.165025	-0.67891	0.702159
O	0.464518	2.538564	0.78875
H	1.449633	-3.407751	-0.702828
H	-2.922835	-1.463874	0.777188
H	0.999515	1.81899	0.429142
H	-1.19883	-3.457271	-0.023564
H	3.609189	0.926548	-0.511208
H	1.056906	3.297416	0.83342
O	4.93161	1.23753	-0.805274
H	5.466779	1.558356	-0.065804
H	5.066277	1.847383	-1.544242
O	2.617337	0.60065	-0.311369
H	3.306004	-1.261063	-0.811466
O	-2.556195	0.369717	-0.158995
H	-2.022577	-0.237159	1.692239
H	-2.880681	-0.003584	-0.988687

54. **R1.1**

C	-5.363226	-2.174094	-0.656263
C	-4.27869	-1.662722	0.289314
C	-4.866991	-0.634912	1.253907
O	-5.42539	0.433442	0.495567
C	-6.469062	0.045181	-0.384493
C	-5.982476	-0.995624	-1.393563
O	-3.720093	-2.711758	1.046774
C	-3.832915	-0.013517	2.169798
O	-2.774655	0.501305	1.368525
O	-6.848008	1.16751	-1.112462
O	-7.05876	-1.455868	-2.175719
O	-4.83713	-3.164204	-1.519669
O	-3.924873	2.123916	-1.156892
H	-7.435639	1.724047	-0.584082
H	-5.644215	-1.111989	1.870121
H	-5.216781	-0.509713	-2.021569
H	-7.425237	-0.701043	-2.656521
H	-7.306952	-0.359142	0.203313
H	-6.140414	-2.683257	-0.071499

55. **R2.1**

C	-4.332746	-0.524138	1.434054
C	-5.607465	0.21829	1.074181
C	-5.828967	0.137402	-0.434703
O	-4.709861	0.723128	-1.094227
C	-3.505927	0.026708	-0.858618
C	-3.163558	0.04022	0.632999
O	-6.739062	-0.334651	1.71561
C	-7.090416	0.858043	-0.884071
O	-7.181708	2.182354	-0.388224
O	-2.508854	0.680505	-1.583782
O	-1.964479	-0.652873	0.915415
O	-4.13128	-0.378085	2.825834
H	-5.920388	-0.920819	-0.731244
H	-2.989151	1.080518	0.934081
H	-1.986765	-1.538238	0.520468
H	-3.612807	-1.016577	-1.207245
H	-4.465699	-1.590505	1.183249
H	-3.306681	-0.824232	3.062813
H	-5.481979	1.275469	1.353469

H	-4.249413	-2.751506	-2.168501
H	-3.503552	-1.164692	-0.316837
H	-3.528539	-3.440651	0.438683
H	-4.308471	0.79684	2.732578
H	-3.442891	-0.760949	2.868576
H	-4.78332	2.280779	-1.575119
H	-2.882328	3.61227	-0.756259
H	-4.14585	1.523758	-0.422232
C	0.019364	0.163061	-0.24676
C	-0.73561	1.496051	-0.267883
C	-0.822122	1.873786	1.228932
O	0.072499	0.996995	1.92731
C	0.901184	0.287451	1.012012
O	-0.003458	2.520374	-0.930949
C	-2.205351	1.724027	1.829806
O	1.226992	-0.954878	1.544482
C	2.199892	1.060424	0.817663
O	3.009059	0.34173	-0.098939
O	-0.857171	-0.935489	-0.082675
H	1.98648	2.058253	0.42522
H	0.60946	-0.004961	-1.150554
H	-1.724383	1.375643	-0.723564
H	-0.492998	2.912055	1.354861
H	-1.586819	-0.656585	0.504805
H	-2.116517	1.7139	2.921859
H	-2.840222	2.564938	1.522667
H	2.688891	1.149694	1.794113
H	0.055677	2.308481	-1.872783
H	0.470039	-1.542081	1.375398
O	-2.255426	4.316581	-0.509371
H	-1.382318	3.968585	-0.744365
C	5.995613	-1.804681	0.098515
C	6.920679	-0.762032	-0.524527
C	6.554306	0.63172	-0.014792
O	5.193542	0.90086	-0.336611
C	4.299876	0.006495	0.286957
C	4.542464	-1.436791	-0.156043
O	8.265229	-1.02285	-0.175518
C	7.410795	1.725452	-0.616023
O	3.704388	-2.30496	0.571844
O	6.335817	-3.104981	-0.353572
H	6.692599	0.658453	1.078874
H	4.3285	-1.491645	-1.236544
H	2.832033	-1.883405	0.6703
H	4.408664	0.073543	1.383733
H	6.168213	-1.82412	1.182675
H	6.080028	-3.197489	-1.282156
H	6.797302	-0.770323	-1.618224
H	8.424979	-1.965247	-0.327869
H	7.038702	2.693655	-0.260291
H	8.439393	1.587522	-0.263781

H	-6.545546	-0.389251	2.661871
H	-7.078162	0.92472	-1.974866
H	-7.958549	0.264035	-0.580875
H	-7.515353	2.15242	0.517034
O	7.337054	0.639352	-0.844361
C	5.304744	1.721104	-0.112691
C	3.875435	1.480154	0.354646
C	3.873666	0.397802	1.434486
O	4.519236	-0.775151	0.940726
C	5.887029	-0.590894	0.58989
C	5.977209	0.421097	-0.544846
O	3.317878	2.645504	0.922918
C	2.475542	0.011854	1.88848
O	1.571278	-0.285012	0.830422
O	6.379262	-1.804703	0.147575
O	5.370091	2.6984	-1.138729
O	-0.336337	1.865955	0.120689
H	6.542713	-2.382549	0.904394
H	4.418129	0.776257	2.314651
H	5.447689	-0.007294	-1.412219
H	6.43473	-0.223927	1.472592
H	5.875862	2.148904	0.721613
H	4.870908	2.392013	-1.910192
H	3.264495	1.13871	-0.496389
H	3.420579	3.368865	0.28908
H	2.544574	-0.836565	2.577598
H	2.031459	0.858355	2.414993
H	0.201069	1.086882	0.338218
H	-1.047812	1.50403	-0.429341
C	-1.016864	-1.133092	-2.050847
C	-1.116469	-2.477789	-1.858697
C	0.002594	-2.853562	-1.037841
C	0.683188	-1.702278	-0.795381
O	0.087856	-0.657382	-1.41478
C	1.919027	-1.374218	-0.022008
O	2.312927	-2.506671	0.677323
C	-1.910725	-0.096274	-2.633069
H	0.262987	-3.836463	-0.675757
H	2.7214	-1.048356	-0.69687
H	-1.348668	0.618224	-3.236922
H	-2.682099	-0.563785	-3.252196
H	-1.897001	-3.118923	-2.24349
H	3.263182	-2.418357	0.854069

O	7.338998	1.639506	-2.030063
H	7.87706	2.342864	-2.410848
C	-5.363226	-2.174094	-0.656263
C	-4.27869	-1.662722	0.289314

56. **R3.1**

C	-6.093021	-1.42508	0.450866
C	-5.251447	-0.487378	1.32636
C	-4.367642	0.218279	0.300573
O	-5.127972	0.264376	-0.910001
C	-6.223521	-0.647633	-0.88035
O	-6.054853	0.50393	1.944447
C	-3.049666	-0.502983	0.011158
O	7.858046	-2.333085	-1.821771
O	-6.19776	-1.490466	-1.98907
C	-7.505446	0.171086	-0.986057
O	-8.642329	-0.664346	-1.057751
O	-5.395181	-2.626905	0.173289
H	-7.607363	0.799369	-0.098984
H	-7.0798	-1.623893	0.880494
H	-4.662891	-1.048618	2.060534
H	-4.189578	1.251743	0.61634
H	-5.614181	-3.298099	0.830585
H	-3.261227	-1.499608	-0.382455
H	-2.501123	0.067605	-0.750868
H	-7.416287	0.812053	-1.873097
H	-6.583968	0.095263	2.641436
H	-5.715956	-2.296902	-1.742857
H	-8.492539	-1.28585	-1.783918
C	5.011344	0.372497	0.844089
C	6.227105	-0.521217	1.098619
C	6.779577	-0.744557	-0.309346
O	5.689008	-0.462273	-1.210307
C	4.512046	-0.208225	-0.487225
O	7.220732	0.068276	1.90891
C	7.303796	-2.150321	-0.531371
O	3.841114	-1.419815	-0.194974
C	3.662801	0.711428	-1.34781
O	2.506397	1.069577	-0.614029
O	4.126344	0.425364	1.926976
H	4.252854	1.598344	-1.60244
H	5.378521	1.388104	0.639294
H	5.880716	-1.466768	1.539422
H	7.569853	-0.008991	-0.506606
H	3.387219	0.185517	-2.274964
H	6.899979	0.090586	2.819606
H	3.716481	-1.905631	-1.023789
H	2.169164	-1.408988	0.837722
O	1.695613	-0.936947	1.541058
H	3.298043	-0.067207	1.758324

57. **TS R3.2** (-227.640)

C	-3.433133	-0.139374	-1.228802
C	-2.385626	-1.242593	-1.49285
C	-1.596113	-1.311916	-0.191423
O	-2.52319	-0.927469	0.830026
C	-3.466902	-0.008639	0.330706
O	-3.006881	-2.505602	-1.725869
C	-0.389216	-0.368693	-0.167212
O	10.137076	3.841826	0.167856
O	-3.117354	1.316295	0.628521
C	-4.782406	-0.406498	0.995495
O	-5.888549	0.405844	0.621588
O	-3.11177	1.074205	-1.878826
H	-4.992095	-1.450926	0.738908
H	-4.40685	-0.460801	-1.61599
H	-1.75329	-0.967165	-2.340252
H	-1.299467	-2.341127	0.026847
H	-2.595326	1.627578	-1.271161
H	-0.716126	0.665985	-0.30237
H	0.093242	-0.442164	0.816539
H	-4.658388	-0.34274	2.081149
H	-3.086087	-2.647706	-2.678674
H	-2.973211	1.40902	1.581307
H	-4.751253	1.955549	-1.785629
O	-5.649582	1.967953	-1.403488
H	-5.692668	1.074081	-0.113238
H	-5.902447	2.892092	-1.284423
O	-5.507589	-3.13247	-0.782052
H	-5.828025	-4.000761	-1.059224
H	-4.579985	-3.035197	-1.093016
C	-9.788081	1.829251	0.535174
C	-9.760907	2.046703	-0.816315
C	-8.811334	1.133813	-1.349571
C	-8.338545	0.423861	-0.279708
O	-8.926531	0.846967	0.871086
C	-7.36792	-0.63086	-0.164832
O	-6.886832	-1.11456	-1.256964
C	-10.56521	2.450853	1.642178
O	-11.41462	1.458299	2.199522
H	-8.509859	1.005522	-2.378787
H	-7.375236	-1.244696	0.736088
H	-9.872029	2.839485	2.397801
H	-11.13810	3.286662	1.22762
H	-10.35530	2.770321	-1.353874
H	-6.35151	-1.991545	-1.104698

H	1.174044	-0.270519	1.06782
C	-1.166733	1.456661	0.935377
C	-1.409936	2.753989	0.614622
C	-0.393737	3.141997	-0.324679
C	0.383886	2.045786	-0.506727
O	-0.071131	1.010815	0.249333
C	1.563232	1.775032	-1.38646
O	2.047245	3.01214	-1.822026
C	-1.832297	0.473305	1.837126
O	-2.251378	-0.706815	1.164842
H	-0.260964	4.099436	-0.804629
H	1.281203	1.152455	-2.249493
H	-1.1404	0.129568	2.611167
H	-2.671153	0.978133	2.332887
H	-2.215883	3.361563	1.001112
H	2.351902	2.948138	-2.73539
H	8.036693	-2.378284	0.254405
H	6.472769	-2.856886	-0.446249
H	8.690672	-1.848224	-1.879396

C	7.875442	-0.298849	-0.378104
C	8.998441	0.443871	-1.104781
C	9.388828	1.529887	-0.101841
O	8.263824	1.66638	0.790911
C	7.194546	0.868395	0.352348
O	10.124892	-0.352858	-1.401045
C	9.715632	2.857418	-0.758829
O	6.415916	1.566964	-0.60124
C	6.384781	0.505026	1.585681
O	5.35265	-0.381098	1.192822
O	7.103759	-1.099306	-1.228382
H	7.050902	0.02942	2.31367
H	8.335986	-0.938629	0.38803
H	8.587074	0.887056	-2.022726
H	10.241661	1.180788	0.493918
H	5.963338	1.420119	2.0291
H	9.897179	-0.948903	-2.125991
H	6.157684	2.419017	-0.219291
H	4.863238	0.71727	-1.457855
O	4.501585	-0.142194	-1.726564
H	6.208406	-0.734169	-1.375741
H	4.031702	-0.455358	-0.938394
C	1.904015	-2.101673	0.133659
C	1.815789	-3.042688	1.109326
C	2.79176	-2.694059	2.105051
C	3.392227	-1.562724	1.658356
O	2.863863	-1.185381	0.463749
C	4.454215	-0.680469	2.235205
O	5.060968	-1.389182	3.276111
C	1.193179	-1.879536	-1.156913
O	0.525035	-0.62354	-1.215192
H	3.015305	-3.208303	3.027127
H	4.028627	0.261539	2.614183
H	1.901386	-1.859424	-1.989439
H	0.502924	-2.716195	-1.319319
H	1.138127	-3.884536	1.117476
H	5.279929	-0.792973	4.002359
H	10.476187	2.686043	-1.532641
H	8.813426	3.247129	-1.239747

The complete reference for Gaussian 16

Gaussian 16, Revision C.01,
M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, G. Scalmani, V. Barone, G. A. Petersson, H. Nakatsuji, X. Li, M. Caricato, A. V. Marenich, J. Bloino, B. G. Janesko, R. Gomperts, B. Mennucci, H. P. Hratchian, J. V. Ortiz, A. F. Izmaylov, J. L. Sonnenberg, D. Williams-Young, F. Ding, F. Lipparini, F. Egidi, J. Goings, B. Peng, A. Petrone, T. Henderson, D. Ranasinghe, V. G. Zakrzewski, J. Gao, N. Rega, G. Zheng, W. Liang, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, T. Vreven, K. Throssell, J. A. Montgomery, Jr., J. E. Peralta, F. Ogliaro, M. J. Bearpark, J. J. Heyd, E. N. Brothers, K. N. Kudin, V. N. Staroverov, T. A. Keith, R. Kobayashi, J. Normand, A. P. Rendell, J. C. Burant, S. S. Iyengar, J. Tomasi, M. Cossi, J. M. Millam, M. Klene, C. Adamo, R. Cammi, J. W. Ochterski, R. L. Martin, K. Morokuma, O. Farkas, J. B. Foresman, and D. J. Fox, Gaussian, Inc., Wallingford CT, **2016**.

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