

# **CHEMISTRY**

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### Supporting Information

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#### **The Electronic Nature of the 1,4- $\beta$ -Glycosidic Bond and Its Chemical Environment: DFT Insights into Cellulose Chemistry**

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## Theoretical methods

### General

All calculations were performed using the Gaussian09 suite of quantum chemical programs.<sup>1</sup> Density functional theory (DFT) was applied using the BB1K,<sup>2</sup> B97-1,<sup>3</sup> B3LYP,<sup>4-7</sup> and M06-2X<sup>8</sup> functionals in combination with the 6-31++G\*\* basis set. Geometry optimizations were carried out in the solvent phase (CPCM, UFF radii, water) for BB1K, B3LYP, and M06-2X without any constraints. Test calculations of  $pK_b$  values were done with the B97-1 functional and the SMD<sup>9</sup> solvation model. The SMD model was generally used for the calculation of solvation energies. All calculations employed the tight convergence criteria and the ultrafine grid in Gaussian09. Harmonic vibrational frequency calculations were performed at the same level as the geometry optimizations. Zero-point energies (EZPC), enthalpies (H), and free energies (G) at 298.15 K and 1 atm were determined from these calculations. The number of imaginary modes was used to verify minima (no imaginary frequency) and transition states (one imaginary frequency). Intrinsic reaction coordinate (IRC)<sup>10,11</sup> calculations were performed to confirm the direct connection between transition states and minima. The programs Molden<sup>12</sup> and Gaussview 3.5<sup>13</sup> were used for visualization.

### Energetics: Comparisons between different functionals

Unless noted otherwise, the results in the main paper come from BB1K/6-31++G(d,p) calculations. For comparison, additional calculations were done at the following levels: L1 = BB1K/6-311++G(3df,3pd), L2 = B3LYP/6-31++G(d,p), and L3 = M06-2X/6-31++G(d,p). The computed total energies are documented in Tables SI2-SI4, and selected energy profiles are shown in Figures SI7-SI10.

As pointed out in the main paper, the Gibbs relative free energies from BB1K/6-31++G(d,p) for structures **1**, **3-6** and **10-16** are well reproduced at the other levels, with small standard deviations of 2.3 (L1), 2.2 (L2), and 1.0 (L3) kcal/mol. In the case of structures **17-25**, geometry optimizations at levels L2-L3 sometimes failed (*e.g.*, when trying to locate the transition state for the required conformational change or C(1)O(1) dissociation); similar problems have been met in related systems.<sup>14</sup> The comparisons for structures **17-25** are thus restricted to single-point calculations, which give standard deviations of 1.7 (L1), 4.2 (L2), and 10.2 (L3) kcal/mol relative to BB1K/6-31++G(d,p). The B3LYP results (L2) are consistent with the well-known tendency of this functional to underestimate barriers. In previous benchmarks for barrier heights, the following mean signed errors (MSE) relative to experiment were reported: BH42/04 database, MSE(B3LYP/MG3S) = -4.4 kcal/mol, MSE(BB1K/MG3S) = -0.61 kcal/mol;<sup>15</sup> BH6 database, MSE(B3LYP/MG3S) = -4.72 kcal/mol, MSE(BB1K/MG3S) = -1.03 kcal/mol;<sup>15</sup> HTBH38/04 and NHTBH38/04 database, MSE(B3LYP/MG3S) = -4.15 kcal/mol, MSE(BB1K/MG3S) = -0.03 kcal/mol.<sup>16</sup> The large deviations of the M06-2X results (L3) for **17-25** are unexpected, however, since this functional usually provides rather accurate results for thermochemistry (TC177 database, mean unsigned errors: MUE(B3LYP) = 1.39 kcal/mol, MUE(M06-2X) = 0.82 kcal/mol) and for barrier heights (DBH76 database, MUE(B3LYP) = 4.50 kcal/mol, MUE(M06-2X) = 1.22 kcal/mol).<sup>17</sup>

## Solvation model

We use the Conductor-like Polarizable Continuum Model (CPCM) for aqueous solvation. In a benchmark study<sup>18</sup> of several solvation models, CPCM was found to give solvation free energies with the lowest mean absolute deviation (MAD) from the experimental values for a set of 70 small neutral and charged organic molecules (MAD = 3 kcal/mol), superior to those from a cluster-continuum model (MAD = 9 kcal/mol), COSMO (MAD = 9 kcal/mol), SM5.24R (MAD = 8 kcal/mol), PCM (MAD = 11 kcal/mol), and IPCM (MAD = 20 kcal/mol). For cations and neutral species that are studied presently, CPCM performs best using UAKS cavities (United Atom Topological Model applied to radii optimized for the PBE1PBE/6-31G(d) level of theory,  $MAD_{\text{cation}} = 4$  kcal/mol,  $MAD_{\text{neutral}} = 1$  kcal/mol). However, when using these UAKS cavities or other United Atom cavities (UAKS, UAHF, or UA0), geometry optimization on some of the charged species failed and the error on total polarization charges (value of the density outside of the generated cavity) exceeded 0.05 by far. On the other hand, these structures could be optimized with Pauling cavities (Merz-Kollman radii) and Bondi radii ( $MAD_{\text{cation}} \approx 5$  kcal/mol,  $MAD_{\text{neutral}} \approx 3$  kcal/mol), but the error on total polarization charges still exceeded 0.05. Only the use of universal force field (UFF) cavities (with explicit cavities for hydrogen atoms) yielded low errors on polarization charges, but led to larger deviations ( $MAD_{\text{cation}} = 15$  kcal/mol,  $MAD_{\text{neutral}} = 8$  kcal/mol) from experimental solvation free energies in the benchmark study.<sup>18</sup> Therefore the CPCM model was used for calculations on the reaction pathway, but was not used for the calculation of the solvation energies (see below).

Table SII lists CPCM solvation free energies for structures **1**, **3-6**, **10-16** and **41**, as obtained with UFF, Pauling, and Bondi cavities. Compared with the UFF-based values, we find standard deviations of 2.0 kcal/mol for Pauling cavities ( $STD_{\text{neutral}} = 0.7$  kcal/mol;  $STD_{\text{cation}} = 2.7$  kcal/mol) and of 1.5 kcal/mol for Bondi cavities ( $STD_{\text{neutral}} = 1.1$  kcal/mol;  $STD_{\text{cation}} = 1.8$  kcal/mol), which are much lower than expected from the errors mentioned above.

**Table SII. Solvation free energies (kcal/mol) relative to structures 1 and 10 (BB1k/6-31++G(d,p), water, 298.15 K, 1 atm) for different choices of CPCM cavities (see text).**

compound	UFF	Pauling	Bondi
41	3.5	2.7	2.7
1	0.0	0.0	0.0
3	0.3	-0.8	-0.7
4	-0.4	-0.8	-1.3
5	7.5	6.7	6.0
6	9.1	9.5	7.5
10	0.0	0.0	0.0
11	-3.2	-1.8	-3.6
12	-13.2	-10.6	-11.9
13	-16.0	-12.6	-13.6
14	-3.4	-1.2	-2.1
15	-14.8	-12.0	-12.6
16	-17.9	-13.7	-15.2

## Transition states with low frequencies

In the transition states for the conformational changes of structure **10** to either **17**, **18**, or **19**, we find small imaginary frequencies ( $\sim 60i \text{ cm}^{-1}$ ) that are typical for such low-barrier processes. The IRC calculations for these three transition states were unsuccessful, since they failed to converge after a few steps, even when the step sizes were varied between 0.05 to 0.2 Bohr. We note, however, that these three transition structures correspond to maxima of relaxed scans (see Figures SI1-SI3) and that optimizations starting from geometries obtained by manually displacing these structures along the transition vector in either direction end up either at **10** or at **17**, **18**, or **19**.

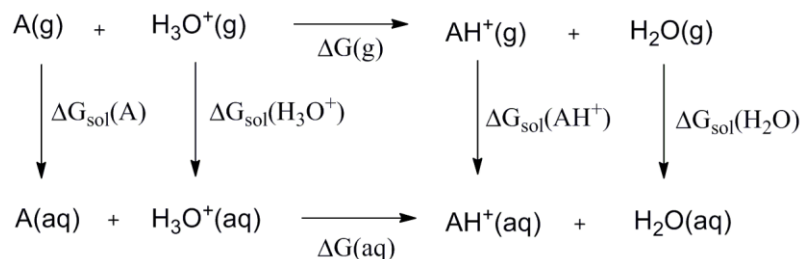
## Calculations with thermodynamic pathways

Thermodynamic cycles were used to determine  $\text{pK}_b$  values, reaction free energies, and energies for bringing reactants together from infinity.

*Calculation of  $\text{pK}_b$  values:* The thermodynamic cycles corresponding to reaction (1) and (2) yield consistent  $\text{pK}_b$  values, with differences of 0.1  $\text{pK}_b$  units or less (A= cellobiose).



Shown below is the thermodynamic pathway for reaction (2):



The required DFT calculations employed the BB1K functional. Previous benchmark calculations indicate that other functionals might provide more accurate solvation free energies: for example, in a comparative study on 30 acids using G-n and CBS methods as well as several DFT functionals, B97-1 performed best among the latter (MAD = 1 kcal/mol relative to experiment).<sup>19</sup> Hence, we also carried out some B97-1 calculations for validation, but the corresponding  $\text{pK}_b$  values showed little improvement over the BB1K results, and therefore we adopted the BB1K functional also here, for the sake of consistency. Changes in solvation free energies were calculated by subtracting the BB1K free energy in vacuum from the BB1K free energy calculated with the SMD solvent model. The latter was chosen because its documented good performance for solvation free energies, for instance, in a benchmark study on a set of 51 drug-like molecules (RMSD = 2.5 kcal/mol relative to experiment).<sup>9</sup> In the case of structure **10**, the gas-phase geometry optimization terminated because of SCF convergence problems, and the gas-phase energy was therefore estimated by a single-point calculation.

For the evaluation of the thermodynamic cycle, we used experimental values for the solvation free energy of hydronium ion,  $H^+$ , and water molecule,<sup>20,21</sup> and for the gas-phase free energy of  $H^+$ :<sup>22</sup>  $\Delta G_{\text{sol},1\text{M}}(H_2O) = -6.32$  kcal/mol,  $\Delta G_{\text{sol},1\text{M}}(H_3O^+) = -110.3$  kcal/mol,  $\Delta G_{\text{sol},1\text{M}}(H^+) = -265.9$  kcal/mol,  $\Delta G_{\text{g},1\text{atm}}(H^+) = -6.28$  kcal/mol. All energy values were converted to the standard state of 298 K and 1 M (1 mol/L). In the gas phase, equation (3), the change of 1 mole of ideal gas from 1 atm (24.46 L/mol) to 1 M gives rise to the following correction term:

$$\begin{aligned}\Delta G_{\text{g},1\text{M}} &= \Delta G_{\text{g},1\text{atm}} - T\Delta S \\ &= \Delta G_{\text{g},1\text{atm}} + RT\ln\left(\frac{V_{\text{g}}}{V_{\text{aq}}}\right) \\ &= \Delta G_{\text{g},1\text{atm}} + RT\ln(24.46) \\ &= \Delta G_{\text{g},1\text{atm}} + 1.89 \text{ kcal/mol}\end{aligned}\tag{3}$$

Likewise, bringing  $n$  water molecules from the concentration of 55.34 M in liquid water to 1M generates another correction term:

$$n \cdot \Delta G_{\text{aq},1\text{M}}^*(H_2O) = -n \cdot RT\ln(55.34) = -2.38 \cdot n \text{ kcal/mol}\tag{4}$$

Combining equations (3) and (4) with the thermodynamic cycle for reaction (2) leads to:

$$\begin{aligned}\Delta G(\text{aq}) &= \Delta G_{\text{g}} + \Delta\Delta G_{\text{sol}} + n\Delta G_{\text{aq},1\text{M}}^*(H_2O) \\ &= G_{\text{g}}(H_2O) + G_{\text{g}}(AH^+) - G_{\text{g}}(A) - G_{\text{g}}(H_3O^+) + \\ &\quad \Delta G_{\text{sol}}(H_2O) + \Delta G_{\text{sol}}(AH^+) - \Delta G_{\text{sol}}(A) - \Delta G_{\text{sol}}(H_3O^+) + 2.38 \text{ kcal/mol}\end{aligned}\tag{5}$$

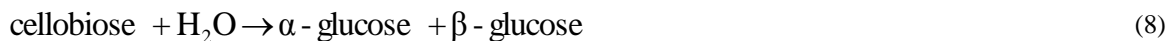
The  $pK_b$  value is defined as:

$$pK_b = \frac{\Delta G(\text{aq})}{RT\ln(10)}\tag{6}$$

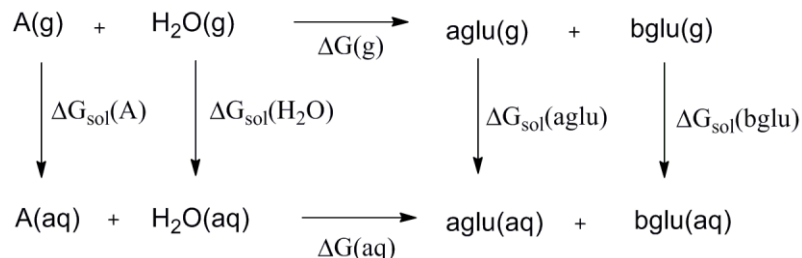
and  $pK_b$  differences between two molecules 1 and 2 are given by:

$$\Delta pK_b = \frac{\Delta G_1(\text{aq}) - \Delta G_2(\text{aq})}{RT\ln(10)}\tag{7}$$

Calculation of reaction free energy: To obtain the reaction free energy of reaction (8),



the following thermodynamic cycle was set up (aglu=  $\alpha$ -glucose, bglu =  $\beta$ -glucose, A=cellobiose):

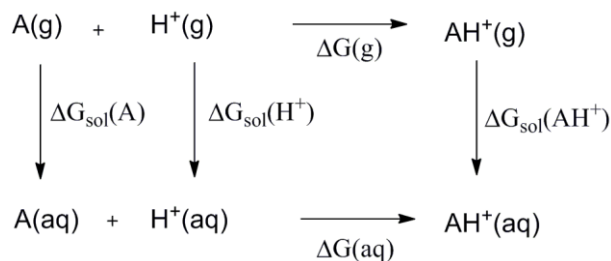


The reaction free energy is given by equation (9)

$$\begin{aligned} \Delta G(\text{aq}) &= \Delta G_{\text{g}} + \Delta \Delta G_{\text{sol}} + n \Delta G_{\text{aq},1\text{M}}^*(\text{H}_2\text{O}) \\ &= G_{\text{g}}(\text{aglu}) + G_{\text{g}}(\text{bglu}) - G_{\text{g}}(\text{A}) - G_{\text{g}}(\text{H}_2\text{O}) + \\ &\quad \Delta G_{\text{sol}}(\text{aglu}) + \Delta G_{\text{sol}}(\text{bglu}) - \Delta G_{\text{sol}}(\text{A}) - \Delta G_{\text{sol}}(\text{H}_2\text{O}) + 2.38 \text{ kcal/mol} \end{aligned} \quad (9)$$

The gas-phase free energies and the solvation free energies in this expression were calculated with the B3LYP functional and the SMD solvent model. For water the experimental solvation energy was used (see above).

Calculation of the free energy needed to bring reactants together from infinity: In this case, the reactants are cellobiose (A) and a proton, which form species **10** in a protonation reaction (10). The gas-phase free energies and the solvation free energies in equation (11) were calculated with the B3LYP functional and the SMD solvent model. For the proton the experimental solvation energy was used (see above).



$$\begin{aligned} \Delta G(\text{aq}) &= \Delta G_{\text{g}} + \Delta \Delta G_{\text{sol}} \\ &= G_{\text{g}}(\text{AH}^+) - G_{\text{g}}(\text{A}) - G_{\text{g}}(\text{H}^+) - 1.89 \text{ kcal/mol} + \\ &\quad \Delta G_{\text{sol}}(\text{AH}^+) - \Delta G_{\text{sol}}(\text{A}) - \Delta G_{\text{sol}}(\text{H}^+) \end{aligned} \quad (11)$$

## Results for the rotated conformer structure 41

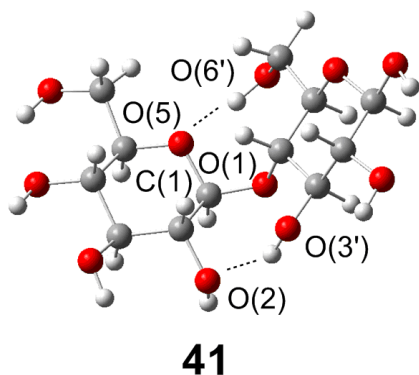


Figure S11. Optimized structure of **41** (BB1K/6-31++G\*\*).

Structure **41** is one of the possible conformers of cellobiose, which can be reached from structure **1** by rotation around the C(1)-O(1) bond. It is often regarded as one of the most stable conformers of cellobiose in vacuum,<sup>23,24</sup> but it is less relevant for the purposes of the present study. Therefore, we present computational results for **41** only in the Supporting Information. Its relative free energy, important bond lengths and dihedral angles (Table SI2), NBO data (Table SI3), and protonation energies (Table SI4) are given below in comparison to the other conformers **1** to **6**.

Conformer **41** contains the atoms H(1) and H(4') located *anti* to each other in the plane formed by the glycosidic linkage C(1)O(1)C(4'). It has two intramolecular H-bonds, O(5)⋯HO(6') and O(2)⋯HO(3'). NBO analysis reveals that the corresponding donor-acceptor interactions,  $n_{O(5)} \rightarrow \sigma^*_{O(6')H}$  and  $n_{O(2)} \rightarrow \sigma^*_{O(3')H}$ , contribute 6.5 and 8.6 kcal mol<sup>-1</sup> to the stabilization of **41**, respectively (Table SI14, entry 41); the occupancies of  $\sigma^*_{O(3')H}$  and  $\sigma^*_{O(6')H}$  are 0.026 and 0.027 electrons ( $e$ ). The *exo*-anomeric effect provides an even stronger interaction stabilizing **41** by 14.1 kcal mol<sup>-1</sup>, with an occupancy of  $\sigma^*_{C(1)O(5)}$  of 0.056  $e$ .

By contrast, the *endo*-anomeric effect is only of marginal importance, as indicated by the low stabilization (3.9 kcal mol<sup>-1</sup>) and the lower occupancy of  $\sigma^*_{C(1)O(1)}$  (0.034  $e$ ). Rotation around the C(1)O(1) bond may convert conformer **41** into **1**. A relaxed scan for this rotation indicates an energy barrier of about 10 kcal mol<sup>-1</sup> (see the computed energy profile, Figure SI5), but the transition state could not be located precisely. Recent dynamic studies do not report transitions between **41** and **1**.<sup>23,25</sup>



Table SI2. Gibbs free energies  $\Delta\Delta G$  (kcal mol<sup>-1</sup>) relative to structure **1**, selected torsional angles and bond lengths for structures **1** to **6** and **41** (BB1K/6-31++G\*\*).

	$\Delta\Delta G$	Torsion angle (degree)			Bond length (Å)	
		$\phi$	$\psi$	$\chi$	C(1)O(1)	C(1)O(5)
1	0.0	-91.9	-144.5	-76.9	1.375	1.413
2	-1.1	-89.5	-139.6	-82.9	1.373	1.410
3	0.3	-77.5	-150.9	-168.9	1.374	1.410
4	-0.4	-73.9	-121.3	53.2	1.376	1.410
5	7.5	0	-141.8	-79.4	1.400	1.392
6	9.1	180	-141.6	-80.2	1.397	1.396
41	3.5	58.3	-121.8	-75.7	1.379	1.408

Table SI3. Selected NBO results for structures **1** to **6** and **41**.

Entry	$E(2)$ donor-acceptor interactions (kcal mol <sup>-1</sup> )							
	Anomeric effect		H-bonding		Occupancy (e)			
	exo	endo			$\sigma^*_{C(1)O(5)}$	$\sigma^*_{C(1)O(1)}$	$\sigma^*_{O(3)H}$	$\sigma^*_{O(2)H}$
<b>1</b>	$n_{O(1)} \rightarrow \sigma^*_{C(1)O(5)}$	$n_{O(5)} \rightarrow \sigma^*_{C(1)O(1)}$	$n_{O(5)} \rightarrow \sigma^*_{O(3)H}$	$n_{O(6')} \rightarrow \sigma^*_{O(2)H}$	0.064	0.035	0.029	0.035
<b>3</b>	18.1	3.8	8.5	14.5	0.062	0.034	0.025	0.005
<b>4</b>	17.8	3.9	6.2	-	0.060	0.040	0.022	0.008
<b>5</b>	17.4	4.2	6.2	-	0.036	0.040	0.008	0.007
<b>6</b>	6.6	4.6	-	-	0.036	0.037	0.004	0.034
<b>2</b>	6.0	5.2	-	-	0.064	0.035	0.030	0.031
			$n_{O(5)} \rightarrow \sigma^*_{O(3)H}$	$n_{O(2)} \rightarrow \sigma^*_{O(6')H}$				$\sigma^*_{O(6')H}$
<b>41</b>	18.4	3.6	9.0	11.9	0.056	0.034	0.026	0.027
			$n_{O(5)} \rightarrow \sigma^*_{O(6')H}$	$n_{O(2)} \rightarrow \sigma^*_{O(3)H}$				$\sigma^*_{O(6')H}$

Table SI4. Relative Gibbs free energy of protonation for the oxygen sites in structures **1** to **6** and **41** (BB1K/6-31++G\*\*, 298.15 K, kcal/mol). The values are relative to the O(1)·1 protonation site of each structure.

	Relative free energy of protonation, $\Delta\Delta G(298.15\text{ K}) / \text{kcal mol}^{-1}$						
	O(1)·1	O(1)·2	O(2)	O(3')	O(5)·1	O(5)·2	O(6')
<b>1</b>	0.0	-3.2*	-13.2*	-16.0	-3.4	-14.8	-17.9
<b>2</b>	0.0	-6.4*	-1.8	-15.6	-3.5	-16.2	-19.5
<b>3</b>	0.0	1.2	-8.4	-19.8	-7.6	-19.3	-13.0
<b>4</b>	0.0	-1.1	-6.1	-18.8	-3.8	-18.4	-18.4
<b>5</b>	0.0	-4.8	-3.9	-5.9	1.6*	9.1*	-5.1
<b>6</b>	0.0*	-15.3*	-1.7	-5.1	-0.6	-6.8	-16.4
<b>41</b>	0.0*	9.3*	-10.6	-11.6	12.1	-2.1*	-3.1

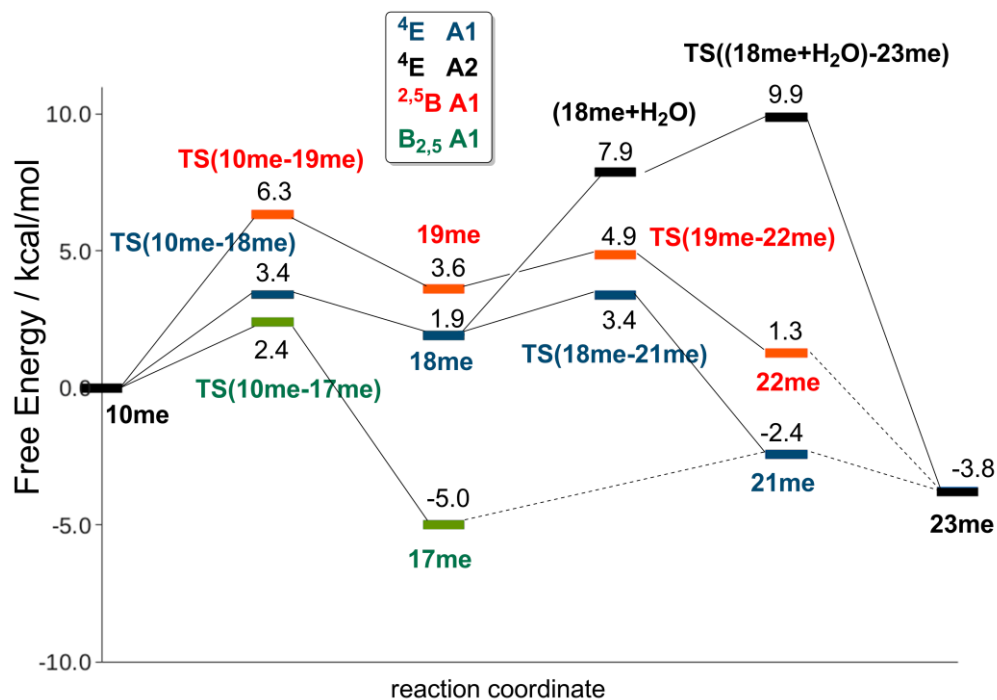
\*[O(X)-H]<sup>+</sup> distance fixed at 0.98 Å. In 5 and 6 the torsional angle  $\phi$  is generally fixed at 0° and 180°, respectively.

## Reaction mechanism A1 and A2 for 4-O-methyl-cellobiose

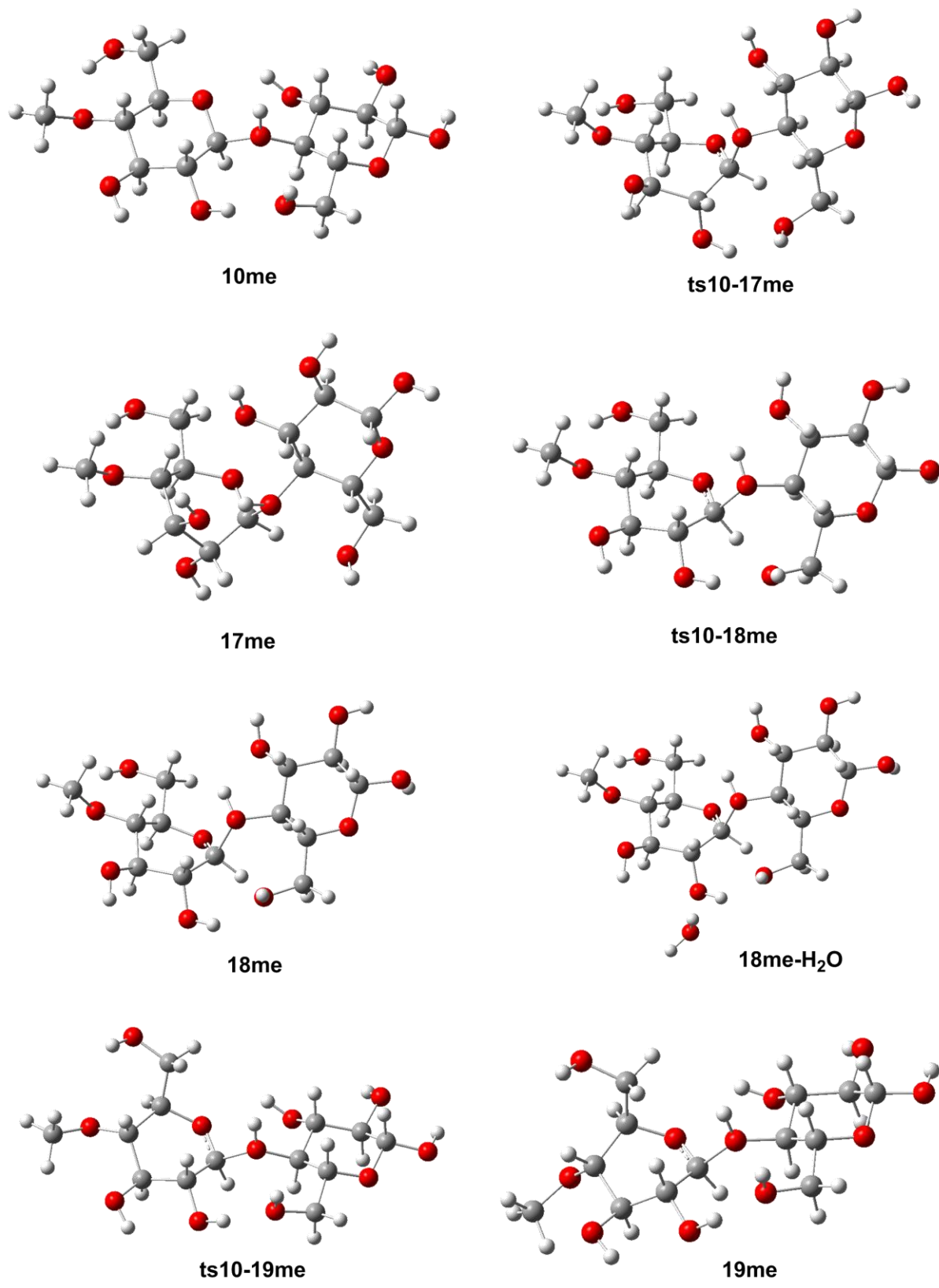
To validate the mechanism found for structure **1**, the A1 and A2 pathways were also calculated with a 4-O-methyl-cellobiose model to assess the influence of an additional methyl group. Results are collected in Table S15 (energies), Figure SI2 (energy profile) and Figure SI3 (structures). The relative free energies of the pathways deviate by at most 1.8 kcal/mol (compared with **1**), and the overall trends are conserved.

**Table S15.** Relative free energies for the A1 and A2 pathways for 4-O-methyl-cellobiose. BB1K/6-31++G\*\*, CPCM water, 298.15 K, 1 atm.

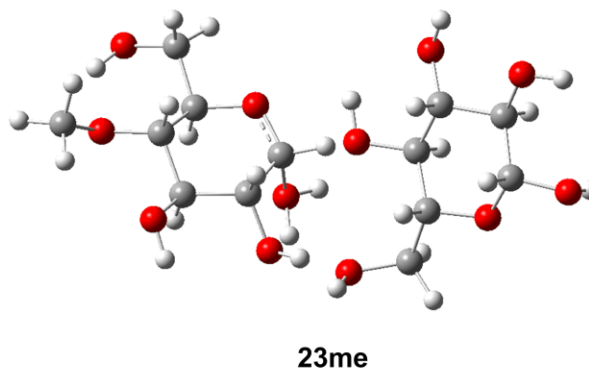
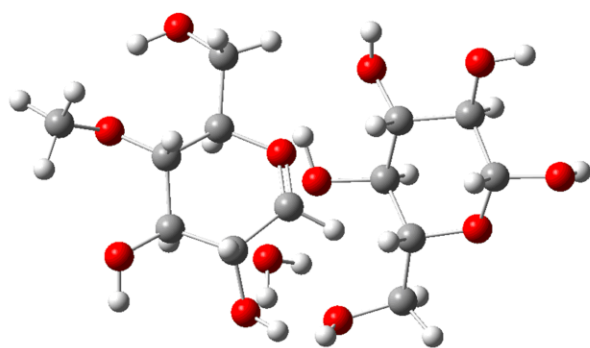
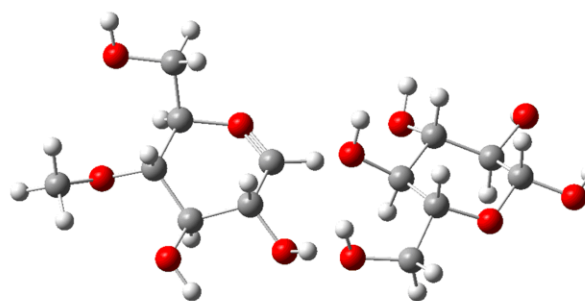
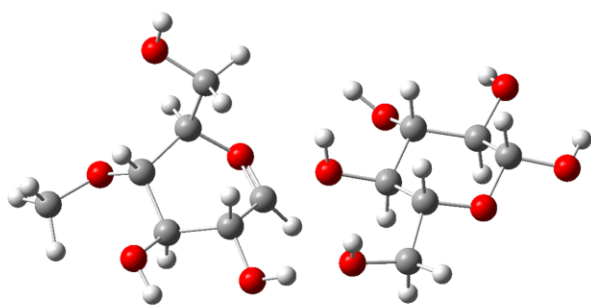
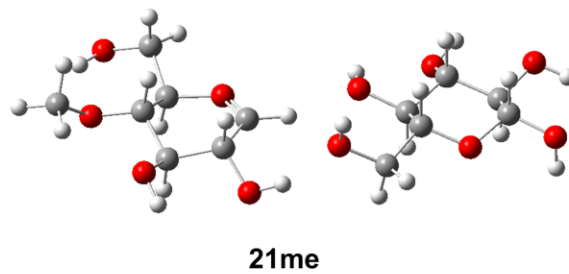
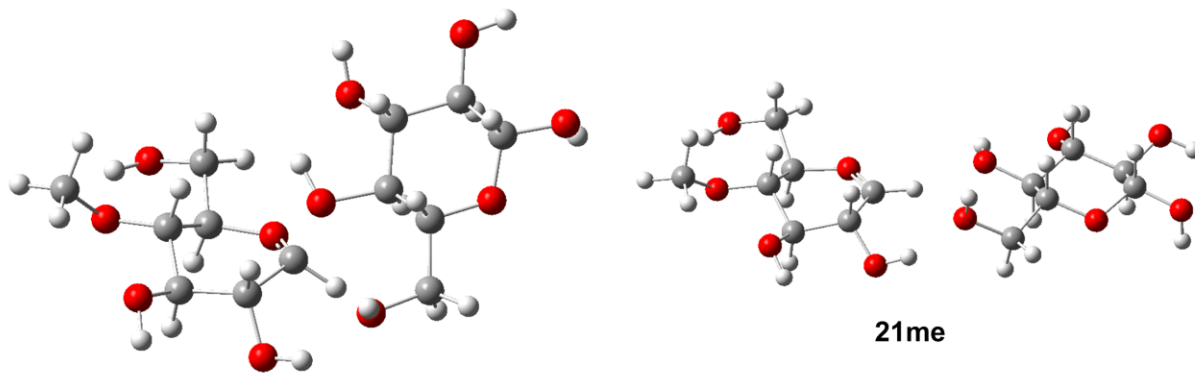
$B_{2,5}, A1$		${}^4E, A1$		${}^{2,5}B, A1$		${}^4E, A2$	
structure	$\Delta G$ (kcal mol <sup>-1</sup> )	structure	$\Delta G$ (kcal mol <sup>-1</sup> )	structure	$\Delta G$ (kcal mol <sup>-1</sup> )	structure	$\Delta G$ (kcal mol <sup>-1</sup> )
<b>10</b>	0.0	<b>10</b>	0.0	<b>10</b>	0.0	<b>10</b>	0.0
<b>Ts(10-17)</b>	2.4	<b>Ts(10-18)</b>	3.4	<b>Ts(10-19)</b>	6.3	<b>Ts(10-18)</b>	3.4
<b>17</b>	-5.0	<b>18</b>	1.9	<b>19</b>	3.6	<b>18</b>	1.9
		<b>Ts(18-21)</b>	3.4	<b>Ts(19-22)</b>	4.9	<b>18+H<sub>2</sub>O</b>	7.9
		<b>21</b>	-2.4	<b>22</b>	1.3	<b>Ts(18+H<sub>2</sub>O - 23)</b>	9.9
		<b>23</b>	-3.8	<b>23</b>	-3.8	<b>23</b>	-3.8



**Figure SI2:** Energy profile (BB1K/6-31++G(d,p)) for the exo-cyclic 4-O-methyl-cellobiose mechanism. Energies refer to structure **10me**.



**Figure SI3-a:** Structures (BB1K/6-31++G(d,p)) for the exo-cyclic 4-O-methyl-cellobiose mechanism.



**Figure S13-b:** Structures (BB1K/6-31++G(d,p)) for the exo-cyclic 4-O-methyl-cellobiose mechanism.

## Results and reaction mechanism A1 for structure 2

To validate the mechanism found for structure **1** (with an O(2)-H···O(6') hydrogen bond) the A1 pathway was also calculated for structure **2** (with an O(2)···H-O(6') hydrogen bond) to assess the influence of different hydrogen bond networks. Results are listed in Table SI6 (energies), Figure SI4 (energy profile), and Figure SI6 (structures). The energies along the pathways deviate by at most 2.6 kcal/mol (compared with **1**), and the overall trends are conserved.

No fully optimized structure for **TS(17'-20')** could be obtained, for the same reasons as discussed in the paper for structure **1**.

Figure SI5 shows the different hydrogen bond networks obtained upon protonation of O(2) in structures **1** and **2**.

**Table SI6. Relative free energies for the A1 pathways for structure 2. BB1K/6-31++G\*\*, CPCM water, 298.15 K, 1 atm.**

$B_{2,5}, A1$		${}^4E, A1$		${}^{2,5}B, A1$	
structure	$\Delta G$ (kcal mol <sup>-1</sup> )	structure	$\Delta G$ (kcal mol <sup>-1</sup> )	structure	$\Delta G$ (kcal mol <sup>-1</sup> )
<b>10'</b>	0.0	<b>10'</b>	0.0	<b>10'</b>	0.0
<b>Ts(10'-17')</b>	2.7	<b>Ts(10'-18')</b>	4.5	<b>Ts(10'-19')</b>	6.9
<b>17'</b>	-5.7	<b>18'</b>	3.2	<b>19'</b>	3.1
		<b>Ts(18'-21')</b>	5.4	<b>Ts(19'-22')</b>	5.7
		<b>21'</b>	-1.2	<b>22'</b>	-0.4
		<b>23</b>	-3.5	<b>23</b>	-3.5

**Table SI7. Selected bond lengths and results from the NBO analysis for structures 10', 17', 18', and 19' (BB1K/6-31++G\*\*).**

Entry	Bond length (Å)		$E(2)$ donor-acceptor interactions (kcal mol <sup>-1</sup> )				Charge at C(1) (e)	Occupancy (e)	
	C(1)O(1)	C(1)O(5)	H-bonding		Anomeric effect			$\sigma^*_{C(1)O(1)}$	$\sigma^*_{C(1)O(5)}$
			$n_{O(5)} \rightarrow \sigma^*_{O(3')H}$	$n_{O(2')} \rightarrow \sigma^*_{O(6)H}$	exo	endo			
<b>2</b>	1.373	1.410	9.0	11.9	18.4	3.6	0.408	0.034	0.061
<b>10'</b>	1.461	1.367	1.6	9.3	5.6	7.8	0.427	0.066	0.028
<b>17'</b>	1.480	1.443	-	-	8.7	29.0	0.421	0.103	0.037
<b>18'</b>	1.559	1.334	-	-	3.2	39.2	0.419	0.144	0.028
<b>19'</b>	1.564	1.331	-	11.4	2.9	38.8	0.419	0.152	0.022

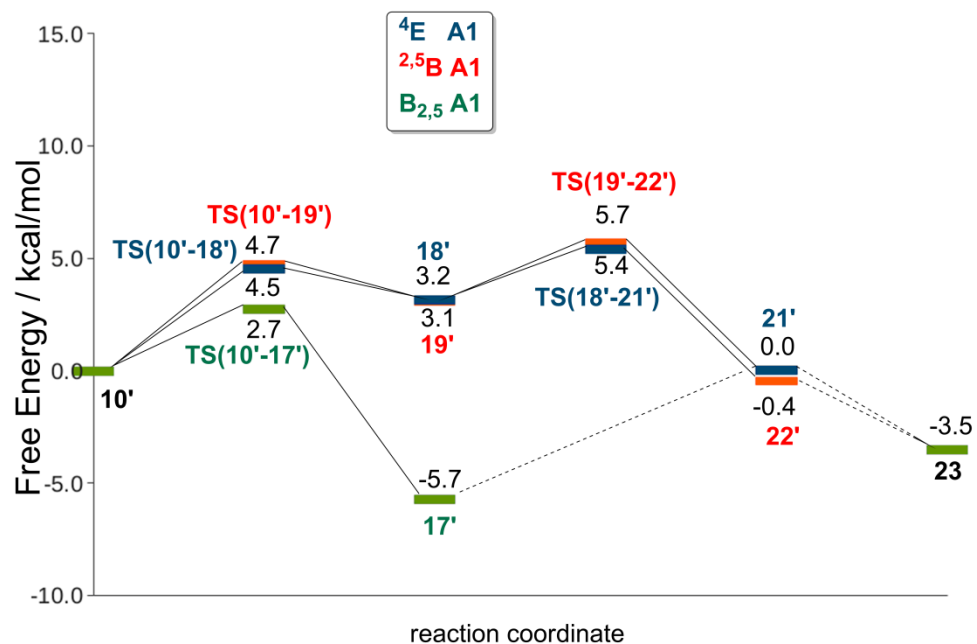


Figure S14: Energy profile (BB1K/6-31++G(d,p)) for the exo-cyclic cellobiose structure 2 mechanism. Energies refer to structure 10'.

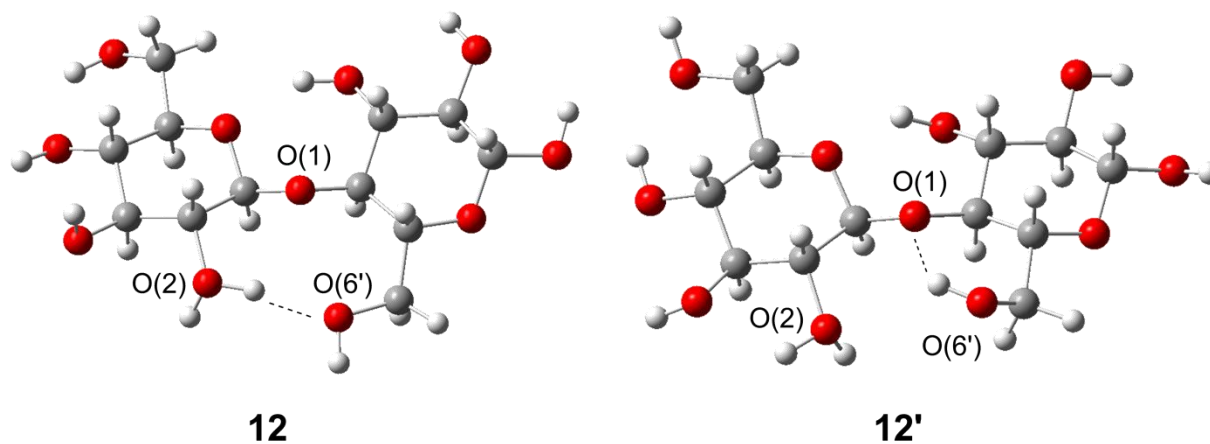
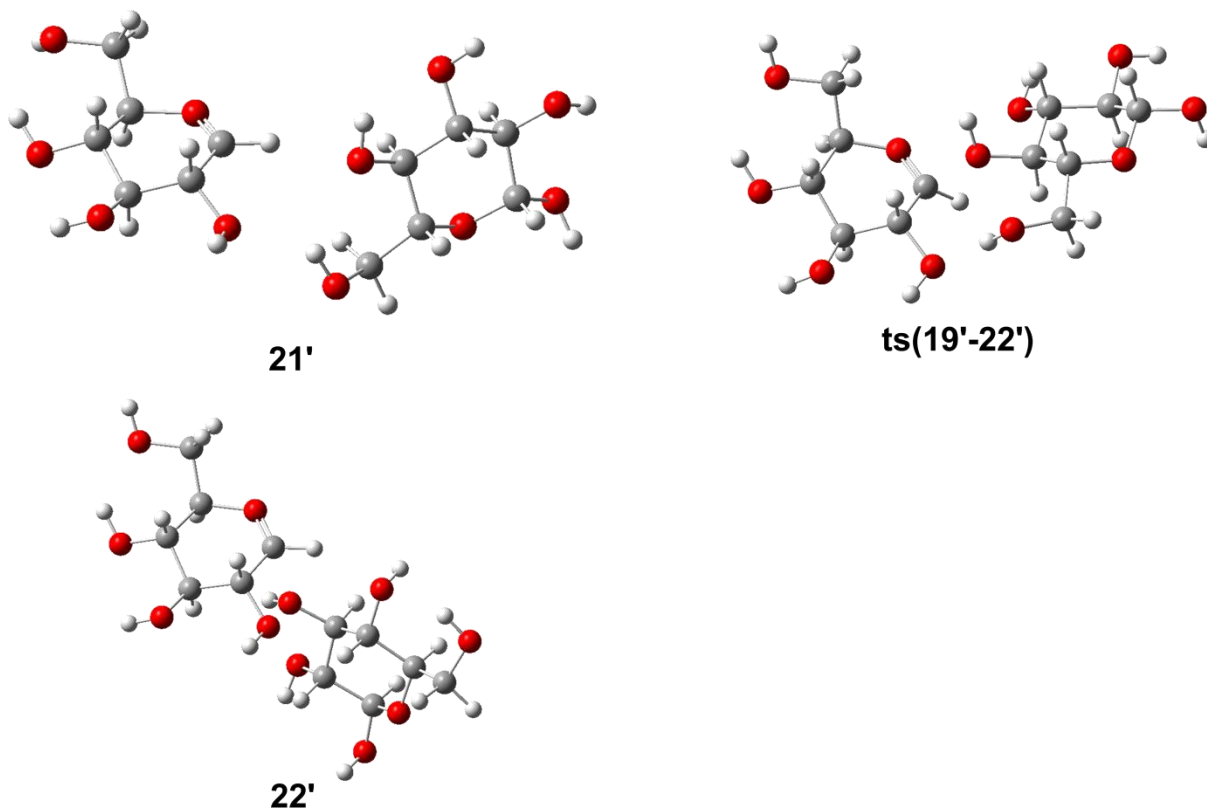


Figure S15: Structures 12 and 12' (BB1K/6-31++G(d,p)) showing the different hydrogen bonds formed upon protonation of O(2) in structures 1 and 2.







**Figure S16-b:** Structures 10' to 22' (BB1K/6-31++G(d,p)) for the exo-cyclic cellobiose structure 2 mechanism.

## Additional NBO data

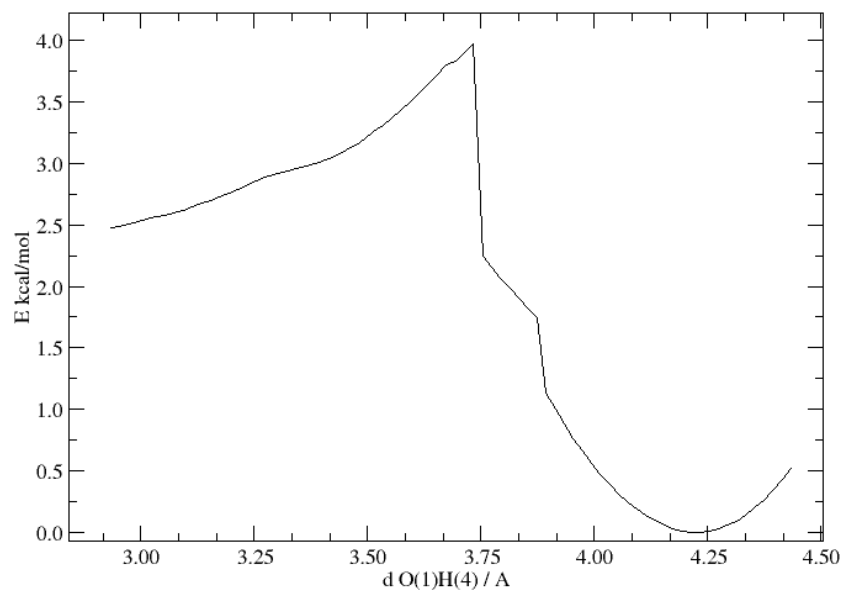
Table SI8. NBO data for 4-O-methyl-cellobiose. BB1K/6-31++G\*\*, CPCM water, 298.15 K, 1 atm.

	$\Delta G$ (kcal mol <sup>-1</sup> )	E(2) (kcal mol <sup>-1</sup> )		H-bonding		Bond length (Å)		Torsion angle (degree)	
		nO(1)→ $\sigma^*C(1)O(5)$	nO(5)→ $\sigma^*C(1)O(1)$	nO(6') → $\sigma^*O(2)H$	nO(3) → $\sigma^*O(X)H$	C(1)O(1)	C(1)O(5)	$\phi$ (O(5)C(1)O(1)C(4'))	$\chi$ (C(4')C(5')C(6')O(6'))
41me	3.5	14.0	4.0	8.1	6.4	1.379	1.406	57.8	-69.8
1me	0.0	18.0	3.9	14.6	2.9	1.375	1.411	-93.1	-76.8
3me	0.3	17.8	3.9	6.1	-	1.375	1.408	-78.0	-168.5
4me	0.0	17.4	4.2	6.26	-	1.376	1.409	-74.2	53.2
5me	9.3	6.6	4.6	-	-	1.400	1.391	0.0	-79.1
6me	9.3	6.0	5.5	-	-	1.398	1.395	-180.0	-80.3
10me	-	4.8	7.5	9.8	0.8	1.467	1.368	-104.9	-65.9
17me	-	7.0	28.7	-	59.6	1.502	1.351	-47.2	-61.3
18me	-	2.5	40.2	6.4	11.2	1.574	1.334	-91.3	-70.6
19me	-	5.7	36.6	12.5	0.5	1.54	1.336	-96.9	-66.3

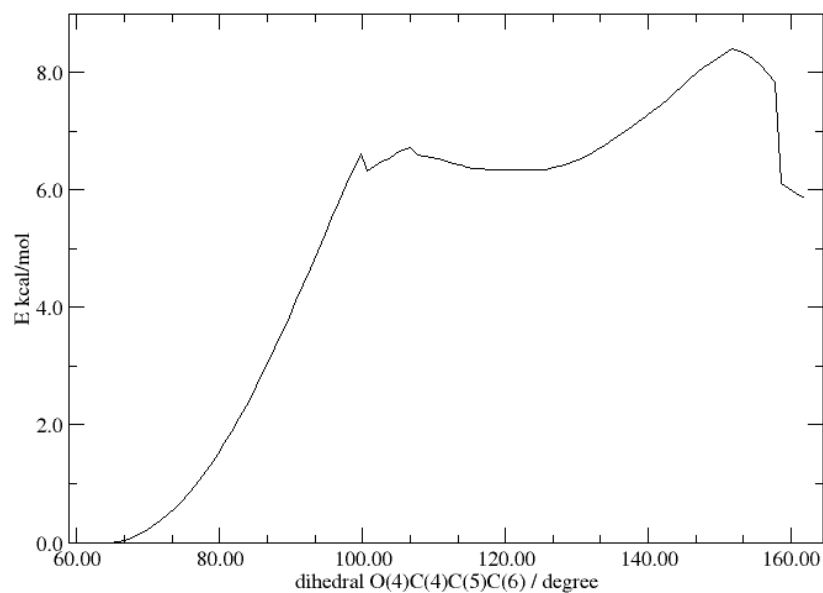
Table SI9: NBO data for structure 1 with water molecules. BB1K/6-31++G\*\*, CPCM water, 298.15 K, 1 atm

Number and position of water molecules	E(2) (kcal mol <sup>-1</sup> )	
	nO(1)→ $\sigma^*C(1)O(5)$	nO(5)→ $\sigma^*C(1)O(1)$
0	18.1	3.8
1 at O(1) (frozen)	17.0	3.7
1 at O(3')	18.0	3.7
1 at O(5)	18.5	4.0
1 at O(6')/O(1)	17.4	4.0
2 at O(6'), O(5)	17.7	4.2
3 at O(1), O(5), O(6)	17.2	3.8

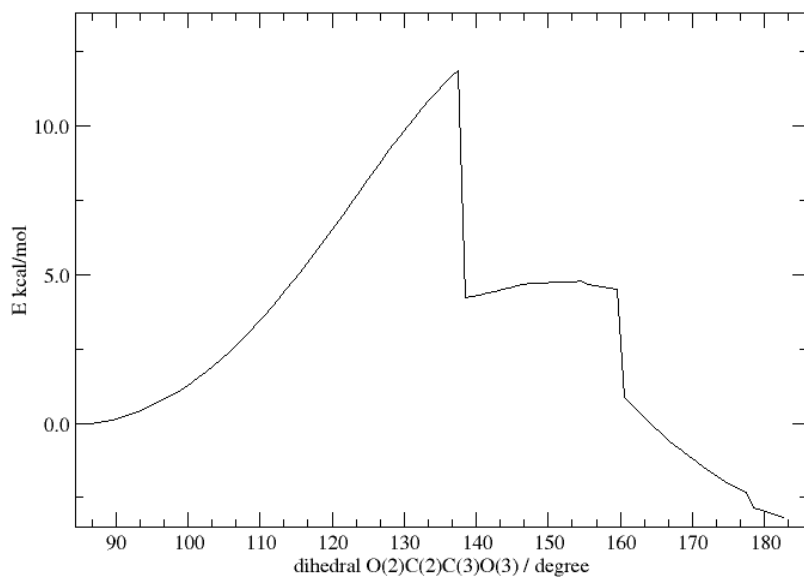
## PES Scans



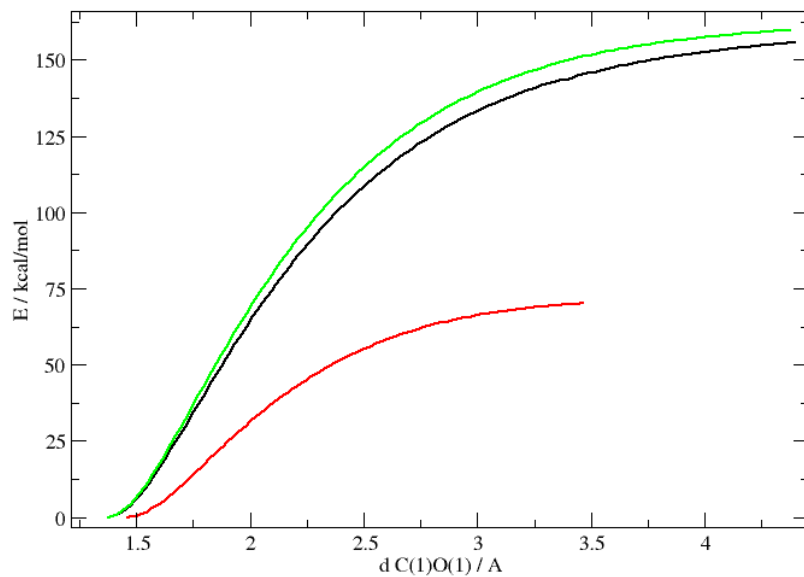
**Figure S17:** Relaxed PES scan energy profile (BB1K/6-31++G(d,p)). Elongation of O(1)H(4) distance in structure **18**. Energies refer to structure **10**. The abrupt change in energy at 3.73 Å is caused by the change from endo-sofa to chair conformation, with a shortening of the C(1)O(1) distance and a flip of C(6) from nearly axial to equatorial position.



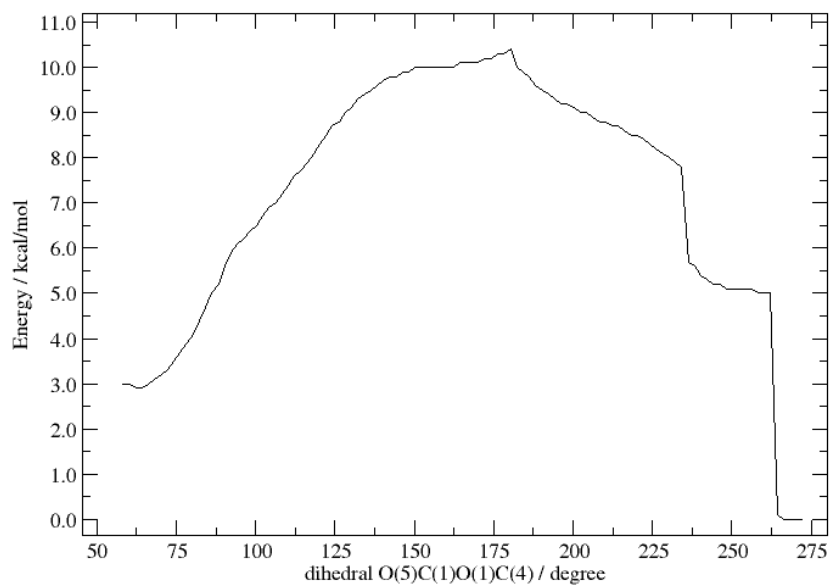
**Figure S18:** Relaxed PES scan energy profile (BB1K/6-31++G(d,p)). Rotation of O(4)C(4)C(5)C(6) dihedral in structure **10**. Energies refer to structure **10**.



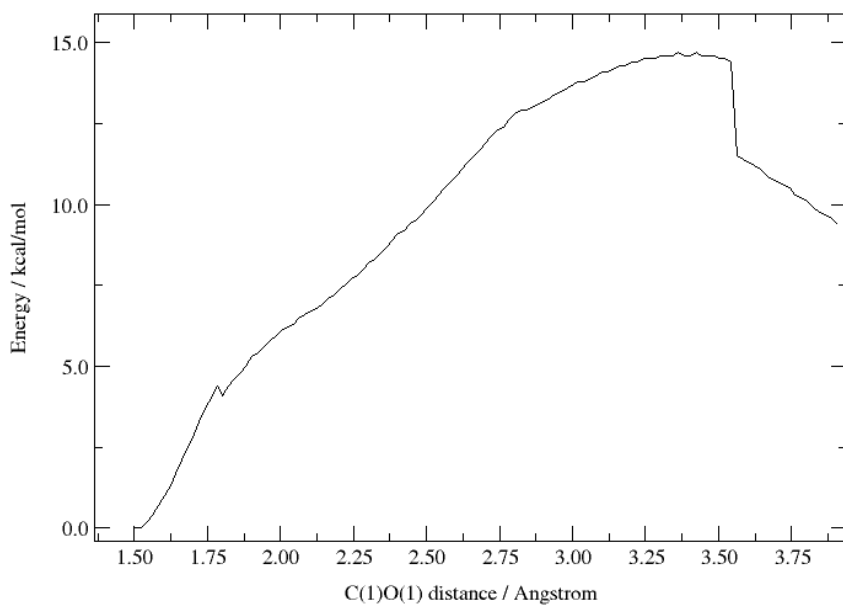
**Figure S19:** Relaxed PES scan energy profile (BB1K/6-31++G(d,p)). Rotation of O(2)C(2)C(3)O(3) dihedral in structure **10**. Energies refer to structure **10**. The abrupt energy change at 138° comes from O(2) moving into axial position and an increase of the C(1)O(1) distance. The abrupt change in energy at 160° is caused by the formation of a hydrogen bond between HO(1) and O(3).



**Figure S110:** Unrelaxed open-shell PES scan energy profile (BB1K/6-31++G(d,p)). Elongation of C(1)O(1) distance in structures **1** (black), **10** (red), and **16** (green). Energies refer to starting structure.



**Figure S111:** Relaxed PES scan energy profile (BB1K/6-31++G(d,p)). Rotation of O(5)C(1)O(1)C(4) dihedral in structure **41**. Energies refer to structure **1**. The abrupt changes in energy at 234° and 254° come from the formation of the O(6')O(2) and O(3')O(5) hydrogen bonds, respectively.



**Figure S112:** Relaxed PES scan energy profile (BB1K/6-31++G(d,p)). Elongation of C(1)O(1) distance in structure **17**. Energies refer to structure **17**. The abrupt energy change at 3.54 Å is caused by the formation of a hydrogen bond between HO(6') and O(1).

## Energy profiles for exo-cyclic mechanisms with different functionals and basis sets

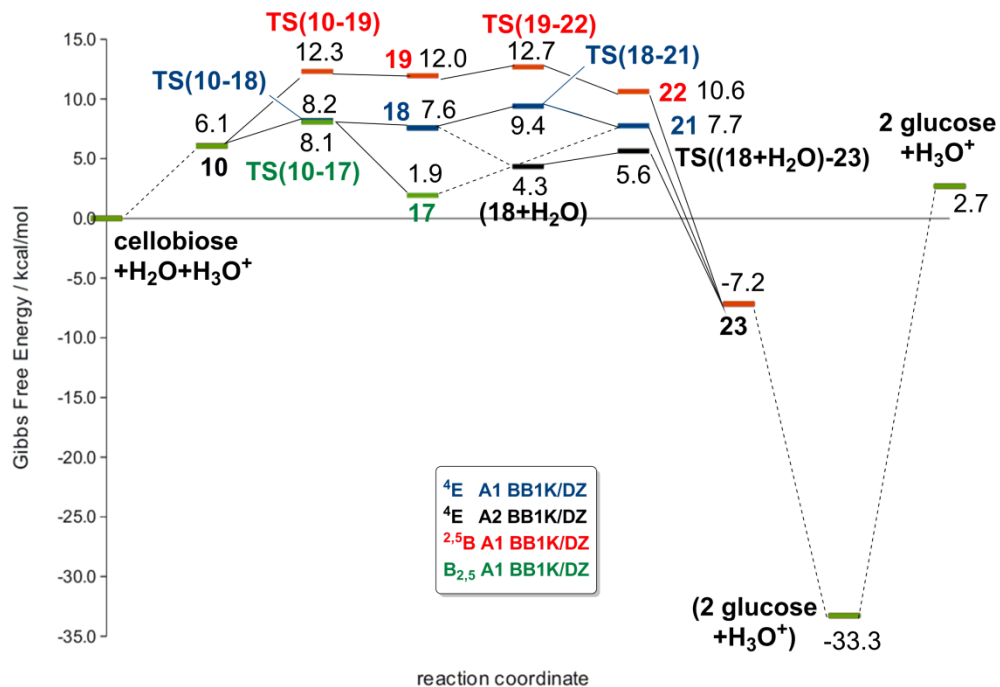


Figure SII3: Energy profile (BB1K/6-31++G(d,p)) for exo-cyclic mechanisms. Energies refer to structure  $1 + \text{H}_2\text{O} + \text{H}_3\text{O}^+$ .

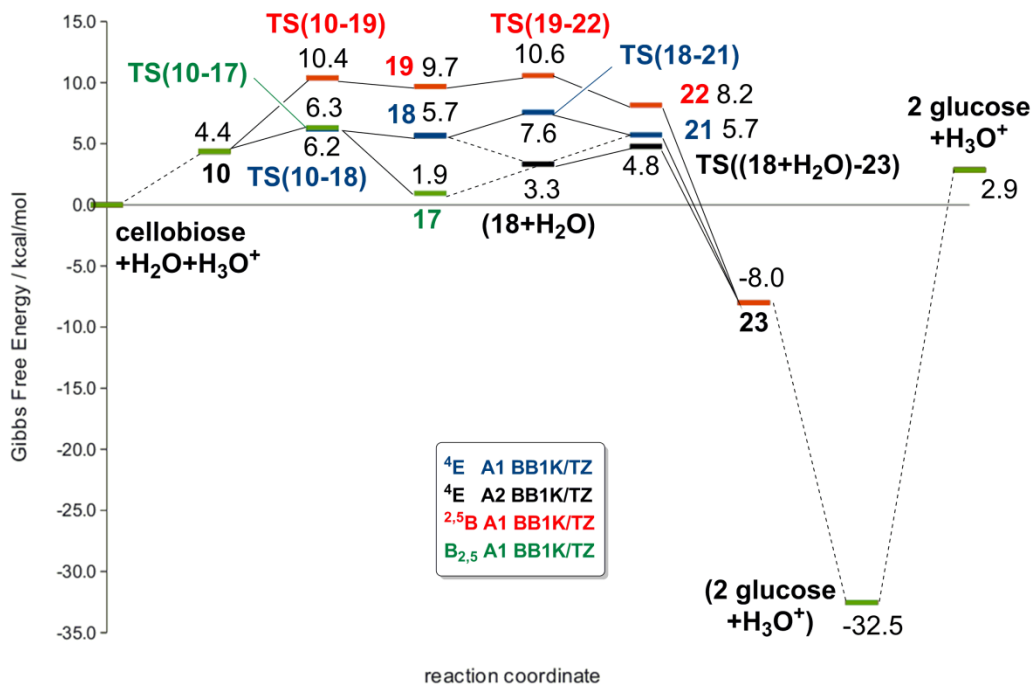


Figure SII4: Single-point energy profile (BB1K/6-311++G(2df,2pd)) for exo-cyclic mechanisms. Energies refer to structure  $1 + \text{H}_2\text{O} + \text{H}_3\text{O}^+$ .

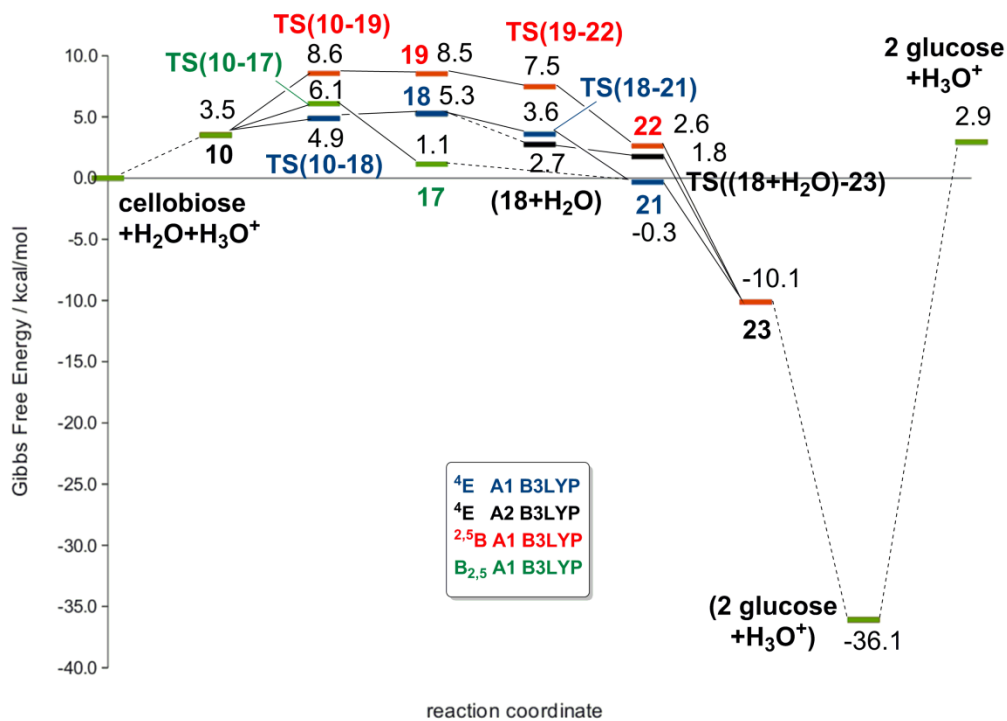


Figure S115: Single-point energy profile (B3LYP/6-31++G(d,p)) for exo-cyclic mechanisms. Energies refer to structure  $1 + \text{H}_2\text{O} + \text{H}_3\text{O}^+$ .

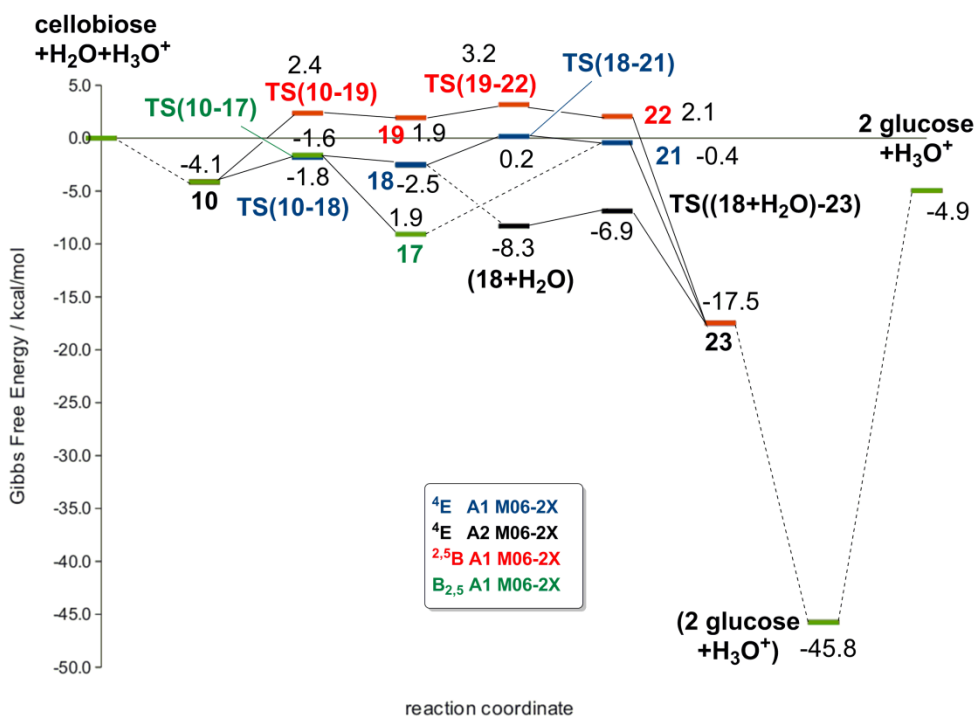
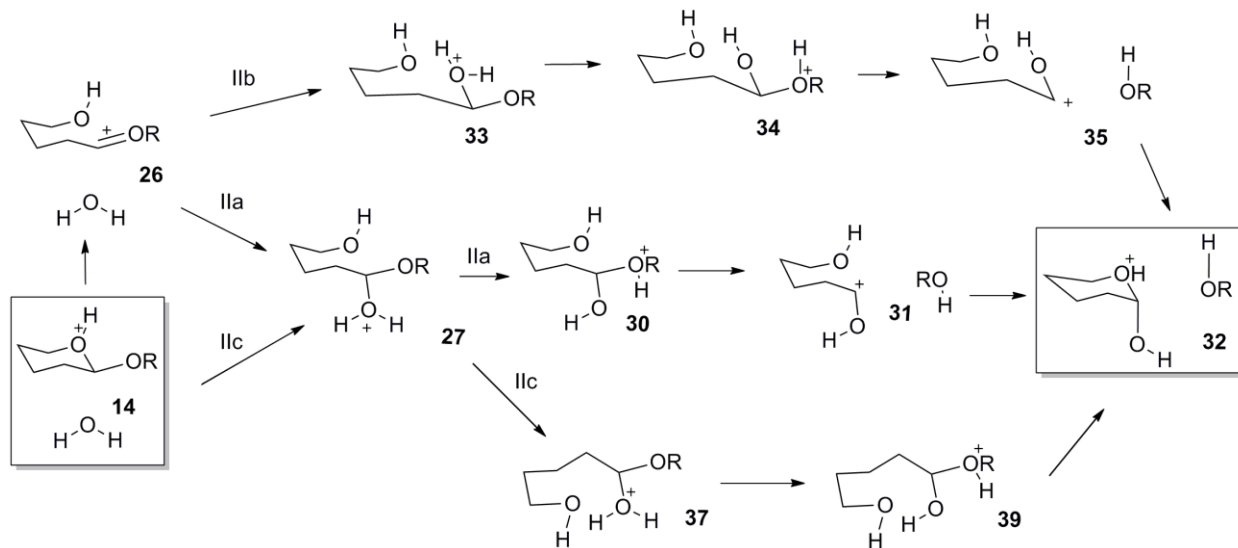


Figure S116: Single-point energy profile (M06-2X/6-31++G(d,p)) for exo-cyclic mechanisms. Energies refer to structure  $1 + \text{H}_2\text{O} + \text{H}_3\text{O}^+$ .

## Reaction scheme and energy profiles for endo-cyclic mechanism for structure 1



Scheme S117. A1 and A2 pathways for cellobiose in the endo-cyclic mechanism.

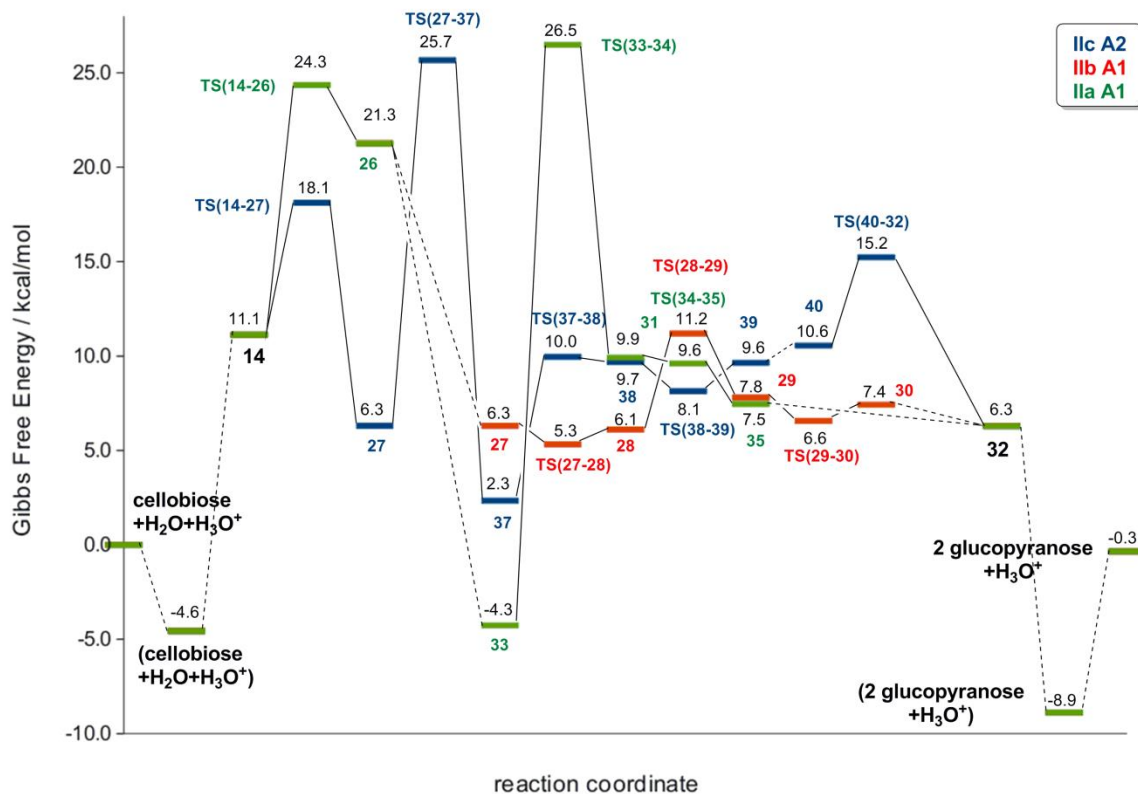


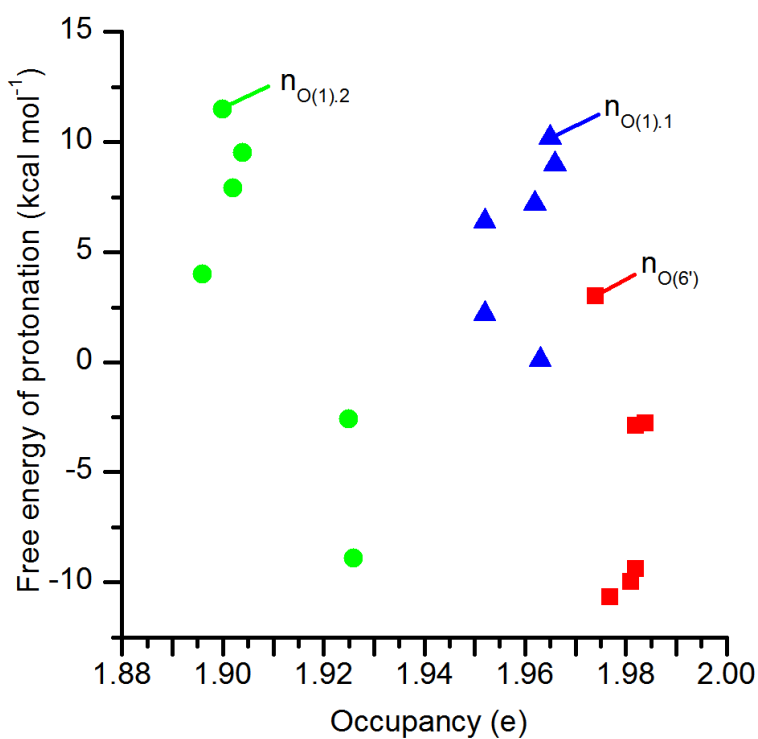
Figure S118. Energy profile for A1 and A2 pathways for cellobiose for the endo-cyclic mechanism (BB1K/6-31++G(d,p)).



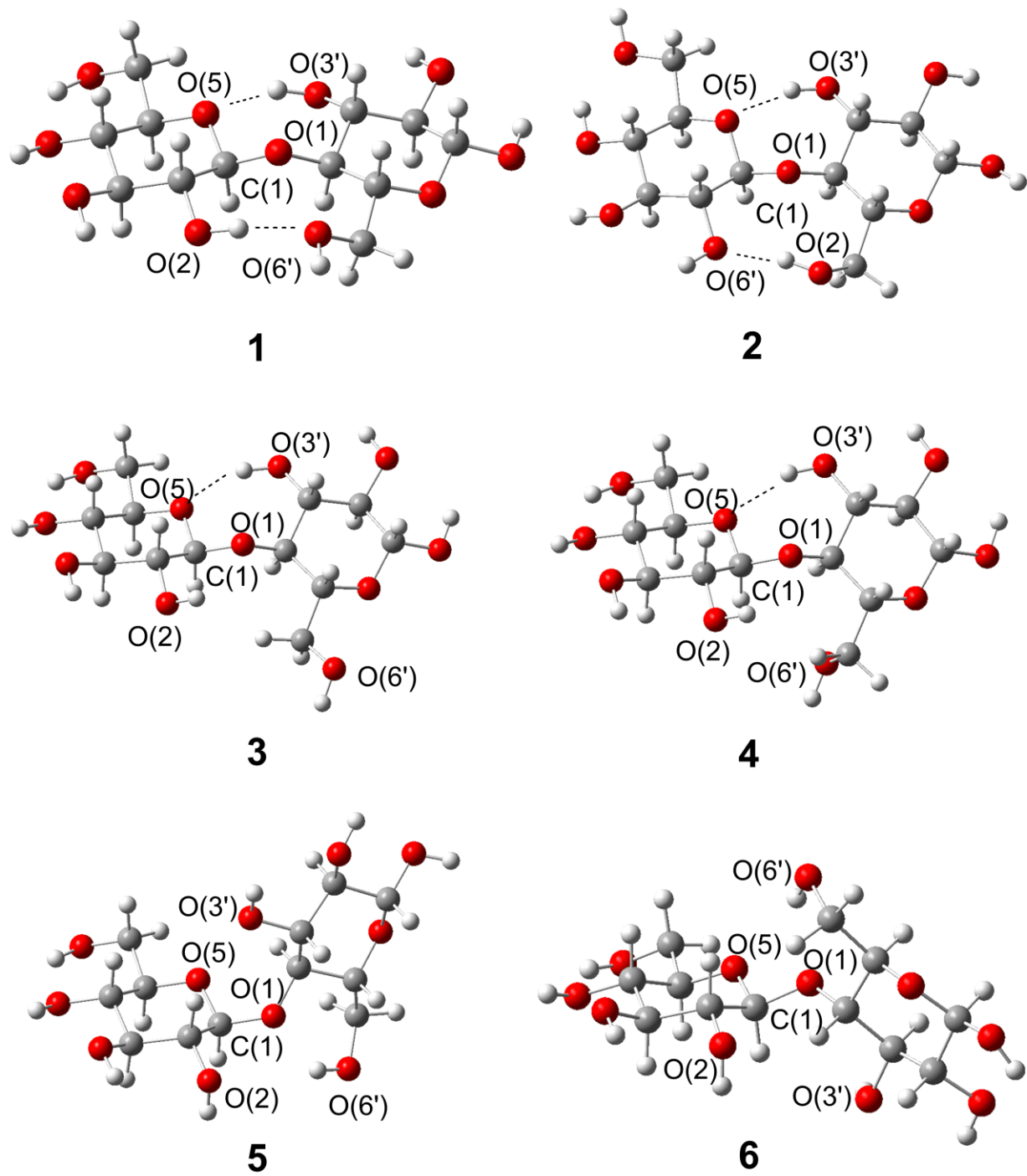
## Additional Figures

Figure SI14 shows an attempt to correlate the computed protonation free energy of structures **1**, **3** to **6** and **41** with the occupancy of the corresponding oxygen lone pairs.

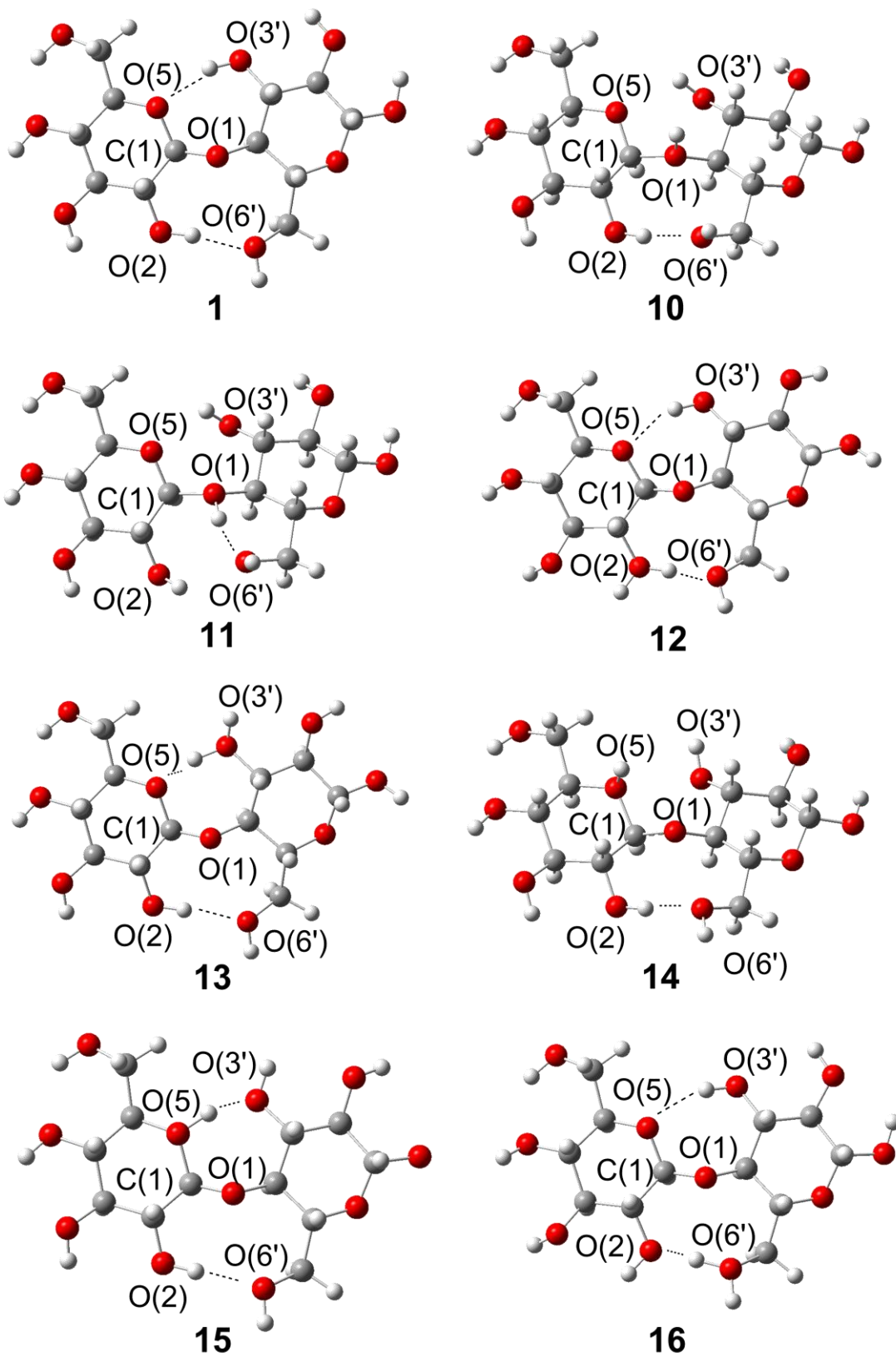
Figures SI15 and SI16 are enlarged versions of Figures 4 and 8 of the main paper, respectively, that are included to provide a better view of these structures.



**Figure SI19.** Correlation of the free energy of protonation versus the occupancy of the O(1)-1, O(1)-2 and O(6) lone pairs in **1**, **3** to **6** and **41**.



**Figure SI20.** Optimized structures of the cellobiose conformers **1** to **6** (BB1K/6-31++G\*\*).



**Figure S121.** Optimized structures of **1** protonated at different sites (BB1K/6-31++G\*\*).

## Total energies of stationary points (Hartree)

Table SI10. BB1K/6-31++G\*\*, CPCM water, 298.15 K, 1 atm.

compound	EZPC	H	G	spE(BB1K/6-311++G(3df,3pd))
H <sub>2</sub> O	-76.381898	-76.378118	-76.399522	-76.4304370347
H <sub>3</sub> O <sup>+</sup>	-76.761283	-76.757457	-76.780387	-76.8212579647
α-glucose	-686.737489	-686.723827	-686.775481	
β-glucose	-686.738926	-686.725169	-686.777114	
1+H <sub>2</sub> O+H <sub>3</sub> O <sup>+</sup>	-1450.281548	-1450.251585	-1450.341078	
α-glucose+ β-glucose+H <sub>3</sub> O <sup>+</sup>	-1450.286306	-1450.256975	-1450.347951	
41	-1297.096401	-1297.072112	-1297.147614	-1297.86818839
1	-1297.100801	-1297.076311	-1297.153244	-1297.87201564
2	-1297.102904	-1297.078618	-1297.154955	
3	-1297.099156	-1297.074911	-1297.152705	-1297.87014789
4	-1297.100289	-1297.075137	-1297.153846	-1297.87115728
5	-1297.087332	-1297.062337	-1297.141286	-1297.85859472
6	-1297.085026	-1297.060044	-1297.138701	-1297.85667333
7	-1221.905189	-1221.881679	-1221.956897	
8	-1221.913720	-1221.889704	-1221.965892	
9	-1146.717775	-1146.695146	-1146.767885	
12	-1297.493630	-1297.469930	-1297.543703	-1298.27988119
13	-1297.496645	-1297.472173	-1297.548188	-1298.28133209
10	-1297.469566	-1297.444240	-1297.522642	-1298.25586652
11	-1297.476602	-1297.452183	-1297.527793	-1298.25586652
14	-1297.474458	-1297.448955	-1297.528006	-1298.26387118
15	-1297.495049	-1297.470633	-1297.546290	-1298.28014517
16	-1297.499624	-1297.475243	-1297.551143	-1298.28391710

Table SI11. B3LYP/6-31++G\*\*, CPCM water, 298.15 K, 1 atm (left) and M06-2X/6-31++G\*\*, CPCM water, 298.15 K, 1 atm (right).

compound	EZPC	H	G	EZPC	H	G
H <sub>2</sub> O	-76.421213	-76.417433	-76.438871	-76.382034	-76.378254	-76.399682
H <sub>3</sub> O <sup>+</sup>	-76.797051	-76.793223	-76.816185	-76.759155	-76.755325	-76.777247
41	-1297.678300	-1297.653557	-1297.730185	-1297.174687	-1297.150342	-1297.225914
1	-1297.684850	-1297.659921	-1297.737390	-1297.177971	-1297.153392	-1297.230200
3	-1297.682899	-1297.657262	-1297.737229	-1297.175367	-1297.150142	-1297.228962
4	-1297.683096	-1297.657522	-1297.737341	-1297.176625	-1297.151438	-1297.230028
5	-1297.670564	-1297.645959	-1297.722258	-1297.163250	-1297.139102	-1297.214311
6	-1297.675816	-1297.650912	-1297.728391	-1297.161215	-1297.136331	-1297.214853
10	-1298.054060	-1298.028305	-1298.107053	-1297.543264	-1297.518301	-1297.595602
11	-1298.059610	-1298.034601	-1298.111879	-1297.550115	-1297.525552	-1297.601624
12	-1298.076750	-1298.052418	-1298.127661	-1297.565098	-1297.540970	-1297.615524
13	-1298.081566	-1298.056666	-1298.133471	-1297.573734	-1297.549358	-1297.624897
14	-1298.060985	-1298.034878	-1298.115447	-1297.548314	-1297.522811	-1297.601789
15	-1298.080713	-1298.055714	-1298.132641	-1297.571686	-1297.547289	-1297.622872
16	-1298.083285	-1298.058455	-1298.135101	-1297.575639	-1297.551306	-1297.626843

**Table SI12. Computed free energies relative to structure 1 in kcal/mol, CPCM water, 298.15 K, 1 atm.**

compound	BB1K/ 6-31++G**	B3LYP/ 6-31++G**	M06-2X/ 6-31++G**	BB1K/ 6-311++G(3pd,3df)
41	3.5	4.5	2.7	2.4
1	0.0	0.0	0.0	0.0
3	0.3	0.1	0.8	1.2
4	-0.4	0.0	0.1	0.5
5	7.5	9.5	10.0	6.4
6	9.1	5.6	9.6	9.6
10	6.8	4.8	7.6	4.4
11	3.6	1.8	3.9	-0.6
12	-6.4	-8.1	-6.3	-10.7
13	-9.2	-11.8	-10.5	-11.6
14	3.4	-0.5	3.7	1.8
15	-8.1	-11.3	-9.5	-10.9
16	-11.1	-12.8	-12.0	-13.2

**Table SI13. Absolute free energies in Hartree for structures 10, 12-14 and 16 (298.15 K, 1atm).**

compound	G(B97-1/6- 31++G**, gas phase)	G(B97-1/6- 31++G**, SMD)	G(BB1K/6- 31++G**, gas phase)
10	-1297.653957	-1297.794645	-1297.419672
12	-1297.664611	-1297.811310	-1297.447881
13	-1297.669348	-1297.810924	-1297.452312
14	-1297.681326	-1297.796008	-1297.425601
16	-1297.667762	-1297.817733	-1297.449656

**Table SI14. BB1K/6-31++G\*\*, CPCM water, 298.15 K, 1 atm: Pathway I.**

compound	EZPC	H	G	spE(B3LYP/6- 311++G(d,p))	spE(M06-2X/6- #11++G(d,p))	spE(BB1K/6- 311++G(3df,3pd))
TS(10-17)	-1297.466285	-1297.441989	-1297.517726	-1298.42199192	-1297.92288382	-1298.25276315
TS(10-18)	-1297.466204	-1297.441869	-1297.517808	-1298.42391927	-1297.92321569	-1298.25293669
TS(10-19)	-1297.459775	-1297.435187	-1297.511056	-1298.41805234	-1297.91657575	-1298.24627009
17	-1297.476617	-1297.451887	-1297.528588	-1298.42988056	-1297.93481896	-1298.26132724
18	-1297.466694	-1297.441683	-1297.519122	-1298.42329589	-1297.92435573	-1298.25381617
18+H <sub>2</sub> O	-1373.849940	-1373.821601	-1373.906685	-1374.86919983	-1374.33668669	-1374.68797338
19	-1297.461441	-1297.435492	-1297.515964	-1298.41809229	-1297.91724589	-1298.24740007
20	-1297.457192	-1297.430081	-1297.515656			
TS(18-21)	-1297.465210	-1297.440329	-1297.517729	-1298.42596100	-1297.92007435	-1298.25077616
TS((18+H <sub>2</sub> O)-23)	-1373.849630	-1373.821370	-1373.906298	-1374.87076504	-1374.33442826	-1374.68565119
TS(19-22)	-1297.461239	-1297.435679	-1297.515119	-1298.41978415	-1297.91527420	-1298.24597866
21	-1297.469130	-1297.442872	-1297.524923	-1298.43219746	-1297.92102355	-1298.25370889
21+H <sub>2</sub> O	-1373.852209	-1373.821775	-1373.916678	-1374.87885536	-1374.32739856	-1374.68686515
22	-1297.465338	-1297.438712	-1297.522359	-1298.42750289	-1297.91706835	-1298.24983439
22+H <sub>2</sub> O	-1373.852649	-1373.823062	-1373.912217	-1374.87881828	-1374.33323958	-1374.68839164
23	-1373.866997	-1373.839451	-1373.924562	-1374.88971587	-1374.35129560	-1374.70602874
24	-1373.860772	-1373.833206	-1373.917710	-1374.87913827	-1374.34803956	-1374.69806765

**Table SI15. BB1K/6-31++G\*\*, CPCM water, 298.15 K, 1 atm: Pathway II.**

compound	EZPC	H	G
TS(14-26)	-1373.836626	-1373.807427	-1373.894834
TS(14-36)	-1373.849442	-1373.821647	-1373.904756
26	-1373.839373	-1373.809056	-1373.899749
27	-1373.869688	-1373.843741	-1373.923586
TS(27-28)	-1373.871420	-1373.845753	-1373.925152
28	-1373.869878	-1373.843803	-1373.923901
TS(28-29)	-1373.861661	-1373.835775	-1373.915780
29	-1373.866626	-1373.840161	-1373.921188
TS(29-30)	-1373.869033	-1373.842950	-1373.923171
30	-1373.867258	-1373.840765	-1373.921799
32	-1373.865198	-1373.837102	-1373.923610
33	-1373.886708	-1373.860750	-1373.940417
TS(33-34)	-1373.835964	-1373.809511	-1373.891439
34	-1373.862317	-1373.835344	-1373.917832
TS(34-35)	-1373.862738	-1373.836199	-1373.918334
35	-1373.864667	-1373.837255	-1373.921744
TS(27-37)	-1373.796689	-1373.771446	-1373.849225
37	-1373.875811	-1373.849729	-1373.929914
TS(37-38)	-1373.864037	-1373.838243	-1373.917753
38	-1373.863950	-1373.837728	-1373.918186
TS(38-39)	-1373.866196	-1373.840286	-1373.920652
39	-1373.863911	-1373.837619	-1373.918257
40	-1373.860199	-1373.832972	-1373.916809
TS(40-32)	-1373.853649	-1373.826647	-1373.909351

**Table SI16. 4-O-methyl-cellobiose, BB1K/6-31++G\*\*, CPCM water, 298.15 K, 1 atm: Pathway I.**

compound	EZPC	H	G
10me	-1336.713408	-1336.686718	-1336.768549
TS(10me-17me)	-1336.711003	-1336.685258	-1336.764724
TS(10me-18me)	-1336.709750	-1336.684094	-1336.763108
TS(10me-19me)	-1336.704616	-1336.678483	-1336.758456
17me	-1336.723099	-1336.697070	-1336.776519
18me	-1336.710273	-1336.683711	-1336.765499
18me+H <sub>2</sub> O	-1413.093766	-1413.063505	-1413.155529
19me	-1336.707080	-1336.679916	-1336.762758
TS(18me-21me)	-1336.708449	-1336.682111	-1336.763164
TS((18me+H <sub>2</sub> O)-23me)	-1413.093559	-1413.063752	-1413.152300
TS(19me-22me)	-1336.705867	-1336.679277	-1336.760814
21me	-1336.712997	-1336.685010	-1336.772411
22me	-1336.708822	-1336.680809	-1336.766539
23me	-1413.112409	-1413.083117	-1413.174083

**Table SI17. BB1K/6-31++G\*\*, CPCM water, 298.15 K, 1 atm: Protonation of structures 1, 41 and 3-6.**

compound	EZPC	H	G
41-O(1)-1	-1297.476248	-1297.451597	-1297.528283
41-O(1)-2	-1297.462110	-1297.437614	-1297.513420
41-O(2)	-1297.494349	-1297.470285	-1297.545157
41-O(3)	-1297.495925	-1297.471824	-1297.546776
41-O(5)-1	-1297.456806	-1297.431807	-1297.508953
41-O(5)-2	-1297.481394	-1297.457424	-1297.531557
41-O(6)	-1297.482503	-1297.458317	-1297.533271
3-O(1)-1	-1297.463731	-1297.438088	-1297.517285
3-O(1)-2	-1297.461924	-1297.436573	-1297.515314
3-O(2)	-1297.477455	-1297.452216	-1297.530710
3-O(3)	-1297.495885	-1297.470862	-1297.548798
3-O(5)-1	-1297.475624	-1297.449970	-1297.529392
3-O(5)-2	-1297.495779	-1297.470843	-1297.548038
3-O(6)	-1297.484562	-1297.459356	-1297.538061
4-O(1)-1	-1297.466624	-1297.440926	-1297.520440
4-O(1)-2	-1297.468759	-1297.443259	-1297.522121
4-O(2)	-1297.477047	-1297.451913	-1297.530092
4-O(3)	-1297.497304	-1297.472353	-1297.550427
4-O(5)-1	-1297.474051	-1297.448837	-1297.526460
4-O(5)-2	-1297.497451	-1297.472485	-1297.549799
4-O(6)	-1297.497997	-1297.473526	-1297.549721
5-O(1)-1	-1297.465373	-1297.440123	-1297.518586
5-O(1)-2	-1297.475277	-1297.451146	-1297.526292
5-O(2)	-1297.472335	-1297.447330	-1297.524857
5-O(3)	-1297.478064	-1297.454315	-1297.528005
5-O(5)-1	-1297.466099	-1297.442364	-1297.516044
5-O(5)-2	-1297.452834	-1297.428297	-1297.504147
5-O(6)	-1297.475229	-1297.451005	-1297.526782
6-O(1)-1	-1297.456759	-1297.431619	-1297.509360
6-O(1)-2	-1297.483111	-1297.459081	-1297.533746
6-O(2)	-1297.459128	-1297.434154	-1297.512045
6-O(3)	-1297.465265	-1297.440596	-1297.517526
6-O(5)-1	-1297.458135	-1297.433054	-1297.510395
6-O(5)-2	-1297.466747	-1297.441621	-1297.520167
6-O(6)	-1297.484199	-1297.459987	-1297.535440

**Table SI18. Total Energies for pathway A1 for structure 2, BB1K/6-31++G\*\*, CPCM water, 298.15 K, 1 atm.**

compound	EZPC	H	G
10'	-1297.470223	-1297.445021	-1297.523070
TS(10'-17')	-1297.466512	-1297.442127	-1297.518287
TS(10'-18')	-1297.464306	-1297.439962	-1297.515844
TS(10'-19')	-1297.463446	-1297.438851	-1297.515519
17'	-1297.479193	-1297.454187	-1297.532172
18'	-1297.464620	-1297.439378	-1297.518023
19'	-1297.463843	-1297.438211	-1297.518099
TS(18'-21')	-1297.461728	-1297.436630	-1297.514439
TS(19'-22')	-1297.460726	-1297.435383	-1297.514040
21'	-1297.465028	-1297.438275	-1297.523043
22'	-1297.468822	-1297.442561	-1297.523787

## Cartesian coordinates (in Angstrom, BB1K/6-31++G\*\*)

<b>10me</b>	1 -7.644519 -2.392640 -2.656119	1 -8.486432 -1.229908 -2.323051
6 -2.475936 2.448619 1.580702	<b>TS(10me-17me) – 1 imaginary</b>	1 -7.911067 -1.790761 -0.738677
6 -2.076821 0.998905 1.736022	<b>frequency</b>	1 -7.857461 -0.061174 -1.147137
6 -1.646356 0.625868 3.150399	6 -3.172911 2.370848 1.985475	<b>TS(10me-18me) – 1 imaginary</b>
8 -0.624538 1.518047 3.505441	6 -2.329115 1.237344 1.454330	<b>frequency</b>
6 -1.041346 2.854231 3.550135	6 -1.519227 0.614767 2.582147	8 0.322937 1.118929 -2.007295
6 -1.359555 3.308326 2.140426	8 -0.709412 1.665438 3.051109	6 1.482695 0.473896 -1.796285
8 -3.206186 0.129345 1.346304	6 -1.422108 2.728058 3.651403	6 2.637763 0.640731 -2.781738
6 -3.457216 -0.292809 -0.035705	6 -2.279521 3.415593 2.603918	6 2.475463 1.864027 -3.662683
8 -4.521170 0.458254 -0.454505	8 -3.323374 0.349505 0.839841	6 1.072988 1.879735 -4.219241
6 -4.953382 0.107779 -1.771545	6 -2.870919 -0.602020 -0.289401	6 0.113980 2.070287 -3.058054
6 -5.373824 -1.357558 -1.801597	8 -3.164228 -0.013181 -1.456492	8 1.089894 -1.019720 -1.828202
6 -4.211506 -2.224102 -1.361023	6 -4.258441 -0.509471 -2.235665	6 0.614811 -1.610340 -0.571589
6 -3.751495 -1.772802 0.013415	6 -5.383843 -0.951942 -1.321908	6 -0.530905 -2.509043 -0.965551
8 -2.620090 -2.502131 0.357314	6 -4.919915 -2.149115 -0.521963	6 -1.148063 -3.072847 0.292607
8 -4.603013 -3.564900 -1.309378	6 -3.502609 -1.949490 0.035527	6 -0.054922 -3.768202 1.098156
8 -5.782352 -1.621969 -3.116289	8 -2.662160 -2.936570 -0.492265	8 1.008726 -2.868862 1.331369
6 -6.080297 1.055584 -2.136158	8 -5.851589 -2.380570 0.498994	6 1.657688 -2.437511 0.161307
8 -6.283945 1.091189 -3.521473	8 -6.482892 -1.245290 -2.136660	8 -1.389231 -1.717868 -1.738885
6 -1.038185 -0.763223 3.264719	6 -4.651039 0.611639 -3.178443	6 2.917980 -1.711392 0.582922
8 -1.961923 -1.787502 2.992784	8 -5.373831 0.128065 -4.275365	8 3.736698 -1.442899 -0.530158
8 0.013287 3.560553 4.086269	6 -0.562431 -0.494964 2.186236	8 -0.513483 -4.231384 2.305167
8 -1.727386 4.652868 2.209818	8 -1.237172 -1.685275 1.863608	8 -2.138521 -3.971281 -0.106247
8 -2.652754 2.776840 0.233454	8 -0.524612 3.650379 4.123174	8 3.846830 0.795703 -2.109257
1 -5.804074 2.058722 -1.823566	8 -3.106860 4.387830 3.166848	8 3.413154 1.816979 -4.698117
1 -0.619682 -0.862349 4.263477	8 -3.919816 2.814385 0.882830	8 0.829340 2.957298 -5.081784
1 -6.989675 0.770962 -1.602157	1 -3.742417 1.067444 -3.562015	6 -1.346875 1.956802 -3.452217
1 -4.128870 0.266725 -2.471063	1 0.132640 -0.639622 3.010061	8 -1.796959 3.125540 -4.079966
1 -6.212541 -1.500092 -1.112683	1 -5.209140 1.375270 -2.631347	1 -1.160775 3.347541 -4.764864
6 -6.764701 -2.633261 -3.253112	1 -3.900237 -1.354720 -2.825117	1 -1.493413 1.076842 -4.083220
1 -3.388866 -2.093910 -2.071575	1 -5.644396 -0.127906 -0.645501	1 -1.935226 1.826073 -2.548286
1 -3.867296 -4.071249 -0.958112	6 -7.754744 -1.073422 -1.538303	1 0.281324 3.061384 -2.635531
1 -4.572513 -1.938632 0.717267	1 -4.871230 -2.995956 -1.208149	1 0.863981 0.938590 -4.738910
1 -2.420406 -2.379434 1.297687	1 -5.769913 -3.281329 0.812533	6 1.097240 2.703508 -6.449852
1 -2.528349 -0.064844 -0.556721	1 -3.562477 -2.015731 1.118043	1 2.624098 2.762234 -3.056364
1 -1.301748 0.739485 1.021648	1 -1.866754 -2.964221 0.047631	1 4.286600 1.779851 -4.303136
1 -2.494397 0.719943 3.836889	1 -1.798845 -0.621765 -0.142827	1 2.655315 -0.234857 -3.434502
1 -0.228324 -0.861466 2.546669	1 -1.674790 1.581322 0.655296	1 4.026318 0.002137 -1.586926
1 -1.932878 2.934381 4.184762	1 -2.193151 0.255589 3.365694	1 1.822178 0.587341 -0.770076
1 -0.087541 4.480543 3.828422	1 0.015563 -0.196606 1.313725	1 0.266394 -0.787160 0.048311
1 -0.460051 3.175101 1.534236	1 -2.051511 2.327228 4.452333	1 1.940547 -3.293907 -0.458720
1 -1.822518 4.999599 1.321600	1 -0.158959 3.358704 4.959073	1 3.434018 -2.328607 1.314888
1 -3.380179 2.654800 2.157719	1 -1.618844 3.838704 1.843494	1 2.685194 -0.759330 1.053354
1 -3.563461 2.634324 -0.028227	1 -2.559197 5.092154 3.516770	1 4.181162 -2.242329 -0.814550
1 -2.495656 -1.974943 3.764940	1 -3.842767 1.984770 2.758975	1 0.309558 -4.637854 0.547780
1 -4.023593 0.242444 1.858340	1 -4.655648 3.353376 1.177786	1 -0.849411 -3.499172 2.827858
1 -6.373048 0.181019 -3.817877	1 -1.439774 -2.167152 2.665593	1 -1.564553 -2.254998 0.888137
1 -7.038846 -2.655540 -4.302037	1 -3.997261 0.979887 0.489692	1 -2.618133 -4.277054 0.664799
1 -6.373942 -3.600743 -2.953795	1 -6.129372 -0.349661 -3.922528	1 -0.148511 -3.340731 -1.564214



1 0.311100 -1.080950 -2.429471  
 1 -2.024942 -2.274299 -2.192186  
 1 0.795097 3.592989 -6.991467  
 1 2.153753 2.514345 -6.611773  
 1 0.512846 1.852701 -6.800491  
**TS(10me-19me) – 1 imaginary frequency**  
 6 -2.225122 2.503012 1.375562  
 6 -2.048909 1.027854 1.664953  
 6 -1.982848 0.691105 3.150921  
 8 -0.980675 1.496853 3.712175  
 6 -1.250066 2.866755 3.615235  
 6 -1.180058 3.271938 2.157482  
 8 -3.144303 0.269040 1.058947  
 6 -3.089137 -0.293362 -0.365502  
 8 -3.759213 0.527037 -1.179946  
 6 -4.918549 0.134741 -1.946884  
 6 -5.154122 -1.375712 -2.078405  
 6 -3.949131 -2.180447 -1.633981  
 6 -3.589903 -1.707380 -0.241356  
 8 -2.607808 -2.530737 0.292875  
 8 -4.284082 -3.535641 -1.599362  
 8 -5.496631 -1.572616 -3.419703  
 6 -6.111115 0.907574 -1.407933  
 8 -7.181808 0.884441 -2.311052  
 6 -1.556108 -0.740954 3.436539  
 8 -2.479324 -1.696866 2.977115  
 8 -0.280136 3.497277 4.364902  
 8 -1.396770 4.650410 2.099371  
 8 -2.037204 2.772760 0.016092  
 1 -5.817593 1.947107 -1.292851  
 1 -1.392783 -0.832860 4.507950  
 1 -6.409843 0.527939 -0.428597  
 1 -4.699635 0.493870 -2.948314  
 1 -5.991394 -1.684336 -1.439490  
 6 -6.261623 -2.726431 -3.697838  
 1 -3.113928 -2.004166 -2.319069  
 1 -3.599242 -3.988028 -1.100089  
 1 -4.495714 -1.731314 0.370900  
 1 -2.557146 -2.389203 1.250439  
 1 -2.019377 -0.253303 -0.547056  
 1 -1.161619 0.657327 1.159809  
 1 -2.948569 0.897845 3.624857  
 1 -0.614052 -0.939139 2.932269  
 1 -2.251073 3.068770 4.017246  
 1 -0.216656 4.405403 4.057792  
 1 -0.185888 3.013051 1.784994  
 1 -1.252820 4.953262 1.201751  
 1 -3.208992 2.839722 1.710279  
 1 -2.858309 2.668935 -0.466826  
 1 -3.208866 -1.783678 3.590989  
 1 -4.031600 0.512444 1.361222  
 1 -7.610128 0.029288 -2.290899  
 1 -6.631074 -2.612135 -4.711290

1 -5.664187 -3.630701 -3.624146  
 1 -7.109305 -2.803989 -3.015338  
**17me**  
 6 -2.848024 -4.488957 -2.206653  
 6 -1.601061 -5.260977 -2.555259  
 6 -1.770387 -6.742245 -2.236014  
 8 -2.115421 -6.842093 -0.876672  
 6 -3.349521 -6.243741 -0.552113  
 6 -3.228702 -4.750466 -0.768013  
 8 -1.363336 -5.075670 -3.979601  
 6 -0.021202 -4.574132 -4.429300  
 6 -0.225558 -4.271953 -5.907787  
 6 -1.248417 -3.150800 -6.033126  
 6 -0.957148 -1.981915 -5.078161  
 6 0.302406 -2.201215 -4.255462  
 8 0.342306 -3.508741 -3.681497  
 8 0.969746 -3.834858 -6.470011  
 6 0.410004 -1.235485 -3.092142  
 8 0.777553 0.048800 -3.521068  
 8 -0.753888 -0.769007 -5.751257  
 8 -2.485848 -3.788766 -5.709664  
 6 -0.506808 -7.570992 -2.383528  
 8 0.005729 -7.570122 -3.688042  
 8 -3.609173 -6.455383 0.778838  
 8 -4.436190 -4.078827 -0.555443  
 8 -2.600256 -3.135473 -2.454253  
 1 -1.261561 -2.804390 -7.063520  
 1 1.168988 -2.078878 -4.901513  
 1 -0.618036 -5.159751 -6.401459  
 1 -0.531408 -1.224303 -2.538359  
 1 1.191569 -1.589832 -2.425347  
 1 -3.212822 -3.163695 -5.661736  
 1 0.222788 0.278289 -4.270942  
 1 -0.740503 -4.837764 -2.043784  
 1 -3.673394 -4.844806 -2.834756  
 1 -2.566073 -7.152565 -2.867356  
 1 -2.443449 -4.377331 -0.105954  
 1 -4.134119 -6.664583 -1.189644  
 1 0.626169 -5.418583 -4.230626  
 1 -1.804713 -1.893732 -4.391227  
 6 -1.931582 -0.186114 -6.266938  
 1 1.520018 -4.584583 -6.698736  
 1 -3.378152 -2.638927 -2.189945  
 1 -4.654877 -4.120196 0.376370  
 1 -3.937466 -7.345096 0.912727  
 1 0.263503 -7.153926 -1.739036  
 1 -0.726896 -8.579226 -2.035243  
 1 -0.539189 -8.119990 -4.250628  
 1 -2.085917 -4.574136 -4.510744  
 1 -1.648414 0.766117 -6.700064  
 1 -2.375274 -0.805139 -7.047085  
 1 -2.661767 -0.023914 -5.473831  
**18me**  
 8 0.583672 1.575408 -1.658484

6 1.602583 0.723221 -1.561644  
 6 2.797329 0.848161 -2.510541  
 6 2.542482 1.823473 -3.645103  
 6 1.090853 1.714824 -4.052277  
 6 0.247567 2.224411 -2.896269  
 8 1.022312 -0.724383 -1.790852  
 6 0.575174 -1.467362 -0.612549  
 6 -0.580715 -2.298848 -1.109612  
 6 -1.176968 -3.049559 0.056043  
 6 -0.067769 -3.853285 0.728332  
 8 0.995335 -2.993826 1.080507  
 6 1.629817 -2.381568 -0.014341  
 8 -1.449503 -1.392178 -1.734483  
 6 2.869642 -1.693009 0.516481  
 8 3.648061 -1.184145 -0.539664  
 8 -0.505566 -4.495822 1.858801  
 8 -2.171885 -3.881987 -0.458392  
 8 3.908174 1.305584 -1.802886  
 8 3.371329 1.540325 -4.734009  
 8 0.750844 2.516784 -5.146089  
 6 -1.246935 2.066010 -3.107702  
 8 -1.741866 3.048903 -3.973217  
 1 -1.176521 3.059645 -4.750574  
 1 -1.474043 1.060262 -3.472361  
 1 -1.742507 2.194165 -2.149327  
 1 0.462744 3.282818 -2.754989  
 1 0.845673 0.668661 -4.279361  
 6 0.873922 1.893082 -6.413535  
 1 2.723932 2.837319 -3.279656  
 1 4.277799 1.727920 -4.487283  
 1 2.978988 -0.134619 -2.944359  
 1 4.209589 0.589201 -1.234318  
 1 1.920926 0.654437 -0.528512  
 1 0.239636 -0.734723 0.119583  
 1 1.928215 -3.128363 -0.756342  
 1 3.427058 -2.407316 1.118125  
 1 2.599305 -0.855700 1.155927  
 1 4.137425 -1.895545 -0.954510  
 1 0.290175 -4.627910 0.047293  
 1 -0.826616 -3.850232 2.493188  
 1 -1.585004 -2.334780 0.776356  
 1 -2.635708 -4.305156 0.265247  
 1 -0.212854 -3.025672 -1.839323  
 1 0.204027 -0.647896 -2.332603  
 1 -2.086137 -1.864696 -2.273758  
 1 0.525910 2.614946 -7.143775  
 1 1.906545 1.629463 -6.617896  
 1 0.247303 1.002422 -6.460439  
**18me+H<sub>2</sub>O**  
 6 0.478418 -1.474143 3.679609  
 6 1.394635 -0.309395 4.013534  
 6 2.659405 -0.836296 4.644143  
 6 3.351480 -1.740541 3.653415  
 6 2.368803 -2.824916 3.221734

8 1.188195 -2.227969 2.728554  
8 0.850671 0.620301 5.005071  
6 0.067703 1.870233 4.467588  
8 0.958803 2.850075 4.315814  
6 1.082947 3.923123 5.262738  
6 0.411185 3.587294 6.580688  
6 -1.041287 3.279598 6.295856  
6 -1.127285 2.045736 5.409372  
8 -2.299821 2.139199 4.650811  
8 -1.728479 3.074590 7.495688  
8 0.582940 4.711052 7.394349  
6 0.682366 4.440160 8.781843  
6 2.560272 4.249155 5.390652  
8 2.750509 5.574544 5.800549  
8 3.392353 0.299671 5.015837  
8 4.461840 -2.284988 4.299525  
8 2.889124 -3.637422 2.246219  
6 -0.851113 -1.109170 3.052316  
8 -1.693192 -0.485928 3.992961  
8 -2.920905 4.337871 2.867961  
1 2.252439 5.696313 6.612310  
1 3.050945 3.547904 6.069657  
1 3.016276 4.144715 4.410094  
1 0.584583 4.787436 4.824364  
1 0.896738 2.720364 7.045031  
1 -1.463269 4.129235 5.754681  
1 -2.670756 3.100143 7.327264  
1 -1.158593 1.172564 6.058545  
1 -2.475098 1.269753 4.269559  
1 -0.249092 1.504832 3.497797  
1 1.621788 0.272326 3.121785  
1 0.294761 -2.063880 4.582938  
1 -1.300548 -2.015161 2.652409  
1 -0.709991 -0.414061 2.227745  
1 -2.077572 -1.144564 4.572684  
1 2.134512 -3.468502 4.071844  
1 3.105166 -3.113338 1.470976  
1 3.644211 -1.155853 2.776515  
1 4.978408 -2.788821 3.669302  
1 2.402526 -1.421134 5.531881  
1 1.650591 0.933942 5.485406  
1 4.088686 0.055876 5.628004  
1 -2.739632 3.607681 3.469374  
1 -3.710192 4.757812 3.205311  
1 0.850079 5.394106 9.269031  
1 -0.232259 3.990853 9.155880  
1 1.527387 3.780856 8.980584

**19me**  
6 -0.651343 0.690908 1.224422  
6 -1.863970 1.238032 0.515206  
8 -1.635509 2.103615 -0.476209  
6 -0.294837 2.251364 -0.984647  
6 0.730731 2.454447 0.127795  
6 0.290695 1.853441 1.458744

8 -2.598477 -0.008214 -0.014936  
6 -4.049552 -0.191530 0.032110  
6 -4.674343 0.295655 -1.257153  
6 -6.151091 -0.044534 -1.224065  
6 -6.322208 -1.519011 -0.923583  
8 -5.745947 -1.794657 0.322060  
6 -4.350096 -1.656714 0.326415  
8 -4.556785 1.681754 -1.391936  
6 -3.888452 -2.119706 1.698856  
8 -2.487331 -2.147452 1.821100  
8 -7.652361 -1.862741 -0.809552  
8 -6.769542 0.202774 -2.451376  
6 0.021130 1.146838 -1.984059  
8 1.177826 1.473951 -2.702824  
8 0.950317 3.834408 0.216762  
8 1.416314 1.410955 2.160397  
8 -0.997393 0.138687 2.449046  
1 -0.805614 1.092054 -2.688745  
1 -4.319423 -3.101405 1.881118  
1 0.124751 0.171631 -1.507556  
1 -0.339323 3.182696 -1.538841  
1 1.661620 1.953764 -0.158928  
6 2.020091 4.199220 1.057679  
1 -0.240491 2.625518 2.024727  
1 1.107912 0.950095 2.944409  
1 -0.141823 -0.043734 0.595482  
1 -1.429929 -0.718393 2.312301  
1 -2.613676 1.618257 1.200048  
1 -4.366602 0.430905 0.864211  
1 -3.901885 -2.288835 -0.448025  
1 -4.263855 -1.438133 2.457465  
1 -5.825001 -2.122194 -1.693570  
1 -8.135896 -1.395331 -1.495581  
1 -6.632034 0.518620 -0.420302  
1 -6.764425 1.146182 -2.619825  
1 -4.224170 -0.223686 -2.107343  
1 -3.715481 1.914523 -1.787481  
1 -2.131861 -2.952381 1.444346  
1 -2.142100 -0.507411 -0.706876  
1 1.937337 1.028246 -2.331239  
1 2.169582 5.265465 0.928140  
1 1.799428 3.990435 2.103601  
1 2.931328 3.667746 0.777970

**TS(18me-21me) – 1 imaginary frequency**  
6 1.867484 1.491198 -2.191202  
6 0.654918 1.129577 -1.362053  
8 -0.523600 1.533757 -1.658633  
6 -0.875560 2.170910 -2.914568  
6 0.265968 2.170820 -3.916917  
6 1.534291 2.574559 -3.201818  
6 -2.155793 1.530919 -3.420379  
8 -2.852744 2.420689 -4.245881  
8 -0.143566 3.072734 -4.905388

8 2.579745 2.705034 -4.115790  
8 2.867375 1.978122 -1.356924  
8 0.571581 -0.764417 -1.579876  
6 0.381072 -1.555826 -0.398141  
6 1.660748 -2.210016 0.100099  
8 1.311129 -2.959844 1.239723  
6 0.435258 -4.031596 0.982967  
6 -0.889565 -3.487869 0.466095  
6 -0.615454 -2.637116 -0.748906  
6 2.752266 -1.262381 0.553337  
8 3.315468 -0.560776 -0.527761  
8 -1.747214 -1.978157 -1.248944  
8 -1.745902 -4.516192 0.062129  
8 0.286180 -4.765176 2.135711  
1 -2.240734 2.754819 -4.906340  
1 -1.936469 0.593546 -3.936183  
1 -2.793103 1.310395 -2.568708  
1 -1.093542 3.200659 -2.639003  
1 0.397357 1.178847 -4.361257  
6 0.372147 2.819692 -6.202331  
1 1.364265 3.516861 -2.673775  
1 3.368507 2.961467 -3.634099  
1 2.187839 0.600759 -2.732042  
1 3.297266 1.218365 -0.939649  
1 0.807546 1.009266 -0.297768  
1 -0.031999 -0.918919 0.386370  
1 2.057197 -2.865019 -0.682833  
1 3.505426 -1.841794 1.083284  
1 2.352444 -0.524148 1.244437  
1 3.889630 -1.137009 -1.033049  
1 0.872663 -4.704130 0.241811  
1 -0.080140 -4.207071 2.825885  
1 -1.348266 -2.870437 1.244149  
1 -2.004997 -5.029675 0.828275  
1 -0.183988 -3.276720 -1.525564  
1 -0.237778 -0.900960 -2.099582  
1 -2.340100 -2.619581 -1.643280  
1 -0.093732 3.543587 -6.861279  
1 1.450340 2.940807 -6.222941  
1 0.107576 1.813354 -6.526875

**TS((18me+H<sub>2</sub>O)-23me) – 1 imaginary frequency**  
8 1.157353 2.972216 4.486367  
6 0.179265 2.136452 4.481621  
6 -1.011737 2.247157 5.418371  
6 -1.004271 3.530805 6.230191  
6 0.414422 3.812534 6.668535  
6 1.251038 4.063854 5.428580  
8 -2.196528 2.200706 4.681360  
8 -1.831293 3.393773 7.348317  
8 0.535954 4.978193 7.432576  
6 2.723699 4.292343 5.712102  
8 2.954337 5.617334 6.100628  
8 0.961056 0.561252 5.074440

6	1.435594	-0.340178	4.061352	6	-1.827913	1.554367	0.579457	6	0.037346	-2.172135	4.636421
6	2.737802	-0.917963	4.563451	6	-0.720676	0.848581	1.288412	6	-0.428760	-1.998970	3.213321
6	3.308389	-1.848095	3.521230	6	0.345315	1.904419	1.558763	6	2.709949	-0.041377	2.118260
6	2.262529	-2.901383	3.182315	6	0.851713	2.479465	0.239784	8	2.756076	-0.001733	0.708205
8	1.073276	-2.266716	2.774080	6	-0.195709	2.449060	-0.871985	8	-1.791281	-1.667826	3.128775
6	0.469198	-1.477393	3.770836	8	-1.550933	2.384343	-0.351675	8	-0.638843	-3.279104	5.166118
8	3.561343	0.176411	4.860580	8	-1.146471	0.305232	2.484104	8	2.047166	-2.489858	5.920490
6	-0.879008	-1.063087	3.217250	6	-0.005966	1.366001	-1.915045	1	-1.908157	2.419531	-5.241020
8	-1.666389	-0.426758	4.194764	8	1.215769	1.655236	-2.531470	1	-1.423645	0.286230	-4.353816
8	2.678284	-3.744940	2.180167	8	1.249075	3.815186	0.359014	1	-2.610934	0.722039	-3.121353
8	4.458155	-2.423298	4.069202	6	2.391764	4.013555	1.160273	1	-1.250541	2.827078	-2.701361
8	-1.146904	4.268922	3.136145	8	1.409503	1.317584	2.244439	1	0.849506	1.153093	-4.164999
1	2.374218	5.804587	6.842588	1	-0.837094	1.413446	-2.618908	6	0.911604	2.795795	-6.016084
1	3.078916	3.585799	6.465148	1	-4.300489	-3.022236	1.963028	1	1.101236	3.629319	-2.408319
1	3.280959	4.121380	4.795373	1	0.013377	0.372282	-1.462411	1	3.299003	3.392673	-2.949643
1	0.854731	4.927689	4.897109	1	-0.169700	3.411462	-1.369474	1	2.277641	0.846648	-2.177043
1	0.813205	2.960208	7.229885	1	1.696743	1.863902	-0.084349	1	2.826021	1.591517	-0.137474
6	0.436873	4.792302	8.834257	1	-0.095902	2.716010	2.144884	1	0.492659	0.547994	-0.263085
1	-1.339709	4.354394	5.596894	1	1.054913	0.898145	3.032244	1	0.123321	0.054377	3.072096
1	-2.740963	3.337837	7.052663	1	-0.279665	0.092420	0.636368	1	2.058332	-2.082953	2.104119
1	-0.953843	1.410531	6.113682	1	-1.579530	-0.549746	2.316817	1	3.706660	-0.175492	2.534195
1	-2.332446	1.285729	4.398592	1	-2.737306	1.782394	1.117923	1	2.330808	0.922877	2.446629
1	-0.017825	1.711041	3.506140	1	-4.435334	0.430038	0.733901	1	3.295984	-0.721264	0.379567
1	1.614613	0.229495	3.147877	1	-3.870354	-2.339967	-0.404326	1	1.793372	-3.310709	4.130779
1	0.315816	-2.063688	4.683136	1	-4.309671	-1.325878	2.436541	1	1.862200	-1.681232	6.404010
1	-1.373815	-1.949729	2.826508	1	-5.826530	-2.298748	-1.664439	1	-0.190790	-1.263528	5.202636
1	-0.754094	-0.361529	2.395415	1	-8.163114	-1.654309	-1.463703	1	-0.405853	-3.375911	6.090235
1	-2.002147	-1.072443	4.817398	1	-6.714660	0.358825	-0.485993	1	-0.236921	-2.928859	2.667680
1	2.071439	-3.527757	4.056285	1	-6.868022	0.885231	-2.728406	1	-1.016110	-0.849890	1.183844
1	2.851875	-3.236562	1.384106	1	-4.322012	-0.382145	-2.191327	1	-2.308261	-2.400840	3.465224
1	3.540317	-1.276402	2.617660	1	-3.930408	1.763014	-2.101880	1	0.472911	3.451202	-6.759557
1	4.890343	-2.959409	3.403149	1	-2.094733	-2.773611	1.476575	1	1.942254	3.081154	-5.831949
1	2.542429	-1.495072	5.472516	1	-2.264713	-0.422337	-0.899533	1	0.869369	1.766443	-6.370951
1	1.763366	0.851148	5.542284	1	1.421514	0.971277	-3.168015		<b>22me</b>		
1	4.325803	-0.124219	5.354180	1	2.669276	5.056206	1.052657	6	-6.217365	-0.129567	0.160959
1	-1.895307	3.681070	3.268331	1	2.189214	3.799355	2.208356	6	-5.329554	0.996287	-0.364897
1	-1.077203	4.407989	2.192833	1	3.214794	3.381735	0.822811	6	-5.933293	1.722014	-1.551896
1	0.608229	5.763699	9.284267		<b>21me</b>			6	-7.395548	2.026094	-1.312705
1	-0.547576	4.426746	9.108911	6	1.746846	1.702566	-1.731560	6	-8.097964	0.738563	-0.932993
1	1.199855	4.095164	9.180321	6	0.495595	1.099717	-1.206492	8	-7.560076	0.282205	0.269327
	<b>TS(19me-22me) - 1 imaginary</b>			8	-0.601484	1.133843	-1.794010	8	-4.042865	0.514789	-0.682397
	<b>frequency</b>			6	-0.827876	1.882532	-3.036350	8	-5.175911	2.893370	-1.743791
6	-4.347106	-1.673966	0.324118	6	0.474540	2.108634	-3.782289	8	-8.029223	2.526047	-2.462526
6	-4.080026	-0.220614	-0.063155	6	1.499082	2.708622	-2.841463	8	-9.444870	0.943213	-0.702909
6	-4.770648	0.164576	-1.357475	6	-1.881202	1.120528	-3.820071	6	-5.850424	-0.545622	1.577861
6	-6.230286	-0.219996	-1.276977	8	-2.558363	1.986861	-4.682397	8	-4.467118	-0.703568	1.792938
6	-6.338239	-1.684251	-0.912360	8	0.126530	2.946340	-4.842672	6	-2.294910	2.507102	-0.251551
8	-5.738614	-1.882240	0.333650	8	2.680567	2.954960	-3.537041	6	-1.945178	1.625516	0.883472
8	-2.675543	0.027627	-0.153097	8	2.478864	2.292458	-0.713659	6	-0.643614	2.127452	1.498912
8	-4.703386	1.547055	-1.581450	8	-0.057803	-0.776388	1.197952	6	0.437385	2.102930	0.440697
8	-6.886978	-0.045307	-2.499316	6	0.334497	-0.880295	2.543348	6	0.014958	2.812330	-0.845115
8	-7.653598	-2.078993	-0.768943	6	1.825178	-1.157017	2.642143	8	-1.431461	3.009992	-0.996662
6	-3.895539	-2.039612	1.729280	8	2.163654	-1.292195	4.006178	8	-2.952969	1.594526	1.826798
8	-2.499873	-2.017954	1.902069	6	1.542372	-2.378896	4.643249	6	0.450971	2.108899	-2.113968

8	1.838682	1.967825	-2.004517	1	1.171444	6.808010	7.137334	1	-3.380316	3.246095	-2.242306
8	1.585783	2.762044	0.882129	1	2.848569	5.181404	6.754817	1	-3.756965	3.106312	-0.525525
6	2.635714	1.904624	1.276990	1	2.832187	5.822721	5.111267	1	-1.342587	3.574058	-0.010371
8	-0.252724	1.289555	2.539021	1	0.335244	5.402363	5.073058	1	-1.050635	3.077361	-2.998052
1	0.165566	2.711339	-2.975699	1	1.061086	3.583360	7.410374	1	-0.031849	5.170766	-2.814126
1	-6.388110	-1.455815	1.837843	6	-0.090073	5.022182	9.055712	1	1.042846	3.451977	-0.837143
1	-0.046614	1.140086	-2.183387	1	-1.491995	4.038037	5.828678	1	2.401900	3.063616	-2.633225
1	0.393813	3.828776	-0.819502	1	-2.263637	2.352692	7.136689	1	0.287834	1.022549	-2.485687
1	0.666894	1.058374	0.215163	1	0.201742	1.525165	6.016750	1	1.844308	0.086802	-1.041364
1	-0.782218	3.151012	1.855555	1	-1.315392	0.801472	4.622594	1	-0.123134	1.596121	0.477872
1	-0.949923	1.289019	3.198464	1	1.204136	2.038605	3.891802	1	-0.266601	-0.147810	1.636937
1	-1.762447	0.637933	0.444420	1	2.103328	-0.873148	3.044166	1	-0.630181	-2.768787	0.121527
1	-3.455059	0.761094	1.764976	1	0.592200	-2.658920	4.985716	1	1.833947	-1.464763	1.352124
1	-3.315163	2.799497	-0.483964	1	-1.173110	-2.407395	3.133527	1	1.690506	-3.185617	0.952620
1	-5.183766	1.727561	0.433257	1	-0.332179	-0.928245	2.670948	1	2.530099	-2.267006	-0.868554
1	-6.142308	-0.981351	-0.524761	1	-1.554728	-1.430295	5.160647	1	-2.173302	-3.531237	1.597847
1	-6.172784	0.244794	2.250384	1	1.967764	-4.507193	4.433417	1	-2.671639	-3.495302	3.981914
1	-7.949352	-0.020982	-1.712460	1	2.405412	-4.762008	1.681527	1	-1.961082	-1.036464	3.319497
1	-9.749589	1.578241	-1.356724	1	3.602986	-2.814220	2.499715	1	-4.238842	-1.013573	2.859204
1	-7.500999	2.720025	-0.477022	1	4.695901	-4.649585	3.369502	1	-2.752969	-1.396382	0.410206
1	-7.930828	3.476687	-2.500170	1	3.031744	-2.457714	5.456938	1	-2.775152	0.903422	0.557645
1	-5.866062	1.080350	-2.435487	1	2.560232	0.124040	5.188118	1	-0.765291	-1.329396	-2.025895
1	-5.164135	3.129079	-2.670772	1	5.027527	-1.579432	4.806014	1	-0.078208	-2.043368	-3.384385
1	-4.118886	-1.379269	1.209688	1	-1.066241	2.829045	3.441464	1	0.582182	-2.103080	-1.793028
1	-4.070143	0.015345	-1.500474	1	0.079416	3.486570	2.489829	8	0.170842	-2.065108	-4.779379
1	2.161056	1.461331	-2.749231	1	-0.356279	5.954694	9.541019	1	-0.462898	-2.552920	-5.308888
1	3.460764	2.542483	1.574569	1	-0.829289	4.261992	9.288913	1	0.293482	-1.212814	-5.201779
1	2.336987	1.281636	2.117640	1	0.890858	4.701224	9.406516				
1	2.947108	1.277614	0.441809								
	<b>23me</b>				<b>1+H<sub>2</sub>O+H<sub>3</sub>O<sup>+</sup></b>				<b>1- H<sub>2</sub>O at O1 (frozen)</b>		
8	1.549113	3.756247	4.819792	6	0.602939	1.490567	-1.548301	6	-0.813135	-1.844774	1.392074
6	0.678838	2.827290	4.416195	6	-0.435231	1.185725	-0.487538	6	0.000857	-0.759488	0.692842
6	-0.309850	2.295613	5.443558	8	-1.684192	1.717803	-0.851226	6	1.064721	-1.378756	-0.193987
6	-0.815087	3.377839	6.379594	6	-1.668967	3.132514	-0.957269	6	0.428454	-2.384346	-1.120762
6	0.350177	4.211113	6.864011	6	-0.700428	3.520547	-2.060894	6	-0.354664	-3.386206	-0.303594
6	1.044994	4.806243	5.649788	6	0.677038	2.984398	-1.756493	8	-1.343196	-2.711899	0.416888
8	-1.409893	1.770269	4.745014	8	-0.563414	-0.193470	-0.396529	8	0.606646	0.036946	1.698573
8	-1.480983	2.798769	7.464268	6	-0.771971	-0.761399	0.888862	6	0.764800	1.391717	1.482680
8	-0.055941	5.287306	7.665132	6	-2.250916	-0.846332	1.212865	6	0.613048	2.087054	2.819834
6	2.230906	5.681249	6.005065	6	-2.431274	-1.600151	2.508871	6	0.872642	3.564106	2.642745
8	1.816493	6.947672	6.438301	6	-1.737965	-2.940955	2.414755	6	2.215674	3.768610	1.985170
8	1.703252	-0.248453	4.963255	8	-0.378379	-2.734940	2.157138	6	2.283877	2.996809	0.678574
6	1.947325	-1.283610	4.047321	6	-0.155413	-2.155369	0.895713	8	2.059591	1.622313	0.963740
6	3.182524	-2.056099	4.449417	8	-2.836623	0.413437	1.385273	8	-0.679536	1.926527	3.317432
6	3.408323	-3.207446	3.502658	6	1.346642	-2.186861	0.700679	6	3.635938	3.109400	0.000142
6	2.152130	-4.060783	3.453042	8	1.671780	-1.893144	-0.658871	8	3.827210	4.375277	-0.569542
8	1.061308	-3.263462	3.071333	8	-1.798018	-3.633743	3.607665	8	2.443321	5.125906	1.703238
6	0.762626	-2.233204	3.989902	8	-3.778918	-1.852139	2.795249	8	0.903320	4.248439	3.867166
8	4.250327	-1.143177	4.454951	6	-3.090504	3.578317	-1.242448	8	1.713120	-0.430897	-0.995157
6	-0.528942	-1.608093	3.495387	8	-3.241419	4.964382	-1.095363	8	1.377234	-3.103286	-1.859939
8	-1.186308	-0.856258	4.489303	8	-0.688132	4.922034	-2.160090	8	-1.019299	-4.293709	-1.106265
8	2.268298	-5.109189	2.566095	8	1.503596	3.327219	-2.836596	6	-2.014924	-1.342301	2.165497
8	4.506050	-3.935913	3.979801	8	1.865868	1.044026	-1.152411	8	-1.605622	-0.787120	3.405559
8	-0.275664	3.436072	3.387877	8	-0.249547	-2.082919	-2.353690	1	3.671675	5.032141	0.114657
				1	-2.572078	5.392053	-1.636340	1	4.426096	2.871792	0.717961
								1	3.685745	2.383550	-0.806909

1 1.513928 3.361712 -0.007384  
1 2.993441 3.385429 2.653721  
1 2.336747 5.623560 2.516428  
1 0.095457 3.983003 1.995684  
1 0.037331 4.191388 4.272933  
1 1.361149 1.670863 3.502973  
1 -0.881400 0.981787 3.377347  
1 0.019661 1.754518 0.768104  
1 -0.664770 -0.140434 0.088338  
1 -0.159273 -2.401323 2.073522  
1 -2.557731 -0.599933 1.581161  
1 -2.665539 -2.196763 2.336877  
1 -2.390070 -0.648170 3.939121  
1 0.314237 -3.903447 0.396985  
1 -0.437507 -4.515667 -1.837459  
1 -0.272868 -1.870970 -1.784407  
1 1.890406 -2.484340 -2.381717  
1 1.786623 -1.899245 0.444877  
1 2.133812 0.226134 -0.430094  
8 2.412065 -1.424462 3.454950  
1 1.833335 -1.691975 4.183519  
1 1.823763 -0.966497 2.847085

**1- H<sub>2</sub>O at O1/O6'**

6 -0.651509 -1.863548 1.444838  
6 0.080137 -0.747931 0.708755  
6 1.110016 -1.331821 -0.238868  
6 0.443333 -2.342160 -1.139189  
6 -0.270983 -3.372852 -0.294065  
8 -1.227466 -2.733563 0.497462  
8 0.701909 0.065456 1.683740  
6 0.812791 1.419576 1.449415  
6 0.697003 2.118342 2.788599  
6 0.944795 3.595714 2.607054  
6 2.266410 3.806504 1.910630  
6 2.290761 3.043979 0.596990  
8 2.075395 1.671351 0.873319  
8 -0.580979 1.953164 3.325607  
6 3.621771 3.157784 -0.121095  
8 3.808053 4.431250 -0.678492  
8 2.482402 5.167751 1.632546  
8 1.005013 4.278759 3.831985  
8 1.694068 -0.362960 -1.064977  
8 1.362234 -3.031595 -1.942797  
8 -0.964662 -4.280427 -1.073017  
6 -1.799469 -1.396503 2.316136  
8 -1.298780 -0.813680 3.507961  
1 3.667929 5.079123 0.017453  
1 4.428598 2.900184 0.569475  
1 3.640240 2.444253 -0.940570  
1 1.501070 3.422272 -0.060020  
1 3.066509 3.419213 2.548597  
1 2.398666 5.658327 2.452581  
1 0.148030 4.012763 1.982701  
1 0.156775 4.195783 4.269698

1 1.463965 1.702951 3.449757  
1 -0.768397 1.007247 3.414035  
1 0.025640 1.760688 0.768063  
1 -0.643031 -0.156774 0.142082  
1 0.064493 -2.407676 2.070964  
1 -2.419020 -0.680011 1.776906  
1 -2.401604 -2.270677 2.551051  
1 -1.967272 -0.880345 4.190221  
1 0.449348 -3.888698 0.354571  
1 -0.419037 -4.484030 -1.836624  
1 -0.305785 -1.836549 -1.755051  
1 1.835859 -2.393708 -2.478964  
1 1.876380 -1.839446 0.356513  
1 2.103362 0.313248 -0.512218  
8 1.486114 -1.271326 4.243518  
1 0.536213 -1.174234 4.118793  
1 1.851727 -0.900914 3.440055

**1- H<sub>2</sub>O at O3'**

6 -0.832354 -1.809379 1.398342  
6 0.000338 -0.745546 0.715034  
8 1.000115 -1.348170 -0.080043  
6 1.926535 -2.100903 0.681576  
6 1.177904 -3.243162 1.347858  
6 0.071232 -2.698741 2.218557  
8 -0.841605 -0.031367 -0.104812  
6 -0.570285 1.333904 -0.333263  
6 0.233855 1.512419 -1.608927  
6 0.337553 2.981280 -1.943027  
6 -1.051117 3.582135 -1.981593  
8 -1.659820 3.413955 -0.738929  
6 -1.905249 2.058307 -0.440762  
8 1.544241 1.014042 -1.484168  
6 -2.718556 2.056660 0.836746  
8 -3.317200 0.790196 1.020742  
8 -1.007319 4.945513 -2.208017  
8 0.916754 3.210580 -3.198938  
6 3.006683 -2.579831 -0.268654  
8 4.113179 -3.102878 0.415745  
8 2.096777 -3.992714 2.103262  
8 -0.612636 -3.799212 2.759722  
8 -1.772076 -1.230528 2.252075  
1 3.791699 -3.773646 1.023632  
1 2.581744 -3.309886 -0.961999  
1 3.362085 -1.732430 -0.848982  
1 2.385422 -1.466885 1.447308  
1 0.734686 -3.865780 0.564939  
1 1.610420 -4.667543 2.581017  
1 0.517198 -2.102116 3.020909  
1 -1.290887 -3.474667 3.353553  
1 -1.314257 -2.405785 0.617696  
1 -2.306555 -0.590914 1.754209  
1 0.474061 -0.091368 1.456080  
1 -0.007561 1.749898 0.506890  
1 -2.502301 1.597070 -1.234188

1 -2.084587 2.311396 1.687357  
1 -3.480244 2.826325 0.731818  
1 -4.098697 0.896608 1.562394  
1 -1.652369 3.079522 -2.751085  
1 -0.324834 5.107902 -2.864068  
1 0.900420 3.491705 -1.155916  
1 1.817208 2.883605 -3.191048  
1 -0.284022 0.997911 -2.423198  
1 1.500454 0.079464 -1.239224  
8 2.821521 2.268115 0.740067  
1 3.596711 2.767770 0.489959  
1 2.502604 1.852610 -0.070843

**1- H<sub>2</sub>O at O5**

6 -0.808628 -1.816115 1.414220  
6 0.002010 -0.741864 0.698174  
6 1.061111 -1.374830 -0.183735  
6 0.418513 -2.390716 -1.094099  
6 -0.365018 -3.380645 -0.262653  
8 -1.348362 -2.697534 0.454008  
8 0.602840 0.065557 1.690143  
6 0.749528 1.410438 1.456792  
6 0.606203 2.118334 2.788356  
6 0.888483 3.590385 2.610829  
6 2.238456 3.772235 1.961710  
6 2.294157 3.007782 0.650523  
8 2.047243 1.636301 0.928166  
8 -0.688479 1.975859 3.285927  
6 3.648400 3.101151 -0.026385  
8 3.861687 4.367544 -0.589014  
8 2.495570 5.127146 1.690386  
8 0.920795 4.275557 3.835600  
8 1.709541 -0.440450 -1.003142  
8 1.361876 -3.121585 -1.830343  
8 -1.034212 -4.296112 -1.054496  
6 -1.996738 -1.292430 2.194845  
8 -1.559128 -0.704767 3.402925  
1 3.717454 5.022186 0.099716  
1 4.431234 2.843969 0.691793  
1 3.685510 2.379707 -0.838254  
1 1.529657 3.388068 -0.033238  
1 3.007048 3.366266 2.627419  
1 2.391056 5.621343 2.505890  
1 0.122121 4.021561 1.958710  
1 0.057891 4.206479 4.246318  
1 1.347030 1.690787 3.471949  
1 -0.903792 1.031456 3.352438  
1 0.006415 1.772592 0.738855  
1 -0.667737 -0.136830 0.082175  
1 -0.151957 -2.359587 2.101482  
1 -2.553861 -0.571834 1.594264  
1 -2.643486 -2.142991 2.399310  
1 -2.278957 -0.726420 4.032814  
1 0.305963 -3.892896 0.439778  
1 -0.452137 -4.531009 -1.781301

1 -0.284196 -1.883803 -1.761427  
1 1.881214 -2.507899 -2.352208  
1 1.784476 -1.885038 0.460600  
1 2.112748 0.236526 -0.448862  
8 4.070667 0.789281 2.883732  
1 4.652035 0.071764 2.636791  
1 3.441310 0.874807 2.162005  
**1- 2H<sub>2</sub>O at O5, O6'**  
6 -0.571212 -1.857698 1.442050  
6 0.083703 -0.715861 0.677011  
6 1.087748 -1.259901 -0.320285  
6 0.415257 -2.292101 -1.191283  
6 -0.220027 -3.349951 -0.316179  
8 -1.159990 -2.748902 0.523419  
8 0.713369 0.109093 1.634211  
6 0.821937 1.457555 1.386207  
6 0.683350 2.167949 2.717455  
6 0.945050 3.642595 2.537351  
6 2.287032 3.837389 1.875669  
6 2.338571 3.074042 0.563767  
8 2.104138 1.700849 0.834829  
8 -0.605954 2.008883 3.228296  
6 3.686614 3.178611 -0.123796  
8 3.886085 4.446618 -0.688157  
8 2.527897 5.194580 1.601308  
8 0.981033 4.328459 3.761452  
8 1.595429 -0.267793 -1.170639  
8 1.319409 -2.946329 -2.039504  
8 -0.917319 -4.280523 -1.064262  
6 -1.691854 -1.427471 2.365896  
8 -1.158606 -0.787231 3.514599  
1 3.740308 5.100319 0.001095  
1 4.477901 2.927296 0.586803  
1 3.722849 2.457433 -0.935992  
1 1.566987 3.453679 -0.112832  
1 3.064647 3.440802 2.536131  
1 2.425017 5.688601 2.417124  
1 0.168377 4.065101 1.891732  
1 0.123938 4.247033 4.181992  
1 1.434055 1.747532 3.394535  
1 -0.776427 1.064398 3.356049  
1 0.055557 1.794203 0.680315  
1 -0.685472 -0.149119 0.146755  
1 0.193779 -2.374212 2.032484  
1 -2.374850 -0.756531 1.845173  
1 -2.235950 -2.323043 2.654694  
1 -1.765624 -0.906318 4.245583  
1 0.549795 -3.840417 0.294192  
1 -0.397329 -4.470669 -1.848923  
1 -0.380378 -1.813388 -1.769231  
1 1.749878 -2.289285 -2.588874  
1 1.900341 -1.740075 0.234476  
1 2.060228 0.388621 -0.640308  
8 3.697481 0.061462 2.873193

1 2.952403 -0.345868 3.336267  
1 3.308329 0.518355 2.125490  
8 1.604254 -1.182771 4.330918  
1 1.596113 -1.137885 5.285773  
1 0.696469 -1.023351 4.045972  
**1- 3H<sub>2</sub>O at O1, O5, O6'**  
6 -0.813135 -1.844774 1.392074  
6 0.000857 -0.759488 0.692842  
6 1.064721 -1.378756 -0.193987  
6 0.428454 -2.384346 -1.120762  
6 -0.354664 -3.386206 -0.303594  
8 -1.343196 -2.711899 0.416888  
8 0.606646 0.036946 1.698573  
6 0.764800 1.391717 1.482680  
6 0.613048 2.087054 2.819834  
6 0.872642 3.564106 2.642745  
6 2.215674 3.768610 1.985170  
6 2.283877 2.996809 0.678574  
8 2.059591 1.622313 0.963740  
8 -0.679536 1.926527 3.317432  
6 3.635938 3.109400 0.000142  
8 3.827210 4.375277 -0.569542  
8 2.443321 5.125906 1.703238  
8 0.903320 4.248439 3.867166  
8 1.713120 -0.430897 -0.995157  
8 1.377234 -3.103286 -1.859939  
8 -1.019299 -4.293709 -1.106265  
6 -2.014924 -1.342301 2.165497  
8 -1.605622 -0.787120 3.405559  
1 3.671675 5.032141 0.114657  
1 4.426096 2.871792 0.717961  
1 3.685745 2.383550 -0.806909  
1 1.513928 3.361712 -0.007384  
1 2.993441 3.385429 2.653721  
1 2.336747 5.623560 2.516428  
1 0.095457 3.983003 1.995684  
1 0.037331 4.191388 4.272933  
1 1.361149 1.670863 3.502973  
1 -0.881400 0.981787 3.377347  
1 0.019661 1.754518 0.768104  
1 -0.664770 -0.140434 0.088338  
1 -0.159273 -2.401323 2.073522  
1 -2.557731 -0.599933 1.581161  
1 -2.665539 -2.196763 2.336877  
1 -2.390070 -0.648170 3.939121  
1 0.314237 -3.903447 0.396985  
1 -0.437507 -4.515667 -1.837459  
1 -0.272868 -1.870970 -1.784407  
1 1.890406 -2.484340 -2.381717  
1 1.786623 -1.899245 0.444877  
1 2.133812 0.226134 -0.430094  
8 4.224881 0.701637 3.050166  
1 3.733585 -0.062545 3.380398  
1 3.733524 0.970178 2.272221

8 2.412065 -1.424462 3.454950  
1 1.833335 -1.691975 4.183519  
1 1.823763 -0.966497 2.847085  
8 0.290386 -2.121936 5.151122  
1 0.207021 -1.786350 6.042650  
1 -0.408624 -1.697669 4.637977  
 **$\alpha$ -glucose+  $\beta$ -glucose+H<sub>3</sub>O<sup>+</sup>**  
6 -2.503334 -2.030059 0.289797  
6 -1.314824 -1.804956 1.193695  
6 -1.343601 -2.824969 2.331650  
8 -2.573409 -2.762182 3.006284  
6 -3.665606 -3.108873 2.189290  
6 -3.782537 -2.076621 1.089698  
8 -0.131751 -1.966399 0.426839  
6 -0.286020 -2.555508 3.379224  
8 0.972287 -2.603640 2.737543  
8 -4.817607 -3.054458 2.935579  
8 -4.801501 -2.373686 0.176366  
8 -2.589998 -0.986643 -0.664767  
8 -0.237819 -0.504648 -1.614935  
8 0.738401 1.843612 -1.583229  
6 0.088998 2.914709 -2.249409  
8 -1.091065 3.203550 -1.599444  
6 -0.957044 3.703585 -0.278800  
6 -0.154674 4.988302 -0.325064  
6 1.204323 4.704423 -0.911713  
6 1.050927 4.097867 -2.287893  
6 -2.362733 3.900695 0.252289  
8 -2.373581 4.115316 1.638944  
8 2.327337 3.654106 -2.685449  
8 1.908841 5.916899 -0.953649  
8 -0.047786 5.488241 0.984170  
1 -1.771235 4.839614 1.827354  
1 -2.842836 4.723408 -0.283566  
1 -2.933708 2.996349 0.060563  
1 -0.440088 2.973543 0.347370  
1 -0.678138 5.706755 -0.963546  
1 0.530947 6.253076 0.967110  
1 1.718743 3.989004 -0.263676  
1 2.813565 5.739876 -1.213872  
1 0.660395 4.850030 -2.971856  
1 2.399134 3.654609 -3.640277  
1 -1.358416 -0.795547 1.608856  
1 -1.187471 -3.821563 1.903963  
1 -0.462706 -1.575144 3.821062  
1 -0.356432 -3.312275 4.158552  
1 1.651078 -2.266702 3.321279  
1 -3.503404 -4.107603 1.770615  
1 -4.900439 -3.844454 3.470414  
1 -3.950265 -1.106858 1.564880  
1 -5.648712 -2.280528 0.613656  
1 -2.372146 -2.983882 -0.227660  
1 -3.418301 -1.093137 -1.141344  
1 0.137889 0.436308 -1.603157

1 -1.223158 -0.509703 -1.514173  
1 0.035889 -1.041650 -0.802364  
1 1.675660 1.884526 -1.814419  
1 -0.189030 2.602316 -3.253325  
1 0.608594 -2.064357 1.047432  
**41**  
6 -2.467330 -0.893550 -2.036196  
6 -0.999468 -0.716468 -1.690091  
6 -0.351532 0.269923 -2.661472  
8 -0.569982 -0.176448 -3.984091  
6 -1.918257 -0.200041 -4.333530  
6 -2.619481 -1.241846 -3.495841  
8 -0.921855 -0.192494 -0.370931  
6 -0.278648 -0.928807 0.601488  
8 1.046667 -1.159682 0.186414  
6 1.862123 -1.766008 1.172714  
6 1.292907 -3.136768 1.486931  
6 -0.133646 -3.004173 1.961898  
6 -0.946143 -2.257999 0.924272  
6 3.271604 -1.827019 0.615971  
8 4.210383 -2.144524 1.608073  
8 2.103121 -3.736555 2.465257  
8 -0.619860 -4.301847 2.175491  
8 -2.280317 -2.083978 1.337121  
6 1.155337 0.405226 -2.530668  
8 1.551842 1.150709 -1.413872  
8 -1.962328 -0.510330 -5.682104  
8 -3.963650 -1.269837 -3.894527  
8 -3.083047 -1.922918 -1.314409  
1 3.920849 -2.953573 2.037820  
1 3.304863 -2.540267 -0.211150  
1 3.534838 -0.847327 0.226255  
1 1.867286 -1.153226 2.079662  
1 1.301158 -3.733058 0.569456  
1 1.713823 -4.580484 2.702739  
1 -0.135394 -2.440435 2.901487  
1 -1.506684 -4.249406 2.534304  
1 -0.998569 -2.861466 0.018969  
1 -2.328934 -1.495942 2.093988  
1 -0.276694 -0.287410 1.487402  
1 -0.479925 -1.673697 -1.756848  
1 -0.807256 1.255408 -2.516603  
1 1.610363 -0.587442 -2.527464  
1 1.505851 0.931993 -3.414782  
1 1.473547 0.578665 -0.646408  
1 -2.360998 0.788034 -4.149223  
1 -2.839141 -0.851918 -5.872988  
1 -2.139293 -2.205526 -3.688634  
1 -4.431193 -1.883955 -3.325673  
1 -2.973087 0.059726 -1.848787  
1 -3.052583 -1.733221 -0.368487  
**1**  
6 0.218348 1.519525 -1.618475  
6 -0.577765 1.341637 -0.339500

6 -1.921868 2.052504 -0.447230  
8 -1.700632 3.407560 -0.772495  
6 -1.087844 3.568512 -2.015700  
6 0.305580 2.986071 -1.958573  
8 -0.841623 -0.025736 -0.106812  
6 0.003427 -0.735214 0.713368  
8 1.009728 -1.330800 -0.079482  
6 1.933133 -2.089110 0.680479  
6 1.182780 -3.234319 1.338476  
6 0.076651 -2.694102 2.210536  
6 -0.826651 -1.804016 1.392755  
6 3.016607 -2.566099 -0.267377  
8 4.115608 -3.101465 0.420439  
8 2.101335 -3.987755 2.091064  
8 -0.607029 -3.796755 2.747993  
8 -1.769339 -1.230610 2.246983  
6 -2.727869 2.068857 0.835658  
8 -3.327346 0.806376 1.043879  
8 -1.063495 4.930278 -2.258066  
8 0.901431 3.210088 -3.208186  
8 1.531578 1.042989 -1.511548  
1 3.784222 -3.767954 1.028615  
1 2.591505 -3.288766 -0.968336  
1 3.380146 -1.716580 -0.839519  
1 2.390176 -1.460573 1.451724  
1 0.741170 -3.853320 0.551775  
1 1.616499 -4.670155 2.559473  
1 0.522237 -2.100211 3.015040  
1 -1.289039 -3.473800 3.338366  
1 -1.306284 -2.398848 0.609454  
1 -2.300997 -0.587549 1.751132  
1 0.470195 -0.078973 1.456849  
1 -0.015719 1.760240 0.499186  
1 -2.518912 1.568763 -1.227374  
1 -2.089082 2.337036 1.678554  
1 -3.490253 2.836920 0.723171  
1 -4.087963 0.918934 1.613310  
1 -1.678783 3.048755 -2.781682  
1 -0.375832 5.096959 -2.907370  
1 0.854801 3.507873 -1.169686  
1 1.777383 2.821027 -3.199956  
1 -0.311678 1.001414 -2.424770  
1 1.507107 0.120493 -1.229474  
**TS(1-3) – 1 imaginary frequency**  
6 -0.930471 -1.899634 1.189661  
6 -0.086350 -0.744344 0.693141  
8 1.048432 -1.232931 0.016177  
6 1.915601 -1.965726 0.861263  
6 1.167777 -3.192118 1.355767  
6 -0.089709 -2.779497 2.083318  
8 -0.850394 -0.024519 -0.193163  
6 -0.499458 1.326576 -0.428723  
6 0.118015 1.459654 -1.804811  
6 0.232081 2.920006 -2.167371

6 -1.124207 3.578152 -2.030595  
8 -1.553768 3.470259 -0.708539  
6 -1.787947 2.130966 -0.328225  
8 1.401613 0.903240 -1.880230  
6 -2.361061 2.117827 1.074906  
8 -3.710664 1.717178 1.004942  
8 -1.061752 4.932690 -2.306110  
8 0.650377 3.110284 -3.492926  
6 3.151165 -2.314699 0.054984  
8 4.182733 -2.808296 0.867235  
8 2.023988 -3.920932 2.199386  
8 -0.758892 -3.956781 2.451655  
8 -2.020885 -1.441459 1.940182  
1 3.823903 -3.529883 1.390816  
1 2.883444 -3.026638 -0.729720  
1 3.522144 -1.411117 -0.421335  
1 2.214551 -1.349672 1.715435  
1 0.887398 -3.796439 0.487741  
1 1.532619 -4.663200 2.556891  
1 0.191188 -2.210695 2.975421  
1 -1.526607 -3.723209 2.974982  
1 -1.261342 -2.474705 0.321567  
1 -2.620681 -0.968978 1.359584  
1 0.236506 -0.116362 1.532535  
1 0.213632 1.665686 0.326597  
1 -2.523718 1.677516 -1.000167  
1 -1.796831 1.429139 1.705562  
1 -2.264596 3.119878 1.491948  
1 -4.100794 1.785970 1.875770  
1 -1.847835 3.081358 -2.691004  
1 -0.470655 5.048187 -3.054211  
1 0.915587 3.414800 -1.471960  
1 1.516308 2.714523 -3.600997  
1 -0.551425 0.973215 -2.522624  
1 1.393416 0.036738 -1.457651  
**3**  
8 1.006838 -1.183920 0.048296  
6 1.852148 -1.913954 0.916614  
6 1.137103 -3.198155 1.298310  
6 -0.189981 -2.880345 1.943510  
6 -1.011092 -1.998855 1.031256  
6 -0.196289 -0.777020 0.659686  
6 3.155547 -2.160233 0.182700  
8 4.153347 -2.648519 1.039152  
8 1.966336 -3.922333 2.172505  
8 -0.828327 -4.101637 2.205914  
8 -2.178533 -1.652097 1.723796  
8 -0.916309 -0.039284 -0.249362  
6 -0.505216 1.301241 -0.462932  
6 -1.725301 2.203502 -0.305426  
8 -1.400442 3.521503 -0.687816  
6 -1.033590 3.614620 -2.028657  
6 0.264775 2.867173 -2.228797  
6 0.066912 1.416619 -1.863029

6	-2.209528	2.243138	1.117764	1	2.239145	-1.349209	1.667398	1	0.292913	1.479753	0.145658
8	-3.470971	2.864086	1.140651	1	0.873656	-3.789760	0.469186	1	-2.555059	1.863263	-0.849954
8	-0.892403	4.964540	-2.299562	1	1.604499	-4.677958	2.497841	1	-2.545536	1.194488	1.421854
8	0.638057	3.031071	-3.571319	1	0.273125	-2.225485	2.994522	1	-2.876790	2.931521	1.340594
8	1.307264	0.779637	-1.996941	1	-1.469154	-3.724918	3.014161	1	-1.251672	2.428203	2.917759
1	3.795972	-3.411530	1.501425	1	-1.283520	-2.462422	0.398152	1	-1.897691	3.251150	-2.545496
1	2.977206	-2.840745	-0.653704	1	-2.664205	-1.090438	1.513367	1	-0.319905	5.040464	-3.002859
1	3.511219	-1.215798	-0.220354	1	0.258731	-0.113653	1.575640	1	1.010299	3.170061	-1.669029
1	2.059050	-1.327687	1.817580	1	0.193257	1.690784	0.380373	1	1.277226	2.540466	-3.870842
1	0.953730	-3.774036	0.386276	1	-2.490093	1.766527	-1.039106	1	-0.869103	0.979108	-2.608934
1	1.494511	-4.708936	2.452889	1	-1.797375	1.540406	1.735769	1	1.120015	-0.155930	-1.651260
1	-0.005639	-2.342923	2.879568	1	-3.395974	1.695713	1.019327	<b>TS(4-1) – 1 imaginary frequency</b>			
1	-1.663296	-3.920774	2.640183	1	-2.926105	3.404663	2.459422	6	-1.873079	2.070383	-0.366567
1	-1.242883	-2.543535	0.113372	1	-1.799062	3.114900	-2.667967	6	-0.556385	1.302132	-0.364392
1	-2.817444	-1.300778	1.103356	1	-0.346892	5.030574	-3.045602	6	0.157543	1.473463	-1.693068
1	0.036632	-0.182363	1.551402	1	0.973152	3.370317	-1.452874	6	0.248964	2.932386	-2.061387
1	0.259278	1.577720	0.267186	1	1.544593	2.592745	-3.567875	6	-1.137505	3.531935	-2.039138
1	-2.527558	1.817972	-0.944124	1	-0.560372	0.955067	-2.466425	8	-1.650270	3.413704	-0.748125
1	-2.267676	1.222029	1.496258	1	1.370340	-0.000020	-1.385453	8	-0.872709	-0.066783	-0.184238
1	-1.485637	2.797231	1.718413	<b>4</b>				6	-0.097355	-0.790368	0.689441
1	-3.766206	2.934120	2.047322	8	0.995886	-1.138931	0.099754	6	-0.924139	-1.949276	1.204595
1	-1.820817	3.174648	-2.655523	6	1.836295	-1.826198	1.005060	6	-0.047781	-2.834398	2.063454
1	-0.324441	5.046538	-3.069640	6	1.173987	-3.148387	1.350535	6	1.179812	-3.255852	1.296004
1	1.010802	3.310434	-1.563739	6	-0.198145	-2.904462	1.930894	6	1.915472	-2.024766	0.797659
1	1.472143	2.581648	-3.714289	6	-1.020268	-2.062029	0.983477	8	1.024673	-1.282840	-0.013873
1	-0.661556	0.979529	-2.554887	6	-0.254093	-0.797884	0.654931	8	-2.016838	-1.516701	1.964935
1	1.286595	-0.056359	-1.517431	6	3.184344	-1.997845	0.333622	6	3.127498	-2.363573	-0.047830
<b>TS(3-4) – 1 imaginary frequency</b>				8	4.165564	-2.438358	1.234440	8	4.178041	-2.875940	0.727963
6	-0.921504	-1.897639	1.260091	8	1.997452	-3.830522	2.263624	8	2.056529	-4.000732	2.105119
6	-0.103585	-0.730362	0.744480	8	-0.783331	-4.159405	2.158373	8	-0.713741	-4.004874	2.463347
8	1.002649	-1.223205	0.018856	8	-2.237717	-1.785779	1.619741	8	1.464369	0.968653	-1.673215
6	1.908506	-1.958805	0.820459	8	-0.960708	-0.097786	-0.295378	8	0.768764	3.121789	-3.350505
6	1.185687	-3.192442	1.331139	6	-0.531933	1.234250	-0.524024	8	-1.117279	4.886010	-2.323598
6	-0.042084	-2.786104	2.108448	6	-1.694595	2.178993	-0.250027	6	-2.565391	2.134382	0.994464
8	-0.896366	0.005675	-0.103541	8	-1.323071	3.494105	-0.602013	8	-1.928702	1.286970	1.932147
6	-0.512841	1.343487	-0.378088	6	-1.041624	3.616307	-1.961633	1	3.828738	-3.601924	1.252052
6	0.118045	1.437067	-1.753726	6	0.189557	2.800107	-2.289267	1	2.835367	-3.060685	-0.837162
6	0.273659	2.887629	-2.141032	6	-0.068243	1.349936	-1.959748	1	3.491212	-1.454194	-0.518883
6	-1.057135	3.592255	-2.013208	6	-2.111042	2.169099	1.196170	1	2.238235	-1.420004	1.651294
8	-1.485618	3.511386	-0.689835	8	-0.982994	2.417022	2.000404	1	0.871289	-3.847241	0.428593
6	-1.781797	2.188363	-0.318861	8	-0.833702	4.964587	-2.194921	1	1.563753	-4.729747	2.487214
8	1.391527	0.858288	-1.824991	8	0.467653	3.002555	-3.650072	1	0.267884	-2.265245	2.943650
6	-2.412814	2.161255	1.081879	8	1.115383	0.636730	-2.198913	1	-1.451107	-3.758495	3.023325
8	-2.517780	3.463588	1.596616	1	3.825717	-3.219303	1.679643	1	-1.270480	-2.519282	0.338107
8	-0.948673	4.941593	-2.302529	1	3.082648	-2.681295	-0.513173	1	-2.121835	-0.558590	1.864318
8	0.702319	3.039108	-3.468292	1	3.506527	-1.032949	-0.048399	1	0.241863	-0.157345	1.517818
6	3.111771	-2.295118	-0.038678	1	1.968528	-1.234223	1.916433	1	0.079848	1.649521	0.450795
8	4.175361	-2.794807	0.726993	1	1.066479	-3.730204	0.430196	1	-2.528567	1.594984	-1.102078
8	2.076080	-3.925820	2.134657	1	1.556320	-4.643134	2.518515	1	-2.506570	3.167397	1.329630
8	-0.701829	-3.963356	2.491809	1	-0.087923	-2.363788	2.876582	1	-3.613972	1.861096	0.897045
8	-1.982645	-1.470106	2.068077	1	-1.646907	-4.024583	2.551437	1	-2.150370	1.583451	2.814428
1	3.838676	-3.522165	1.257390	1	-1.177648	-2.612619	0.053125	1	-1.789479	2.997449	-2.743118
1	2.814501	-2.999287	-0.819749	1	-2.851884	-1.430798	0.976632	1	-0.473040	5.025448	-3.021970
1	3.462773	-1.386001	-0.519732	1	-0.098833	-0.187892	1.553151	1	0.854152	3.460415	-1.319344



1	1.637856	2.719352	-3.388784	6	1.497548	-2.954885	1.969534	6	-0.100525	-2.007110	0.914655
1	-0.436063	0.960738	-2.458032	6	0.251833	-2.430837	2.633724	6	1.408251	-1.920925	0.815433
1	1.449337	0.078756	-1.300553	8	-1.031922	-1.024685	-0.605543	8	1.792417	-1.690033	-0.525028
<b>5</b>				6	-2.313638	-0.429138	-0.502535	8	-1.788514	-3.606709	3.541319
6	0.171155	1.239228	-2.390197	6	-2.278086	1.026349	-0.916580	8	-3.835636	-1.976825	2.659448
6	0.273170	-0.169284	-1.817748	6	-3.695010	1.554064	-0.914852	6	-3.076982	3.734456	-0.929952
6	-0.495782	-1.113015	-2.715227	6	-4.569371	0.683886	-1.792924	8	-3.145570	5.128668	-0.780746
6	0.023532	-0.992783	-4.130581	8	-4.538754	-0.631795	-1.329531	8	-0.770963	4.972494	-2.195142
6	-0.011521	0.451457	-4.580703	6	-3.249683	-1.194244	-1.429130	8	1.234311	3.277565	-3.159108
8	0.732919	1.237850	-3.683206	8	-1.530326	1.823630	-0.028373	8	1.719109	0.976685	-1.518486
8	-0.280177	-0.146913	-0.516134	6	-3.345782	-2.664554	-1.072502	1	-2.530834	5.519675	-1.407486
6	0.286334	-0.891460	0.525260	8	-2.250424	-3.392503	-1.568682	1	-3.527693	3.411314	-1.871873
6	-0.747134	-1.872096	1.060304	8	-5.895009	1.077496	-1.739599	1	-3.646324	3.293718	-0.116126
6	-0.123443	-2.717547	2.152182	8	-3.776744	2.859813	-1.416587	1	-1.172359	3.651649	0.032698
6	1.145927	-3.358396	1.651827	6	3.167392	-2.412901	0.149266	1	-1.331662	3.145701	-2.961352
6	2.073446	-2.283862	1.114123	8	4.333542	-2.394294	0.929576	1	-0.195516	5.189719	-2.931089
8	1.400021	-1.597721	0.080845	8	2.532537	-3.151228	2.901108	1	1.057268	3.425859	-1.116585
8	-1.919054	-1.250736	1.520342	8	-0.204504	-3.416755	3.520817	1	2.128685	2.941749	-3.087635
6	3.349199	-2.846048	0.518808	8	-1.943935	-1.567315	2.278030	1	-0.033957	1.017197	-2.607346
8	4.221085	-3.325594	1.508323	1	4.153888	-2.882880	1.737464	1	1.648556	0.050261	-1.238427
8	1.814713	-4.051081	2.677902	1	2.974192	-3.408326	-0.258523	1	-0.002202	1.654088	0.365844
8	-0.984835	-3.744485	2.569269	1	3.323171	-1.732152	-0.683075	1	-0.374479	-0.011278	1.609789
8	-0.373553	-2.428538	-2.248055	1	2.197029	-0.998954	1.423023	1	-0.470617	-2.645523	0.105041
8	-0.786147	-1.809188	-4.934148	1	1.261418	-3.893268	1.459701	1	1.782119	-1.128481	1.466186
8	0.571713	0.515948	-5.826195	1	2.228189	-3.768287	3.568895	1	1.808400	-2.870500	1.165828
6	0.905265	2.272452	-1.560014	1	0.522125	-1.523986	3.189000	1	2.702906	-1.963919	-0.632292
8	0.159337	2.657894	-0.433059	1	-1.017600	-3.110203	3.926211	1	-2.076656	-3.498639	1.514882
1	3.726085	-3.934170	2.063539	1	-1.149212	-2.995299	1.120691	1	-2.690366	-3.522884	3.861517
1	3.098510	-3.625272	-0.205230	1	-1.706932	-0.769579	2.756284	1	-2.108534	-1.030876	3.270175
1	3.865161	-2.048717	-0.008984	1	0.009031	-0.177185	0.950034	1	-4.342404	-1.212778	2.932661
1	2.336377	-1.590396	1.920267	1	-2.695082	-0.512544	0.511373	1	-2.746395	-1.414089	0.312475
1	0.897542	-4.040625	0.833774	1	-2.888033	-1.117315	-2.461015	1	-2.793486	0.124706	1.167669
1	1.218624	-4.710412	3.037478	1	-3.440025	-2.777968	0.011134	<b>8</b>			
1	0.131413	-2.075268	3.004117	1	-4.240535	-3.073824	-1.533401	6	0.364693	1.167994	-1.696080
1	-1.822031	-3.350994	2.821836	1	-1.452127	-2.911342	-1.336798	6	-0.567150	1.309912	-0.497450
1	-1.042683	-2.505818	0.225910	1	-4.197681	0.713575	-2.826088	6	-1.734011	2.221417	-0.818417
1	-1.707920	-0.628167	2.218683	1	-5.913946	2.037159	-1.766632	6	-2.393792	1.772612	-2.098803
1	0.592483	-0.186771	1.309676	1	-4.092046	1.506439	0.103488	6	-1.353063	1.684481	-3.192357
1	1.320441	-0.458463	-1.781619	1	-3.205240	3.419042	-0.887311	8	-0.383708	0.754901	-2.823120
1	-0.883034	1.535523	-2.442403	1	-1.869624	1.103463	-1.926751	8	0.165864	1.879447	0.575471
1	1.888718	1.891635	-1.273584	1	-0.642761	1.936375	-0.364829	6	0.175018	1.180882	1.758429
1	1.051017	3.160248	-2.169281	<b>7</b>				6	1.277056	1.742364	2.632933
1	-0.138496	1.854810	-0.000187	6	0.436992	1.485641	-1.737424	6	1.227713	1.065980	3.983001
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<b>6</b>				6	-0.820160	-0.666629	0.856465	8	-0.260231	0.477069	5.779674
6	-0.816468	-2.080226	1.610908	6	-2.301894	-0.844823	1.130228	8	2.126424	1.643345	4.892609
6	-0.234265	-1.161552	0.533688	6	-2.498543	-1.602802	2.424680	8	-3.380820	2.669639	-2.536329
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6 -2.186213 0.945057 1.882716  
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8	-1.824157	4.633922	2.569368	1	-6.007332	-2.092214	-3.112837	1	-2.351626	0.668259	3.942381
8	-2.681798	2.774801	0.437124	1	-3.510294	-2.095572	-1.782497	1	-0.351894	-0.827152	2.191460
1	-0.700525	-0.903102	4.370152	1	-4.549376	-3.983325	-1.079642	1	-1.790707	2.835164	4.498797
1	-7.015931	1.003997	-1.633950	1	-4.924386	-1.719789	0.885394	1	-0.103432	4.515518	3.998747
8	-6.214085	1.225879	-3.525888	1	-2.775147	-2.411702	1.580166	1	-0.784567	3.421772	1.690619
1	-4.103262	0.448926	-2.317098	1	-2.476615	-0.303839	-0.267699	1	-2.324253	5.133837	1.916326
1	-6.243366	-1.311838	-1.029810	1	-1.382132	0.814082	1.187549	1	-3.523964	2.577589	2.698075
1	-5.956157	-2.416098	-3.073188	1	-2.440433	0.507191	4.027207	1	-3.842658	2.485406	0.380066
1	-3.402809	-1.925168	-1.916954	1	-0.153987	-0.842749	2.542856	1	-1.708113	-2.496569	3.590695
1	-4.004515	-3.959662	-1.050098	1	-1.990055	2.813703	4.516067	1	-6.033071	0.299529	-3.796643
1	-4.677769	-1.806634	0.843957	1	0.553173	3.610842	3.663439	1	-2.442012	-1.969500	2.191074
1	-2.537935	-2.284474	1.466192	1	-0.868942	3.268313	1.716292	<b>3-O(1)-1</b>			
1	-2.582357	0.048480	-0.421412	1	-1.678618	5.186802	2.640449	6	0.303899	1.580100	-1.618934
1	-1.321384	0.795425	1.183954	1	-3.604644	2.310844	2.622809	6	-0.547004	1.478136	-0.369046
1	-2.627830	0.607887	3.927651	1	-3.507653	3.498113	0.611321	6	-1.882746	2.208236	-0.485419
1	-0.318543	-0.904417	2.645377	1	-1.445654	-2.653511	3.581139	8	-1.603764	3.527782	-0.868507
1	-2.102470	2.804684	4.439084	1	-6.016058	0.679028	-3.793506	6	-1.017061	3.616330	-2.133993
1	-0.270956	4.390456	4.225081	1	-3.955353	1.563099	0.008062	6	0.376110	3.034588	-2.048485
1	-0.522328	3.194545	1.872911	<b>16</b>				8	-0.861106	0.043035	-0.086371
1	-1.688877	5.085137	1.736491	6	-2.715343	2.549601	1.960948	6	-0.047877	-0.791497	0.793227
1	-3.465134	2.595642	2.336804	6	-2.210742	1.126926	1.850063	8	0.977582	-1.270404	0.015906
1	-3.415669	3.376942	0.324505	6	-1.584683	0.683320	3.161505	6	1.890092	-2.105541	0.736423
1	-1.853806	-2.597162	3.644043	8	-0.544433	1.561089	3.502310	6	1.117176	-3.301443	1.259581
1	-6.452408	0.333701	-3.791379	6	-1.011296	2.862974	3.726470	6	-0.030424	-2.841881	2.127832
1	-5.272842	0.734088	0.295078	6	-1.581164	3.425111	2.439783	6	-0.927697	-1.893738	1.347599
<b>15</b>				8	-3.266798	0.226950	1.590913	6	2.996798	-2.490709	-0.226989
6	-4.028944	-1.732824	0.258579	6	-3.487050	-0.184195	0.297429	8	4.079873	-3.064407	0.448757
6	-3.389186	-0.369767	0.325489	8	-4.452489	0.640356	-0.295472	8	2.011429	-4.102619	1.982560
8	-4.337638	0.617942	-0.254470	6	-4.747097	0.267581	-1.632583	8	-0.731914	-3.983016	2.525473
6	-4.672215	0.399166	-1.656048	6	-5.337514	-1.136920	-1.628607	8	-1.887905	-1.355082	2.202840
6	-5.327120	-0.968085	-1.704003	6	-4.354495	-2.103746	-0.994745	6	-2.630885	2.248015	0.821923
6	-4.413823	-2.050490	-1.168259	6	-4.018449	-1.592694	0.380588	8	-3.922414	2.721574	0.552306
8	-3.207907	-0.036612	1.618638	8	-3.003937	-2.385544	0.978373	8	-0.987340	4.959129	-2.446760
6	-2.178138	0.882400	1.931532	8	-4.886295	-3.394325	-0.838380	8	0.963102	3.163203	-3.308519
6	-2.743826	2.277916	1.953100	8	-5.619239	-1.489833	-2.960025	8	1.615615	1.156609	-1.415774
6	-1.703172	3.257564	2.423760	6	-5.703072	1.304630	-2.190304	1	3.751000	-3.804353	0.966212
6	-1.183306	2.796772	3.780289	1	-5.311841	2.292792	-1.964340	1	2.596137	-3.158295	-0.992911
8	-0.664989	1.495068	3.652429	6	-0.947148	-0.687236	3.087415	1	3.365777	-1.594281	-0.717690
6	-1.622711	0.524693	3.300341	8	-1.986545	-1.705142	3.115336	1	2.321096	-1.540380	1.565863
8	-3.176059	2.594397	0.632327	8	0.082024	3.586373	4.157198	1	0.712510	-3.853734	0.406226
6	-0.900621	-0.806774	3.337296	8	-1.992598	4.734291	2.721661	1	1.522746	-4.838862	2.356616
8	-1.829666	-1.862085	3.204810	8	-3.151353	3.056395	0.731131	1	0.368628	-2.314244	2.998522
8	-0.195744	3.619778	4.264378	1	-0.337880	-0.847525	3.967536	1	-1.338807	-3.752060	3.229693
8	-2.332654	4.504063	2.486595	1	-6.675027	1.204964	-1.701087	1	-1.378027	-2.448413	0.523033
6	-5.596625	1.516967	-2.110418	8	-5.815398	1.211299	-3.584456	1	-2.762970	-1.454904	1.830329
8	-5.683865	1.533151	-3.504267	1	-3.831158	0.278505	-2.231830	1	0.281669	-0.106336	1.572693
8	-5.656979	-1.200881	-3.043801	1	-6.254953	-1.123594	-1.035359	1	0.005292	1.793301	0.510906
8	-5.133509	-3.246833	-1.263689	1	-6.230120	-2.227278	-2.972004	1	-2.509261	1.722680	-1.241122
8	-3.098936	-2.668405	0.702552	1	-3.447240	-2.136650	-1.601672	1	-2.657054	1.247044	1.252991
1	-5.187084	2.477409	-1.808992	1	-4.636275	-3.944364	-1.579882	1	-2.096242	2.907567	1.507270
1	-0.387606	-0.865191	4.294892	1	-4.906557	-1.595418	1.012597	1	-4.404945	2.797757	1.374531
1	-6.573381	1.399957	-1.638321	1	-3.253367	-3.314482	0.919373	1	-1.621681	3.057195	-2.859193

1 -0.324354 5.086793 -3.130078  
1 0.928673 3.602017 -1.295884  
1 1.885237 2.908365 -3.253933  
1 -0.172431 1.018813 -2.430278  
1 1.640072 0.207293 -1.272555  
1 -1.208300 -0.445849 -0.850566

**3-O(1)-2**

6 -4.630879 -1.491332 0.736954  
6 -3.614819 -0.391688 0.436818  
6 -4.105885 0.583845 -0.616373  
6 -5.488230 1.075009 -0.235053  
6 -6.384343 -0.112694 0.034120  
8 -5.827511 -0.847619 1.085125  
8 -2.345939 -0.955818 -0.096663  
6 -1.113833 -0.950323 0.691789  
6 -0.095337 -1.644317 -0.182660  
6 1.237745 -1.592010 0.541354  
6 1.520992 -0.141420 0.896151  
6 0.377321 0.482517 1.680529  
8 -0.817722 0.360707 0.906265  
8 -0.571697 -2.906829 -0.548716  
6 0.579006 1.961405 1.947413  
8 1.541175 2.175282 2.941924  
8 2.678551 -0.033407 1.677186  
8 2.295350 -2.016937 -0.268690  
8 -3.280423 1.704068 -0.715786  
8 -6.070410 1.817208 -1.264310  
8 -7.635770 0.276293 0.463167  
6 -4.242669 -2.377090 1.893373  
8 -5.162038 -3.431726 1.936778  
1 -0.358149 2.376164 2.307395  
1 -3.229092 -2.754821 1.749719  
1 0.840701 2.467156 1.015336  
1 0.251167 -0.034731 2.635078  
1 1.637925 0.415287 -0.038529  
1 3.408035 -0.421899 1.189549  
1 1.193815 -2.179810 1.461933  
1 2.375771 -2.970037 -0.239700  
1 -0.010135 -1.073680 -1.106366  
1 -1.326589 -1.486986 1.619082  
1 -3.301093 0.136792 1.332609  
1 -4.785966 -2.111726 -0.152850  
1 -4.263334 -1.784379 2.809018  
1 -6.453649 -0.746513 -0.859099  
1 -7.907024 1.029884 -0.067106  
1 -5.422399 1.660316 0.685395  
1 -5.562337 2.618880 -1.397305  
1 -4.182548 0.065827 -1.575266  
1 -2.525244 1.517318 -1.273755  
1 -4.986922 -3.968418 2.708906  
1 -2.399310 -1.784077 -0.613609  
1 2.347919 1.726036 2.676650  
1 -0.499054 -3.533058 0.175817

**3-O(2)**

6 -2.686318 2.306408 1.940349  
6 -2.152006 0.886231 2.017074  
6 -1.665589 0.552206 3.414845  
6 -2.754862 0.857000 4.413591  
6 -3.259612 2.271941 4.203808  
8 -3.720691 2.435435 2.884905  
8 -1.079248 0.789407 1.097340  
6 -0.933103 -0.350568 0.352942  
6 -0.388661 0.076753 -0.987409  
6 -0.110998 -1.097545 -1.878708  
6 0.854191 -2.011581 -1.142510  
6 0.257471 -2.377825 0.211879  
8 0.025990 -1.183131 0.944084  
8 -1.403093 0.888485 -1.642476  
6 1.180542 -3.250173 1.041490  
8 1.198509 -4.571948 0.576255  
8 1.067858 -3.200905 -1.856598  
8 0.394219 -0.567252 -3.073881  
8 -1.324076 -0.801553 3.518659  
8 -2.241079 0.711008 5.707185  
8 -4.311915 2.457072 5.070634  
6 -3.299919 2.668965 0.603569  
8 -2.279348 2.860026 -0.371644  
1 0.808772 -3.273387 2.061984  
1 -3.854493 3.592852 0.733743  
1 2.182228 -2.814430 1.055012  
1 -0.686346 -2.911563 0.063660  
1 1.796875 -1.485577 -0.977875  
1 1.742077 -3.064031 -2.522453  
1 -1.037390 -1.645838 -2.062108  
1 0.190832 -1.148539 -3.806928  
1 0.493243 0.695909 -0.847984  
1 -1.701786 1.670690 -1.154687  
1 -1.881960 -0.885982 0.244500  
1 -2.944686 0.189328 1.736050  
1 -1.876499 3.011288 2.155521  
1 -3.987770 1.892660 0.271919  
1 -2.455499 2.991679 4.392618  
1 -4.485441 3.392027 5.182897  
1 -3.595438 0.177118 4.245537  
1 -2.935680 0.950386 6.323539  
1 -0.800932 1.185008 3.639436  
1 -0.625060 -0.995872 2.887062  
1 -2.503876 3.602297 -0.933864  
1 1.410162 -4.547940 -0.360547  
1 -1.150064 1.078024 -2.560349

**3-O(3)**

6 0.198521 1.352183 -1.548041  
6 -0.551017 1.308184 -0.240962  
6 -1.763894 2.229053 -0.362862  
8 -1.326866 3.509230 -0.749571  
6 -0.758263 3.545693 -2.034391  
6 0.529812 2.744285 -2.000257  
8 -0.998592 -0.011300 -0.005121

6 -0.230295 -0.805880 0.804550  
8 0.901083 -1.262180 0.040151  
6 1.810558 -2.081548 0.788382  
6 1.048140 -3.331592 1.185291  
6 -0.174759 -2.970380 1.993335  
6 -1.048113 -2.012083 1.215159  
6 3.016278 -2.380714 -0.084873  
8 4.057112 -2.934295 0.668532  
8 1.920932 -4.145394 1.922337  
8 -0.846348 -4.165770 2.275423  
8 -2.105239 -1.636947 2.048434  
6 -2.496595 2.356630 0.945394  
8 -3.719369 2.998957 0.693953  
8 -0.424001 4.838868 -2.345361  
8 1.138393 2.605116 -3.249401  
8 1.456821 0.639996 -1.377325  
1 3.716000 -3.711274 1.120013  
1 2.718666 -3.033113 -0.908530  
1 3.396858 -1.453802 -0.506429  
1 2.138103 -1.535788 1.675277  
1 0.727710 -3.843473 0.273248  
1 1.433022 -4.914515 2.224088  
1 0.144789 -2.484928 2.920935  
1 -1.601017 -3.969240 2.832746  
1 -1.407266 -2.501822 0.308348  
1 -2.837052 -1.323473 1.517209  
1 0.144188 -0.255653 1.671660  
1 0.087264 1.647814 0.577172  
1 -2.446097 1.816683 -1.113419  
1 -2.649907 1.360193 1.359338  
1 -1.879391 2.931995 1.637736  
1 -4.189013 3.108131 1.519761  
1 -1.460410 3.122451 -2.759976  
1 -1.200630 5.318691 -2.635026  
1 1.195493 3.222091 -1.278689  
1 1.520209 3.443676 -3.512204  
1 -0.367383 0.825805 -2.314184  
1 1.928201 0.548145 -2.217760  
1 1.328155 -0.261130 -0.831238

**3-O(5)-1**

6 -3.584983 -1.856690 -0.105516  
6 -3.208604 -0.420755 0.195082  
8 -4.478876 0.424296 -0.030205  
6 -5.050471 0.361693 -1.378604  
6 -5.406837 -1.085801 -1.641997  
6 -4.192896 -1.975911 -1.491356  
8 -2.870204 -0.242478 1.472189  
6 -1.911025 0.771199 1.805396  
6 -2.343358 2.152628 1.365451  
6 -1.458131 3.208023 1.992090  
6 -1.398133 3.022806 3.489822  
8 -0.902950 1.732718 3.747255  
6 -1.779901 0.719190 3.324534  
8 -2.268621 2.231807 -0.033969

6	-1.235262	-0.598090	3.808943	6	-2.588840	2.331717	0.874786	1	-6.158385	-2.172131	-2.998199
8	-1.343121	-0.619601	5.210134	8	-3.809155	2.959401	0.577341	1	-3.431563	-2.179363	-1.604886
8	-0.517486	3.951681	3.991838	1	3.726894	-3.776789	1.019342	1	-4.664852	-3.937400	-1.620591
8	-2.005211	4.442023	1.619239	1	2.634546	-3.164085	-0.965262	1	-4.881589	-1.624744	1.006150
6	-6.213537	1.334127	-1.469632	1	3.343230	-1.574065	-0.669956	1	-3.343010	-3.416832	0.843435
8	-6.514007	1.588822	-2.808989	1	2.189129	-1.552487	1.580555	1	-2.458959	-0.273004	-0.236813
8	-5.922134	-1.136620	-2.939990	1	0.669997	-3.873750	0.311734	1	-1.490257	1.167245	0.994046
8	-4.631218	-3.280330	-1.731409	1	1.442586	-4.904088	2.259568	1	-2.189306	0.646641	3.917560
8	-2.423228	-2.629547	-0.106629	1	0.223302	-2.432557	2.944100	1	-1.314337	-1.404631	2.926513
1	-5.918756	2.276493	-1.017222	1	-1.526350	-3.902473	2.988685	1	-1.821641	2.829147	4.540372
1	-1.811551	-1.404825	3.358919	1	-1.449521	-2.499722	0.404944	1	-0.300472	4.688933	3.988710
1	-7.075713	0.941247	-0.927105	1	-2.842885	-1.354420	1.658293	1	-0.969184	3.575918	1.717643
1	-4.244468	0.704000	-2.022125	1	0.191778	-0.232576	1.636980	1	-2.669395	5.118587	2.018065
1	-6.165471	-1.402243	-0.918539	1	0.018369	1.669745	0.610465	1	-3.582936	2.447167	2.780547
1	-6.104653	-2.053841	-3.157020	1	-2.448911	1.784494	-1.179647	1	-3.899596	2.369797	0.423636
1	-3.442650	-1.680907	-2.230695	1	-2.746374	1.334667	1.285628	1	0.805735	-1.274619	4.185643
1	-3.872624	-3.866526	-1.737165	1	-2.004925	2.915317	1.588768	1	-5.878276	0.381321	-3.785947
1	-4.298577	-2.208342	0.641420	1	-4.303746	3.076814	1.387270	1	0.471148	0.285780	4.382774
1	-2.207304	-2.904510	0.784585	1	-1.397967	3.094891	-2.788724	<b>4-O(1)-1</b>			
1	-2.524656	0.015574	-0.526059	1	-1.192325	5.298538	-2.655186	6	0.109625	1.471193	-1.915123
1	-0.963793	0.513085	1.330883	1	1.176757	3.244041	-1.174441	6	-0.534892	1.353353	-0.554305
1	-2.771435	0.873581	3.764282	1	1.571007	3.507916	-3.398629	6	-1.805221	2.177884	-0.406669
1	-0.195116	-0.688074	3.489904	1	-0.313080	0.843054	-2.292583	8	-1.450348	3.508846	-0.679462
1	-2.392032	3.127621	3.938192	1	1.251597	-0.509838	-0.610093	6	-1.058387	3.678714	-2.011055
1	-0.627720	4.028312	4.939981	1	1.984748	0.629366	-2.071096	6	0.252863	2.953243	-2.227415
1	-0.440795	3.096990	1.607969	<b>3-O(6)</b>				8	-0.904747	-0.058908	-0.254473
1	-1.402237	5.139056	1.880248	6	-1.462298	0.753441	3.107468	6	-0.149692	-0.830952	0.721863
1	-3.371336	2.323412	1.702552	6	-2.189866	1.143177	1.832473	8	0.994218	-1.227319	0.078685
1	-2.475078	3.134313	-0.286831	6	-2.802837	2.520361	2.015452	6	1.882795	-1.952631	0.928773
1	-1.004638	-1.453153	5.533868	6	-1.740706	3.489072	2.487692	6	1.167814	-3.210355	1.386824
1	-6.755336	0.758968	-3.228590	6	-1.079476	2.968077	3.745656	6	-0.117976	-2.847385	2.093451
1	-5.124396	0.273619	0.679531	8	-0.497166	1.720960	3.448787	6	-0.995382	-1.998160	1.186958
<b>3-O(5)-2</b>				8	-3.180684	0.164595	1.621942	6	3.136149	-2.234985	0.123940
6	-1.804312	2.210387	-0.403636	6	-3.393853	-0.273624	0.334562	8	4.174623	-2.695922	0.942546
6	-0.578779	1.318919	-0.233369	6	-3.976407	-1.666405	0.393526	8	2.033415	-3.909992	2.239184
6	0.238834	1.350986	-1.500717	6	-4.342706	-2.111184	-1.005870	8	-0.756859	-4.041715	2.436595
6	0.556461	2.757251	-1.930418	6	-5.270347	-1.098499	-1.640708	8	-2.097568	-1.550450	1.914748
6	-0.740071	3.534986	-2.031894	6	-4.607140	0.269003	-1.622494	6	-2.375422	2.077275	0.986594
8	-1.375029	3.497239	-0.777856	8	-4.317055	0.599360	-0.276165	8	-1.314458	2.132252	1.907297
8	-1.016875	-0.013231	0.006841	8	-3.025370	-2.518969	0.962821	8	-0.916134	5.037712	-2.197290
6	-0.258603	-0.789234	0.814259	6	-5.495479	1.365367	-2.178133	8	0.628845	3.164113	-3.555458
6	-1.047305	-1.992727	1.282964	8	-5.614473	1.280889	-3.572775	8	1.399511	0.941825	-1.959898
6	-0.141978	-2.938447	2.045259	8	-5.558702	-1.425568	-2.979295	1	3.852575	-3.456528	1.433461
6	1.039495	-3.345784	1.195408	8	-4.946177	-3.378804	-0.897650	1	2.904105	-2.944114	-0.673878
6	1.820270	-2.131976	0.734799	8	-3.325526	3.033074	0.825240	1	3.472516	-1.307911	-0.331566
8	0.863002	-1.320410	0.002203	8	-2.269588	4.745726	2.805344	1	2.145874	-1.335174	1.790943
8	-2.058718	-1.587984	2.154803	8	-0.049202	3.778449	4.164717	1	0.927301	-3.813601	0.506338
6	2.976175	-2.477096	-0.189205	6	-0.687366	-0.524471	2.951698	1	1.572154	-4.683691	2.569746
8	4.041710	-3.001694	0.546239	8	0.107373	-0.603981	4.191314	1	0.121299	-2.269375	2.990665
8	1.929509	-4.152667	1.913902	1	-5.045132	2.328430	-1.952364	1	-1.482972	-3.849637	3.031490
8	-0.812857	-4.116708	2.385420	1	0.007984	-0.493224	2.121142	1	-1.288684	-2.604745	0.328638
8	1.455993	0.640197	-1.265315	1	-6.471759	1.324694	-1.688746	1	-2.899282	-1.644314	1.401710
8	1.229862	2.647731	-3.150506	1	-3.682308	0.237098	-2.207503	1	0.022982	-0.115396	1.526062
8	-0.418118	4.834778	-2.334743	1	-6.192693	-1.041936	-1.057119	1	0.167194	1.603698	0.233329

1 -2.563756 1.840986 -1.118833  
1 -2.921098 1.138780 1.077129  
1 -3.075810 2.900271 1.122238  
1 -1.662945 2.092888 2.797097  
1 -1.832535 3.269931 -2.673309  
1 -0.368056 5.170786 -2.974979  
1 0.984849 3.381907 -1.538684  
1 1.523434 2.846307 -3.684802  
1 -0.533280 1.021899 -2.678265  
1 1.387682 -0.010028 -1.847835  
1 -1.228031 -0.575568 -1.009959

**4-O(1)-2**

6 -0.987005 -2.123927 0.782588  
6 -0.169553 -0.874275 0.601077  
8 1.110967 -1.132444 0.216718  
6 1.816647 -1.792096 1.269445  
6 1.117943 -3.112166 1.561846  
6 -0.344445 -2.899949 1.916826  
8 -0.799900 -0.165895 -0.515084  
6 -0.442441 1.253740 -0.746355  
6 -0.263083 1.436776 -2.236275  
6 0.016411 2.907272 -2.487026  
6 -1.057172 3.756397 -1.839309  
8 -1.079096 3.489099 -0.465916  
6 -1.507850 2.184065 -0.178435  
8 0.825331 0.714177 -2.728796  
6 -1.690447 2.046043 1.310972  
8 -0.424962 2.063931 1.918058  
8 -0.779369 5.102150 -1.956450  
8 0.016249 3.209072 -3.850097  
6 3.246726 -1.968426 0.798605  
8 4.091185 -2.335539 1.853965  
8 1.804794 -3.734498 2.612401  
8 -0.924377 -4.165297 2.073568  
8 -2.293161 -1.668685 1.009544  
1 3.723631 -3.119970 2.269726  
1 3.275289 -2.697238 -0.014454  
1 3.602065 -1.016664 0.414077  
1 1.813080 -1.162420 2.162974  
1 1.162696 -3.729536 0.659307  
1 1.368139 -4.567496 2.803282  
1 -0.411270 -2.324593 2.842174  
1 -1.585280 -4.143467 2.764608  
1 -0.930100 -2.715461 -0.132751  
1 -2.926833 -2.367872 0.841756  
1 -0.219599 -0.201467 1.459684  
1 0.499211 1.372889 -0.219756  
1 -2.470875 1.991573 -0.663646  
1 -2.221290 1.113957 1.525042  
1 -2.316927 2.870385 1.647099  
1 -0.525539 2.146487 2.865846  
1 -2.037476 3.518436 -2.272064  
1 -0.468079 5.260671 -2.851209  
1 0.972372 3.168897 -2.025790

1 0.745674 2.751141 -4.270575  
1 -1.185331 1.163148 -2.755307  
1 0.554772 -0.170323 -2.974458  
1 -1.760637 -0.356198 -0.471686

**4-O(2)**

8 -0.746544 0.615336 0.346995  
6 -1.126334 -0.733288 0.366069  
6 -0.050116 -1.439871 -0.416828  
6 1.275469 -1.302262 0.273485  
6 1.627647 0.165210 0.386146  
6 0.455821 0.894937 1.048727  
8 -2.312164 -0.886663 -0.296691  
6 -3.489281 -0.435869 0.370587  
6 -4.483731 -1.591651 0.430698  
8 -5.727945 -1.121454 0.895659  
6 -6.300673 -0.178142 0.044648  
6 -5.444127 1.067243 0.058651  
6 -4.056638 0.723825 -0.426680  
6 -4.031788 -2.679683 1.366313  
8 -4.842620 -3.807526 1.158079  
8 -3.282096 1.885136 -0.316309  
8 -6.072981 2.014881 -0.761315  
8 -7.568302 0.069749 0.539811  
8 -0.286700 -2.890789 -0.469592  
8 2.161419 -2.072528 -0.491437  
8 2.793340 0.226654 1.152229  
6 0.606157 2.398816 1.005977  
8 1.826334 2.714746 1.635816  
1 -0.236078 2.859790 1.520024  
1 -4.113965 -2.315299 2.391875  
1 0.604532 2.723473 -0.035025  
1 0.369699 0.556373 2.085013  
1 1.786179 0.575739 -0.615625  
1 2.950125 1.152854 1.366217  
1 1.200216 -1.707522 1.286032  
1 2.967191 -2.232353 0.002710  
1 -0.028017 -1.079903 -1.440516  
1 -0.960877 -3.160973 -1.113093  
1 -1.181623 -1.093739 1.398927  
1 -3.238454 -0.098466 1.378068  
1 -4.593415 -2.009027 -0.575926  
1 -2.985628 -2.911013 1.164024  
1 -6.355151 -0.586946 -0.973156  
1 -7.847275 0.925580 0.204932  
1 -5.389822 1.423029 1.090864  
1 -5.571036 2.830474 -0.731580  
1 -4.121943 0.406254 -1.472804  
1 -2.354155 1.663390 -0.434454  
1 -4.605844 -4.482743 1.792476  
1 2.016350 3.645469 1.523840  
1 0.573704 -3.320829 -0.669328

**4-O(3)**

6 1.540974 0.065476 1.934590  
8 2.180409 -1.034423 1.332203  
6 2.092879 -1.016750 -0.069899  
6 0.640466 -1.211863 -0.467385  
8 -0.603228 1.111187 2.167487  
6 -1.808053 0.914271 2.788375  
8 -2.790337 0.653910 1.771282  
6 -4.092928 0.362054 2.291097  
6 -4.567379 1.617243 2.999301  
6 -3.596071 2.010976 4.086525  
6 -2.205821 2.181320 3.514423  
6 -4.995216 -0.041111 1.138706  
8 -6.192320 -0.593743 1.607905  
8 -5.840078 1.354359 3.527400  
8 -4.071767 3.202753 4.646706  
8 -1.345892 2.443582 4.584184  
6 1.842730 0.060891 3.409507  
8 1.192922 -1.036996 3.998396  
8 2.794140 -2.078513 -0.582676  
8 0.428018 -1.100490 -1.842429  
8 -1.582160 -0.437770 -0.053344  
1 -6.597325 0.039910 2.206659  
1 -5.172322 0.821916 0.493136  
1 -4.506374 -0.812451 0.549298  
1 -4.019377 -0.469721 2.994310  
1 -4.618219 2.427050 2.265687  
1 -6.128591 2.127004 4.017647  
1 -3.571332 1.219223 4.841941  
1 -3.500303 3.447393 5.376325  
1 -2.207884 2.999125 2.791394  
1 -0.546566 2.858560 4.260095  
1 -1.775351 0.053290 3.461345  
1 -0.332293 -0.936060 2.165114  
1 1.918591 1.001657 1.511695  
1 1.496049 1.001569 3.836367  
1 2.924024 0.001626 3.532850  
1 1.370056 -1.039765 4.937882  
1 2.471414 -0.061194 -0.448110  
1 3.730676 -1.878520 -0.594979  
1 0.325222 -2.186299 -0.088232  
1 0.836144 -1.846994 -2.283514  
1 0.022917 0.833452 -0.288175  
1 -2.212849 0.036658 0.648235  
1 -1.840121 -0.302106 -0.975164

**4-O(5)-1**

6 -0.901409 -0.859220 2.430671  
6 -0.500457 -0.593499 0.996192  
8 -0.684550 -1.869562 0.189784  
6 -0.033869 -3.079969 0.710956  
6 -0.522226 -3.294511 2.128230  
6 -0.216386 -2.088273 2.987862  
8 -1.320680 0.310783 0.439081  
6 -0.740076 1.426194 -0.231149  
6 -0.305683 1.111530 -1.640343

6	0.170797	2.406929	-2.274334	8	1.231562	2.667155	-3.166344	1	-5.842925	2.213555	-1.592395
6	-0.897628	3.476424	-2.141623	8	-0.379703	4.856337	-2.307484	1	-0.604059	-0.840630	4.188282
8	-1.202091	3.673684	-0.792656	8	-2.051150	-1.560637	2.171697	1	-6.956857	0.863443	-1.379317
6	-1.789641	2.524728	-0.227790	8	-0.802101	-4.080381	2.421893	1	-4.043557	0.553809	-2.180635
8	0.727541	0.160499	-1.579920	8	1.937887	-4.118786	1.937296	1	-6.061254	-1.394901	-0.996555
6	-2.301743	2.827747	1.159687	6	2.970015	-2.469575	-0.193547	1	-5.988846	-2.283527	-3.047069
8	-1.245336	2.752511	2.098272	8	4.040704	-2.984054	0.541725	1	-3.177679	-1.781663	-1.870076
8	-0.450995	4.694231	-2.617543	1	3.728901	-3.752300	1.027856	1	-3.975596	-3.783283	-1.974946
8	0.435900	2.267830	-3.644872	1	2.623725	-3.167090	-0.958098	1	-4.448341	-1.843238	0.892367
6	-0.312548	-4.229039	-0.242202	1	3.333510	-1.573179	-0.689117	1	-2.535509	-3.156305	0.549570
8	0.600676	-5.260957	-0.020434	1	2.193208	-1.523450	1.569747	1	-2.556986	0.201485	-0.329764
8	0.132574	-4.437527	2.596092	1	0.669947	-3.861855	0.337989	1	-1.367658	1.002545	1.195504
8	-0.682315	-2.392853	4.270799	1	1.453612	-4.866049	2.295431	1	-2.453353	1.002527	4.034482
8	-0.499955	0.236581	3.189640	1	0.234915	-2.388378	2.954231	1	-2.252852	-1.250115	3.670026
1	0.500184	-5.564493	0.885622	1	-1.515232	-3.858497	3.022836	1	-1.657610	3.048229	4.408974
1	-1.344108	-4.568788	-0.131181	1	-1.452758	-2.487768	0.426068	1	0.145015	4.518754	3.781673
1	-0.168903	-3.882589	-1.261660	1	-2.829845	-1.304486	1.677689	1	-0.636410	3.302708	1.558366
1	1.025581	-2.840709	0.685556	1	0.191696	-0.202176	1.620512	1	-2.036915	5.132001	1.644251
1	-1.605159	-3.454516	2.114553	1	0.015623	1.678887	0.582573	1	-3.437862	2.732419	2.589954
1	-0.078621	-4.543763	3.526873	1	-2.443005	1.814152	-1.204541	1	-3.799040	2.540633	0.338442
1	0.864619	-1.923303	3.001845	1	-3.072884	1.347273	1.031913	1	-1.561510	-1.663702	1.538365
1	-0.405978	-1.703554	4.876433	1	-3.380518	3.058174	0.703371	1	-6.330944	0.317486	-3.597427
1	-1.985047	-1.001119	2.465782	1	-2.239018	2.709187	2.716437	1	-0.062582	-1.765869	2.281780
1	-0.908556	1.054336	2.861999	1	-1.385153	3.137738	-2.784630	<b>5-O(1)-1</b>			
1	0.556461	-0.380197	0.866838	1	-1.147126	5.334884	-2.622452	6	-0.710458	-2.617301	0.835756
1	0.114858	1.769236	0.350962	1	1.197253	3.225863	-1.179005	6	-0.078375	-1.288416	0.483978
1	-2.645140	2.216119	-0.837293	1	1.570513	3.531187	-3.404109	8	1.238639	-1.438960	0.163309
1	-3.072085	2.102614	1.414461	1	-0.316738	0.854656	-2.327595	6	1.994927	-1.818756	1.312742
1	-2.746911	3.819428	1.150033	1	1.242912	-0.508324	-0.629703	6	1.495865	-3.176345	1.780528
1	-1.386646	3.392451	2.794603	1	1.972302	0.602695	-2.110071	6	0.005564	-3.150401	2.064436
1	-1.805362	3.160308	-2.673566	<b>4-O(6)</b>			8	-0.782188	-0.787565	-0.717907	
1	0.020458	4.523900	-3.437132	6	-3.652753	-1.574543	0.197860	6	-0.087265	-0.528937	-1.991422
1	1.057156	2.757340	-1.741199	6	-3.427534	-0.083223	0.272123	6	-1.135559	-0.825675	-3.036982
1	1.314094	1.909211	-3.769423	8	-4.563240	0.596927	-0.181033	6	-0.486777	-0.659986	-4.396302
1	-1.155041	0.721810	-2.204895	6	-4.890180	0.309520	-1.531001	6	0.082482	0.749715	-4.465370
1	0.686516	-0.416064	-2.341658	6	-5.213386	-1.172975	-1.649396	8	0.985369	0.950280	-3.416236
1	-1.614862	-1.982777	-0.064104	6	-4.016872	-1.990143	-1.203345	6	0.386747	0.907291	-2.144175
<b>4-O(5)-2</b>			8	-3.226033	0.234757	1.599473	8	-1.612279	-2.114276	-2.752554	
8	0.857613	-1.311852	-0.003185	6	-2.187836	1.136430	1.903690	6	1.424666	1.364831	-1.150744
6	-0.261675	-0.770762	0.807643	6	-2.619507	2.584436	1.879527	8	0.778969	1.478552	0.091384
6	-1.045359	-1.969963	1.295527	6	-1.428735	3.416951	2.303411	8	0.807643	0.946526	-5.621342
6	-0.134314	-2.905586	2.063454	6	-0.888477	2.925077	3.634838	8	-1.416759	-0.778738	-5.434843
6	1.043153	-3.322137	1.213007	8	-0.543959	1.569985	3.547426	6	3.453733	-1.834117	0.899993
6	1.819572	-2.113110	0.733102	6	-1.680472	0.784566	3.290321	8	4.299362	-1.914959	2.013265
8	-1.021345	-0.005467	-0.007797	8	-2.996190	3.002658	0.596697	8	2.222562	-3.526842	2.926467
6	-0.575340	1.321819	-0.260880	6	-1.363425	-0.680675	3.433807	8	-0.366767	-4.465691	2.359455
6	-1.796526	2.219458	-0.419421	8	-0.843855	-1.211297	2.176719	8	-2.098640	-2.505484	0.940926
8	-1.355658	3.510304	-0.768967	8	0.271015	3.588165	3.983594	1	4.037761	-2.681289	2.530674
6	-0.719632	3.556926	-2.022200	8	-1.749058	4.768705	2.482846	1	3.625654	-2.655418	0.200689
6	0.567003	2.759923	-1.940007	6	-6.061064	1.197122	-1.908584	1	3.678613	-0.901707	0.390102
6	0.237478	1.350259	-1.529711	8	-6.263067	1.227459	-3.295532	1	1.856630	-1.074900	2.101771
6	-2.599732	2.311929	0.850357	8	-5.544348	-1.437136	-2.989982	1	1.673583	-3.900530	0.979882
8	-1.738687	2.665125	1.903065	8	-4.289847	-3.368048	-1.172826	1	1.915931	-4.384517	3.227993
8	1.450163	0.627879	-1.300696	8	-2.440972	-2.199979	0.597253	1	-0.179495	-2.494763	2.919929



1 -1.223174 -4.477422 2.786760  
1 -0.528684 -3.304821 0.009166  
1 -2.348740 -1.990920 1.712208  
1 -0.238468 -0.500932 1.218289  
1 0.743385 -1.224641 -2.044875  
1 -0.472767 1.581653 -2.093143  
1 2.244580 0.647695 -1.114477  
1 1.809523 2.324438 -1.494344  
1 1.414040 1.753824 0.751416  
1 -0.735510 1.477411 -4.384883  
1 0.268880 0.644638 -6.356913  
1 0.333590 -1.369448 -4.510442  
1 -1.426422 -1.674705 -5.769394  
1 -1.948909 -0.100143 -2.950729  
1 -2.473521 -2.246305 -3.152223  
1 -1.525618 -1.403133 -0.921602

**5-O(1)-2**

6 -0.726126 -1.688207 1.191972  
6 0.375726 -0.802660 0.642820  
8 1.410211 -1.534152 0.129038  
6 2.064546 -2.334440 1.104699  
6 1.062653 -3.346486 1.626637  
6 -0.131101 -2.634781 2.219689  
8 -0.211077 -0.030855 -0.459440  
6 0.320471 -0.124016 -1.827507  
6 -0.464461 -1.136315 -2.620409  
6 0.063299 -1.091018 -4.048466  
6 -0.015204 0.324942 -4.591766  
8 0.703647 1.187121 -3.750933  
6 0.135725 1.247476 -2.477096  
8 -0.324511 -2.401778 -2.047837  
6 0.797252 2.356448 -1.690390  
8 0.226423 2.334769 -0.374835  
8 0.580583 0.430036 -5.830295  
8 -0.706053 -1.905065 -4.892318  
6 3.256422 -2.973561 0.419480  
8 4.130865 -3.555352 1.347047  
8 1.708705 -4.144556 2.583124  
8 -1.045819 -3.624067 2.603301  
8 -1.796488 -0.944979 1.695373  
1 3.624030 -4.167237 1.887300  
1 2.905595 -3.701353 -0.315711  
1 3.808623 -2.199640 -0.106096  
1 2.423864 -1.704642 1.923377  
1 0.721310 -3.957414 0.785918  
1 1.068524 -4.761445 2.943495  
1 0.204088 -2.068220 3.095167  
1 -1.763434 -3.224328 3.095662  
1 -1.111750 -2.270525 0.356641  
1 -1.531000 -0.462620 2.480931  
1 0.714933 -0.053280 1.361834  
1 1.371385 -0.380813 -1.755620  
1 -0.935409 1.464944 -2.549385  
1 1.862981 2.184034 -1.580590

1 0.631826 3.318053 -2.162127  
1 -0.480300 2.978394 -0.284142  
1 -1.062542 0.651056 -4.629125  
1 0.239571 -0.282563 -6.376449  
1 1.110767 -1.395485 -4.056816  
1 -0.271008 -2.746275 -5.023945  
1 -1.514923 -0.832570 -2.623227  
1 -0.997704 -2.977891 -2.412112  
1 -0.149186 1.005384 -0.233141

**5-O(2)**

6 -0.532672 -1.962315 1.007738  
6 0.391165 -0.848962 0.533031  
6 1.676542 -1.460152 0.027062  
6 1.358037 -2.464653 -1.056702  
6 0.350262 -3.472379 -0.545975  
8 -0.799722 -2.796754 -0.096180  
8 0.653030 0.014685 1.631460  
6 0.768770 1.389508 1.442415  
6 2.183033 1.796410 1.785281  
6 2.358692 3.279426 1.693317  
6 2.027328 3.712602 0.281188  
6 0.646233 3.163330 -0.089347  
8 0.602428 1.761218 0.119612  
8 2.474756 1.459514 3.190687  
6 0.319392 3.350401 -1.553806  
8 0.407470 4.729367 -1.831735  
8 2.059328 5.109410 0.280756  
8 3.678864 3.524861 2.094390  
8 2.521196 -0.447139 -0.447791  
8 2.568239 -3.071913 -1.418898  
8 0.007433 -4.289492 -1.598426  
6 -1.857069 -1.459038 1.546190  
8 -1.751905 -1.027544 2.878767  
1 0.330717 4.874451 -2.773996  
1 1.034535 2.781948 -2.148844  
1 -0.682218 2.970252 -1.749646  
1 -0.107726 3.659745 0.528255  
1 2.771973 3.296950 -0.404475  
1 1.701898 5.406438 -0.563532  
1 1.658122 3.775389 2.370941  
1 3.798054 4.460967 2.261690  
1 2.878982 1.239243 1.163545  
1 0.042215 1.890268 2.088470  
1 -0.102267 -0.297074 -0.262525  
1 -0.040319 -2.535807 1.801224  
1 -2.249770 -0.669133 0.901783  
1 -2.561612 -2.285740 1.534432  
1 -1.046784 -0.380736 2.926364  
1 0.775339 -4.046631 0.284606  
1 -0.422372 -5.080387 -1.271656  
1 0.909616 -1.946394 -1.908642  
1 2.413480 -3.641113 -2.173749  
1 2.156954 -1.986933 0.858917  
1 3.295201 -0.870450 -0.824883

1 3.277926 1.943008 3.469631  
1 2.570413 0.506439 3.347110

**5-O(3)**

6 -0.724050 -1.643125 1.207519  
6 0.400217 -0.847494 0.565015  
8 1.349239 -1.744860 0.006407  
6 2.014637 -2.531035 1.006867  
6 0.971260 -3.413409 1.664187  
6 -0.132085 -2.568706 2.258453  
8 -0.087513 0.014349 -0.417739  
6 0.359282 -0.071071 -1.749001  
6 -0.274121 -1.192547 -2.535836  
6 0.209586 -1.162095 -3.959943  
6 -0.161449 0.182424 -4.558250  
8 0.438022 1.185081 -3.772450  
6 -0.047981 1.225727 -2.452828  
8 0.079545 -2.490737 -1.967177  
6 0.530815 2.459215 -1.783111  
8 -0.210965 2.852018 -0.661101  
8 0.367099 0.221031 -5.821486  
8 -0.377446 -2.260540 -4.589333  
6 3.133752 -3.304754 0.335688  
8 4.024826 -3.816020 1.286299  
8 1.620227 -4.176978 2.643937  
8 -1.088808 -3.454081 2.768313  
8 -1.718390 -0.821714 1.742961  
1 3.524678 -4.362061 1.898716  
1 2.718954 -4.098928 -0.289753  
1 3.692468 -2.625063 -0.301448  
1 2.451375 -1.847749 1.736496  
1 0.535656 -4.068452 0.902948  
1 0.965319 -4.715387 3.093068  
1 0.296825 -1.964891 3.066209  
1 -1.773911 -2.955179 3.215627  
1 -1.212790 -2.240060 0.437572  
1 -1.355861 -0.267390 2.437032  
1 0.924617 -0.241886 1.307301  
1 1.445848 -0.152137 -1.784980  
1 -1.139087 1.313471 -2.447442  
1 1.580689 2.291927 -1.533654  
1 0.480023 3.272977 -2.500561  
1 -0.203490 2.131899 -0.029127  
1 -1.246948 0.322484 -4.565187  
1 -0.050419 0.914469 -6.333487  
1 1.300211 -1.229752 -3.982778  
1 0.022024 -2.383984 -5.452116  
1 -1.358309 -1.152746 -2.480897  
1 0.266422 -3.159296 -2.646255  
1 0.750339 -2.398113 -1.195248

**5-O(5)-1**

6 -0.738492 -1.674224 1.144953  
6 0.363000 -0.809055 0.552153  
8 1.416764 -1.706502 0.044900  
6 2.050221 -2.551006 1.070918

6	0.963203	-3.435152	1.645248	8	0.466922	1.207294	-3.760715	6	3.262640	-2.974789	0.430646
6	-0.166886	-2.601381	2.208785	6	-0.043616	1.261246	-2.450118	8	4.140954	-3.523680	1.376000
8	-0.099939	0.004563	-0.448165	8	0.092521	-2.404083	-1.874127	8	1.728614	-4.101894	2.625788
6	0.380445	-0.024382	-1.788326	6	0.532172	2.493345	-1.776947	8	-1.032520	-3.587268	2.648864
6	-0.192834	-1.178970	-2.581838	8	-0.261551	2.933713	-0.706847	8	-1.800089	-0.957734	1.689500
6	0.202098	-1.034184	-4.036888	8	0.345864	0.356119	-5.807771	1	3.634176	-4.115123	1.938774
6	-0.213735	0.337285	-4.535505	8	-0.449002	-2.109080	-4.748719	1	2.922128	-3.726578	-0.285271
8	0.400426	1.314345	-3.751710	6	3.230617	-3.132349	0.355026	1	3.809725	-2.211183	-0.115219
6	-0.054716	1.293503	-2.421789	8	4.034345	-3.871281	1.222848	1	2.413074	-1.670856	1.893890
8	0.327050	-2.386694	-2.048077	8	1.511253	-4.374548	2.281230	1	0.733779	-3.973393	0.827108
6	0.514690	2.513078	-1.718882	8	-1.102937	-3.562014	2.506291	1	1.095232	-4.713868	3.005432
8	-0.241089	2.884597	-0.597905	8	-1.731233	-0.841488	1.784289	1	0.220730	-2.016511	3.078564
8	0.222389	0.557004	-5.826941	1	3.490673	-4.545445	1.639227	1	-1.788709	-3.155172	3.048374
8	-0.437527	-1.998418	-4.829700	1	2.798287	-3.744279	-0.437242	1	-1.118227	-2.291221	0.357663
6	3.212170	-3.295219	0.435720	1	3.870274	-2.382706	-0.105655	1	-1.512744	-0.422144	2.431692
8	4.064603	-3.768198	1.435042	1	2.516942	-1.970476	2.031167	1	0.735034	-0.095184	1.341650
8	1.574102	-4.215846	2.629538	1	0.569201	-3.792565	0.544716	1	1.362091	-0.378727	-1.763545
8	-1.128170	-3.509151	2.659950	1	0.788834	-4.912374	2.615074	1	-0.959847	1.459812	-2.502860
8	-1.776539	-0.888270	1.638951	1	0.270096	-2.140564	3.077001	1	1.830411	2.169437	-1.497981
1	3.571823	-4.378176	1.990076	1	-1.799018	-3.146281	3.017013	1	0.623492	3.317267	-2.153799
1	2.843951	-4.102462	-0.199694	1	-1.116969	-2.104731	0.367127	1	-0.127323	1.369650	-0.180220
1	3.780475	-2.602297	-0.177768	1	-1.434463	-0.388688	2.576711	1	-1.097285	0.673218	-4.601508
1	2.431934	-1.849894	1.808022	1	0.690459	0.115455	1.391816	1	0.242290	-0.251720	-6.354400
1	0.560653	-4.071898	0.850823	1	1.410651	-0.128327	-1.758519	1	1.110909	-1.344782	-4.064337
1	0.901974	-4.762302	3.043431	1	-1.133467	1.362886	-2.471600	1	-0.266307	-2.722447	-5.018835
1	0.223712	-2.007204	3.041652	1	1.561435	2.308026	-1.461903	1	-1.521482	-0.836247	-2.623172
1	-1.820246	-3.039356	3.127412	1	0.544498	3.293389	-2.511221	1	-1.012373	-2.975164	-2.452917
1	-1.168853	-2.272316	0.341582	1	-0.340868	2.222902	-0.070622	1	0.520047	2.856054	0.292908
1	-1.479291	-0.358635	2.382261	1	-1.235240	0.365091	-4.508027	<b>6-O(1)-1</b>			
1	0.880866	-0.215955	1.303900	1	0.161420	-0.461443	-6.277232	6	-0.793700	-2.079941	1.580457
1	1.470711	-0.066776	-1.792741	1	1.273130	-1.268115	-3.983781	6	-0.123531	-1.131074	0.603029
1	-1.146911	1.361511	-2.392119	1	0.085032	-2.900634	-4.798853	8	0.998899	-1.691286	0.060970
1	1.561808	2.344882	-1.458860	1	-1.370129	-1.096986	-2.483814	6	2.034946	-1.934012	1.009930
1	0.470166	3.341966	-2.419188	1	-0.481516	-3.108318	-2.177174	6	1.513903	-2.982892	1.969861
1	-0.227964	2.163551	0.031720	1	2.278091	-0.771767	0.043585	6	0.241228	-2.495226	2.625536
1	-1.304314	0.444758	-4.467222	<b>5-O(6)</b>				8	-0.948283	-0.972631	-0.630086
1	-0.045720	-0.198911	-6.355016	6	-0.724161	-1.693694	1.177329	6	-2.316869	-0.382531	-0.568187
1	1.286403	-1.104120	-4.127201	6	0.364358	-0.807139	0.596833	6	-2.238738	1.051010	-1.022261
1	0.175294	-2.694645	-5.061330	8	1.399469	-1.568823	0.096642	6	-3.650677	1.614851	-0.969591
1	-1.279158	-1.177344	-2.488209	6	2.061726	-2.327526	1.091675	6	-4.575176	0.712322	-1.768123
1	-0.221571	-3.140447	-2.272720	6	1.073041	-3.334936	1.647857	8	-4.528096	-0.583338	-1.240067
1	1.088950	-2.172990	-0.727452	6	-0.119934	-2.611239	2.223066	6	-3.276091	-1.198252	-1.418563
<b>5-O(5)-2</b>				8	-0.210217	-0.035100	-0.461286	8	-1.347254	1.702705	-0.164156
6	-0.691789	-1.581745	1.220732	6	0.305699	-0.130145	-1.799123	6	-3.411496	-2.658618	-1.019059
6	0.343273	-0.612242	0.661984	6	-0.468543	-1.132827	-2.626834	8	-2.496128	-3.480196	-1.692134
8	1.561304	-1.387917	0.265824	6	0.057638	-1.059786	-4.052541	8	-5.889857	1.113302	-1.660491
6	2.119605	-2.456522	1.143071	6	-0.045583	0.359683	-4.577916	8	-3.711042	2.892474	-1.538041
6	0.967576	-3.372766	1.473299	8	0.667212	1.221470	-3.730508	6	3.252438	-2.384004	0.227100
6	-0.130497	-2.614065	2.175845	6	0.112314	1.239442	-2.450729	8	4.394722	-2.408696	1.036876
8	-0.190192	0.017972	-0.430566	8	-0.326276	-2.414830	-2.089174	8	2.507990	-3.234737	2.924282
6	0.325465	-0.044799	-1.755950	6	0.778461	2.355570	-1.683373	8	-0.239840	-3.551100	3.404783
6	-0.282786	-1.209007	-2.506608	8	0.064605	2.374149	-0.408970	8	-1.950310	-1.568551	2.171205
6	0.189021	-1.147930	-3.947483	8	0.536873	0.490337	-5.820194	1	4.207319	-2.959280	1.801708
6	-0.147534	0.213196	-4.525633	8	-0.691760	-1.872012	-4.918307	1	3.054534	-3.358566	-0.224686

1 3.434759 -1.670097 -0.571005  
1 2.276822 -1.012622 1.544894  
1 1.287584 -3.889546 1.401603  
1 2.177975 -3.891966 3.540388  
1 0.486652 -1.632856 3.254201  
1 -0.892238 -3.233053 4.029097  
1 -1.091965 -2.974588 1.035561  
1 -1.737044 -0.896187 2.822655  
1 0.025161 -0.121007 0.985950  
1 -2.577202 -0.428296 0.482876  
1 -2.976492 -1.161961 -2.470297  
1 -3.350886 -2.775250 0.064231  
1 -4.402595 -2.975003 -1.329972  
1 -1.620646 -3.399030 -1.317425  
1 -4.255995 0.686646 -2.818025  
1 -5.916288 2.062079 -1.808311  
1 -3.998170 1.623105 0.064240  
1 -3.669422 3.561285 -0.855661  
1 -1.888913 1.101671 -2.058135  
1 -1.038995 2.514598 -0.568027  
1 -0.385724 -0.526347 -1.267234

**6-O(1)-2**

6 -0.692846 -1.916844 1.847125  
6 -0.210758 -1.363945 0.521403  
8 0.776665 -2.150729 -0.016885  
6 1.961264 -2.186165 0.770738  
6 1.617422 -2.791040 2.119388  
6 0.516846 -1.987386 2.769665  
8 -1.231398 -1.418884 -0.522026  
6 -2.526014 -0.724498 -0.437582  
6 -2.319449 0.764136 -0.402597  
6 -3.662927 1.444546 -0.581768  
6 -4.364437 0.935737 -1.823973  
8 -4.505855 -0.467892 -1.709017  
6 -3.276115 -1.126914 -1.707667  
8 -1.746469 1.130417 0.825184  
6 -3.549493 -2.617240 -1.756562  
8 -2.316358 -3.320326 -1.619344  
8 -5.609860 1.504437 -1.859022  
8 -3.385964 2.812645 -0.644274  
6 2.978709 -2.997169 -0.007128  
8 4.262565 -2.869035 0.539175  
8 2.783743 -2.794127 2.899822  
8 0.188422 -2.617636 3.974262  
8 -1.732401 -1.185703 2.427061  
1 4.212272 -3.092362 1.472362  
1 2.658290 -4.040918 -0.044888  
1 3.019227 -2.617756 -1.024208  
1 2.344448 -1.171122 0.905553  
1 1.259825 -3.812970 1.962271  
1 2.569691 -3.148237 3.765117  
1 0.887959 -0.974605 2.959252  
1 -0.490020 -2.103160 4.415125  
1 -1.065845 -2.928511 1.689939

1 -1.603662 -0.240028 2.290930  
1 0.068636 -0.313588 0.579421  
1 -3.033295 -1.080514 0.454165  
1 -2.675843 -0.836980 -2.576515  
1 -4.184281 -2.908369 -0.925003  
1 -4.041915 -2.876329 -2.687423  
1 -1.984560 -3.599462 -2.474736  
1 -3.785374 1.163522 -2.724128  
1 -5.984183 1.428619 -2.737378  
1 -4.299703 1.207812 0.274263  
1 -4.206056 3.302428 -0.571868  
1 -1.663586 1.055076 -1.227753  
1 -1.739571 2.089759 0.878706  
1 -1.408924 -2.329782 -0.894515

**6-O(2)**

6 -0.689253 -2.093898 1.680798  
6 -0.276972 -1.174703 0.530819  
8 0.825963 -1.839292 0.001095  
6 1.970460 -1.906549 0.830541  
6 1.664918 -2.821928 2.011485  
6 0.418306 -2.298498 2.683119  
8 -1.151186 -1.151812 -0.543374  
6 -2.436678 -0.556658 -0.458027  
6 -2.366672 0.948812 -0.659754  
6 -3.762054 1.516150 -0.834400  
6 -4.510429 0.750597 -1.905460  
8 -4.539825 -0.603323 -1.575860  
6 -3.252516 -1.170694 -1.592771  
8 -1.665294 1.629900 0.352505  
6 -3.402307 -2.676447 -1.487025  
8 -2.270964 -3.353766 -1.968972  
8 -5.831244 1.151258 -1.988281  
8 -3.740470 2.855207 -1.246087  
6 3.071080 -2.440579 -0.058370  
8 4.209306 -2.626714 0.751553  
8 2.666242 -2.818055 2.984878  
8 -0.141468 -3.170128 3.630159  
8 -1.852868 -1.634426 2.488905  
1 4.891032 -3.073722 0.251483  
1 2.740705 -3.382729 -0.496922  
1 3.265842 -1.729190 -0.859568  
1 2.237352 -0.912449 1.199513  
1 1.474567 -3.832292 1.637000  
1 3.502736 -2.983796 2.537316  
1 0.671820 -1.342831 3.151945  
1 0.372911 -3.154049 4.438730  
1 -1.042710 -3.037869 1.279875  
1 -1.741850 -0.754861 2.886000  
1 -0.028070 -0.166082 0.868556  
1 -2.925803 -0.807411 0.483478  
1 -2.755849 -0.948600 -2.543803  
1 -3.631740 -2.962413 -0.457770  
1 -4.240824 -2.971752 -2.111225  
1 -1.498615 -2.996573 -1.526745

1 -4.001606 0.881405 -2.869708  
1 -5.845863 2.111256 -1.988725  
1 -4.325230 1.406044 0.098364  
1 -3.253886 3.377096 -0.606713  
1 -1.798225 1.131888 -1.571976  
1 -2.193682 1.677554 1.152054  
1 -1.916400 -2.272338 3.234502

**6-O(3)**

6 -0.792720 -2.078952 1.658538  
6 -0.238044 -1.176199 0.557366  
8 0.881521 -1.782827 -0.000707  
6 1.958986 -1.945195 0.897700  
6 1.530621 -2.937352 1.960314  
6 0.300845 -2.415161 2.658548  
8 -1.082745 -1.054999 -0.557402  
6 -2.357409 -0.477066 -0.436563  
6 -2.374995 0.952316 -0.904941  
6 -3.761829 1.524457 -1.015870  
6 -4.601053 0.613781 -1.896722  
8 -4.565847 -0.679764 -1.344361  
6 -3.280557 -1.242898 -1.391664  
8 -1.595827 1.846681 0.001647  
6 -3.369581 -2.711076 -1.013260  
8 -2.301275 -3.453977 -1.537823  
8 -5.883210 1.092386 -1.857854  
8 -3.586392 2.811805 -1.526299  
6 3.147674 -2.419739 0.085497  
8 4.336500 -2.376613 0.828691  
8 2.592644 -3.116850 2.862699  
8 -0.117824 -3.404151 3.559722  
8 -1.910891 -1.545429 2.322883  
1 4.189206 -2.857803 1.647291  
1 2.948541 -3.424596 -0.295073  
1 3.272639 -1.755482 -0.765090  
1 2.212042 -0.987984 1.364691  
1 1.283200 -3.883281 1.470012  
1 2.309184 -3.724358 3.548433  
1 0.580938 -1.504497 3.201633  
1 -0.873379 -3.082065 4.053278  
1 -1.133881 -3.002001 1.189490  
1 -1.653096 -0.781991 2.844569  
1 0.018247 -0.185282 0.951046  
1 -2.754448 -0.575021 0.571035  
1 -2.874395 -1.181055 -2.406995  
1 -3.433525 -2.814082 0.073238  
1 -4.281957 -3.112285 -1.444429  
1 -1.482399 -3.015143 -1.298144  
1 -4.204434 0.586336 -2.916297  
1 -6.390258 0.736797 -2.588509  
1 -4.246303 1.544373 -0.036928  
1 -4.391677 3.319108 -1.415145  
1 -1.827871 1.058100 -1.837109  
1 -1.879423 1.838101 0.930547  
1 -1.665545 2.762960 -0.328051

**6-O(5)-1**

6 -0.750185 -1.877625 1.804777  
6 -0.328524 -1.310482 0.455817  
8 0.820561 -2.127291 -0.012872  
6 2.014023 -2.166039 0.860243  
6 1.575117 -2.726929 2.195462  
6 0.442696 -1.897338 2.753781  
8 -1.207026 -1.451332 -0.582566  
6 -2.477356 -0.792138 -0.509359  
6 -2.318020 0.712533 -0.443637  
6 -3.671012 1.377367 -0.591264  
6 -4.366067 0.874814 -1.839766  
8 -4.487524 -0.512836 -1.742292  
6 -3.243624 -1.172471 -1.773876  
8 -1.738559 1.063204 0.792921  
6 -3.553710 -2.654556 -1.897301  
8 -2.486866 -3.394654 -2.424236  
8 -5.651201 1.369126 -1.942818  
8 -3.566375 2.776076 -0.556809  
6 3.108519 -2.945581 0.152773  
8 4.338536 -2.652262 0.742595  
8 2.707150 -2.689718 3.014953  
8 0.081975 -2.476349 3.971418  
8 -1.801996 -1.170072 2.387363  
1 4.305509 -2.917603 1.665446  
1 2.889429 -4.014452 0.176778  
1 3.159260 -2.623203 -0.883210  
1 2.308805 -1.123310 0.941749  
1 1.231772 -3.758877 2.066938  
1 2.458997 -2.994735 3.890546  
1 0.798898 -0.873123 2.905748  
1 -0.649828 -1.976194 4.339243  
1 -1.103251 -2.898488 1.652606  
1 -1.743161 -0.229656 2.171039  
1 0.095642 -0.312433 0.524712  
1 -3.023732 -1.150838 0.360830  
1 -2.669348 -0.864326 -2.653388  
1 -3.883962 -3.053096 -0.936509  
1 -4.377105 -2.746764 -2.599511  
1 -1.794259 -3.447344 -1.768831  
1 -3.782989 1.120768 -2.737812  
1 -5.655640 2.268623 -1.606957  
1 -4.293601 1.105845 0.260384  
1 -3.038402 3.090555 -1.294713  
1 -1.659924 1.026881 -1.259919  
1 -1.778266 2.017157 0.897861  
1 0.541286 -2.988142 -0.364527

**6-O(5)-2**

6 -0.704604 -1.905523 1.835504  
6 -0.321329 -1.289439 0.502742  
8 0.795419 -2.137108 0.003903  
6 2.041170 -2.136905 0.803709  
6 1.628169 -2.735737 2.130998  
6 0.508847 -1.935456 2.754126

8 -1.213847 -1.417520 -0.522954  
6 -2.474545 -0.742311 -0.457965  
6 -2.313438 0.756061 -0.347657  
6 -3.652246 1.434390 -0.524229  
6 -4.297987 0.977540 -1.812468  
8 -4.433712 -0.422841 -1.766143  
6 -3.197580 -1.092985 -1.754722  
8 -1.773992 1.075839 0.915405  
6 -3.508584 -2.572630 -1.901477  
8 -2.400255 -3.332038 -2.301174  
8 -5.546290 1.547293 -1.879007  
8 -3.396763 2.810488 -0.503323  
6 3.092097 -2.947516 0.063438  
8 4.345900 -2.684610 0.614989  
8 2.779725 -2.732336 2.923061  
8 0.194000 -2.562632 3.960907  
8 -1.759161 -1.225937 2.444726  
1 4.332561 -2.950139 1.538471  
1 2.837823 -4.007348 0.096992  
1 3.133974 -2.636944 -0.978073  
1 2.364143 -1.102787 0.901876  
1 1.277637 -3.757827 1.961131  
1 2.548668 -3.063134 3.794014  
1 0.857928 -0.913170 2.931360  
1 -0.523798 -2.080461 4.376685  
1 -1.041002 -2.925511 1.650994  
1 -1.712714 -0.278630 2.258431  
1 0.076029 -0.280660 0.593526  
1 -3.041685 -1.123446 0.389787  
1 -2.581102 -0.778468 -2.603404  
1 -3.943724 -2.953264 -0.975238  
1 -4.254301 -2.666887 -2.685558  
1 -1.750991 -3.323360 -1.598557  
1 -3.682466 1.252352 -2.675690  
1 -5.886781 1.488120 -2.772153  
1 -4.313689 1.143987 0.296130  
1 -4.230177 3.281323 -0.466577  
1 -1.636578 1.100209 -1.135038  
1 -1.799983 2.030131 1.023301  
1 0.940832 -1.943525 -0.938551

**6-O(6)**

6 -0.717144 -1.894357 1.822044  
6 -0.248764 -1.390048 0.466476  
8 0.747625 -2.228419 -0.014252  
6 1.927746 -2.205929 0.766577  
6 1.595507 -2.750420 2.143639  
6 0.487732 -1.925687 2.748243  
8 -1.227989 -1.478094 -0.551159  
6 -2.460673 -0.759182 -0.476470  
6 -2.282693 0.739201 -0.441688  
6 -3.631167 1.402907 -0.640738  
6 -4.302202 0.912251 -1.912540  
8 -4.423449 -0.494656 -1.833984  
6 -3.185535 -1.133529 -1.768251

8 -1.738516 1.126514 0.795137  
6 -3.483214 -2.614623 -1.852469  
8 -2.185069 -3.289798 -1.853104  
8 -5.550715 1.448543 -2.092678  
8 -3.374958 2.777916 -0.675414  
6 2.962195 -3.034840 0.031696  
8 4.242384 -2.873535 0.581477  
8 2.761407 -2.707067 2.927888  
8 0.154926 -2.492596 3.985646  
8 -1.750346 -1.147580 2.403686  
1 4.180652 -3.039063 1.526133  
1 2.653933 -4.083242 0.033059  
1 3.007457 -2.697304 -1.000023  
1 2.296967 -1.179482 0.857325  
1 1.248887 -3.782413 2.034855  
1 2.547503 -3.021615 3.808134  
1 0.854240 -0.902579 2.889567  
1 -0.577873 -1.994187 4.352813  
1 -1.090756 -2.910442 1.693544  
1 -1.652864 -0.213255 2.183328  
1 0.101902 -0.357707 0.521176  
1 -3.032633 -1.092982 0.387279  
1 -2.555220 -0.848503 -2.617289  
1 -4.056902 -2.961110 -1.000568  
1 -3.968766 -2.869324 -2.784781  
1 -1.557165 -2.752533 -1.237408  
1 -3.712840 1.186243 -2.789220  
1 -6.107100 1.235383 -1.339594  
1 -4.273713 1.143373 0.206309  
1 -4.195387 3.262316 -0.579768  
1 -1.614375 1.039497 -1.253892  
1 -1.784886 2.084438 0.854423  
1 -2.231549 -4.226611 -1.621706

**TS(10-17) – 1 imaginary frequency**

8 -3.113802 -0.033999 -1.419403  
6 -2.893413 -0.637107 -0.241778  
6 -3.597559 -1.957591 0.021056  
6 -5.051369 -1.989191 -0.468266  
6 -5.383780 -0.784229 -1.316668  
6 -4.219599 -0.463421 -2.224267  
8 -3.354674 0.308065 0.886685  
6 -2.361515 1.216546 1.472723  
6 -1.555466 0.628742 2.620674  
8 -0.730363 1.687336 3.043196  
6 -1.427246 2.781492 3.604198  
6 -2.293584 3.431826 2.538744  
6 -3.199134 2.368903 1.970495  
6 -0.618648 -0.511626 2.266940  
8 -1.314377 -1.692502 1.958146  
8 -3.959606 2.773802 0.862641  
8 -3.109187 4.429792 3.072900  
8 -0.516567 3.715912 4.023983  
8 -2.878696 -2.937049 -0.676088

8	-5.984965	-2.007052	0.576821	1	2.473188	2.714857	-0.045903	1	-4.681678	-1.648073	0.348947
8	-6.516279	-0.999230	-2.109411	1	0.118151	3.596234	-0.001458	1	-2.761894	-2.369613	1.280638
6	-4.500813	0.670791	-3.190588	1	0.002442	2.005630	2.586694	1	-2.112647	-0.309520	-0.559984
8	-5.296473	0.249396	-4.262088	1	-0.911890	4.097459	3.161632	1	-1.191222	0.630050	1.108089
1	-3.554678	1.010791	-3.602293	1	-2.150139	3.112439	0.753285	1	-2.927188	0.933533	3.604274
1	0.061447	-0.651586	3.104205	1	-3.497411	2.566981	2.469137	1	-0.690685	-1.001607	2.861756
1	-4.955183	1.505093	-2.651003	1	-1.747690	0.334387	1.860088	1	-2.156031	3.076633	3.984713
1	-3.914872	-1.349066	-2.783137	1	-3.208286	-0.073192	0.124960	1	-0.082971	4.352942	3.978083
1	-5.557896	0.077591	-0.660708	1	-1.159102	0.448627	-0.961957	1	-0.143571	2.959470	1.707788
1	-7.265322	-1.180310	-1.538675	1	0.598251	-0.837519	-1.490067	1	-1.181104	4.923840	1.141678
1	-5.144059	-2.874954	-1.097860	1	-0.642541	-3.292756	-0.155993	1	-3.171585	2.863261	1.698253
1	-6.056363	-2.890333	0.939023	1	-2.345760	-3.102791	-1.984170	1	-2.872723	2.711137	-0.482854
1	-3.583808	-2.130350	1.093045	1	-1.821603	-1.449522	-2.274362	1	-3.287620	-1.727129	3.634131
1	-2.058068	-3.108868	-0.208133	1	-3.009359	-2.455876	0.071145	1	-4.051937	0.531800	1.403860
1	-1.830386	-0.698653	-0.051524	1	1.143365	-4.633008	-0.877118	1	-7.778525	0.078335	-1.994757
1	-1.707265	1.532992	0.662417	1	2.003568	-4.054364	-3.477051	<b>17</b>			
1	-2.232368	0.312421	3.419856	1	2.598980	-2.213860	-2.033055	6	-0.222001	-4.150602	-5.901474
1	-0.021254	-0.244003	1.397266	1	3.966874	-3.915975	-1.340448	6	-0.020189	-4.524830	-4.439184
1	-2.050022	2.421594	4.429487	1	1.479664	-2.717715	0.740358	8	0.399881	-3.510409	-3.650921
1	-0.139278	3.455372	4.865018	1	0.699988	-0.398057	0.961335	6	0.400551	-2.176344	-4.162521
1	-1.639548	3.821840	1.755168	1	3.187609	-1.258699	0.866186	6	-0.859654	-1.876385	-4.956077
1	-2.554194	5.145404	3.386506	<b>TS(10-19) – 1 imaginary</b>				6	-1.196821	-2.983124	-5.966845
1	-3.859345	2.014343	2.767031	<b>frequency</b>				8	-1.381898	-4.980300	-3.996272
1	-4.685880	3.331145	1.147183	8	-3.802611	0.544263	-1.212459	6	-1.613138	-5.211571	-2.577967
1	-1.534538	-2.157413	2.765134	6	-3.181740	-0.290440	-0.373303	6	-1.814950	-6.697874	-2.305542
1	-4.048358	0.922185	0.546631	6	-3.755611	-1.677840	-0.234369	8	-2.140996	-6.831619	-0.944320
1	-6.121492	-0.081385	-3.898834	6	-4.083677	-2.122631	-1.642987	6	-3.356927	-6.217251	-0.583080
<b>TS(10-18) – 1 imaginary</b>				6	-5.245526	-1.286903	-2.127478	6	-3.208650	-4.721074	-0.757579
<b>frequency</b>				6	-5.030579	0.210685	-1.896898	6	-2.838174	-4.423063	-2.191906
6	1.697403	-2.056049	-0.102801	8	-3.185178	0.292763	1.047182	6	-0.576272	-7.552811	-2.502281
6	0.408031	-1.482945	-0.634863	6	-2.059045	1.024947	1.628370	8	-0.097635	-7.532830	-3.819604
6	-0.520898	-2.623778	-1.013553	6	-1.976826	0.692691	3.115212	8	-2.558647	-3.068613	-2.398320
8	0.139168	-3.284931	-2.064158	8	-0.939622	1.466921	3.655706	8	-4.399860	-4.032465	-0.510202
6	1.340955	-3.918440	-1.678569	6	-1.170506	2.844449	3.561203	8	-3.600286	-6.461574	0.745438
6	2.342401	-2.872268	-1.197860	6	-1.122096	3.244928	2.101706	6	0.551151	-1.270483	-2.956208
8	-0.102973	-0.624499	0.438995	6	-2.203393	2.503810	1.342338	8	0.950960	0.022082	-3.327013
6	-1.892803	-2.229594	-1.519951	6	-1.602901	-0.753494	3.397965	8	-0.621958	-0.634301	-5.572729
8	-2.690337	-1.733669	-0.471134	8	-2.591501	-1.662328	2.980229	8	-2.459078	-3.582312	-5.666642
8	1.817088	-4.642994	-2.741586	8	-2.036310	2.772348	-0.019933	8	0.987721	-3.739197	-6.452968
8	3.478669	-3.467581	-0.648631	8	-1.303905	4.628522	2.045025	1	-1.202550	-2.577785	-6.975237
8	2.450026	-0.957939	0.332635	8	-0.165967	3.447242	4.287671	1	1.264620	-2.053414	-4.812242
6	-0.747671	0.718814	0.005778	8	-2.830334	-2.542280	0.329173	1	-0.653989	-4.998731	-6.430434
6	-1.870354	1.008228	1.009781	8	-4.490813	-3.456742	-1.680133	1	-0.383674	-1.259477	-2.390931
6	-1.803451	2.427242	1.530401	8	-5.478682	-1.469312	-3.496972	1	1.329450	-1.678356	-2.316788
6	-0.378158	2.756123	1.886218	6	-6.194602	0.900093	-1.205311	1	-3.160157	-2.929228	-5.606134
6	0.453622	2.769624	0.624245	8	-7.318177	0.915557	-2.043083	1	0.383568	0.311451	-4.046253
8	0.282737	1.566285	-0.136795	1	-5.919883	1.933640	-1.014654	1	-0.739408	-4.826882	-2.058371
8	-3.113226	0.846483	0.405245	1	-1.405564	-0.846451	4.463403	1	-3.678160	-4.738007	-2.822573
6	1.941624	2.920597	0.878908	1	-6.426297	0.425057	-0.250665	1	-2.630531	-7.067841	-2.936135
8	2.259538	4.230508	1.260544	1	-4.902138	0.664573	-2.874773	1	-2.408250	-4.383367	-0.094627
8	-0.269254	4.033524	2.450826	1	-6.117767	-1.620429	-1.555301	1	-4.160112	-6.603629	-1.219149
8	-2.566726	2.574874	2.694384	1	-5.687664	-2.393715	-3.644066	1	0.588158	-5.407140	-4.283062
1	1.704043	4.471606	2.006201	1	-3.218088	-1.963688	-2.292926	1	-1.691555	-1.805999	-4.253292
1	2.265667	2.192677	1.626654	1	-3.791465	-3.997834	-1.308036	1	-1.451571	-0.231491	-5.831588

1 1.505080 -4.500682 -6.716980  
1 -3.322400 -2.561202 -2.114200  
1 -4.609320 -4.099097 0.422276  
1 -3.946649 -7.347237 0.858944  
1 0.220410 -7.170725 -1.868213  
1 -0.812592 -8.563433 -2.172154  
1 -0.667785 -8.059045 -4.379818  
1 -2.086623 -4.427371 -4.501181

**18**

6 -0.634382 -2.312629 -1.043845  
6 0.544546 -1.478098 -0.608968  
6 1.626373 -2.388271 -0.053806  
8 1.041836 -2.995522 1.071272  
6 -0.034061 -3.859382 0.773357  
6 -1.174728 -3.059916 0.151086  
8 0.933105 -0.745154 -1.815057  
6 1.537823 0.696141 -1.627174  
6 2.699298 0.794823 -2.625398  
6 2.383109 1.724695 -3.779535  
6 0.906568 1.652407 -4.076876  
6 0.144242 2.220069 -2.901678  
8 0.522437 1.559068 -1.682257  
8 3.827106 1.280857 -1.966431  
6 -1.362979 2.104393 -3.032456  
8 -1.867044 3.033766 -3.949394  
8 0.565821 2.413529 -5.197257  
8 3.057948 1.358010 -4.950958  
6 2.887115 -1.697799 0.423191  
8 3.624146 -1.193035 -0.663889  
8 -0.415603 -4.497968 1.926191  
8 -2.190592 -3.895023 -0.316279  
8 -1.533369 -1.409869 -1.630418  
1 -1.411133 2.911649 -4.785620  
1 -1.638020 1.081843 -3.304976  
1 -1.809719 2.325577 -2.067260  
1 0.406903 3.270378 -2.784804  
1 0.623473 0.603606 -4.242200  
1 1.193427 2.203737 -5.894280  
1 2.636653 2.746362 -3.490772  
1 3.949772 1.704308 -4.935761  
1 2.869416 -0.202628 -3.028159  
1 4.148073 0.583621 -1.384394  
1 1.901659 0.633986 -0.608771  
1 0.245209 -0.738119 0.131216  
1 1.892583 -3.138014 -0.804881  
1 3.467166 -2.410631 1.004769  
1 2.642499 -0.858588 1.070497  
1 4.106734 -1.903728 -1.087704  
1 0.293173 -4.636350 0.079736  
1 -0.706875 -3.850150 2.572498  
1 -1.550889 -2.344190 0.887676  
1 -2.625277 -4.313353 0.427867  
1 -0.301856 -3.042632 -1.787216  
1 0.086646 -0.663805 -2.310859

1 -2.192340 -1.885410 -2.139406

**18+H<sub>2</sub>O**

6 1.716022 -2.012034 -0.080887  
6 0.449463 -1.435910 -0.663057  
6 -0.520914 -2.563225 -0.971471  
8 0.126669 -3.342163 -1.945883  
6 1.297304 -3.986591 -1.490875  
6 2.335729 -2.941191 -1.096795  
8 -0.029632 -0.493754 0.349245  
6 -1.852592 -2.141934 -1.556621  
8 -2.638361 -1.489212 -0.587906  
8 1.750911 -4.821787 -2.480456  
8 3.448450 -3.527071 -0.492076  
8 2.506039 -0.906511 0.262818  
6 -0.755386 0.804421 -0.159925  
6 -1.924997 1.026078 0.812513  
6 -1.762542 2.266929 1.670991  
6 -0.296688 2.524479 1.907116  
6 0.357091 2.829310 0.580770  
8 0.203217 1.719603 -0.316105  
8 -3.116500 1.144408 0.088265  
6 1.843798 3.114987 0.682275  
8 2.080170 4.406423 1.170324  
8 -0.100329 3.633889 2.734239  
8 -2.367017 2.114566 2.926401  
8 -2.318681 3.412701 -1.390543  
1 1.647628 4.485347 2.023930  
1 2.332152 2.357990 1.300405  
1 2.271413 3.063034 -0.315151  
1 -0.140711 3.681485 0.120856  
1 0.167505 1.637239 2.356748  
1 -0.676918 3.537832 3.496697  
1 -2.181749 3.122979 1.140021  
1 -3.298970 2.322802 2.867715  
1 -1.960505 0.160980 1.472639  
1 -3.323985 0.277590 -0.282563  
1 -1.115262 0.466830 -1.125696  
1 0.667169 -0.857452 -1.559193  
1 -0.700932 -3.148374 -0.064186  
1 -2.351221 -3.026953 -1.944874  
1 -1.708131 -1.449735 -2.383211  
1 -3.028839 -2.134092 0.003126  
1 1.064938 -4.618069 -0.631066  
1 1.964763 -4.308473 -3.263520  
1 2.617168 -2.367770 -1.984686  
1 3.921971 -4.049592 -1.140661  
1 1.471790 -2.589266 0.815478  
1 0.792352 -0.211528 0.810250  
1 3.221886 -1.181337 0.838196  
1 -2.854169 2.654792 -1.134859  
1 -2.250978 3.379594 -2.343335

**19**

6 -4.685916 0.283065 -1.241668  
6 -4.043977 -0.205805 0.038815

6 -4.300997 -1.681976 0.321242  
8 -5.690853 -1.869260 0.297506  
6 -6.265749 -1.595806 -0.949065  
6 -6.149045 -0.110957 -1.222462  
8 -2.598111 0.016999 -0.014410  
6 -1.907192 1.286383 0.516632  
8 -1.683699 2.155776 -0.473160  
6 -0.349633 2.340985 -0.990407  
6 0.713494 2.428231 0.105297  
6 0.179176 2.011294 1.459354  
6 -0.695815 0.790262 1.267929  
8 -1.055548 0.268681 2.500148  
8 1.274183 1.737929 2.279908  
8 1.204862 3.740752 0.127489  
6 -0.067814 1.303095 -2.066084  
8 1.080612 1.651744 -2.786342  
6 -3.849633 -2.134605 1.701130  
8 -2.453798 -2.086262 1.866060  
8 -7.582615 -1.992402 -0.853633  
8 -6.769501 0.135052 -2.449090  
8 -4.614239 1.675618 -1.344353  
1 -0.904296 1.297694 -2.760095  
1 -4.231181 -3.140171 1.862587  
1 0.027296 0.300731 -1.642663  
1 -0.399552 3.313304 -1.469076  
1 1.523162 1.732078 -0.133025  
1 1.920699 3.786356 0.763612  
1 -0.420824 2.826124 1.875059  
1 0.947697 1.429718 3.127621  
1 -0.147346 0.054631 0.671044  
1 -1.464631 -0.601582 2.377573  
1 -2.681013 1.653388 1.181859  
1 -4.372766 0.400143 0.878406  
1 -3.818898 -2.294740 -0.448412  
1 -4.284135 -1.482262 2.453874  
1 -5.738982 -2.166507 -1.724143  
1 -8.078633 -1.527907 -1.532728  
1 -6.655190 0.419259 -0.411923  
1 -6.802328 1.080941 -2.599310  
1 -4.216080 -0.200704 -2.101822  
1 -3.799436 1.943988 -1.770960  
1 -2.042462 -2.858880 1.478547  
1 -2.139163 -0.449982 -0.726593  
1 1.852982 1.236883 -2.405069

**TS(17-20)**

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**TS(18-21) – 1 imaginary frequency**

6 1.607330 -2.095159 0.104890  
6 0.322246 -1.527594 -0.477563  
6 -0.576295 -2.666391 -0.901943  
6 -0.861889 -3.558821 0.279802  
6 0.464485 -4.017607 0.868244  
8 1.238966 -2.891962 1.205839

8	0.547395	-0.717759	-1.636213	6	-1.051564	1.145366	1.203388	8	0.982914	0.620680	-3.874748
8	-1.720573	-2.072002	-1.453273	8	-1.858231	0.918342	2.302871	8	-0.383317	-0.517465	-6.262387
8	-1.615046	-4.638299	-0.191501	8	0.737523	1.882784	2.630641	8	-1.697274	-3.718034	-5.257691
8	0.298563	-4.793832	1.990801	8	1.703672	3.415096	0.269662	8	1.333403	-3.067119	-6.946336
6	2.585157	-1.071427	0.646300	6	0.538896	0.804467	-1.772600	1	-1.313238	-2.720529	-7.049718
8	3.190444	-0.331400	-0.386269	8	1.921738	0.798514	-1.981869	1	1.584817	-1.438164	-5.308781
6	0.745644	1.211906	-1.339814	6	-3.647445	-2.166116	1.458998	1	0.126279	-4.737740	-6.674740
8	-0.425683	1.690604	-1.498680	8	-2.332124	-1.738165	1.710286	1	-0.020985	-0.829373	-2.787781
6	-0.866103	2.290759	-2.745758	8	-7.615605	-2.058155	-0.648475	1	1.741825	-0.931653	-2.850927
6	0.100025	1.948955	-3.855922	8	-7.149019	0.315927	-2.020502	1	-2.571045	-3.334188	-5.174039
6	1.495273	2.354002	-3.445984	8	-4.718142	1.757296	-1.149086	1	0.276789	0.823964	-4.491481
6	1.911817	1.498033	-2.266668	1	-0.012898	0.806915	-2.712320	1	3.445106	-6.933624	-3.215818
8	2.870733	2.174632	-1.516261	1	-3.726227	-3.249325	1.522055	1	1.628557	-8.271003	-1.191634
8	2.322880	2.153721	-4.555212	1	0.222287	-0.060616	-1.184465	1	0.967241	-8.653653	-3.598213
8	-0.333494	2.640196	-4.987808	1	0.522367	2.936155	-1.648644	1	4.506299	-8.871276	-1.949607
6	-2.291794	1.831611	-2.990449	1	1.623463	1.368475	0.423145	1	1.938600	-10.425780	-2.438172
8	-2.929358	2.680663	-3.899886	1	2.271505	3.449952	1.040948	1	1.036425	-4.942673	-4.355806
1	-2.428282	2.681455	-4.718978	1	-0.466156	3.186515	1.598203	1	-1.355619	-1.391012	-4.671737
1	-2.301719	0.794517	-3.331754	1	0.131549	1.822447	3.372269	1	-1.239260	-0.231796	-6.585446
1	-2.839733	1.887236	-2.054391	1	-0.539439	0.233207	0.891999	1	1.968330	-3.674708	-7.328321
1	-0.865045	3.363492	-2.566200	1	-2.065737	-0.028154	2.318273	1	3.166023	-7.349451	0.219993
1	0.082511	0.868170	-4.044374	1	-2.830602	2.078137	0.192091	1	4.110442	-10.545004	-0.429747
1	0.358508	2.579862	-5.651917	1	-4.096394	0.342528	0.786163	1	3.381493	-11.855784	-3.332034
1	1.491831	3.403439	-3.146757	1	-3.788676	-2.279984	-0.705652	1	2.810109	-7.256099	-5.571616
1	3.106180	2.698871	-4.483275	1	-4.265210	-1.734426	2.241866	1	1.816825	-8.649462	-5.990727
1	2.280051	0.543998	-2.638012	1	-5.906020	-2.022062	-1.772987	1	0.004126	-7.362366	-5.507754
1	3.306772	1.525421	-0.950492	1	-8.210198	-1.549646	-1.206380	1	1.803408	-5.727301	-1.990343
1	0.988889	1.016641	-0.304677	1	-6.679798	0.331917	-0.009254	<b>21</b>			
1	-0.186419	-0.927699	0.280063	1	-7.593217	1.136743	-1.812229	6	1.817120	-2.634824	0.226525
1	2.110190	-2.702711	-0.654958	1	-4.591314	-0.019038	-2.177480	6	0.515246	-1.859396	0.093987
1	3.327605	-1.594142	1.245976	1	-4.991319	2.145173	-1.980537	6	-0.508425	-2.735223	-0.591259
1	2.073493	-0.363117	1.294723	1	-1.711002	-2.215811	1.160059	6	-0.690367	-4.023626	0.169719
1	3.834145	-0.877060	-0.839700	1	-2.505081	-0.121193	-1.481320	6	0.664109	-4.694289	0.326763
1	0.997207	-4.634593	0.141101	1	2.174086	-0.017070	-2.413431	8	1.549286	-3.809369	0.963803
1	-0.143947	-4.282069	2.672134	<b>20</b>				8	0.688942	-0.676792	-0.654894
1	-1.409941	-2.991244	1.038084	6	0.366873	-3.776859	-6.234492	8	-1.690477	-1.982114	-0.679991
1	-1.856443	-5.198738	0.547129	6	0.837340	-3.977751	-4.822724	8	-1.579023	-4.819130	-0.564645
1	-0.059883	-3.258306	-1.664071	8	1.015395	-2.982779	-4.093726	8	0.590750	-5.855249	1.064464
1	-0.251273	-0.832296	-2.175892	6	0.774563	-1.636131	-4.614809	6	2.919285	-1.923269	0.989891
1	-2.240085	-2.739017	-1.904149	6	-0.547311	-1.591146	-5.377523	8	3.572160	-0.947084	0.211134
<b>TS(19-22) – 1 imaginary</b>				6	-0.878935	-2.920023	-6.070974	6	1.149826	1.765023	0.186756
<b>frequency</b>				8	1.565723	-6.212637	-2.784746	8	0.146120	2.394352	-0.203336
6	-4.885466	0.365435	-1.195080	6	2.463511	-7.289201	-2.886943	6	0.154626	3.321562	-1.338172
6	-3.966792	-0.215949	-0.141223	6	1.960998	-8.302818	-3.902029	6	1.371367	3.091855	-2.207285
6	-4.210418	-1.702224	0.122795	8	2.868730	-9.383506	-3.933423	6	2.623813	3.008985	-1.364574
8	-5.588105	-1.957869	0.245084	6	2.941845	-10.083559	-2.716579	6	2.485307	1.794628	-0.466577
6	-6.340051	-1.578588	-0.866814	6	3.500272	-9.171726	-1.644867	8	3.479146	1.741232	0.495830
6	-6.316528	-0.066200	-0.957263	6	2.617977	-7.954291	-1.538062	8	3.693636	2.870349	-2.248089
8	-2.602016	-0.005203	-0.529511	6	1.893029	-7.787488	-5.328174	8	1.404900	4.167823	-3.097554
6	-1.828109	1.693995	0.056624	8	0.834624	-6.887688	-5.540548	6	-1.172091	3.147583	-2.054148
8	-1.202330	2.225296	-0.920738	8	3.141430	-6.985095	-0.665596	8	-1.422340	4.254115	-2.869917
6	0.242468	2.091224	-1.030012	8	3.517463	-9.793461	-0.389109	1	-0.697214	4.352616	-3.491791
6	0.959626	2.229252	0.314182	8	3.810427	-11.141725	-2.859788	1	-1.171278	2.213661	-2.618403
6	0.005160	2.205929	1.491468	6	0.852343	-0.699136	-3.429069	1	-1.966017	3.103057	-1.314627

1 0.192773 4.304899 -0.876189  
1 1.257134 2.149806 -2.753458  
1 2.205146 4.092795 -3.623388  
1 2.728486 3.911338 -0.758794  
1 4.517069 3.035970 -1.788086  
1 2.487683 0.894507 -1.093544  
1 3.738583 0.810892 0.587166  
1 1.002503 1.208841 1.103917  
1 0.156659 -1.614624 1.098098  
1 2.186509 -2.894360 -0.772020  
1 3.624404 -2.675298 1.338798  
1 2.511056 -1.413414 1.858792  
1 4.172846 -1.364469 -0.406279  
1 1.054244 -4.976809 -0.654126  
1 0.268827 -5.650686 1.945560  
1 -1.089213 -3.802022 1.164547  
1 -1.759600 -5.621976 -0.074263  
1 -0.145795 -2.975121 -1.596497  
1 -0.167938 -0.491328 -1.053293  
1 -2.325582 -2.464684 -1.210615

**21-h2o**

6 -1.174933 3.415224 6.037017  
6 -0.929039 2.108395 5.309837  
6 0.420317 2.062106 4.682976  
8 1.363081 2.823613 4.967262  
6 1.251444 3.949539 5.901227  
6 0.073471 3.742417 6.826227  
8 -1.908835 1.875611 4.353946  
6 2.592694 4.063611 6.602934  
8 2.719310 5.326320 7.186537  
8 -0.060821 4.932952 7.541918  
8 -2.214927 3.303025 6.958507  
8 -2.741386 3.787632 2.313201  
8 -1.004803 -0.568865 3.686521  
6 -1.020309 -1.094252 2.375753  
6 0.303657 -1.726439 1.989245  
6 1.395353 -0.733698 1.627489  
6 2.612985 -1.482453 1.138197  
6 2.245714 -2.389570 -0.008682  
6 1.108565 -3.299511 0.424411  
8 0.024482 -2.515594 0.852528  
8 3.565418 -0.515298 0.776803  
8 1.736002 0.049403 2.743804  
8 0.682915 -4.125556 -0.592896  
8 3.392650 -3.120381 -0.345924  
1 2.002090 5.451981 7.812608  
1 2.701276 3.260291 7.333342  
1 3.382305 3.966112 5.863941  
1 1.099374 4.815582 5.261713  
1 0.287696 2.910964 7.505471  
1 -0.844945 4.861980 8.092245  
1 -1.371703 4.206865 5.312613  
1 -3.058318 3.407762 6.517787  
1 -0.901396 1.307055 6.062763

1 -1.845842 0.947535 4.063651  
1 0.656320 1.305736 3.929891  
1 1.025816 -0.096947 0.817820  
1 0.650755 -2.362481 2.811509  
1 -1.799625 -1.846534 2.271494  
1 -1.252098 -0.267701 1.709297  
1 -1.050648 -1.282566 4.323680  
1 1.442596 -3.954280 1.233014  
1 0.354186 -3.590068 -1.318864  
1 1.904093 -1.781244 -0.852084  
1 3.205710 -3.661213 -1.114088  
1 2.998864 -2.096572 1.958500  
1 2.571855 0.476360 2.536458  
1 4.383933 -0.958453 0.550122  
1 -2.494903 3.149770 2.990129  
1 -3.631675 4.059240 2.529630

**22**

6 -1.698862 2.807269 -0.906834  
6 -0.563582 2.070186 -0.310673  
8 0.615801 2.280243 -0.661884  
6 0.975392 3.325538 -1.625744  
6 -0.135210 3.662100 -2.620401  
6 -1.400069 2.857086 -2.406142  
6 1.463514 4.503764 -0.808382  
8 1.972232 5.409358 -1.743996  
8 0.395604 3.447919 -3.896902  
8 -2.422620 3.500851 -3.093350  
8 -2.896136 2.173124 -0.673398  
8 -1.274280 2.958536 1.892262  
6 -1.571175 2.198179 3.041741  
6 -2.925509 2.585884 3.632200  
8 -3.158163 1.861005 4.818882  
6 -2.218398 2.099003 5.834052  
6 -0.863997 1.615926 5.353977  
6 -0.482745 2.338887 4.083204  
6 -4.116197 2.245829 2.752026  
8 -4.187997 2.993021 1.561755  
8 0.715252 1.839662 3.557573  
8 0.152919 1.881660 6.281234  
8 -2.632350 1.453801 6.978194  
1 1.802520 2.877899 -2.165041  
1 -0.396033 4.714786 -2.489489  
1 -0.220582 3.793289 -4.544979  
1 -1.255688 1.842071 -2.784251  
1 -3.229092 2.991501 -2.990751  
1 -1.680217 3.833638 -0.525584  
1 -3.307133 2.511031 0.144863  
1 -0.704073 1.218736 0.340559  
1 -1.613557 1.159445 2.714026  
1 -2.924668 3.661558 3.848163  
1 -5.018320 2.383984 3.345773  
1 -4.061764 1.200937 2.457874  
1 -4.352628 3.916524 1.753133  
1 -2.179839 3.163485 6.076346

1 -2.707464 0.513210 6.800412  
1 -0.935467 0.543333 5.147748  
1 0.015879 1.347087 7.063949  
1 -0.370783 3.402968 4.328532  
1 -1.064343 3.861293 2.142005  
1 1.363663 1.846704 4.264668  
1 0.635335 4.934950 -0.243076  
1 2.225418 4.162711 -0.108413  
1 2.203637 6.225363 -1.301481

**TS(21-25) – 1 imaginary frequency**

6 2.761653 -0.949436 4.603784  
6 1.485102 -0.330085 4.085675  
6 0.490635 -1.436242 3.769013  
8 1.087484 -2.237255 2.777756  
6 2.248613 -2.910948 3.203982  
6 3.320237 -1.891814 3.565853  
8 1.017436 0.572269 5.100543  
6 -0.835857 -0.978879 3.197170  
8 -1.619079 -0.329092 4.169813  
8 2.655045 -3.763584 2.205729  
8 4.443043 -2.504453 4.129095  
8 3.612910 0.119030 4.916663  
6 0.177161 2.127687 4.496289  
6 -0.959454 2.236461 5.504169  
6 -0.838420 3.469493 6.378867  
6 0.623045 3.741127 6.635066  
6 1.298293 4.075058 5.326663  
8 1.124190 2.988505 4.387559  
8 -2.169969 2.281937 4.808286  
6 2.787184 4.341552 5.442537  
8 3.020291 5.626272 5.946763  
8 0.802503 4.842718 7.474899  
8 -1.448066 3.281636 7.625185  
8 -1.261246 4.495355 3.366371  
1 2.598434 5.691921 6.806792  
1 3.263891 3.576684 6.058539  
1 3.224003 4.299231 4.448854  
1 0.811056 4.931839 4.865678  
1 1.087614 2.851394 7.076901  
1 0.234259 4.724742 8.240532  
1 -1.268161 4.325375 5.857635  
1 -2.383139 3.474880 7.564341  
1 -0.907606 1.356393 6.142357  
1 -2.341872 1.397098 4.460083  
1 -0.076180 1.654504 3.556937  
1 1.697095 0.244151 3.181969  
1 0.302891 -2.023464 4.674361  
1 -1.349731 -1.847564 2.791116  
1 -0.678901 -0.275018 2.382412  
1 -1.979851 -0.973977 4.779387  
1 2.022216 -3.534191 4.071828  
1 2.857021 -3.258444 1.414314  
1 3.584123 -1.322862 2.669418



1 4.870325 -3.048930 3.466670  
1 2.536363 -1.523737 5.507757  
1 1.819685 0.853964 5.572938  
1 4.362955 -0.206414 5.416468  
1 -1.933877 3.827379 3.526322  
1 -1.241155 4.635134 2.420938

**20 – h2o**

6 -0.375953 -1.992149 1.810586  
6 -0.640254 -2.661266 0.487855  
6 -0.584853 -1.616229 -0.625616  
8 -1.508692 -0.593129 -0.351923  
6 -1.203076 0.117737 0.824223  
6 -1.309918 -0.822566 2.005840  
8 0.329289 -3.668387 0.300283  
6 -0.971908 -2.188477 -1.975179  
8 -0.123835 -3.261197 -2.335019  
8 -2.133753 1.113748 0.999909  
8 -0.934833 -0.208454 3.207457  
8 -0.532215 -2.935334 2.848039  
6 0.489361 -5.562229 1.694094  
6 -0.973963 -5.845902 1.850045  
6 -1.292063 -7.277052 1.456095  
6 -0.596191 -7.544037 0.140383  
6 0.904904 -7.469316 0.300815  
8 1.288876 -6.271062 1.044340  
8 -1.337767 -5.599097 3.170942  
6 1.677856 -7.446576 -1.004774  
8 1.681190 -8.720975 -1.579670  
8 -0.868302 -8.830224 -0.332928  
8 -2.651308 -7.471484 1.244635  
1 -0.909924 -7.956999 2.222181  
1 1.260056 -8.291427 0.917321  
1 -1.498419 -5.185609 1.155985  
1 1.255651 -6.696821 -1.675928  
1 2.710323 -7.181425 -0.797625  
1 -3.088197 -7.574813 2.107486  
1 0.773713 -9.009539 -1.704075  
1 -1.646704 -3.093631 0.499022  
1 0.654407 -1.625423 1.812575  
1 0.432358 -1.211108 -0.675824  
1 -2.341287 -1.181668 2.052466  
1 -0.188895 0.524074 0.746400  
1 0.946368 -4.785268 2.291138  
1 -0.928077 -6.797004 -0.588487  
1 -1.822110 -8.948098 -0.311747  
1 -1.372050 -4.641749 3.293798  
1 0.343949 -3.879292 -0.646526  
1 -0.412796 -2.470726 3.680424  
1 -1.575525 0.470922 3.421166  
1 -1.934990 1.853964 0.425978  
1 -1.982850 -2.585171 -1.920444  
1 -0.953884 -1.399444 -2.723124  
1 0.652429 -2.923974 -2.782758  
8 -3.469635 -7.407506 3.846688

1 -3.353251 -8.144312 4.445383  
1 -2.779608 -6.770616 4.055803

**22 – h2o**

6 -1.548172 2.685329 -0.907310  
6 -0.272308 2.004197 -0.410562  
6 0.935902 2.595769 -1.106100  
6 0.931136 4.101798 -1.012239  
6 -0.375070 4.636152 -1.565454  
8 -1.424793 4.087234 -0.813355  
8 -0.320534 0.608180 -0.585680  
8 2.105443 2.066048 -0.532720  
8 2.043589 4.544307 -1.740668  
8 -0.455246 6.008949 -1.498282  
6 -2.784953 2.379668 -0.079677  
8 -3.183283 1.030897 -0.105618  
6 0.134206 -1.439538 1.030308  
8 0.997716 -2.300821 0.754619  
6 0.663999 -3.597169 0.160481  
6 -0.740197 -4.096164 0.496839  
6 -1.518118 -3.140021 1.374271  
6 -1.305549 -1.718049 0.852285  
8 -2.090855 -0.822761 1.541528  
8 -2.859089 -3.499382 1.297703  
8 -0.586101 -5.345379 1.108027  
1 1.390580 -4.264706 0.609715  
8 1.925133 0.820258 1.978613  
6 0.934271 -3.450823 -1.323304  
1 -1.292953 -4.198028 -0.439980  
1 -1.450388 -5.751433 1.192562  
1 -1.155368 -3.208668 2.402539  
1 -3.365676 -2.900473 1.850395  
1 -1.516310 -1.720878 -0.223032  
1 -2.428565 -0.141546 0.930878  
1 0.529384 -0.533785 1.490570  
1 -0.179556 2.166288 0.663063  
1 -1.722124 2.396089 -1.951560  
1 -3.589368 3.023854 -0.430903  
1 -2.587162 2.623021 0.960941  
1 -3.471325 0.782252 -0.984124  
1 -0.479311 4.371386 -2.620160  
1 -0.400691 6.284800 -0.580169  
1 1.006891 4.397474 0.038781  
1 2.161858 5.484629 -1.602949  
1 0.900419 2.326532 -2.168220  
1 -0.300946 0.399070 -1.521990  
1 2.851362 2.567136 -0.871500  
1 2.079902 1.326864 1.169870  
1 1.858724 1.459030 2.686356  
8 0.771690 -4.733458 -1.854486  
1 0.228101 -2.741881 -1.761092  
1 1.944753 -3.070239 -1.467275  
1 0.846466 -4.693337 -2.807320

**24**

6 1.193505 2.022701 -1.276957

6 -0.225495 1.563472 -1.021676  
8 -1.152070 2.107521 -1.839708  
6 -0.993302 3.471303 -2.269113  
6 -0.025145 4.223842 -1.374179  
6 1.308537 3.529779 -1.096883  
1 -1.965541 3.933644 -2.112593  
8 -0.733869 4.344491 -0.128950  
8 2.297723 4.095489 -1.905858  
8 2.098979 1.381898 -0.435766  
8 -0.548371 1.951174 0.412243  
8 1.142890 -0.947345 -2.262749  
6 1.233792 -1.795974 -1.141272  
6 2.513255 -2.626159 -1.200348  
8 2.540374 -3.614533 -0.194732  
6 1.460174 -4.507606 -0.229874  
6 0.188853 -3.725515 0.041758  
6 0.009539 -2.674289 -1.026253  
6 3.762425 -1.797904 -0.939243  
8 3.769608 -0.546605 -1.586435  
8 -1.093075 -1.848914 -0.759968  
8 -0.952667 -4.537622 -0.004418  
8 1.676682 -5.498357 0.703423  
6 -0.742683 3.513150 -3.754314  
1 0.153597 5.212990 -1.785519  
1 -0.330588 5.014672 0.428650  
1 1.546682 3.708481 -0.044640  
1 3.143306 3.712505 -1.669057  
1 1.368670 1.793405 -2.325409  
1 2.602946 0.709799 -0.920657  
1 -0.328957 0.486310 -1.020332  
1 1.271820 -1.142487 -0.267791  
1 2.568273 -3.102415 -2.186335  
1 4.642852 -2.378935 -1.210906  
1 3.807031 -1.589946 0.126685  
1 3.542366 -0.659277 -2.510780  
1 1.401688 -5.005898 -1.200469  
1 1.785368 -5.097102 1.569015  
1 0.286041 -3.239381 1.017610  
1 -0.915788 -5.174420 0.710176  
1 -0.138347 -3.199861 -1.978494  
1 0.802661 -1.437046 -3.013282  
1 -1.856434 -2.412961 -0.621680  
1 -1.320697 1.474370 0.743111  
1 -0.721277 2.969800 0.419248  
8 0.453231 2.858676 -4.075497  
1 -1.593068 3.030597 -4.237081  
1 -0.727486 4.560217 -4.062381  
1 0.561535 2.851319 -5.025464

**23**

6 -0.834126 2.126938 5.127539  
6 0.430299 2.420139 4.329505  
8 1.432148 3.045873 4.954294  
6 1.098701 4.154620 5.794242  
6 0.041654 3.720657 6.787580

6 -1.194577 3.274460 6.045139  
6 2.394174 4.595333 6.447322  
8 2.272143 5.864885 7.026296  
8 -0.235482 4.814695 7.618528  
8 -2.142455 2.893625 7.001785  
8 -1.883867 1.922967 4.216287  
8 -0.131035 3.349111 3.239463  
8 1.791937 -0.109480 2.765097  
6 1.480187 -0.844935 1.610821  
6 0.273326 -1.734097 1.859642  
8 0.017646 -2.478031 0.686574  
6 1.055131 -3.356097 0.334015  
6 2.305670 -2.554054 0.017215  
6 2.658082 -1.702537 1.210341  
6 -1.014040 -0.985503 2.153087  
8 -1.084290 -0.529844 3.486883  
8 3.728602 -0.830562 0.951341  
8 3.402577 -3.387025 -0.240623  
8 0.642199 -4.123205 -0.733838  
1 1.538489 5.838308 7.645660  
1 2.708938 3.846495 7.177694  
1 3.160211 4.661537 5.679799  
1 0.717832 4.969936 5.177018  
1 0.430376 2.882844 7.374939  
1 -0.969885 4.578688 8.189544  
1 -1.566166 4.114010 5.451299  
1 -3.005569 2.831549 6.592100  
1 -0.643728 1.235982 5.724373  
1 -1.822692 1.003826 3.891539  
1 0.809740 1.553542 3.796358  
1 1.241141 -0.169570 0.782871  
1 0.490012 -2.412790 2.692502  
1 -1.848115 -1.647123 1.926745  
1 -1.092756 -0.106908 1.518393  
1 -1.251230 -1.266677 4.075404  
1 1.255729 -4.051379 1.152825  
1 0.428025 -3.547276 -1.471551  
1 2.094995 -1.904703 -0.838538  
1 3.226597 -3.901236 -1.029432  
1 2.909560 -2.362307 2.047514  
1 2.680774 0.233760 2.640856  
1 4.513554 -1.351226 0.776518  
1 -1.050825 3.005863 3.092488  
1 0.380463 3.355511 2.418659

**TS(14-26) – 1 imaginary**

**frequency**

1 -3.387932 0.057566 -1.016280  
6 -2.259379 -0.955377 0.790946  
6 -3.088409 -2.161648 0.579547  
6 -3.518962 -2.448868 -0.849042  
6 -4.719882 -1.625158 -1.285328  
6 -4.411956 -0.132149 -1.373593  
8 -2.413135 -0.325061 1.855494  
6 -1.379517 0.567675 2.344992

6 -1.073243 0.137032 3.774636  
8 -0.137817 1.048012 4.285333  
6 -0.647947 2.348501 4.376151  
6 -0.914731 2.879381 2.979953  
6 -1.911660 1.977093 2.274098  
6 -0.442160 -1.242375 3.870231  
8 -1.342502 -2.265487 3.500174  
8 -2.052690 2.322308 0.923877  
8 -1.396944 4.184286 3.127267  
8 0.318604 3.090446 5.021946  
8 -2.079709 -3.093225 0.909190  
8 -3.926128 -3.784710 -0.918199  
8 -5.161256 -2.094227 -2.531428  
6 -4.484794 0.426885 -2.783148  
8 -4.334206 1.828745 -2.730935  
8 0.607200 -1.523887 0.698585  
1 -5.469183 0.234377 -3.197005  
1 -0.088869 -1.383632 4.889065  
1 -3.740517 -0.038747 -3.425251  
8 -5.313505 0.551663 -0.543618  
1 -5.507690 -1.749151 -0.537885  
1 -5.215642 -3.050844 -2.470764  
1 -2.679582 -2.266095 -1.526087  
1 -3.177591 -4.355730 -0.735994  
1 -3.930074 -2.198041 1.267665  
1 -1.868614 -3.034379 1.856970  
1 -1.390798 -0.762974 0.166646  
1 -0.506175 0.444405 1.708127  
1 -1.997867 0.163607 4.360544  
1 0.403048 -1.306660 3.191969  
1 -1.580247 2.329815 4.955090  
1 0.149274 4.016360 4.829132  
1 0.030326 2.869454 2.432960  
1 -1.299650 4.658733 2.301659  
1 -2.869147 2.029221 2.794597  
1 -2.889327 2.762725 0.781147  
1 -1.939925 -2.454760 4.224223  
1 -3.406125 2.049867 -2.652332  
1 1.496632 -1.248431 0.477542  
1 0.557087 -2.450578 0.462727  
1 -5.242891 1.483299 -0.771098

**TS(14-36) – 1 imaginary**

**frequency**

6 -2.062346 0.161014 4.146937  
6 -2.213122 0.442759 2.655189  
6 -2.607607 1.880413 2.369401  
6 -1.671390 2.805358 3.116330  
6 -1.653419 2.425327 4.580098  
8 -1.185440 1.112655 4.688996  
8 -3.286998 -0.417056 2.184229  
6 -3.297907 -0.840111 1.005865  
6 -4.385937 -1.836109 0.685147  
6 -4.454438 -2.155698 -0.805503  
6 -5.163632 -1.096650 -1.635229

6 -4.522053 0.277216 -1.595519  
8 -4.594311 0.767009 -0.262378  
8 -4.114684 -3.033647 1.352967  
6 -5.159302 1.257402 -2.569004  
8 -4.751419 1.035118 -3.889763  
8 -5.193215 -1.509428 -2.975959  
8 -5.217215 -3.313179 -0.996459  
8 -2.503069 2.174418 1.007113  
8 -2.087428 4.136820 3.032825  
8 -0.769938 3.203680 5.299508  
6 -1.426144 -1.177081 4.460913  
8 -2.208998 -2.216372 3.911762  
8 -1.378236 -2.193349 1.275439  
1 -4.834919 2.258060 -2.295963  
1 -1.357755 -1.267785 5.541697  
1 -6.248581 1.216170 -2.475321  
1 -3.461211 0.209853 -1.833802  
1 -6.186367 -1.010775 -1.250294  
1 -5.567945 -2.392520 -3.009826  
1 -3.441824 -2.299763 -1.195254  
1 -4.901115 -3.991022 -0.394611  
1 -5.326532 -1.403760 1.027424  
1 -4.384230 -2.973422 2.271101  
1 -2.566339 -0.478577 0.296544  
1 -1.314893 0.172513 2.103036  
1 -3.048551 0.224797 4.616271  
1 -0.417065 -1.195060 4.046842  
1 -2.664280 2.488259 5.002567  
1 -0.842571 4.105122 4.975892  
1 -0.656499 2.686084 2.728016  
1 -2.058068 4.411859 2.114972  
1 -3.623845 2.049510 2.732624  
1 -3.320720 1.958192 0.545480  
1 -2.114146 -3.001818 4.449910  
1 -4.997902 0.135533 -4.118433  
1 -5.501368 0.979511 -0.024719  
1 -1.317908 -2.961801 0.707740  
1 -1.631175 -2.521178 2.151578

**26**

1 -1.664475 0.290177 -1.730908  
6 -0.036580 -0.853176 -0.353520  
6 -0.854069 -2.068335 -0.555819  
6 -1.362121 -2.350886 -1.958289  
6 -2.589779 -1.535664 -2.348964  
6 -2.309180 -0.059929 -2.550491  
8 -0.102322 -0.300793 0.763222  
6 0.945870 0.592293 1.218029  
6 1.386744 0.087141 2.587043  
8 2.349094 0.988181 3.064106  
6 1.823703 2.267556 3.282280  
6 1.413722 2.872216 1.952690  
6 0.373736 1.986540 1.289484  
6 2.040636 -1.283919 2.546769  
8 1.113212 -2.303909 2.240795

8 0.092453 2.423037 -0.011339  
8 0.919064 4.151976 2.222782  
8 2.832069 2.994595 3.879077  
8 0.206484 -2.969936 -0.310650  
8 -1.782409 -3.686664 -1.988059  
8 -3.123791 -2.054035 -3.535645  
6 -1.624592 0.262490 -3.866753  
8 -1.561537 1.662303 -4.032592  
8 2.832664 -1.300578 -0.755279  
1 -2.229127 -0.120090 -4.682337  
1 2.512866 -1.462977 3.509937  
1 -0.634921 -0.188834 -3.925952  
8 -3.532604 0.620956 -2.482358  
1 -3.320389 -1.619553 -1.538629  
1 -3.192178 -3.005253 -3.426416  
1 -0.553300 -2.192917 -2.675637  
1 -1.026150 -4.259612 -1.849488  
1 -1.650169 -2.148631 0.180952  
1 0.462478 -2.944247 0.629203  
1 0.757903 -0.586936 -1.045748  
1 1.763625 0.536445 0.502541  
1 0.518739 0.061274 3.254421  
1 2.800348 -1.308462 1.771656  
1 0.951341 2.189795 3.943843  
1 2.627979 3.925799 3.759665  
1 2.302864 2.920012 1.320030  
1 0.884211 4.659572 1.411592  
1 -0.527470 1.976471 1.904110  
1 -0.792866 2.781584 -0.055616  
1 0.587116 -2.513838 3.013016  
1 -0.845312 2.016445 -3.505023  
1 3.687737 -0.983133 -1.044848  
1 2.803768 -2.225934 -0.999643  
1 -3.380864 1.495170 -2.852338

**TS(27-28) – 1 imaginary**

**frequency**

6 -1.826785 0.189261 4.129791  
6 -2.220174 0.441812 2.672316  
6 -2.712301 1.864408 2.458092  
6 -1.804796 2.862420 3.135404  
6 -1.631555 2.479078 4.583299  
8 -1.014790 1.224547 4.620681  
8 -3.280814 -0.450721 2.333138  
6 -3.097777 -1.260989 1.239674  
6 -4.442426 -1.836131 0.771624  
6 -4.444160 -2.125071 -0.748309  
6 -5.127909 -1.054206 -1.588119  
6 -4.463682 0.313626 -1.546779  
8 -4.695785 0.895218 -0.278881  
8 -4.627150 -3.032001 1.484397  
6 -4.943277 1.236855 -2.658379  
8 -4.373589 0.931503 -3.901166  
8 -5.142996 -1.475571 -2.927851  
8 -5.177230 -3.314348 -0.971267

8 -2.739716 2.208477 1.103618  
8 -2.336278 4.157325 3.095274  
8 -0.785045 3.340935 5.251830  
6 -0.949950 -1.026749 4.329072  
8 -1.657848 -2.207363 3.909878  
8 -2.278379 -2.385224 1.606534  
1 -4.633283 2.246831 -2.402632  
1 -0.722866 -1.141802 5.381730  
1 -6.036232 1.220082 -2.706690  
1 -3.382482 0.213094 -1.641011  
1 -6.155290 -0.945452 -1.222228  
1 -5.584547 -2.326364 -2.967450  
1 -3.423306 -2.255354 -1.108959  
1 -4.603380 -3.999916 -1.312665  
1 -5.216263 -1.122439 1.037652  
1 -5.115431 -3.628780 0.902467  
1 -2.568208 -0.737438 0.446615  
1 -1.361439 0.270930 2.019753  
1 -2.739442 0.093962 4.724724  
1 -0.030412 -0.935662 3.758181  
1 -2.604737 2.420927 5.087131  
1 -0.932119 4.224421 4.905170  
1 -0.817768 2.833736 2.665035  
1 -2.496087 4.385040 2.177409  
1 -3.709035 1.945827 2.901367  
1 -3.495014 1.797885 0.658581  
1 -1.237770 -3.007285 4.243339  
1 -4.629507 0.030170 -4.112215  
1 -5.613359 1.162332 -0.193704  
1 -2.907636 -3.142678 1.623447  
1 -1.904029 -2.290663 2.787456

**28**

8 -1.012320 1.228646 4.624226  
6 -1.830834 0.196540 4.138257  
6 -2.218949 0.441640 2.678318  
6 -2.709639 1.864071 2.460061  
6 -1.797607 2.862547 3.130741  
6 -1.622602 2.486636 4.580455  
6 -0.962763 -1.023578 4.349138  
8 -1.683307 -2.204443 3.937485  
8 -3.276051 -0.452975 2.339267  
6 -3.086915 -1.262196 1.241515  
8 -2.255470 -2.371399 1.601941  
8 -2.740839 2.203172 1.104482  
8 -2.324643 4.159075 3.085225  
8 -0.769946 3.347548 5.242036  
6 -4.429990 -1.841318 0.775328  
8 -4.609648 -3.039621 1.484705  
6 -4.432267 -2.125523 -0.745511  
8 -5.158991 -3.318052 -0.973579  
6 -5.123803 -1.056561 -1.581397  
8 -5.138975 -1.474763 -2.922259  
6 -4.468705 0.315629 -1.538487  
6 -4.954797 1.236788 -2.649041

8 -4.383015 0.937087 -3.892293  
8 -4.704141 0.894889 -0.270244  
1 -4.651996 2.248634 -2.392049  
1 -0.741200 -1.138286 5.402584  
1 -6.047604 1.212296 -2.697401  
1 -3.386902 0.222435 -1.633184  
1 -6.151276 -0.955052 -1.213505  
1 -5.567443 -2.332333 -2.960926  
1 -3.411036 -2.248509 -1.107852  
1 -4.579194 -4.002206 -1.307609  
1 -5.206619 -1.131138 1.043190  
1 -5.102103 -3.633891 0.904362  
1 -2.569130 -0.725465 0.449018  
1 -1.356779 0.269628 2.030466  
1 -2.745183 0.110900 4.732026  
1 -0.042108 -0.950002 3.778455  
1 -2.594787 2.436340 5.086966  
1 -0.912299 4.229773 4.890235  
1 -0.811670 2.828101 2.658399  
1 -2.488063 4.381460 2.166664  
1 -3.704925 1.948896 2.906028  
1 -3.499459 1.793392 0.664177  
1 -1.278104 -3.009676 4.278777  
1 -4.632286 0.034074 -4.104138  
1 -5.623641 1.154709 -0.183768  
1 -2.865987 -3.140688 1.606285  
1 -1.895072 -2.284464 2.851726

**TS(28-29) – 1 imaginary**

**frequency**

8 -1.090158 1.259719 4.689009  
6 -1.949857 0.260247 4.220535  
6 -2.189653 0.417215 2.724225  
6 -2.687004 1.818631 2.439958  
6 -1.764820 2.845420 3.066892  
6 -1.604032 2.571979 4.547195  
6 -1.229252 -1.019242 4.575943  
8 -2.100105 -2.138721 4.200139  
8 -3.162897 -0.551902 2.349466  
6 -2.945267 -1.182482 1.108817  
8 -1.925106 -2.117237 1.269394  
8 -2.726144 2.112012 1.072560  
8 -2.280564 4.131511 2.889501  
8 -0.747585 3.435455 5.176665  
6 -4.240428 -1.881806 0.705485  
8 -4.240441 -3.105579 1.393307  
6 -4.299099 -2.120005 -0.817271  
8 -4.946468 -3.356364 -1.054389  
6 -5.113536 -1.081149 -1.577269  
8 -5.164020 -1.451084 -2.932040  
6 -4.571529 0.339276 -1.513024  
6 -5.178538 1.250815 -2.570942  
8 -4.632353 1.043937 -3.844360  
8 -4.794326 0.862765 -0.217899  
1 -4.953737 2.275988 -2.288093

1	-1.086430	-1.108863	5.644106	1	-5.113364	6.438493	-2.271410	1	-4.671663	2.848473	-0.303518
1	-6.266150	1.132986	-2.581463	1	-2.938821	5.204884	-0.952649	1	-3.345739	2.645359	-2.379713
1	-3.491138	0.338478	-1.656900	1	-3.275579	4.834182	-3.012504	1	-3.003940	3.986105	1.357301
1	-6.126322	-1.076264	-1.157830	1	-4.709796	2.861195	-0.249536	1	-1.560026	2.226200	2.641927
1	-5.500699	-2.348394	-2.979669	1	-3.395407	2.554877	-2.308537	1	-3.459724	-0.156355	2.846659
1	-3.290573	-2.150287	-1.232081	1	-3.045904	4.017127	1.389563	1	-0.625080	-0.022432	1.736643
1	-4.326935	-3.992126	-1.411389	1	-1.588057	2.274116	2.671774	1	-3.628030	-0.012779	5.091411
1	-5.077964	-1.269940	1.031268	1	-3.407571	-0.171036	2.816523	1	-2.349180	0.665318	7.025779
1	-4.755524	-3.725183	0.865058	1	-0.596301	0.117517	1.667723	1	-1.853194	2.454503	5.122851
1	-2.627763	-0.442922	0.378366	1	-3.586101	-0.069416	5.066724	1	-3.810529	3.321744	6.036218
1	-1.257302	0.238936	2.184690	1	-2.320292	0.614559	7.014843	1	-4.436256	1.905768	3.617111
1	-2.912238	0.292752	4.741444	1	-1.881695	2.445864	5.148247	1	-4.284382	4.021956	3.104303
1	-0.291520	-1.122183	4.041584	1	-3.875485	3.233022	6.074555	1	-1.816671	-0.307025	-0.217017
1	-2.562859	2.647458	5.063410	1	-4.450559	1.846445	3.638122	1	-5.521233	8.090482	0.001113
1	0.061263	3.520419	4.667723	1	-4.332673	3.983345	3.126024	1	-6.201033	4.227599	1.494719
1	-0.776567	2.754518	2.600899	1	-1.824836	-0.353104	-0.258164	1	-1.361257	2.850747	-0.553700
1	-2.542757	4.199889	1.968055	1	-5.448342	8.118048	-0.071074	1	-2.764222	0.947813	0.707307
1	-3.680761	1.926942	2.884251	1	-6.241913	4.312176	1.500327	<b>30</b>			
1	-3.535422	1.763107	0.671902	1	-1.384569	2.861830	-0.490382	8	-1.855079	0.042960	4.115457
1	-1.695618	-3.006031	4.346885	1	-2.729770	0.780153	0.586597	6	-2.449681	0.242876	2.867786
1	-4.814904	0.131420	-4.081132	<b>TS(29-30) – 1 imaginary</b>				6	-2.548966	1.748463	2.625801
1	-5.727554	1.035155	-0.078051	<b>frequency</b>				6	-3.435844	2.362997	3.685989
1	-2.339128	-2.992533	1.261158	8	-1.843103	0.041553	4.097837	6	-2.839074	2.002539	5.034630
1	-2.399299	-2.043963	3.263205	6	-2.449619	0.268505	2.862193	6	-2.671347	0.502113	5.158552
<b>29</b>				6	-2.551594	1.774836	2.627560	6	-1.616501	-0.465244	1.825258
6	-2.626526	0.458072	5.139242	6	-3.446074	2.360778	3.699684	8	-2.303354	-0.235515	0.594349
8	-1.802224	0.052647	4.078036	6	-2.839852	1.989236	5.040789	8	-3.134027	1.940602	1.300955
6	-2.414473	0.292095	2.846583	6	-2.654166	0.489272	5.151425	6	-2.775397	3.214740	0.589968
6	-2.567321	1.795665	2.636371	6	-1.631175	-0.425082	1.798219	8	-1.468201	3.208259	0.268262
6	-3.474145	2.330035	3.727458	8	-2.346151	-0.147959	0.571126	8	-3.506049	3.757121	3.618352
6	-2.854890	1.954045	5.059269	8	-3.106207	1.950599	1.306493	8	-3.663464	2.411370	6.085661
6	-1.563505	-0.359623	1.781282	6	-2.789939	3.211803	0.636024	8	-2.019453	0.154743	6.323107
8	-2.328751	-0.181013	0.547452	8	-1.470296	3.265501	0.312100	6	-3.692726	3.250431	-0.616878
8	-3.124445	1.973985	1.334201	8	-3.541509	3.755296	3.661710	8	-3.079640	2.406771	-1.550841
6	-2.829709	3.223473	0.688891	8	-3.661854	2.376376	6.102848	6	-3.829911	4.683385	-1.161200
6	-3.726036	3.231392	-0.533934	8	-1.988082	0.140198	6.307414	8	-3.999700	4.592884	-2.560865
6	-3.845456	4.630850	-1.146229	6	-3.693233	3.236705	-0.581956	6	-5.052524	5.423570	-0.630501
6	-5.052391	5.411782	-0.639433	8	-3.069622	2.376538	-1.497544	8	-5.135949	6.669096	-1.274529
6	-5.044337	5.731344	0.851374	6	-3.830196	4.656415	-1.151129	6	-5.047682	5.689192	0.869243
8	-5.319216	4.556863	1.592913	8	-4.005895	4.547355	-2.550228	6	-6.079726	6.729219	1.284304
8	-3.615170	3.722235	3.717378	6	-5.050978	5.406764	-0.630642	8	-5.679318	8.039743	0.995354
8	-3.683348	2.294987	6.133249	8	-5.133461	6.642604	-1.294504	8	-5.261628	4.473861	1.564639
8	-1.953435	0.103238	6.289428	6	-5.048654	5.694923	0.865515	1	-6.198248	6.660645	2.362642
8	-1.503126	3.308209	0.356944	6	-6.067633	6.755774	1.260069	1	-1.573711	-1.528805	2.038138
8	-3.107373	2.331487	-1.418162	8	-5.648933	8.056438	0.952291	1	-7.043743	6.496340	0.821696
8	-4.032771	4.487547	-2.541739	8	-5.284010	4.495384	1.580499	1	-4.067704	6.049368	1.183252
8	-5.118229	6.633443	-1.331831	1	-6.190658	6.705650	2.338923	1	-5.938930	4.824192	-0.866752
6	-6.031315	6.830958	1.220456	1	-1.607792	-1.497005	1.951171	1	-5.162361	6.513713	-2.220876
8	-5.576235	8.111518	0.880740	1	-7.033356	6.528799	0.797850	1	-2.933616	5.261587	-0.934537
1	-6.153709	6.810486	2.300337	1	-4.065143	6.045626	1.178776	1	-3.263010	5.005180	-3.011191
1	-1.462472	-1.424767	1.941095	1	-5.938414	4.805340	-0.858597	1	-4.669489	2.861564	-0.334534
1	-7.004251	6.620619	0.765360	1	-5.139601	6.470793	-2.238479	1	-3.339197	2.712094	-2.426901
1	-4.051593	6.058440	1.160471	1	-2.932624	5.237120	-0.936093	1	-2.971771	3.972330	1.332725
1	-5.949432	4.819161	-0.853126	1	-3.260068	4.934383	-3.007612	1	-1.558548	2.199966	2.609353

1 -3.459379 -0.182183 2.850165  
1 -0.610607 -0.054121 1.787624  
1 -3.649558 0.009278 5.092722  
1 -2.380103 0.690200 7.034055  
1 -1.847800 2.457442 5.116169  
1 -3.779564 3.361602 6.025766  
1 -4.432219 1.921462 3.609351  
1 -4.266391 4.026081 3.085805  
1 -1.750879 -0.443715 -0.161647  
1 -5.555355 8.090902 0.044430  
1 -6.176570 4.196767 1.484793  
1 -1.379482 2.797482 -0.603743  
1 -2.858571 1.098443 0.751768

**32**

6 4.130217 -2.745579 -1.435756  
8 3.917656 -1.368322 -1.242948  
6 2.562307 -0.999552 -1.376975  
6 1.765217 -1.683852 -0.279978  
6 1.948074 -3.180326 -0.378580  
6 3.415980 -3.525995 -0.352234  
6 2.540561 0.512773 -1.315891  
8 1.311857 1.000900 -1.827924  
8 0.419452 -1.326146 -0.418955  
6 -1.059897 1.012389 0.634161  
6 -2.281099 0.383976 1.263353  
6 -3.537760 1.094775 0.796190  
6 -3.501965 2.542446 1.245352  
6 -2.280778 3.256260 0.700337  
8 -1.144048 2.478028 1.203198  
8 1.248061 -3.757381 0.693554  
8 3.527473 -4.909236 -0.549194  
8 5.476199 -3.009579 -1.321163  
8 -1.108782 1.060294 -0.683343  
8 -2.272206 -0.956797 0.880455  
8 -4.631027 0.436987 1.384218  
8 -4.606811 3.266494 0.778617  
6 -2.151985 4.690015 1.185619  
8 -3.000565 5.518658 0.448703  
1 -1.137998 5.047228 1.017702  
1 3.363857 0.873889 -1.927299  
1 -2.356878 4.739519 2.256031  
1 -2.246585 3.221116 -0.386017  
1 -3.459210 2.570215 2.337349  
1 -5.390591 2.975413 1.247342  
1 -3.594247 1.050499 -0.291317  
1 -5.304329 0.265359 0.727472  
1 -2.194610 0.480840 2.347757  
1 -3.093436 -1.346184 1.190223  
1 -0.122609 0.673054 1.059350  
1 2.155155 -1.349425 0.687314  
1 2.176384 -1.311909 -2.353364  
1 2.690548 0.855861 -0.292040  
1 3.750006 -3.032068 -2.422721  
1 5.930102 -2.748521 -2.122811

1 3.843450 -3.230698 0.609769  
1 4.451261 -5.153632 -0.479401  
1 1.525098 -3.522645 -1.329037  
1 1.322891 -4.710299 0.627253  
1 1.448748 1.883113 -2.172935  
1 -3.898737 5.195449 0.561817  
1 -0.304680 2.940603 1.063679  
1 -0.210318 0.957983 -1.074416  
1 -0.112204 -1.845837 0.189202

**33**

6 1.848366 2.483106 2.575863  
6 0.861483 1.847698 1.631970  
6 1.124860 0.366597 1.517980  
6 1.120424 -0.267108 2.900466  
8 2.091513 0.384220 3.684132  
6 1.805556 1.746643 3.901158  
8 0.963603 2.413452 0.335932  
8 0.111469 -0.242492 0.744773  
6 0.335032 -0.409251 -0.591047  
6 -0.515052 -1.582403 -1.033307  
6 -0.483318 -1.807601 -2.562801  
6 -1.864361 -1.631210 -3.203731  
6 -2.273465 -0.187069 -3.404531  
6 -3.656685 -0.054797 -4.010905  
8 -4.103934 1.273493 -3.849844  
6 1.490895 -1.741192 2.897669  
8 0.486692 -2.568882 2.358236  
8 2.781988 2.285909 4.702270  
8 1.479868 3.826712 2.701087  
8 -0.053116 0.782626 -1.317144  
8 -0.009922 -2.721039 -0.408224  
8 -0.050530 -3.104484 -2.875246  
8 -1.857380 -2.189458 -4.487212  
8 -2.311348 0.474745 -2.137159  
1 -1.536590 0.309784 -4.038427  
1 -4.356341 -0.684694 -3.466443  
1 1.720384 -2.028535 3.922319  
1 -3.642302 -0.362005 -5.052097  
1 -2.606072 -2.130501 -2.569831  
1 -1.387057 -3.025342 -4.417376  
1 0.210664 -1.104997 -3.031324  
1 0.092333 -3.577678 -2.048258  
1 -1.538645 -1.389059 -0.704838  
1 0.043327 -2.596247 0.555128  
1 1.387524 -0.563429 -0.819818  
1 2.098421 0.199686 1.051634  
1 0.126653 -0.144698 3.346108  
1 2.381840 -1.897617 2.295147  
1 0.813857 1.837456 4.357211  
1 2.627902 2.044792 5.616159  
1 2.859338 2.384915 2.172516  
1 2.145696 4.284744 3.215760  
1 -0.150558 2.000303 2.012996  
1 0.827776 3.363273 0.391731

1 -0.245136 -2.636081 2.972008  
1 -3.767825 1.819779 -4.560978  
1 -2.914330 1.227055 -2.240293  
1 0.250677 1.587656 -0.787492  
1 -1.071296 0.776587 -1.622486

**TS(33-34) – 1 imaginary frequency**

6 0.337967 2.326393 3.531306  
6 -0.703173 2.087882 2.464693  
6 -1.005570 0.616135 2.339139  
6 -1.348507 -0.006714 3.686926  
8 -0.312074 0.303437 4.584948  
6 -0.132535 1.682014 4.817690  
8 -0.299518 2.531379 1.200524  
8 -2.132601 0.468205 1.442748  
6 -1.931536 0.280499 0.017268  
6 -2.420093 -1.079174 -0.406001  
6 -2.367642 -1.231355 -1.945874  
6 -3.740668 -1.567489 -2.538020  
6 -4.630977 -0.352001 -2.693092  
6 -6.007658 -0.705772 -3.216834  
8 -6.859624 0.409825 -3.072059  
6 -1.390453 -1.526064 3.688325  
8 -2.324980 -2.079214 2.794807  
8 0.856027 1.846839 5.755557  
8 0.475926 3.712656 3.648593  
8 -2.792356 1.349153 -0.316028  
8 -1.596803 -2.037176 0.179570  
8 -1.467118 -2.237601 -2.315790  
8 -3.577709 -2.082327 -3.828911  
8 -4.802066 0.270143 -1.424389  
1 -4.144660 0.350830 -3.373628  
1 -6.436088 -1.500219 -2.609814  
1 -1.581862 -1.856993 4.706940  
1 -5.945200 -1.044288 -4.247180  
1 -4.233873 -2.301214 -1.889938  
1 -2.805861 -2.655734 -3.796875  
1 -2.015075 -0.304841 -2.405876  
1 -1.277612 -2.764926 -1.531313  
1 -3.448154 -1.187834 -0.058963  
1 -1.895206 -2.193892 1.092519  
1 -0.904269 0.503208 -0.249201  
1 -0.169117 0.091061 1.882151  
1 -2.301409 0.403770 4.037662  
1 -0.415133 -1.900235 3.388439  
1 -1.080477 2.120321 5.147184  
1 0.508795 1.685300 6.633366  
1 1.281112 1.854669 3.244234  
1 1.192180 3.901688 4.256193  
1 -1.617629 2.606552 2.774156  
1 -0.119854 3.472055 1.250688  
1 -3.220388 -1.927889 3.098405  
1 -6.731827 1.012180 -3.805530  
1 -5.615661 0.788979 -1.484298

1 -2.778235 1.363732 0.942734  
 1 -3.643002 1.019605 -0.761223  
**34**  
 6 1.501570 1.951307 1.776679  
 6 1.040616 0.522944 1.624127  
 6 0.699625 -0.117778 2.969218  
 8 1.789253 0.075784 3.833772  
 6 2.094433 1.426122 4.104728  
 6 2.588262 2.055044 2.821423  
 8 -0.136473 0.505623 0.758121  
 6 0.034933 0.454715 -0.833462  
 8 -0.750726 1.403639 -1.312814  
 6 0.539874 -1.629517 2.929060  
 8 -0.421885 -2.088630 2.013371  
 8 3.116317 1.473617 5.018093  
 8 2.861320 3.418901 2.958524  
 8 1.926849 2.396298 0.522793  
 6 -0.342501 -0.967032 -1.161153  
 8 0.520124 -1.841666 -0.505136  
 6 -0.251359 -1.199383 -2.691014  
 8 0.753515 -2.127528 -2.990934  
 6 -1.576588 -1.708614 -3.267366  
 8 -1.348258 -2.272463 -4.528535  
 6 -2.589438 -0.602576 -3.483265  
 8 -2.826510 0.059777 -2.250855  
 6 -3.913817 -1.126549 -3.998273  
 8 -4.877774 -0.097008 -3.939481  
 1 -2.172108 0.108329 -4.201491  
 1 -4.271759 -1.918638 -3.344068  
 1 0.315865 -1.970751 3.937304  
 1 -3.801021 -1.523777 -5.003420  
 1 -1.993913 -2.456332 -2.582470  
 1 -0.519562 -2.756516 -4.462275  
 1 0.009550 -0.270481 -3.201710  
 1 0.956825 -2.605863 -2.178630  
 1 -1.370181 -1.122833 -0.835444  
 1 0.127015 -2.087114 0.349561  
 1 1.088175 0.691525 -0.932044  
 1 1.775653 -0.072512 1.088067  
 1 -0.201978 0.353257 3.375482  
 1 1.488866 -2.065185 2.627827  
 1 1.196774 1.934433 4.471416  
 1 2.778391 1.321735 5.901260  
 1 3.472147 1.501787 2.495316  
 1 3.627222 3.527955 3.523571  
 1 0.658069 2.557543 2.130446  
 1 2.248113 3.295676 0.615863  
 1 -1.309706 -1.894481 2.315072  
 1 -4.782402 0.476120 -4.700672  
 1 -3.679439 0.501987 -2.339645  
 1 -0.749654 1.232624 0.946072  
 1 -1.610840 1.027096 -1.616097

**TS(34-35) – 1 imaginary  
 frequency**

6 -0.676774 2.105127 2.584457  
 6 -1.095003 0.662308 2.428018  
 6 -1.353025 -0.007590 3.777003  
 8 -0.266399 0.233526 4.636693  
 6 -0.020692 1.595102 4.896986  
 6 0.424325 2.246735 3.607071  
 8 -2.263319 0.588446 1.603890  
 6 -2.040054 0.580978 -0.304265  
 8 -2.806102 1.497750 -0.743637  
 6 -1.421728 -1.525070 3.706821  
 8 -2.324286 -2.023689 2.748899  
 8 1.011534 1.695440 5.797400  
 8 0.654236 3.619396 3.750707  
 8 -0.288868 2.569904 1.322345  
 6 -2.401991 -0.861755 -0.480278  
 8 -1.491433 -1.656776 0.201193  
 6 -2.367106 -1.218828 -1.999279  
 8 -1.509925 -2.300189 -2.222033  
 6 -3.753036 -1.607013 -2.524232  
 8 -3.610735 -2.233851 -3.767329  
 6 -4.675319 -0.430623 -2.765545  
 8 -4.873931 0.265326 -1.540266  
 6 -6.036773 -0.865835 -3.270361  
 8 -6.930165 0.223129 -3.187649  
 1 -4.210581 0.242956 -3.489567  
 1 -6.436137 -1.641223 -2.620357  
 1 -1.657951 -1.907655 4.697651  
 1 -5.959222 -1.257889 -4.280206  
 1 -4.217524 -2.286430 -1.800028  
 1 -2.877341 -2.849590 -3.681902  
 1 -1.996574 -0.376646 -2.588127  
 1 -1.240237 -2.639630 -1.359665  
 1 -3.414162 -1.009093 -0.105414  
 1 -1.836159 -1.854318 1.092280  
 1 -0.996648 0.852919 -0.205584  
 1 -0.326297 0.113596 1.885012  
 1 -2.275773 0.399411 4.205374  
 1 -0.440021 -1.895935 3.424685  
 1 -0.934676 2.064417 5.276189  
 1 0.693112 1.523955 6.684140  
 1 1.322056 1.727562 3.262312  
 1 1.406133 3.747952 4.330358  
 1 -1.534603 2.682580 2.952152  
 1 0.010983 3.476339 1.414998  
 1 -3.226683 -1.812878 2.990955  
 1 -6.824365 0.787060 -3.954380  
 1 -5.709862 0.742554 -1.631623  
 1 -2.884780 1.293763 1.817627  
 1 -3.701639 1.127429 -1.028972  
**35**  
 6 1.385270 1.989397 1.925074  
 6 0.960989 0.547535 1.765166  
 6 0.804430 -0.158717 3.109907  
 8 1.918774 0.087762 3.934489

6 2.150202 1.449390 4.196902  
 6 2.531179 2.122696 2.897520  
 8 -0.239264 0.470201 1.017184  
 6 0.029704 0.501243 -1.250985  
 8 -0.745619 1.374784 -1.685650  
 6 0.778462 -1.674136 2.983820  
 8 -0.095946 -2.157859 1.990300  
 8 3.215970 1.561545 5.058260  
 8 2.765983 3.494286 3.054378  
 8 1.718161 2.473490 0.651923  
 6 -0.297451 -0.954654 -1.283469  
 8 0.663871 -1.655250 -0.571645  
 6 -0.303918 -1.456441 -2.768526  
 8 0.438590 -2.634224 -2.865818  
 6 -1.714685 -1.783625 -3.267095  
 8 -1.615566 -2.507154 -4.460483  
 6 -2.567945 -0.579824 -3.601697  
 8 -2.766577 0.191046 -2.417156  
 6 -3.941592 -0.973257 -4.111244  
 8 -4.787427 0.154543 -4.061909  
 1 -2.057208 0.035654 -4.344510  
 1 -4.378561 -1.716936 -3.448840  
 1 0.539674 -2.109431 3.952346  
 1 -3.868722 -1.390496 -5.110690  
 1 -2.218424 -2.376062 -2.494960  
 1 -0.962000 -3.196478 -4.315735  
 1 0.141310 -0.711033 -3.432745  
 1 0.815844 -2.812157 -1.994399  
 1 -1.291441 -1.091914 -0.857176  
 1 0.344794 -1.837806 0.333742  
 1 1.030559 0.825243 -0.986546  
 1 1.713699 0.026748 1.171616  
 1 -0.110503 0.204384 3.591845  
 1 1.773784 -2.003655 2.698180  
 1 1.244653 1.899987 4.617601  
 1 2.935766 1.369379 5.953574  
 1 3.414472 1.612742 2.504432  
 1 3.532534 3.612410 3.616914  
 1 0.543668 2.561626 2.335504  
 1 2.027855 3.376188 0.746595  
 1 -0.999965 -1.921006 2.200901  
 1 -4.671491 0.683806 -4.851610  
 1 -3.588840 0.686841 -2.549328  
 1 -0.863298 1.135900 1.316928  
 1 -1.661796 0.973752 -1.991640  
**27**  
 6 -1.795738 0.175176 4.130490  
 6 -2.198822 0.438219 2.676214  
 6 -2.704938 1.856364 2.458854  
 6 -1.834218 2.866807 3.164742  
 6 -1.683005 2.468474 4.610545  
 8 -1.027592 1.235418 4.641484  
 8 -3.264988 -0.458650 2.342675  
 6 -3.121291 -1.251842 1.246972

6 -4.478811 -1.802550 0.783510  
6 -4.485346 -2.125524 -0.729182  
6 -5.135661 -1.051756 -1.591169  
6 -4.430509 0.295772 -1.565806  
8 -4.643408 0.894249 -0.301749  
8 -4.687869 -2.980282 1.523237  
6 -4.883954 1.222672 -2.685027  
8 -4.329997 0.884814 -3.926283  
8 -5.154818 -1.494656 -2.923353  
8 -5.249728 -3.299389 -0.918702  
8 -2.702677 2.207856 1.105494  
8 -2.395631 4.149137 3.126286  
8 -0.880137 3.347915 5.310516  
6 -0.871168 -1.009483 4.309647  
8 -1.511445 -2.203249 3.867802  
8 -2.351518 -2.444565 1.604263  
1 -4.539206 2.224330 -2.441411  
1 -0.634709 -1.110440 5.363563  
1 -5.977049 1.242305 -2.728768  
1 -3.352910 0.161836 -1.660491  
1 -6.160920 -0.908106 -1.232238  
1 -5.651756 -2.314092 -2.961583  
1 -3.468324 -2.292760 -1.084728  
1 -4.704841 -3.995948 -1.284671  
1 -5.236480 -1.068108 1.036658  
1 -5.168333 -3.589469 0.945062  
1 -2.559561 -0.766074 0.453665  
1 -1.347233 0.271912 2.013749  
1 -2.706238 0.036753 4.720492  
1 0.046005 -0.847817 3.747343  
1 -2.665094 2.372257 5.090915  
1 -1.050342 4.231081 4.973745  
1 -0.837006 2.866314 2.715867  
1 -2.533247 4.386965 2.207454  
1 -3.713487 1.920117 2.877089  
1 -3.447503 1.801123 0.640600  
1 -1.023981 -2.972059 4.173938  
1 -4.616744 -0.009545 -4.127175  
1 -5.550850 1.196010 -0.221494  
1 -3.061950 -3.138488 1.698381  
1 -1.909028 -2.330528 2.578953

**TS(36-37) – 1 imaginary**

**frequency**

6 -1.286479 0.453545 3.571357  
6 -2.610653 0.954402 3.014211  
6 -3.554360 1.264686 4.149935  
6 -2.913072 2.222789 5.123499  
6 -1.596599 1.640230 5.596608  
8 -0.780309 1.413317 4.460028  
8 -3.258666 -0.023741 2.227714  
6 -3.204252 0.079820 0.856369  
6 -4.622837 0.094891 0.244427  
6 -5.123388 -1.243092 -0.343161  
6 -4.971889 -1.339688 -1.855512

6 -3.550684 -1.290306 -2.396063  
8 -3.006609 -0.007425 -2.200792  
8 -5.489075 0.542061 1.246757  
6 -3.489859 -1.682875 -3.866490  
8 -3.623081 -3.057793 -4.079323  
8 -5.553108 -2.544676 -2.278860  
8 -6.519297 -1.335334 -0.131064  
8 -4.732936 1.846928 3.688090  
8 -3.742481 2.439448 6.224468  
8 -0.914918 2.450831 6.461061  
6 -0.182368 0.297436 2.547455  
8 -0.387522 -0.921464 1.781797  
8 -2.400344 -0.996367 0.385495  
1 -2.510655 -1.386974 -4.237076  
1 0.759960 0.170459 3.064242  
1 -4.239630 -1.109620 -4.424726  
1 -2.916931 -1.982079 -1.844768  
1 -5.517508 -0.487495 -2.282339  
1 -6.426570 -2.583254 -1.882990  
1 -4.645443 -2.111616 0.111121  
1 -6.690134 -1.876908 0.639076  
1 -4.594372 0.818207 -0.568759  
1 -6.378267 0.358026 0.930928  
1 -2.668604 0.972250 0.544013  
1 -2.442549 1.861815 2.430883  
1 -1.445845 -0.506821 4.072449  
1 -0.123319 1.139117 1.865195  
1 -1.768423 0.693924 6.114980  
1 -0.894218 3.340839 6.105226  
1 -2.694181 3.159016 4.594901  
1 -4.617854 2.615752 5.873881  
1 -3.760225 0.326712 4.680011  
1 -5.071257 1.302481 2.963922  
1 0.412900 -1.197740 1.319888  
1 -4.466322 -3.301742 -3.690309  
1 -3.436243 0.598499 -2.806911  
1 -2.814335 -1.831708 0.627611  
1 -1.229248 -0.950270 1.127918

**37**

6 -0.289334 -1.936965 3.517053  
6 -1.600630 -1.215050 3.246420  
6 -2.504917 -1.234698 4.459547  
6 -1.752187 -0.713958 5.657407  
6 -0.475693 -1.515714 5.810660  
8 0.305117 -1.369628 4.659779  
8 -2.306334 -1.868055 2.202185  
6 -2.658662 -1.144421 1.104861  
6 -4.022474 -1.600774 0.619319  
6 -4.122946 -3.146076 0.458756  
6 -4.443013 -3.586331 -0.973720  
6 -3.227806 -3.608499 -1.886873  
8 -2.642613 -2.313197 -1.972514  
8 -4.907684 -1.132427 1.596051  
6 -3.538785 -4.128240 -3.282657

8 -3.672335 -5.520955 -3.317643  
8 -4.920066 -4.904136 -0.967970  
8 -5.189948 -3.610759 1.257205  
8 -3.635641 -0.435441 4.255416  
8 -2.468765 -0.859216 6.852861  
8 0.297712 -1.048225 6.855136  
6 0.743139 -1.773246 2.422337  
8 0.280675 -2.409916 1.232947  
8 -1.647288 -1.353332 0.084376  
1 -2.702946 -3.870575 -3.928013  
1 1.665764 -2.245409 2.744593  
1 -4.433309 -3.631674 -3.670289  
1 -2.463943 -4.246148 -1.445962  
1 -5.201515 -2.913961 -1.390477  
1 -5.565544 -4.977389 -0.259779  
1 -3.196567 -3.618558 0.781580  
1 -4.854036 -4.064087 2.030740  
1 -4.238206 -1.107474 -0.329717  
1 -5.523651 -1.854451 1.776375  
1 -2.671262 -0.075696 1.301340  
1 -1.396347 -0.179593 2.967275  
1 -0.489883 -3.001418 3.671876  
1 0.929639 -0.717140 2.234841  
1 -0.718572 -2.577198 5.950037  
1 -0.295590 -0.817183 7.574401  
1 -1.477013 0.331302 5.493326  
1 -3.267129 -0.331995 6.802424  
1 -2.796828 -2.271886 4.653327  
1 -4.121259 -0.760587 3.487189  
1 1.025964 -2.620834 0.667198  
1 -4.348612 -5.762293 -2.679553  
1 -3.134996 -1.726149 -2.551970  
1 -1.995254 -1.753692 -0.794490  
1 -0.808961 -1.815912 0.497843

**TS(37-38) – 1 imaginary**

**frequency**

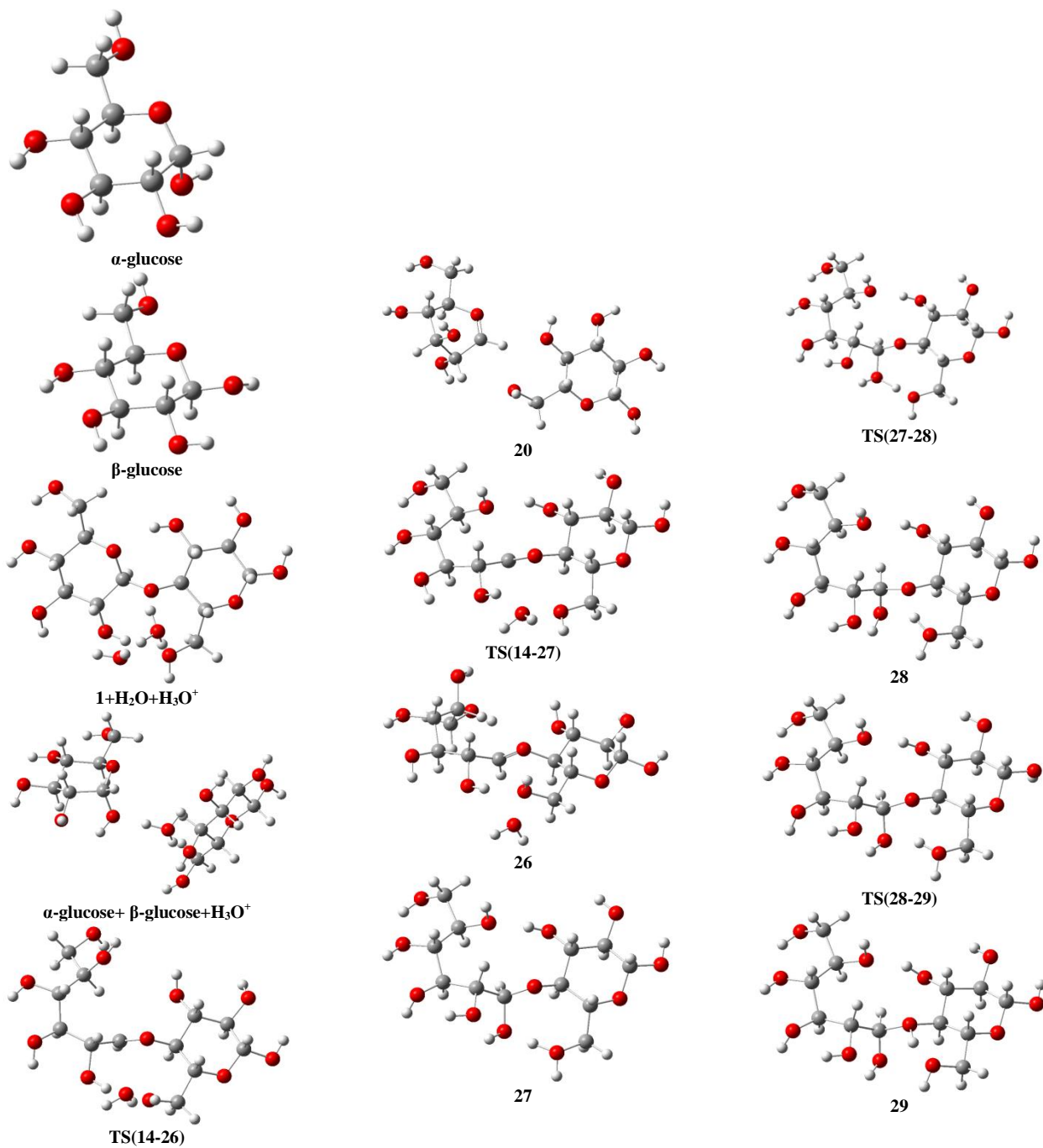
8 -0.258873 -2.241795 3.518124  
6 -1.420399 -1.535163 3.190617  
6 -2.241491 -1.274332 4.446591  
6 -2.563199 -2.578906 5.145166  
6 -1.276191 -3.341782 5.363437  
6 -0.549846 -3.509468 4.045783  
6 -0.934073 -0.257414 2.543458  
8 -2.124822 0.484466 2.114357  
8 -3.422726 -0.608329 4.019039  
6 -4.016161 0.334693 4.893074  
8 -3.800460 1.567349 4.301536  
8 -3.152383 -2.377418 6.396534  
8 -1.501768 -4.626105 5.872083  
8 0.667089 -4.137368 4.206926  
6 -5.490589 0.000973 5.034916  
8 -5.611157 -1.214279 5.722843  
6 -6.195885 -0.072237 3.655979  
8 -6.572113 -1.410073 3.403945

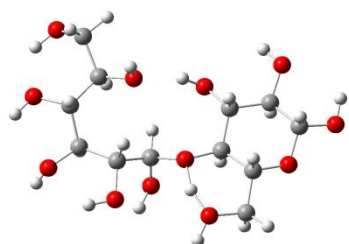
6	-7.470786	0.773024	3.595093	8	0.928422	-1.717549	2.369119	6	-2.554742	-2.475704	5.172475
8	-8.303875	0.318277	2.561688	8	2.536941	-3.990520	1.878674	6	-1.295698	-3.292196	5.394207
6	-7.172366	2.231858	3.274785	8	4.736560	-3.552616	0.228152	6	-0.578150	-3.533400	4.082746
6	-8.424743	3.089857	3.183133	6	-1.403415	0.587914	0.968584	6	-0.950570	-0.346469	2.402240
8	-9.164276	2.851674	2.016188	8	-1.524610	-0.656717	1.600361	8	-2.164163	0.385525	2.135093
8	-6.265528	2.776741	4.214744	6	-2.088106	0.566840	-0.422253	8	-3.331028	-0.472274	3.986438
1	-8.114547	4.131561	3.158131	8	-2.414298	-0.767148	-0.749964	6	-4.014345	0.408528	4.944320
1	-0.366059	-0.455118	1.644476	6	-3.389311	1.373497	-0.452736	8	-3.815067	1.681066	4.510182
1	-9.038299	2.942281	4.077660	8	-4.205085	0.940273	-1.508512	8	-3.106940	-2.226671	6.430986
1	-6.662602	2.268098	2.312667	6	-3.129126	2.851910	-0.709254	8	-1.584876	-4.545627	5.940911
1	-7.993398	0.704403	4.555987	6	-4.401522	3.683476	-0.749160	8	0.621704	-4.186535	4.268429
1	-8.296629	-0.642629	2.581078	8	-5.152288	3.473680	-1.914400	6	-5.471180	-0.014781	4.985640
1	-5.518178	0.265369	2.873336	8	-2.223304	3.372936	0.245055	8	-5.559899	-1.279399	5.576890
1	-5.965165	-1.814159	2.783414	1	-4.116411	4.732566	-0.736817	6	-6.127325	-0.020442	3.577757
1	-5.945440	0.781526	5.642400	1	3.692652	0.086925	-2.452455	8	-6.419309	-1.354097	3.224277
1	-6.056209	-1.826351	5.120554	1	-4.998418	3.485885	0.147029	6	-7.444819	0.761396	3.538292
1	-3.522101	0.271723	5.862939	1	-2.631260	2.942043	-1.674076	8	-8.237312	0.326227	2.467024
1	-1.679352	-0.628027	5.123852	1	-3.912498	1.248606	0.502164	6	-7.207538	2.246012	3.300170
1	-2.029113	-2.095688	2.473671	1	-4.170142	-0.019926	-1.531705	6	-8.490077	3.061882	3.280703
1	-0.375607	0.361145	3.236691	1	-1.414936	0.971106	-1.177054	8	-9.248549	2.851173	2.120911
1	-1.181417	-4.055345	3.333620	1	-1.795444	-1.113222	-1.393239	8	-6.300731	2.761880	4.256890
1	0.558989	-4.819174	4.874883	1	-1.876641	1.336020	1.602370	1	-8.218682	4.114497	3.298901
1	-0.627616	-2.768084	6.031725	1	-1.918727	-1.256325	0.951605	1	-0.484719	-0.611610	1.460576
1	-1.977440	-4.544270	6.700561	1	0.550223	0.841561	1.840059	1	-9.075607	2.848875	4.180732
1	-3.219549	-3.168111	4.497244	1	2.438057	0.000880	1.072176	1	-6.717093	2.355553	2.333622
1	-4.058659	-2.060453	6.270368	1	2.063406	-1.530001	-1.541186	1	-7.976969	0.614935	4.484973
1	-1.945238	1.399504	1.857915	1	3.759277	0.923707	-0.873033	1	-8.208081	-0.634053	2.447899
1	-9.313621	1.904348	1.955795	1	2.896057	-3.469168	-0.662305	1	-5.450148	0.410829	2.840882
1	-6.714723	3.006886	5.030612	1	4.614343	-4.231189	0.896859	1	-5.809621	-1.668097	2.556462
1	-4.614875	2.098959	4.282541	1	3.443656	-2.146979	2.019834	1	-5.981462	0.700493	5.629325
1	-2.838886	0.432895	2.815407	1	2.049171	-3.886536	2.697773	1	-5.931006	-1.872091	4.907819
<b>38</b>				1	0.853251	-2.522370	0.476251	1	-3.526560	0.226224	5.899280
8	3.833725	-1.660962	-0.499263	1	0.010185	-1.439725	2.237652	1	-1.568350	-0.562907	5.066006
6	2.680931	-0.951966	-0.845308	1	2.104328	1.986054	-2.064892	1	-2.049505	-2.175463	2.515496
6	1.865043	-0.647437	0.406694	1	-5.275444	2.526002	-2.014858	1	-0.278252	0.257769	3.003781
6	1.516137	-1.936716	1.120395	1	-2.671515	3.571208	1.069721	1	-1.226965	-4.089563	3.394630
6	2.790939	-2.718734	1.353875	1	-0.557159	2.715797	0.311175	1	0.485424	-4.870700	4.928570
6	3.526659	-2.917250	0.045922	1	1.246980	0.879295	-1.187648	1	-0.619373	-2.730063	6.044467
6	3.163469	0.305115	-1.534672	<b>TS(38-39) – 1 imaginary</b>				1	-2.049484	-4.413623	6.769524
8	1.956438	1.043984	-1.909094	<b>frequency</b>				1	-3.246119	-3.050693	4.550146
8	0.696216	0.045686	-0.037350	8	-0.253661	-2.295984	3.507740	1	-4.041991	-2.005270	6.319168
6	0.067433	0.952241	0.869387	6	-1.397852	-1.576605	3.160932				
8	0.273050	2.210932	0.347749	6	-2.166579	-1.216203	4.431103				
1	-2.004020	1.319781	1.972134	6	-0.583657	-3.532953	4.078159	6	-6.138576	-0.028734	3.579728
1	-9.359351	1.903015	2.011420	6	-0.923745	-0.345116	2.387275	8	-6.434397	-1.360314	3.225347
1	-6.746780	2.960912	5.082737	8	-2.114685	0.387259	2.091197	6	-7.452924	0.759980	3.535650
1	-4.661648	2.139478	4.356876	8	-3.330976	-0.460413	3.993265	8	-8.243267	0.328321	2.462122
1	-2.917288	0.119992	3.065795	6	-4.041162	0.419854	4.979101	6	-7.207905	2.242765	3.296950
<b>39</b>				8	-3.838377	1.690904	4.578028	6	-8.485169	3.066681	3.278671
8	-0.250556	-2.298893	3.503282	8	-3.088560	-2.194159	6.432715	8	-9.245117	2.859880	2.119359
6	-1.385867	-1.566698	3.150157	8	-1.592766	-4.530534	5.944228	8	-6.297214	2.751270	4.254400
6	-2.146765	-1.202974	4.424919	8	0.610610	-4.198136	4.257855	1	-8.207200	4.117573	3.296112
6	-2.543456	-2.454969	5.173558	6	-5.489564	-0.030624	4.992929	1	-0.429170	-0.638644	1.466903
6	-1.290966	-3.282775	5.392941	8	-5.556522	-1.303402	5.566280	1	-9.071409	2.857621	4.179083



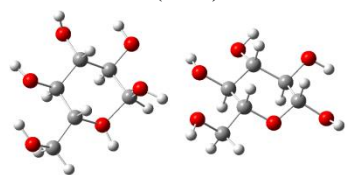
1	-6.717037	2.350104	2.330432	6	-2.794412	1.915774	1.360835	8	-4.412373	-1.470044	3.167953
1	-7.988495	0.616435	4.480746	8	-4.100777	2.437690	1.390728	6	-5.247403	0.275640	3.696849
1	-8.235508	-0.632400	2.454390	6	-1.904688	2.967847	0.729411	6	-6.366583	-0.186987	4.604223
1	-5.456999	0.400696	2.845672	6	-2.197873	4.358911	1.277065	6	-7.620744	0.701534	4.485055
1	-5.845336	-1.668238	2.536548	8	-3.343449	4.936123	0.709104	6	-7.579212	2.002005	5.274961
1	-6.015498	0.668865	5.642055	8	-0.588070	2.580451	1.051835	6	-6.582170	3.017049	4.757606
1	-5.931442	-1.891086	4.894578	1	-1.360940	5.007349	1.024643	8	-5.320741	2.455438	5.047602
1	-3.546022	0.201721	5.921580	1	3.535007	0.794805	-2.098990	8	-3.736757	-3.630750	4.653232
1	-1.553564	-0.540156	5.053141	1	-2.268163	4.315615	2.367162	8	-1.334299	-4.960116	3.892869
1	-2.044133	-2.160815	2.507229	1	-2.054849	2.983835	-0.352516	8	0.727438	-3.178540	3.091453
1	-0.249683	0.250919	2.997364	1	-2.436815	1.749276	2.382523	8	-5.568129	0.701286	2.548290
1	-1.241953	-4.082918	3.394008	1	-4.687664	1.721941	1.648286	8	-6.701329	-1.488145	4.210096
1	0.469625	-4.884322	4.914889	1	-3.176935	0.722348	-0.380776	8	-8.679984	-0.060547	5.029273
1	-0.606015	-2.725799	6.038377	1	-4.163049	-0.856167	0.824478	8	-8.848532	2.601189	5.221429
1	-2.042430	-4.391599	6.779911	1	-1.102158	-0.240549	1.633796	6	-6.741332	4.371129	5.434906
1	-3.241756	-3.026990	4.556855	1	-2.000115	-2.133047	1.100869	8	-7.826085	5.101018	4.928263
1	-4.032288	-2.011036	6.328788	1	0.297718	0.726161	0.024097	1	-5.847250	4.960897	5.242268
1	-1.923287	1.302335	1.875960	1	1.665773	-1.017429	0.540817	1	-1.213977	0.515871	1.608682
1	-9.364104	1.912553	2.011472	1	2.276848	-1.331643	-2.441034	1	-6.820572	4.229432	6.515919
1	-6.741212	2.957525	5.079724	1	2.675788	1.038226	-0.574314	1	-6.710264	3.149987	3.679424
1	-4.681409	2.138541	4.369536	1	3.717520	-3.113471	-2.042946	1	-7.314817	1.771254	6.311580
1	-2.994450	0.098421	3.164100	1	5.813954	-2.919240	-1.355380	1	-9.484516	1.983134	5.586650
<b>40</b>				1	3.228336	-3.026509	0.960410	1	-7.813603	0.914229	3.434908
6	2.967941	-3.384324	-0.038765	1	3.838689	-5.092528	0.202188	1	-9.349761	-0.213233	4.363202
6	3.924750	-2.753536	-1.029917	1	1.317654	-3.355835	-1.373887	1	-5.992993	-0.174622	5.628340
8	3.760056	-1.351289	-0.997354	1	0.554921	-4.319759	0.547136	1	-7.532276	-1.699681	4.647823
6	2.502512	-0.918845	-1.453257	1	1.705474	1.959484	-2.602735	1	-4.289546	0.535828	4.117737
6	1.493674	-1.449070	-0.443304	1	-4.073024	4.340249	0.898383	1	-2.788631	-1.250761	4.420272
6	1.562727	-2.954203	-0.385459	1	0.030637	3.158728	0.604757	1	-2.407582	-1.683673	1.424573
8	5.201083	-3.058516	-0.632639	1	-0.365635	1.035805	-2.031690	1	-2.034334	0.801239	3.142742
6	2.611213	0.585683	-1.565095	1	-0.526907	-1.832255	-0.479587	1	-0.856055	-3.382924	1.809644
8	1.500406	1.081403	-2.281072		<b>TS(40-32) – 1 imaginary</b>			1	1.275431	-3.046825	2.317069
8	0.123733	-1.144340	-0.831888		<b>frequency</b>			1	-1.123409	-3.132132	4.830214
8	0.608874	-3.362462	0.553019	6	-0.590994	-2.950948	2.780691	1	-0.433662	-5.198774	4.116556
8	2.986534	-4.779532	-0.104184	8	-0.816467	-1.560059	2.741257	1	-3.186218	-3.702553	2.677578
6	-0.521978	0.157472	-0.394086	6	-2.133287	-1.217478	2.376136	1	-3.742469	-4.588028	4.694824
8	-1.086545	0.702657	-1.477188	6	-3.052782	-1.732632	3.475455	1	-3.021100	1.441986	0.891999
6	-1.565772	-0.263270	0.650496	6	-2.884108	-3.227313	3.616536	1	-8.609679	4.559450	5.055432
8	-1.916104	-1.597174	0.310606	6	-1.437088	-3.564896	3.876753	1	-4.629159	3.018644	4.696533
6	-2.848912	0.570885	0.647037	6	-2.104683	0.285899	2.185074	1	-4.727065	0.882723	2.034122
8	-3.824620	-0.146536	1.370648	8	-3.256119	0.718413	1.473388	1	-4.978628	-2.120684	3.614822

## Figures of optimized structures (BB1K/6-31++G\*\*)

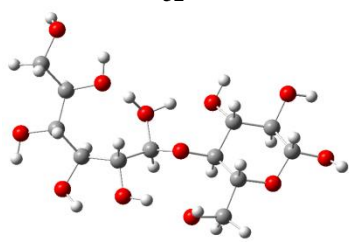




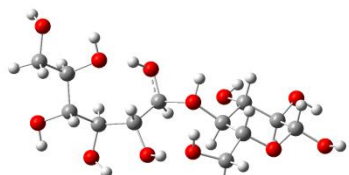
TS(29-30)



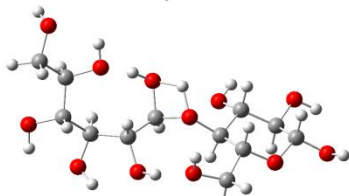
32



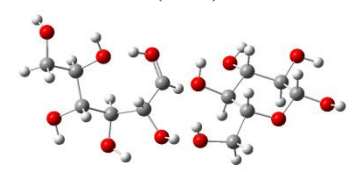
33



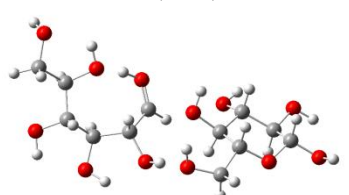
34



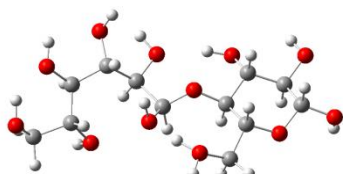
TS(33-34)



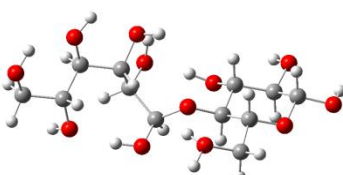
TS(34-35)



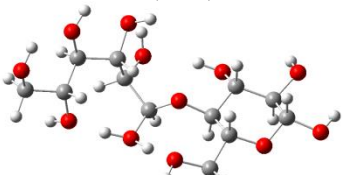
35



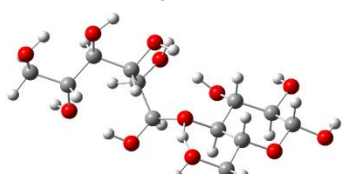
TS(27-37)



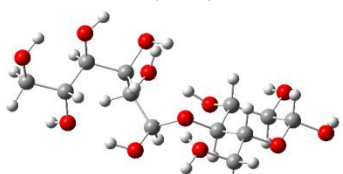
TS(37-38)



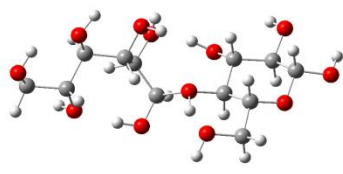
37



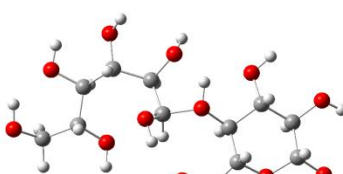
TS(38-39)



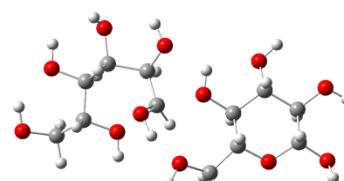
38



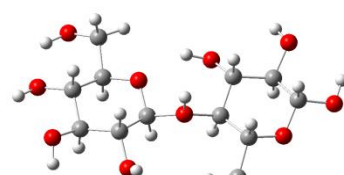
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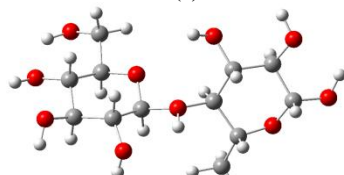
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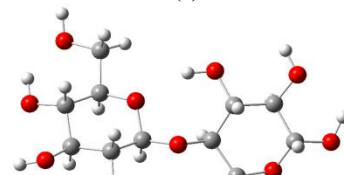
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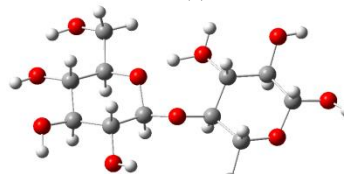
3-O(1)-1



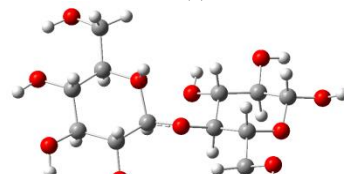
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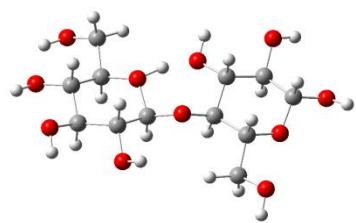
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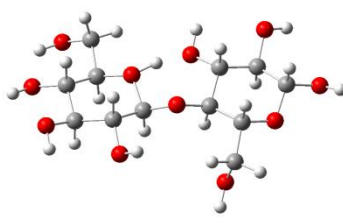
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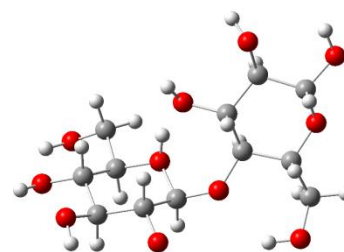
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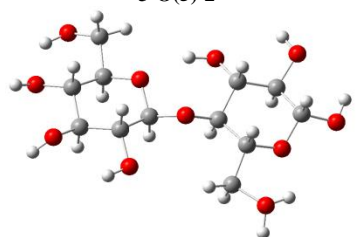
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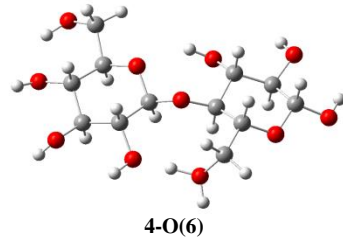
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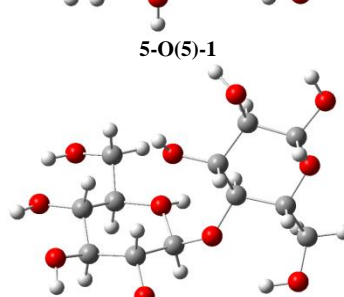
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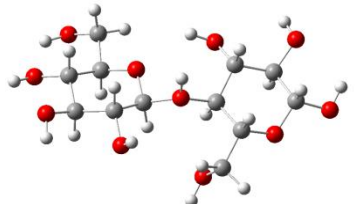
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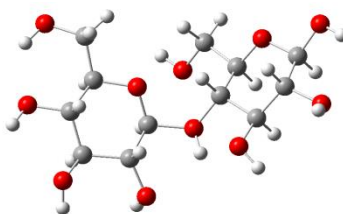
4-O(6)



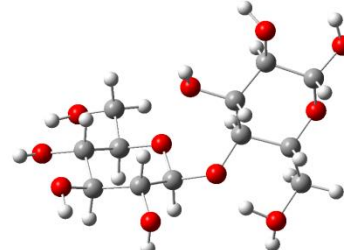
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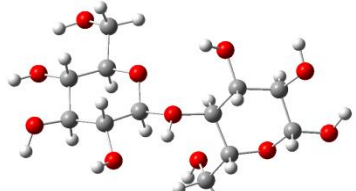
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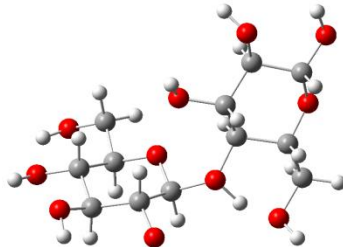
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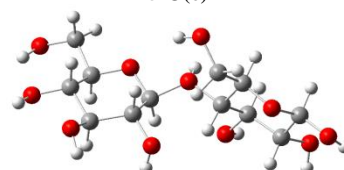
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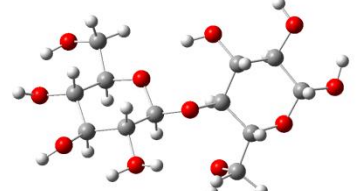
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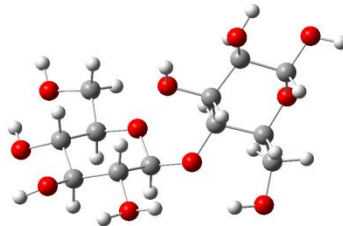
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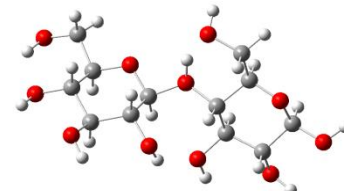
6-O(1)-1



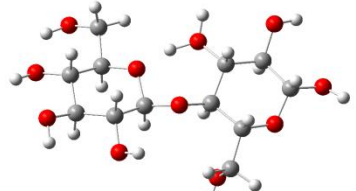
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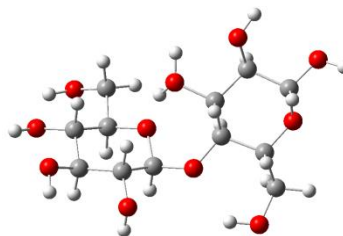
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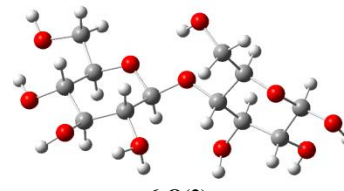
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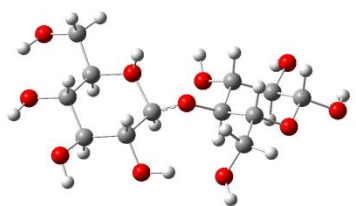
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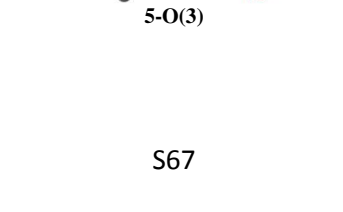
5-O(3)



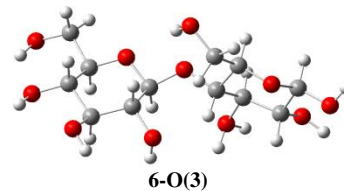
6-O(2)



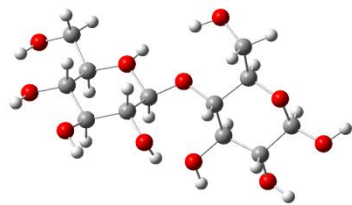
4-O(5)-1



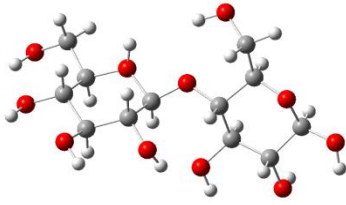
5-O(3)



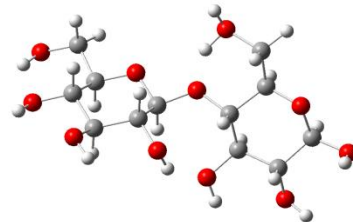
6-O(3)



6-O(5)-1



6-O(5)-2



6-O(6)

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