Supporting information for:

Mechanistic insights in the selective catalytic oxidation of glycolaldehyde: an industrially feasible route from biomass to bio-glycolic acid

Mojgan Heshmat*, Lotte Bruurs, Frits van der Klis*, Rajeesh Pazhavelikkakath Purushothaman, Carolien de kovel, Erik Hagberg, Daan S. van Es*

[a]Wageningen Food & Biobased Research, Bornse Weilanden 9, 6708 WG Wageningen, The Netherlands

[b]Archer Daniels Midland Company, 1001 N Brush College Road, Decatur, IL, 62521, USA

[c]Biometris, Wageningen University & Research, POBox 16, 6700 AA Wageningen, The Netherlands

Table S1. DoE experiments: 1wt% glycolaldehyde substrate concentration in 20 mL water, 100 mg 1wt% Pt/C (0.32 mEq Pt), 10 bar oxygen, stirring at 750 rpm.

Entry	Variables		Response
	Temperature (°C)	Reaction time (h)	Glycolic acid yield (mol%)
1	74.9	1.52	57.6
2	61	4.28	73.1
3	74.2	6.68	85.5
4	46.2	1.43	34.2
5	60.1	4.12	83.5
6	47.9	6.9	68.0
7	60.2	4.2	70.2
8	41.4	4.23	46.7
9	60.2	8	82.9
10	61.3	0.47	29.4
11	60.3	4.19	70.5
12	80	4.1	73.8

The equation presenting the estimated surface is:

Glycolic acid yield (mol%) = -139.5 + 4.63 * temperature + 18.86 * time - 0.031 * temperature^2 + 1.18 * time^2 - 0.04 * temperature * time.

Analytical methods

HPLC analyses were performed on a Waters e2695 HPLC instrument, equipped with a Concise Corogel Ion 300 (30 cm length) column, maintained at 65 °C, using H2SO4 (3 mM) in MilliQ water as the eluent, with a flow rate of 0.4 mL min−1. The components were identified using a Waters 2489 UV/Vis Detector (210 nm) and a Waters 2414 RI detector. Glycolaldehyde, glycolic acid, glyoxylic acid, oxalic acid, formaldehyde and formic acid concentrations were determined based on calibration curves of the corresponding components. An overview of all HPLC spectra are displayed in SI **Figure S1 A-C**.

Table1 – entry 1

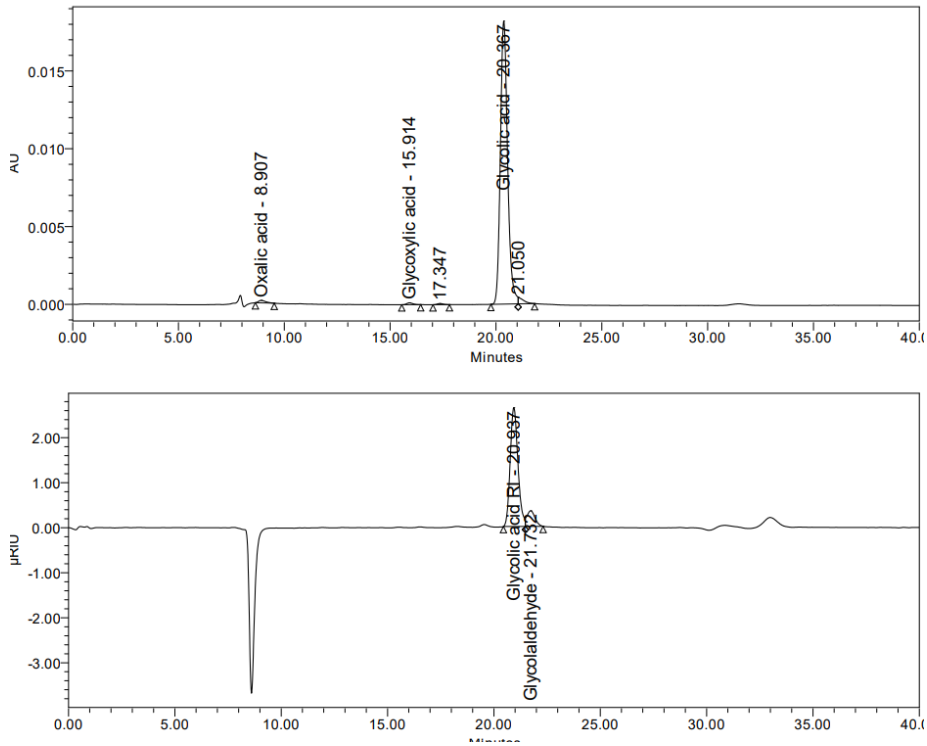
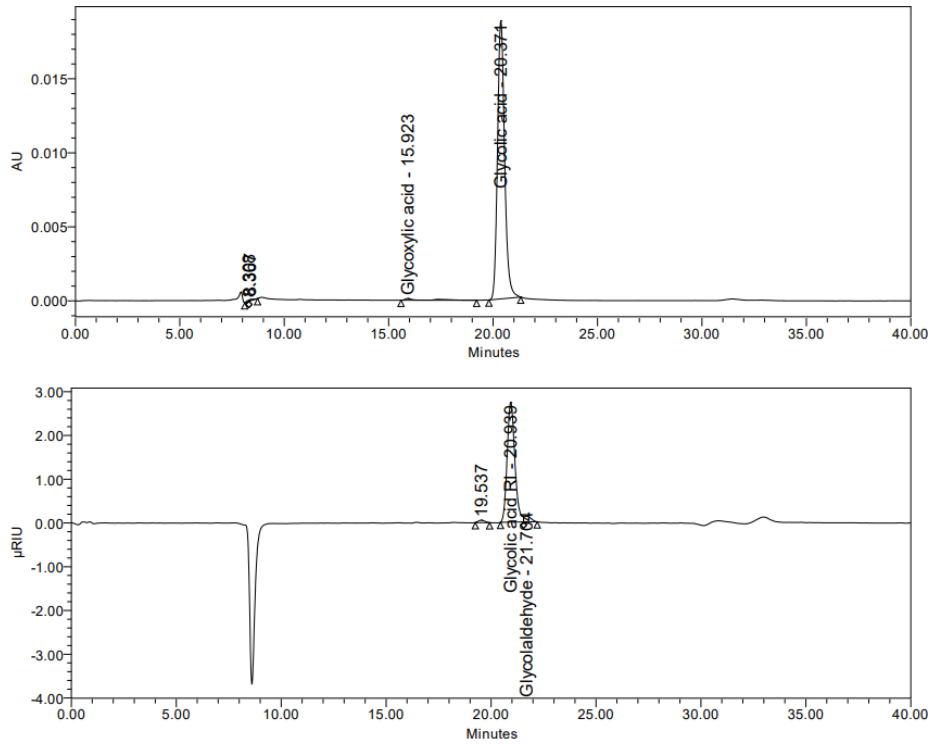


Table1 – entry 2



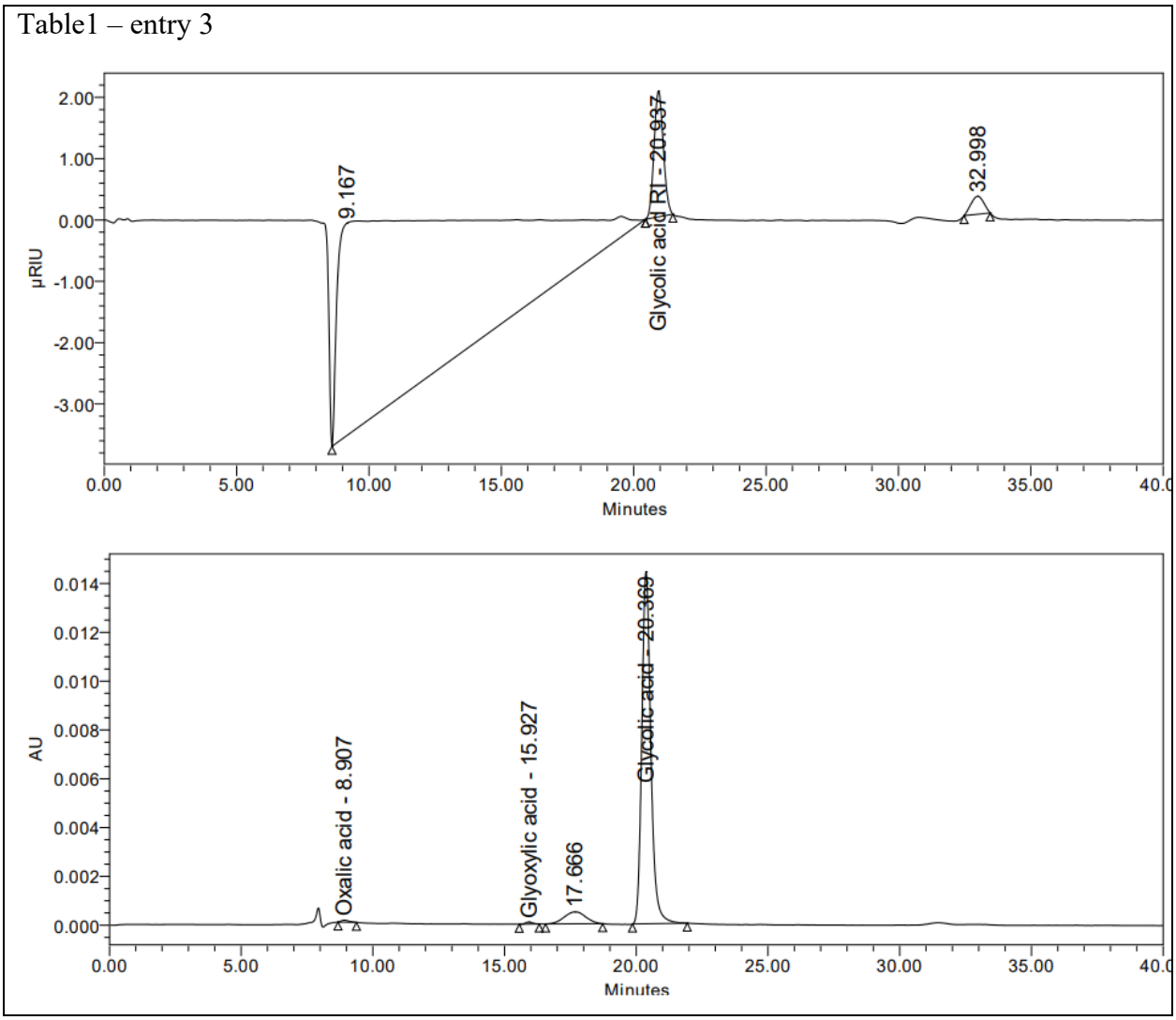


Figure S1A. HPLC chromatograms corresponding to entries 1 - 3 of Table 1 in the main text.

Table3 – entry 1

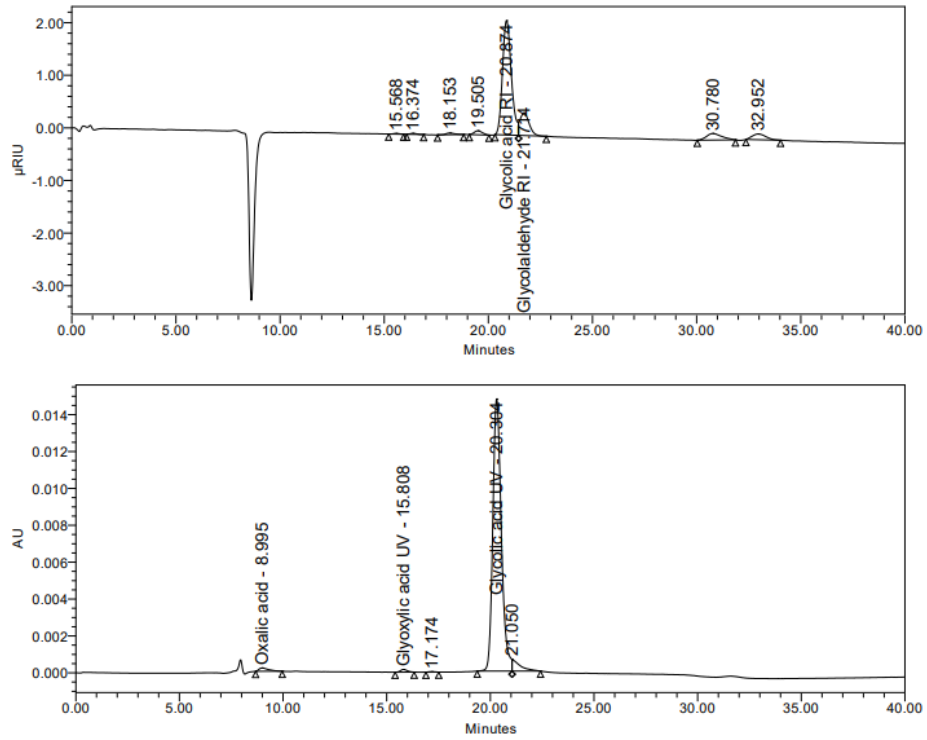


Table3 – entry 2

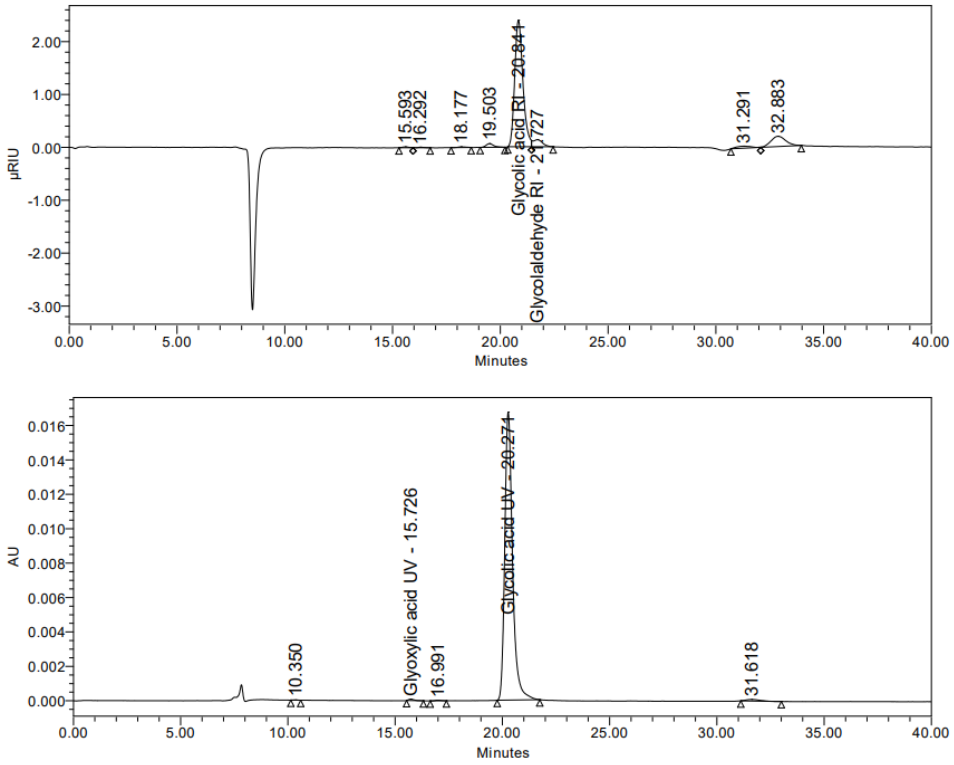


Table3 – entry 3

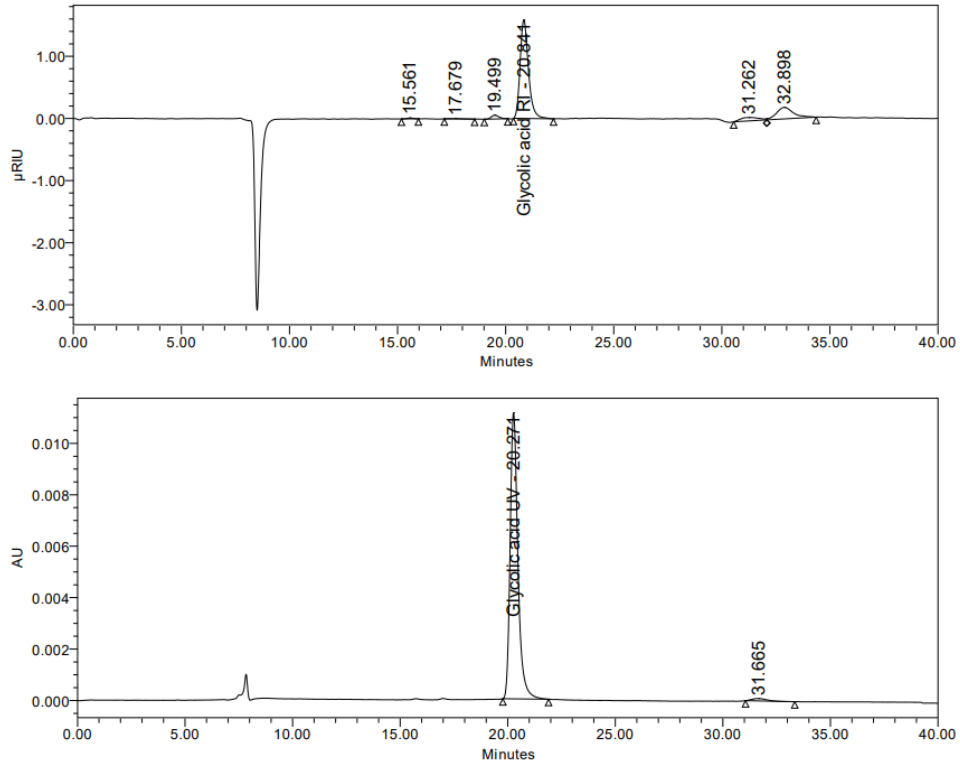


Table 3 – entry 4

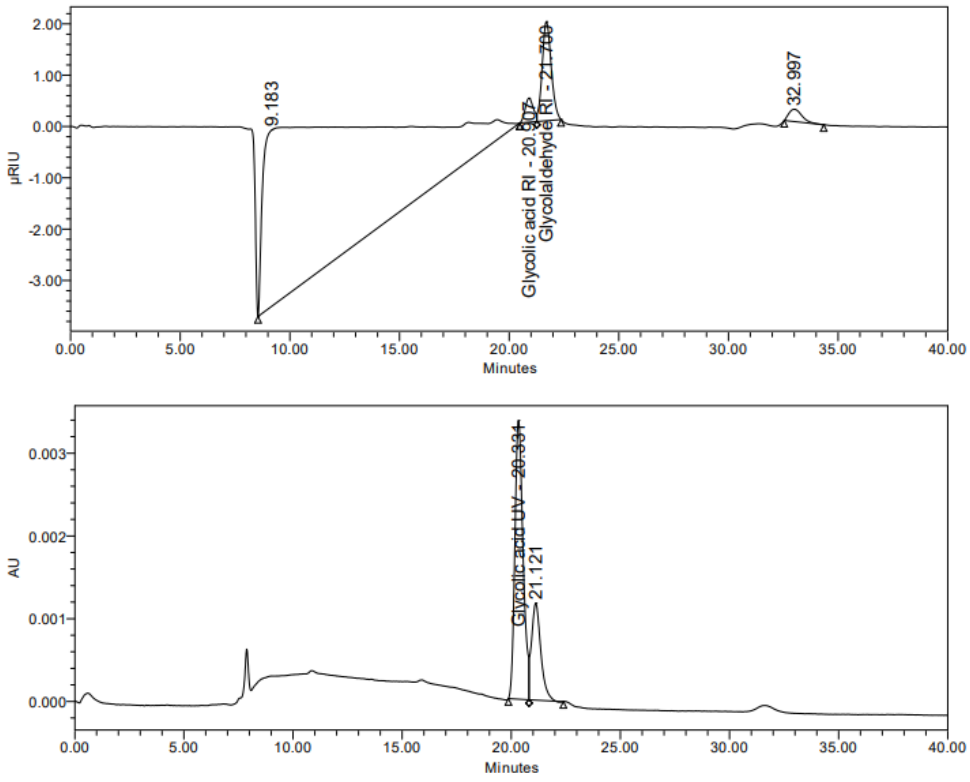


Table 3 – entry 5

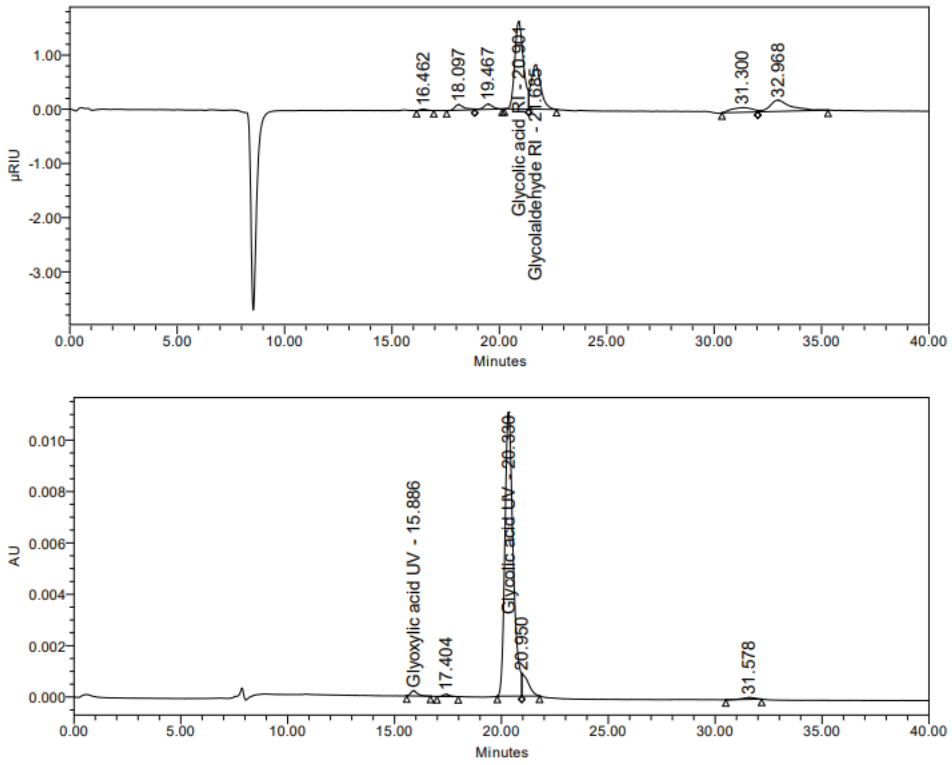


Table 3 – entry 6

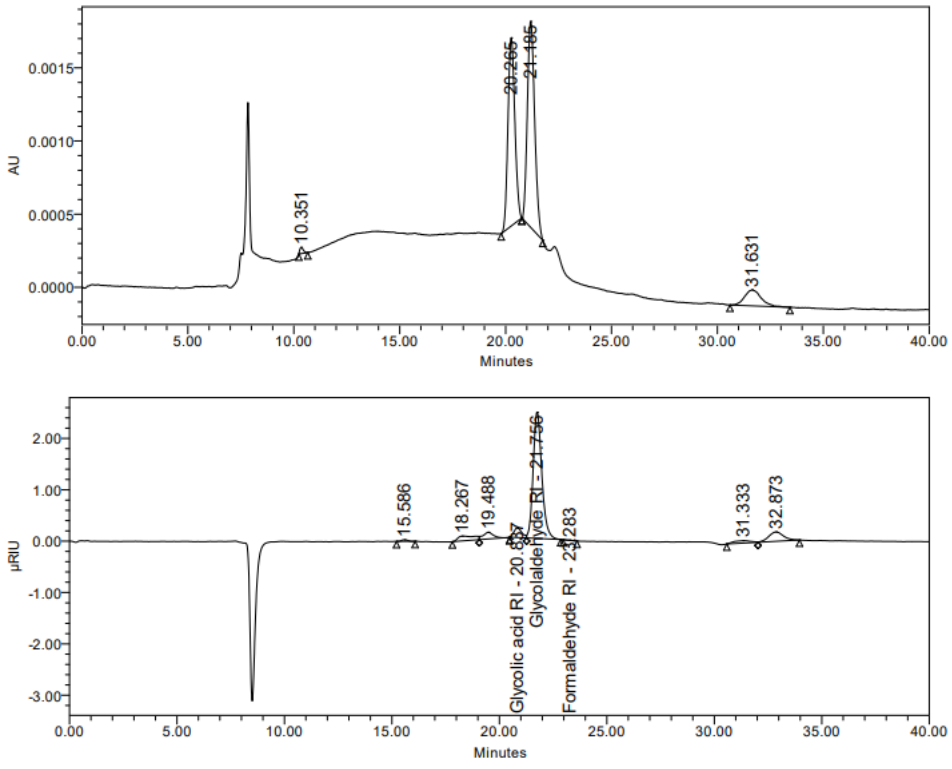


Table 3 – entry 7

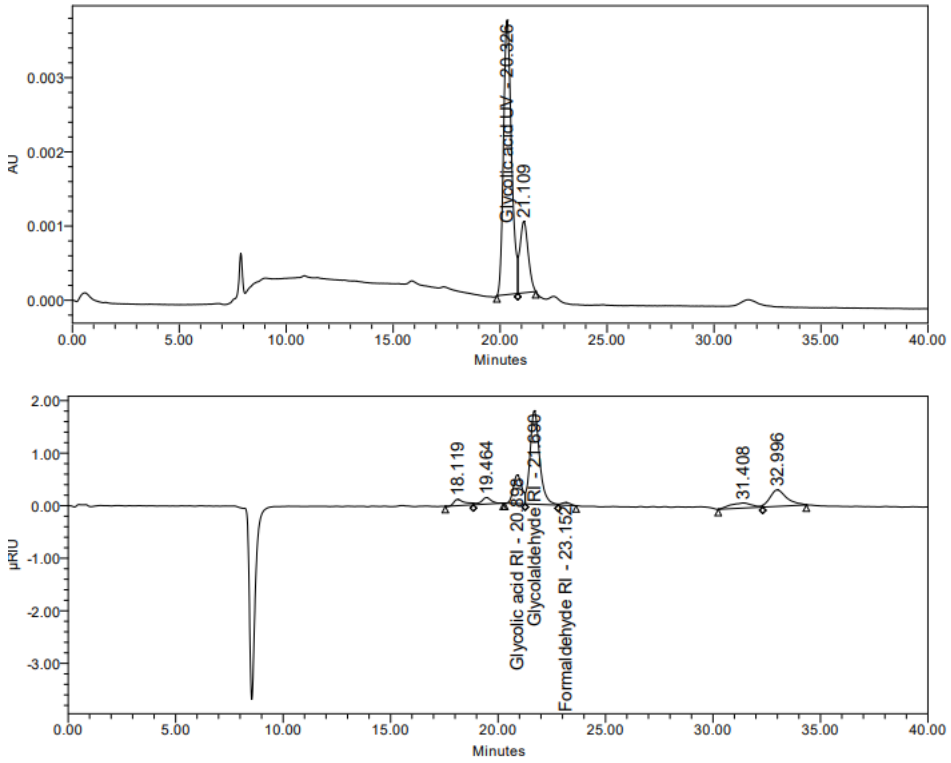


Figure S1B. HPLC chromatograms corresponding to entries 1 – 7 of Table 3 in the main text.

Table4 – entry 2

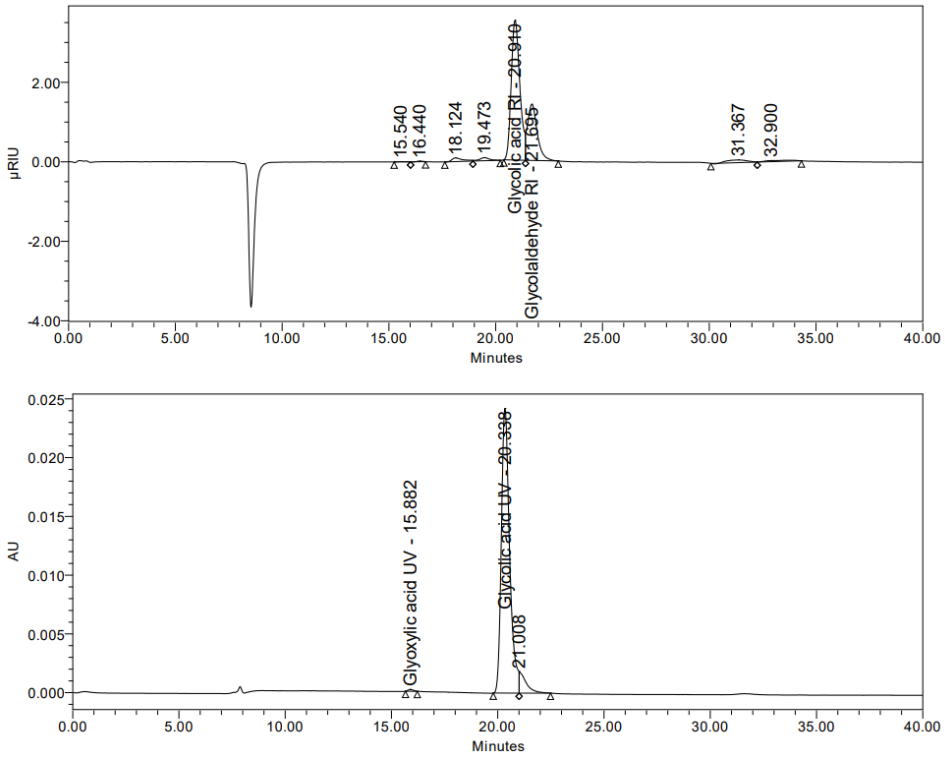


Table4 – entry 3

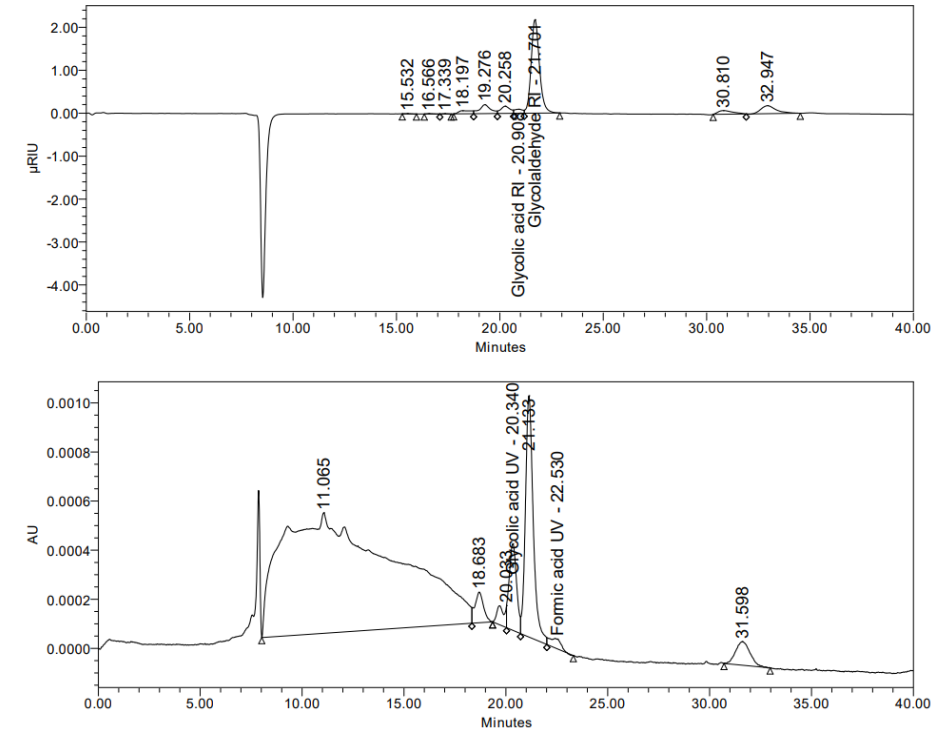


Table4 – entry 4

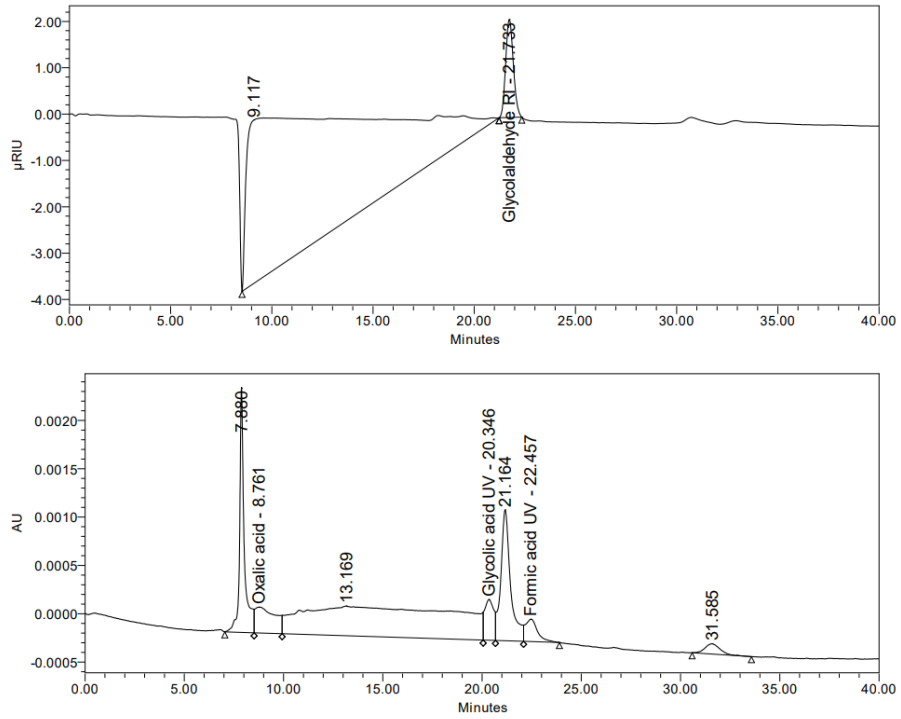


Table4 – entry 5

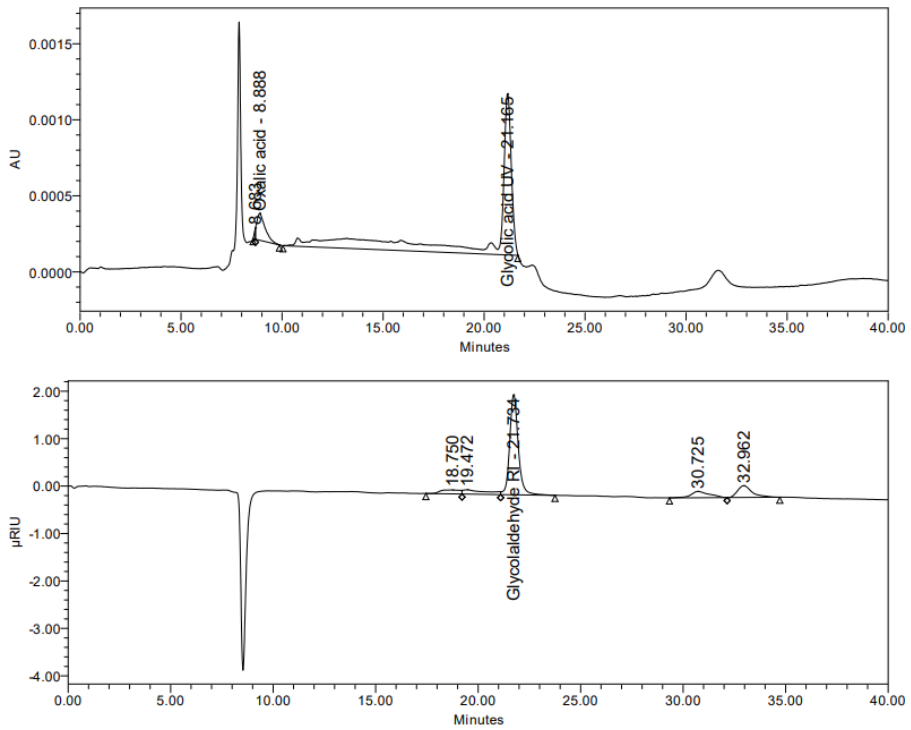


Figure S1C. HPLC chromatograms corresponding to entries 2 - 5 of Table 4 in the main text.

The calibration curves were made by making 1, 2, 4, 6, 8 and 10 mM solutions of the substrates. The corresponding areas in the UV or RI chromatograms were plotted against their respective concentrations. Concentrations of the reaction components can then be calculated from the trendlines of the calibration curves, two examples are show in Figures **S1D** and **S1E**.

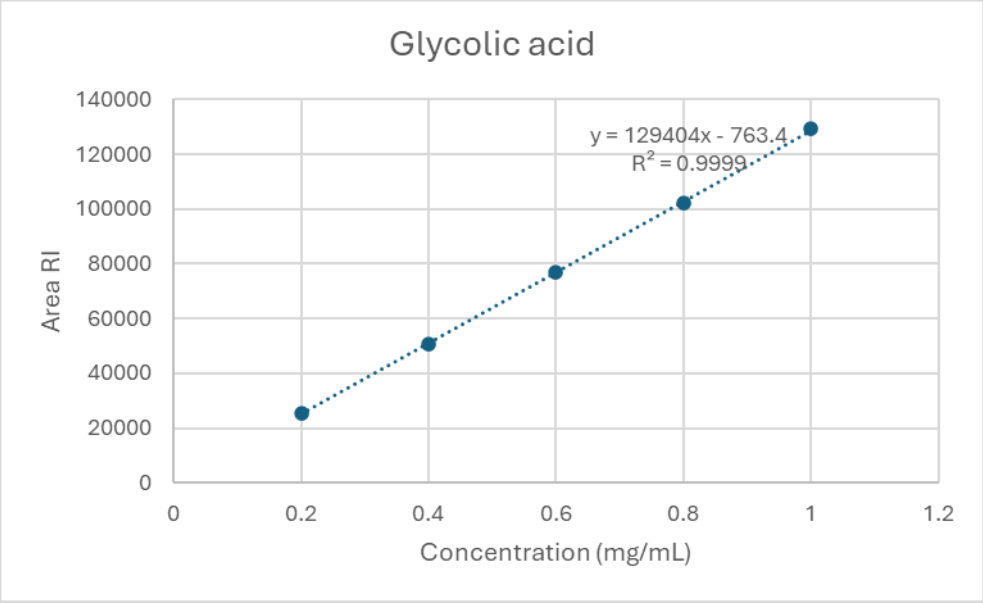


Figure S1D. Calibration curve for glycolic acid. Concentration can be calculated using the formula: C = (Area+763.4)/129404.

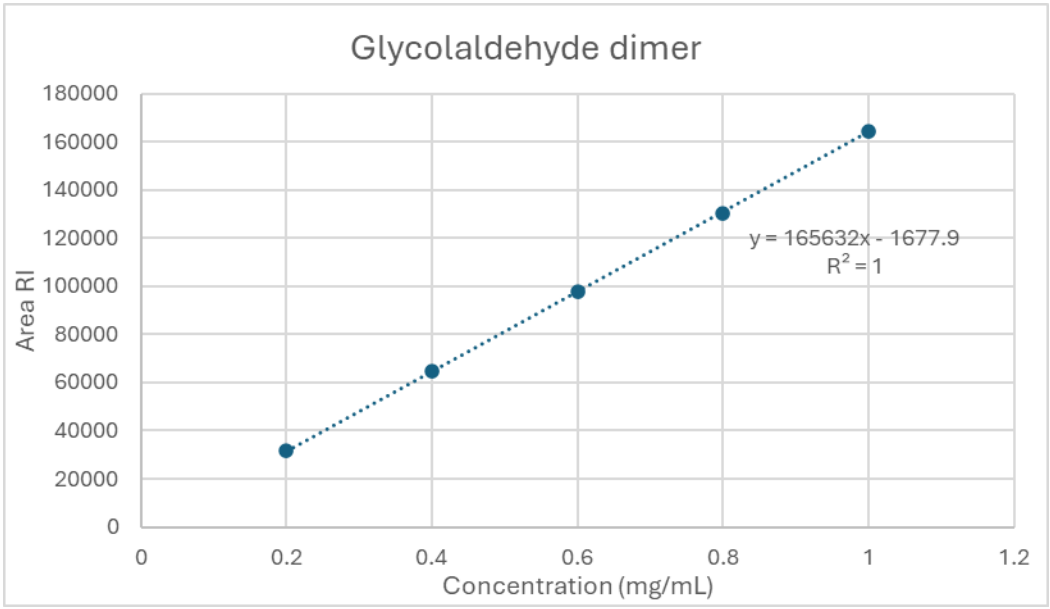


Figure S1E. Calibration curve for glycolaldehyde dimer. Concentration can be calculated using the formula: C = (Area+1677.9)/165632.

The replication error for these measurements lies between 0.4 and 0.7%, **Table S2**.

Table S2. Replication errors for glycolaldehyde dimer and glycolic acid.

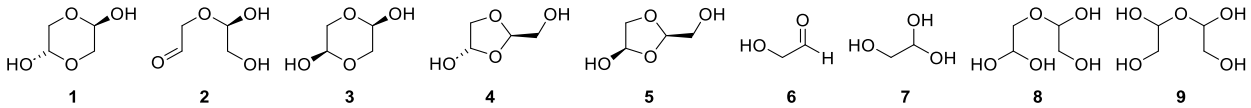
Sample	Glycolaldehyde	Glycolic acid
1	0.91	6.15
2	0.91	6.09
3	0.93	6.12
4	0.91	6.09
5	0.91	6.09
Average	0.92	6.11
Standard Deviation	0.01	0.02
Percent Error	0.7	0.4

Both solvent and eluent are water, which is a neutral, non-interacting solvent, we think they should not result in a serious interaction with the column. Hence, the recovery rate is supposed to be quite high.

All calculations related to the thermodynamics and kinetics of various equilibria of glycolaldehyde in aqueous/acidic solution and in the absence of Pt/C catalyst (the results reported in Table **S2**) were performed using the ADF software package.[1,2] For each reaction the lowest energy structures of ground and transition states were obtained. The calculations were carried out with the BLYP functional, augmented with Grimme's D3 dispersion correction and the TZ2P basis set. The optimized geometries have been verified to have zero imaginary frequency modes. The transition states were searched based on potential energy scans using linear transit (LT) calculations by employing the corresponding reaction coordinates (distances) for each reaction, starting from and ending at fully converged stable minima in a series of steps. In each LT calculation, all degrees of freedom are fully optimized except the reaction coordinate, which are scanned stepwise.

Table S2 reports the ΔG and $\Delta G^{\neq}$ from Ref. 47, which have been calculated with including explicit H_2O molecules. In comparison, we calculated free energy values including explicit glycolic acid and water molecules, since glycolic acid is continuously produced during the reaction. In **Scheme S1** molecule **1** is the starting cyclic glycolaldehyde dimer that can partially hydrolyze to a linear dimer **2** (a thermodynamically favorable and kinetically not very demanding transformation), which can undergo cyclic rearrangements and generate species **3** - **5**. The cyclic rearrangement of glycolaldehyde dimer according to the literature and our calculations (entries **2**, **3** and **4** in **Table**

S1) show an unfavorable thermodynamic with slightly higher barrier than **1 → 2**. In fact, entries **2 - 4** have the highest barriers (especially in the presence of glycolic acid) within the equilibria shown in **Scheme 1**. Generation of glycolaldehyde monomer by hydrolysis of the dimer (entry **5**) has the most favorable thermodynamics and rather favorable kinetics and therefore is the most dominant equilibrium amongst the others. This implies that in a dilute aqueous solution the dimer is not a stable hydrolyses to the monomer. Formation of glycolaldehyde monomer is followed by a nucleophilic attack by a water molecule on the carbonyl, forming the glycolaldehyde hydrate that is slightly less favorable transformation thermodynamically (0.66 and 1.45 kcal/mol in neutral and acidic environments), however, kinetically favorable due to a lower barrier (16.05 and 15.45 kcal/mol).



Scheme S1. Various forms of glycolaldehyde in solution reported in ref. 47.

In **Figure S2** we have plotted the results of **Table S2** for explicit water molecules.

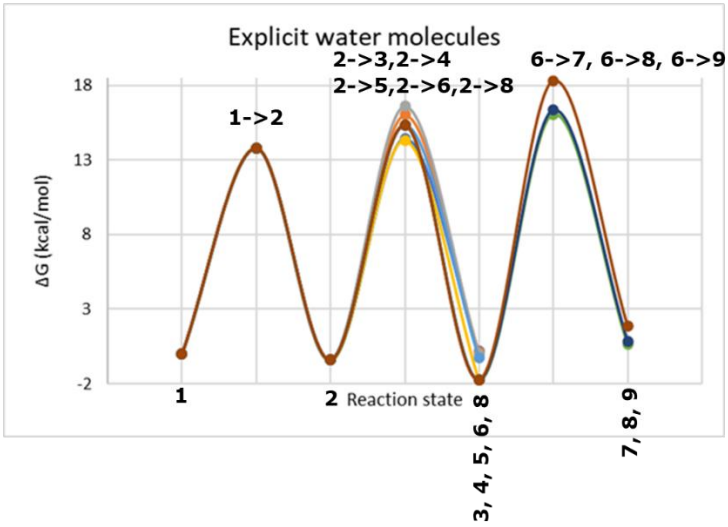
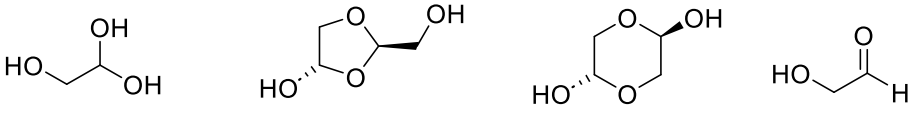


Figure S2. The results of **Table S2** for explicit water molecules (ref. 47).

Table S2. The ΔG and $\Delta G^{\neq}$ values reported in Ref. 47 for the species shown in **Scheme 1**, which have been calculated including the explicit and implicit H_2O environment in comparison to calculated values in this work with explicit glycolic acid (GA) molecules instead of water.

Entry	Reaction	ΔG (thermodynamics)		$\Delta G^{\neq}$ (Kinetics)	
		Ref.[47] (H_2O)	Calculated in this work (explicit GA)	Ref.[47] (H_2O)	Calculated in this work (explicit GA)
1	**1 -> 2**	**-0.42**	**-1.44**	**13.79**	**12.92**
2	2 -> 3	0.16	0.46	14.43	20.07
3	2 -> 4	0.12	3.80	16.01	25.81
4	2 -> 5	0.02	1.85	16.61	24.31
5	**2 -> 6 + 6**	**-1.76**	**-2.81**	**14.31**	**13.40**
6	2 + H2O(GA) -> 8	-0.24	-1.13	15.34	18.21
7	6 + H_2O(GA) -> 7	0.66	1.45	16.05	15.45
8	6 + 7 -> 8	0.86	1.76	16.37	18.25
9	6 + 7 -> 9	1.86	3.11	18.31	23.7

According to the reported data in **Table S2** and previous experimental studies, glycolaldehyde dimer hydrolyses in water to the monomeric hydrate (entry 5 in **Table S2**). Studies performed by NMR and FTIR spectroscopies at room temperature in D_2O identified the presence of at least four molecular species as shown in **Scheme 2.** As can be seen in **Scheme 2**, the predominant species in the mixture is the hydrate form of glycolaldehyde (70%).



70% **17%** **9%** **4%**

Scheme S2. Various forms of glycolaldehyde in solution reported by NMR and FTIR spectroscopies (ref. 51 and 52). The hydrated species has the highest percentage (70%) and the dominant form of glycolaldehyde in aqueous solution.

Interactions between Pt atoms and reacting species

The optimized geometries obtained by CP2K and using the same computational method (periodic calculations) described in the main text. We removed $^3O_2$ and water molecules in order to calculate the pure interaction between substrate and product molecules with the catalyst. Analysis of the

Mulliken atomic charges for the hexagonal C support as well as Pt_4 cluster are provided in **Figure S3** for free support and free Pt_4 cluster and when they complexed. In a free symmetric C support structure (**Figure S3A**), according to the atomic charges, three types of carbon atoms are distinguished and shown. Upon Pt_4 complexation the charge distribution is perturbed and as can be seen in **Figure S3B** each carbon atom has a different charge and the symmetric pattern of charge distribution completely changes. The increase of positive and negative atomic charges on the C support can also increase the electronic interaction with the present species (reactant, intermediate and product) in the reaction medium. Similarly, for Pt_4 cluster atomic charge perturbation has been shown in Figure **S3 C** and **D**.

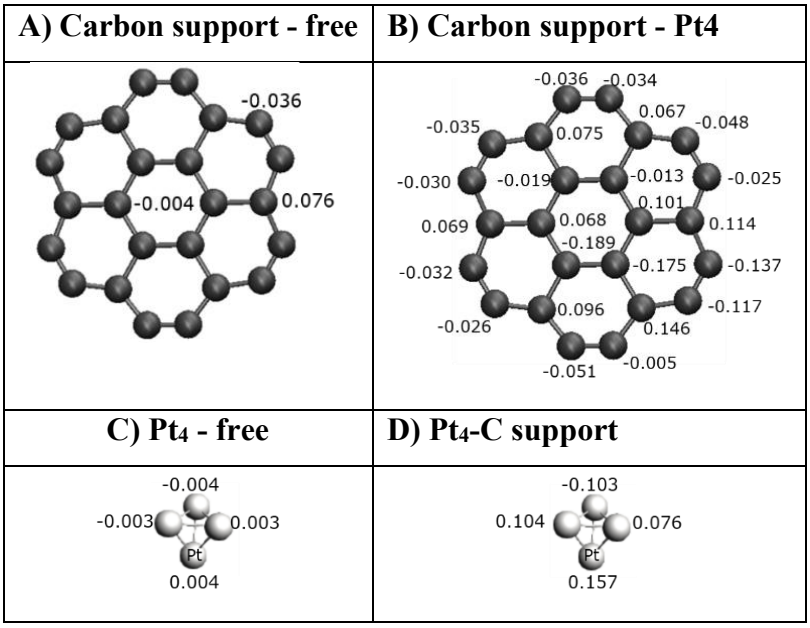


Figure S3. A) Symmetric free carbon support and three atomic charges correlated to the surface, **B)** perturbation of the carbon atomic charges after Pt_4 complexation., **C)** free Pt_4 cluster, **D)** Pt_4 cluster after complexation to the support.

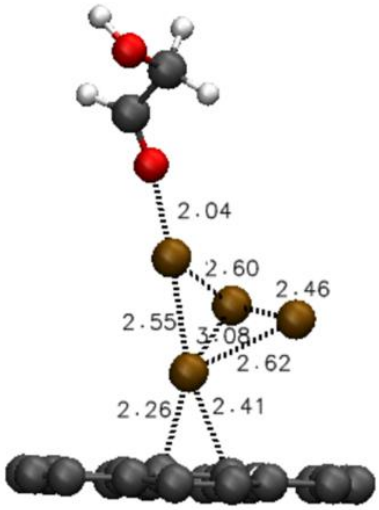
In **Table S3** we have summarized the atomic charges of the interacting atoms with the Pt_4 in comparison to those in the free molecules. The corresponding molecular complexes are shown in Figure **S4**.

Table S3. The atomic charges of the interacting atoms with the Pt_4 in comparison to the atomic charge (for the same atom) in free molecules

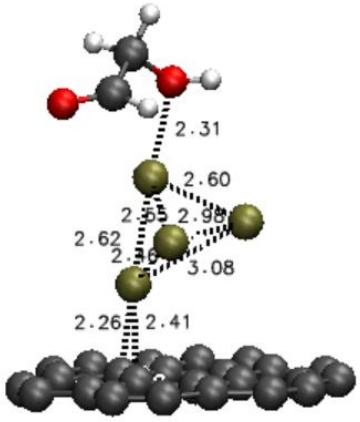
Atomic charge (bold atom in the functional group)	Free molecule (FM)	Molecular complex with Pt (MC)	Difference MC vs. FM
Glycolaldehyde (C=O)			
C(C=O)	+0.560	+0.600	**+0.040**
H(C=O)	-0.171	-0.180	-0.009
Glycolaldehyde (OH)			
O(OH)	-0.528	-0.563	-0.035
H(OH)	+0.226	+0.312	**+0.086**
Glycolaldehyde Hydrate			
$\mathbf{H^+}$(OH)	+0.221	+0.268	**+0.047**
$\mathbf{H^-}$(C-H)	-0.167	-0.182	-0.015
O(OH)	-0.528	-0.593	-0.065
Glycolic acid (OH)			
$\mathbf{H^+}$(OH)	+0.245	+0.281	+0.036
$\mathbf{H^-}$(CH_2)	-0.078 / -0.099	-0.132 / -0.151	-0.054/-0.052
Glycolic acid (COOH)			
C(C=OOH)	+0.639	+0.728	+0.089
O(C=**O**OH)	-0.497	-0.528	-0.031
Glycolic acid (COO^-)			
C(C=OO)	+0.639 (COOH)	+0.665	+0.026
O(C=OO)	-0.497 (COOH)	-0.699	-0.202
Glyoxylic acid (C=O)			
H(C=O)	-0.096	-0.107	-0.011
C(C=O)	+0.542	+0.647	**+0.105**
Glyoxylic acid (COOH)			
C(C=OOH)	+0.646	+0.693	+0.047
O(C=**O**OH)	-0.463	-0.611	-0.148

Glyoxylic acid (COO^-)			
C(C=OO)	+0.646 (COOH)	+0.677	+0.031
O(C=OO)	-0.463 (COOH)	-0.634	-0.171
Formaldehyde			
C(C=O)	+0.722	+0.843	**+0.121**
H(C=O)	-0.438	-0.533	-0.095
Formaldehyde hydrate			
$\mathbf{H}^+$(OH)	+0.245	+0.308	+0.063
$\mathbf{H}^-$(C-H)	-0.161	-0.198	-0.037
O(OH)	-0.543	-0.595	-0.052
Formic acid (COOH)			
C(C=OOH)	+0.772	+0.854	**+0.082**
O(C=OOH)	-0.431	-0.612	-0.181
Formic acid (COO^-)			
C(C=OO)	+0.772	+0.915	**+0.143**
O(C=OO)	-0.431	-0.649	-0.218
Oxalic acid (COOH)			
C(C=OOH)	+0.640	+0.719	+0.079
O(C=**O**OH)	-0.452	-0.533	-0.081
Oxalic acid (COO^-)			
C(C=OO)	+0.640	+0.611	-0.290
O(C=OO)	-0.452	-0.646	-0.194

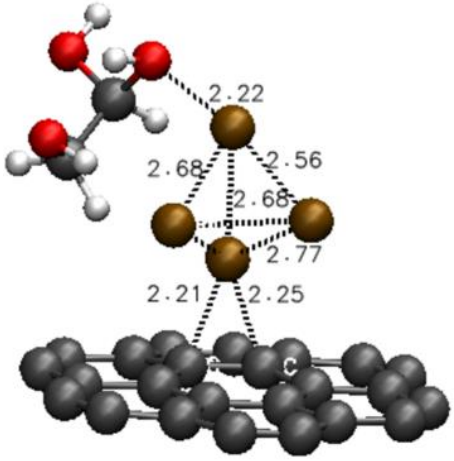
A) Glycolaldehyde – via C=O (-19.78 kcal/mol)



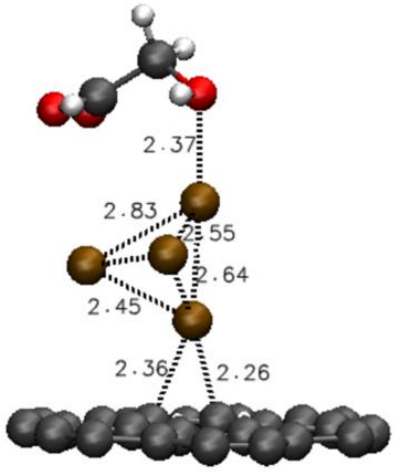
B) Glycolaldehyde - via OH (-23.25 kcal/mol)



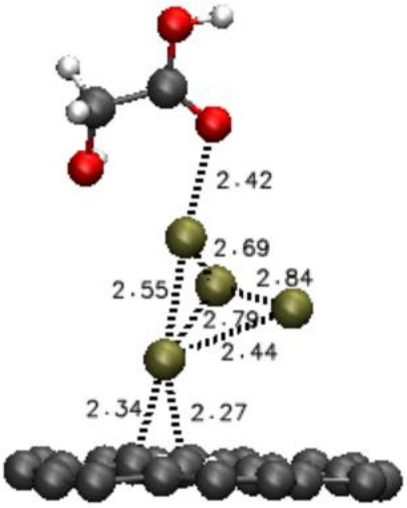
C) Glycolaldehyde hydrate (-25.18 kcal/mol)



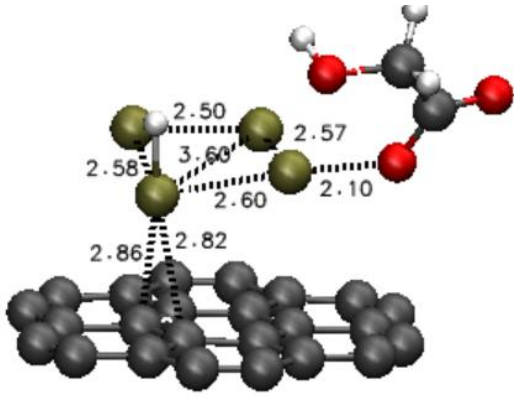
D) Glycolic acid – via OH (-19.00 kcal/mol)



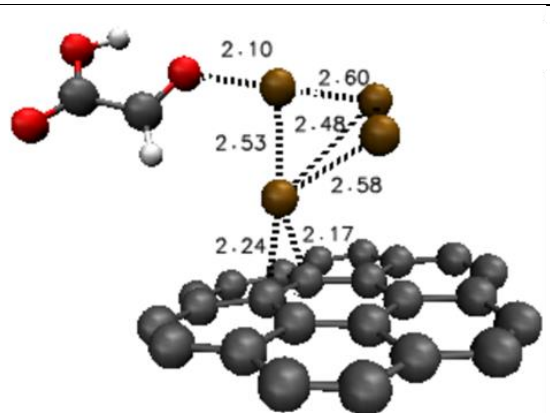
E) Glycolic acid – via (COOH)C=O (-16.08 kcal/mol)



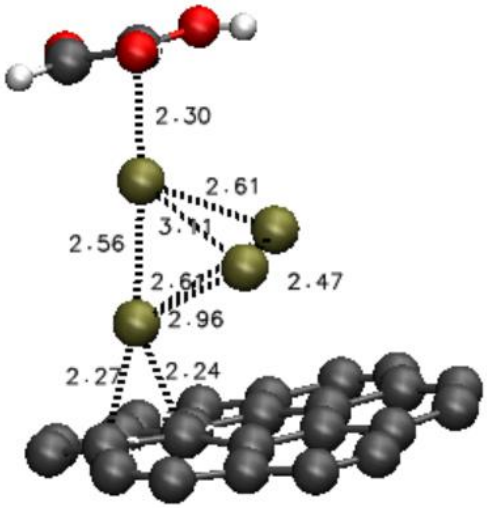
F) Glycolic acid – via COO^- (-33.09 kcal/mol)



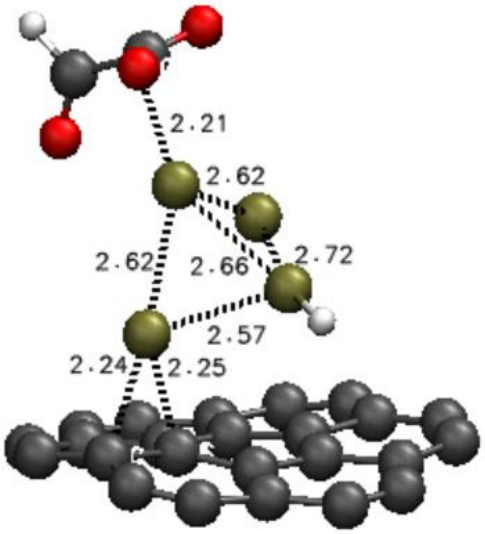
G) Glyoxylic acid - via (CHO)C=O (-28.83 kcal/mol)



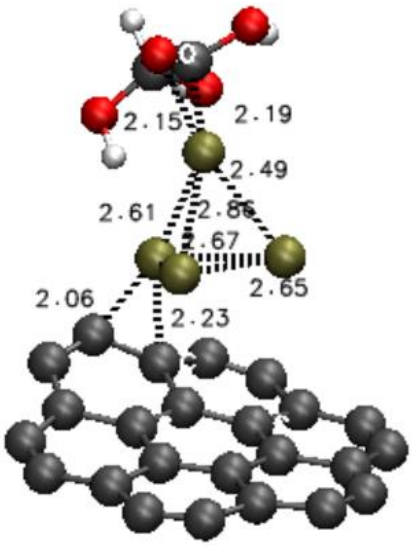
H) Glyoxylic acid – via (COOH)C=O (-19.12 kcal/mol)



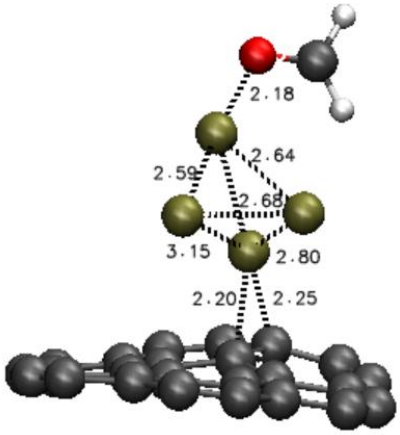
I) Glyoxylic acid – via COO^- (-32.07 kcal/mol)



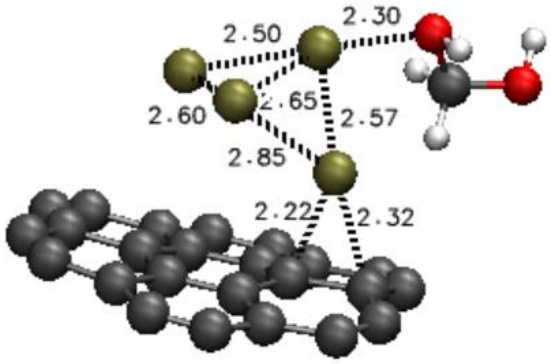
J) Glyoxylic acid – hydrate (-33.66 kcal/mol)



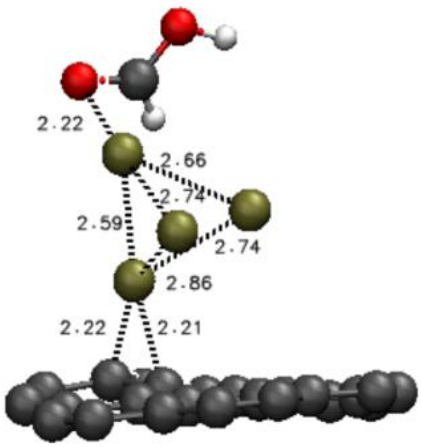
K) Formaldehyde (-16.33 kcal/mol)



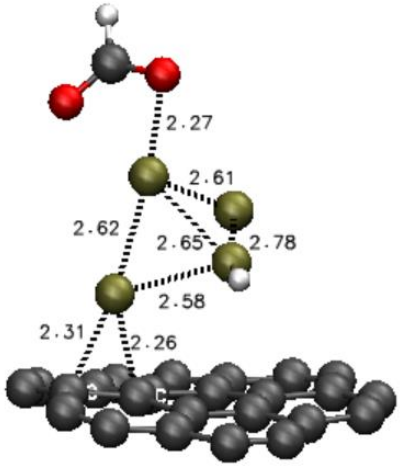
L) Formaldehyde-hydrate (-14.33 kcal/mol)



M) Formic acid COOH (-13.9 kcal/mol)



N) Formic acid COO^- (-29.9 kcal/mol)



O) Oxalic acid COOH (23.08 kcal/mol)

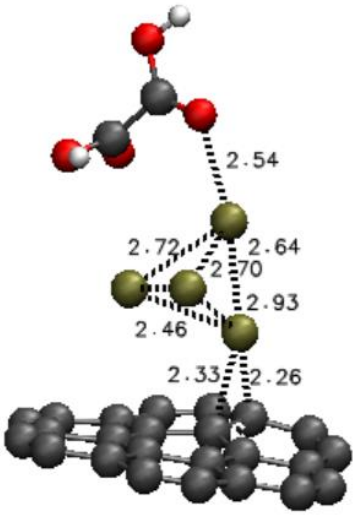


Figure S4. Complexation of the reactant molecules to the Pt4, the corresponding atomic charges of the functional groups are listed in **Table S3**. The numbers in parentheses show the complexation energies in kcal/mol obtained from eq. 1.

$$\Delta E_{Complexation} = E_{Complex} - (E_{substarte} + E_{Catalyst}) \quad \text{eq. 1}$$

We note that the binding energy of Pt4 on the C6 cluster is -88.31 kcal/mol (Pt-C distances between 2.00 – 2.40 Å), which is stronger than Pt_4 cluster formation energy, and this prohibits agglomeration of Pt atoms. For comparison, we calculated the complexation energies of all functional groups present in the molecular structures such as OH, C=O, COOH and COO^- that can be generated via acidic proton transfer to the Pt4 catalyst. As seen in **Figure S4**, the structures with carbonyl group, i.e., glycolaldehyde and glyoxylic acid have the shortest O-Pt bond distances (2.04 Å and 2.10 Å, respectively). **Table S3** shows upon complexation to the Lewis acidic Pt sites the C(C=O) gain positive charge and H^- in H(C=O) atomic charge become more negative versus the free glycolaldehyde. In case of glycolaldehyde hydrate the similar effect related to the complexation to the Pt center can be observed for the O-H group, i.e., increase of the positive and negative charge of H^+ and oxygen (respectively) on the OH and increase of the negative charge on the H^-. Glycolic acid is complexed to the Pt atom via the OH group and due to this complexation the positive charge on the H^+ and negative charges on $H(CH_2)$ increase. Glyoxylic acid with the strongest energy of complexation amongst the other molecules shows the highest atomic charge perturbation (highest activation) due to complexation to the Pt centers. To summarize, the interaction between glycolaldehyde hydrate…Pt and glyoxylic acid…Pt are the strongest and this facilitates the easier activation of these molecules in the entire reaction process and results in a faster conversion of glycolaldehyde to glycolic acid.

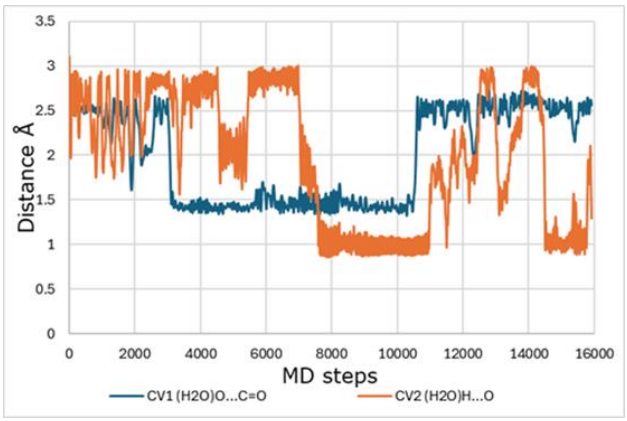


Figure S5. Variation of the CVs corresponds to the Figure **8A**, glyoxylic acid to glyoxylic acid hydrate.

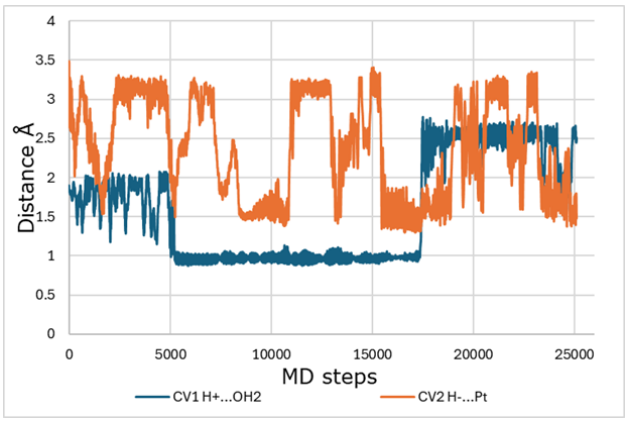


Figure S6. Variation of the CVs corresponds to the Figure **8B**, glyoxylic acid hydrate to oxalic acid.

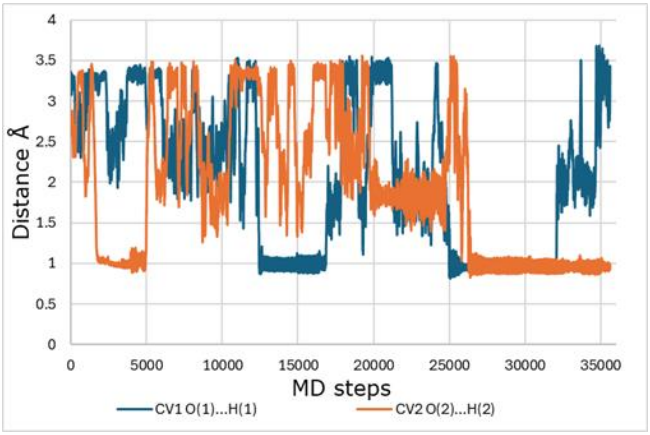


Figure S7. Variation of the CVs corresponds to the Figure 13A, Pt…H+/H- interaction with O2 and formation of H2O2.

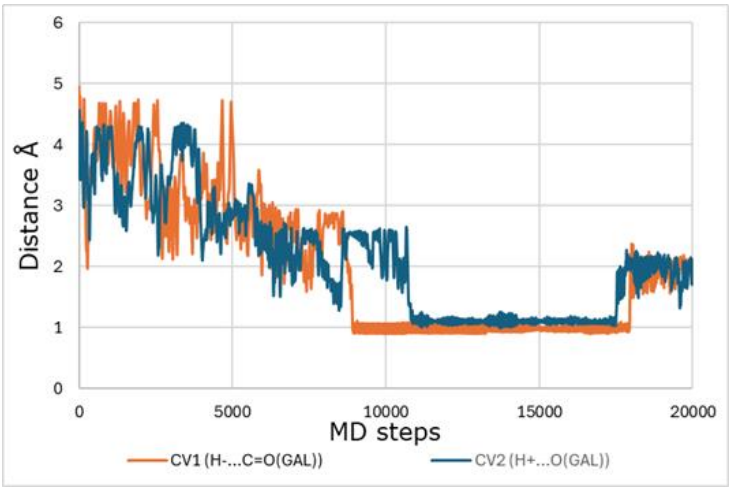
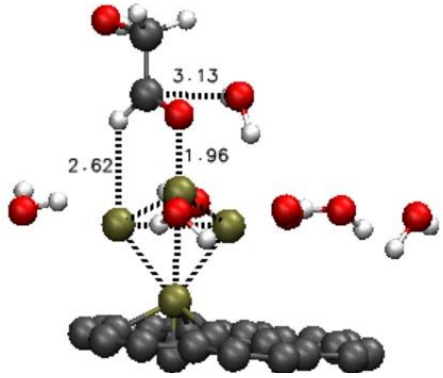


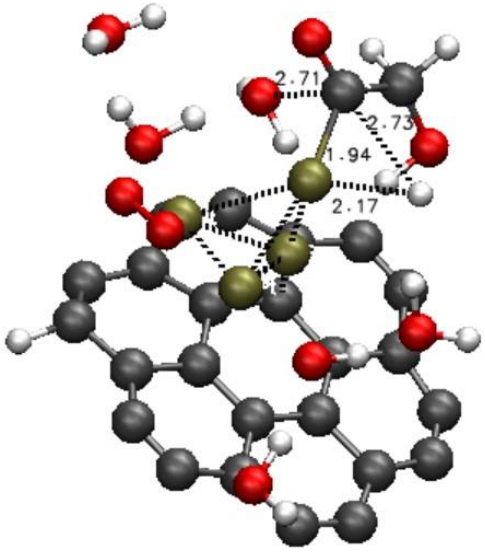
Figure S8. Variation of the CVs corresponds to the Figure **13B**, $Pt^{\cdots}H^{+}/H^{-}$ interaction with glycolaldehyde and formation of ethylene glycol.

Oxygen and water molecules available in the reaction environment can strongly interact with the Lewis acidic Pt atoms and make Pt-O bonds. Due to this interaction O2 and H2O molecules are activated and dissociate to oxygen, hydrogen and OH atoms on the Pt surface and further react with the reactant and product species in the reaction environment. To investigate the energetic of O2 and H2O dissociation on the Pt atoms we performed MTD simulations and calculated the corresponding free energetics for these transformations. It turned out that at 343 K H2O and O2 dissociations need 16.0 and 14.0 kcal/mol activation energies, respectively, which is achievable under the current reaction conditions.

Glycolaldehyde (GAl) monomer



TS – GAl to Glycolic acid (GAc)



Glycolic acid

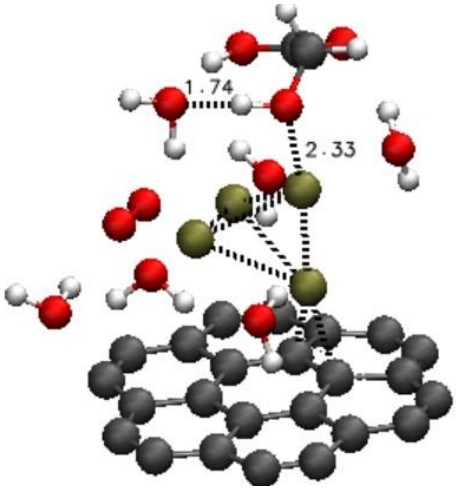
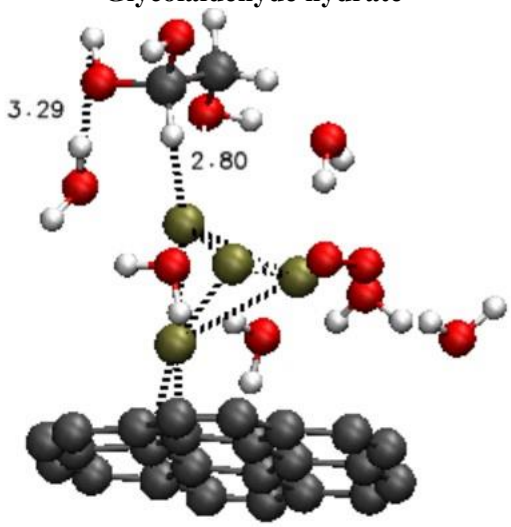


Figure S9. Molecular structures corresponding to the FESs of **Figure 2** in the main text.

Glycolaldehyde hydrate



TS Glycolaldehyde hydrate to glycolic acid

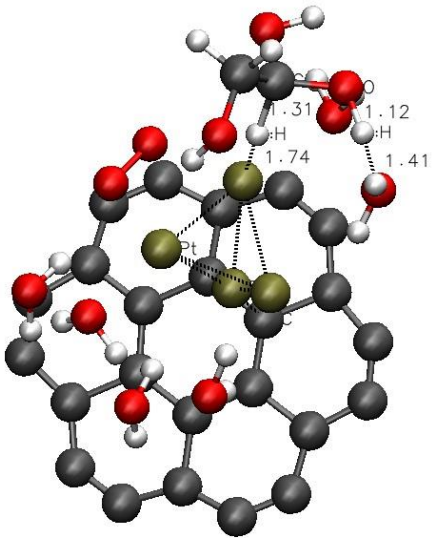
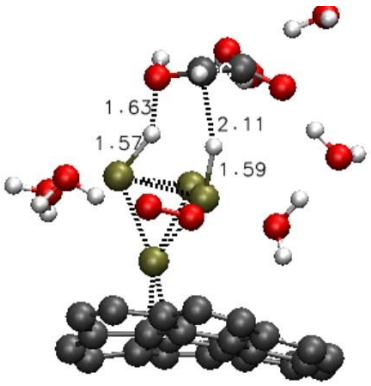


Figure S10. Molecular structures corresponding to the FESs of **Figure 4** in the main text.

TS Glycolic acid to Glyoxylic acid



Glyoxylic acid

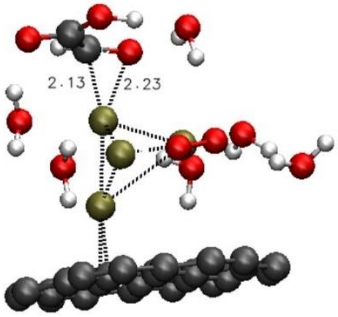


Figure S11. Molecular structures corresponding to the FESs of **Figure 5** in the main text.

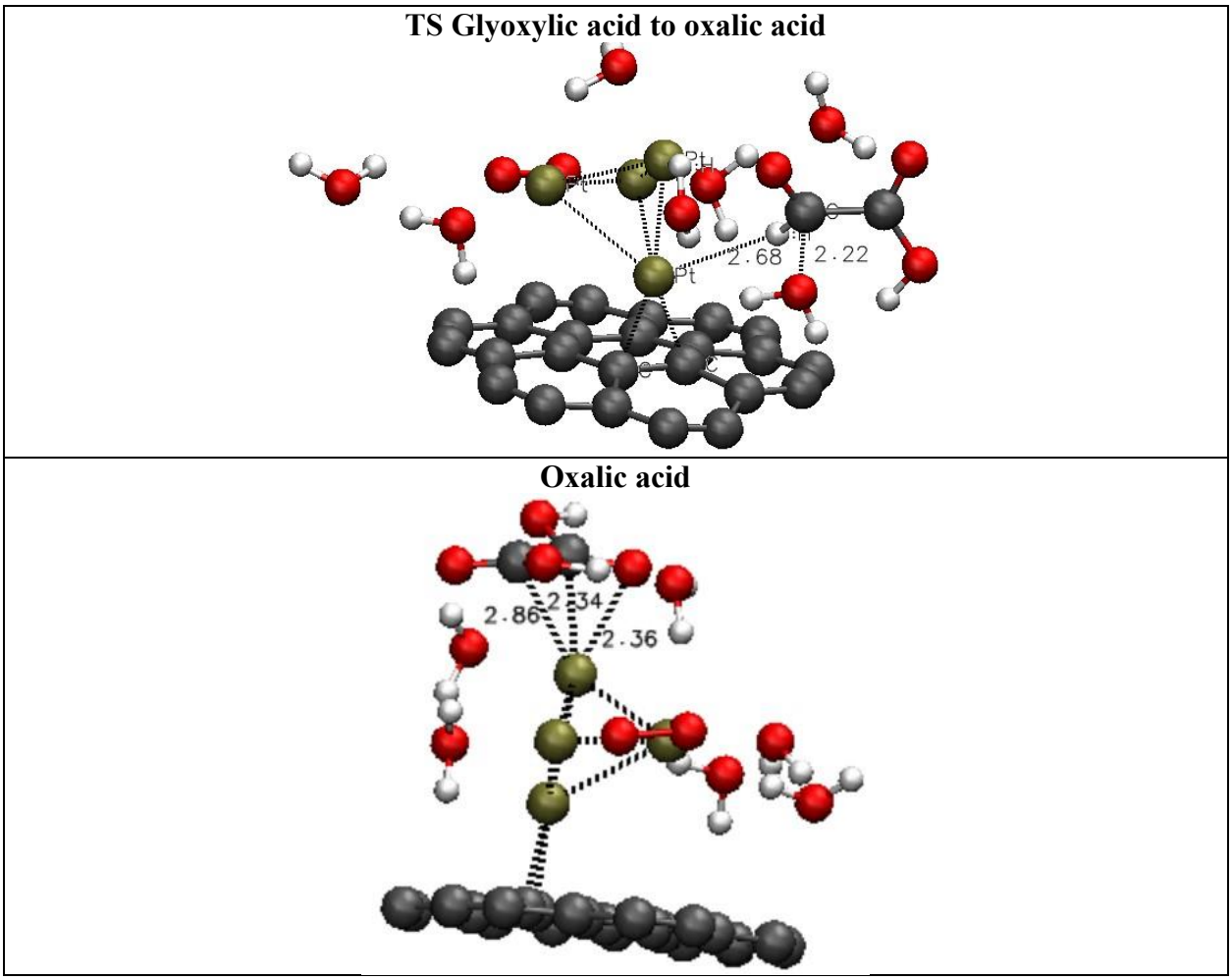


Figure S12. Molecular structures corresponding to the FESs of **Figure 7A** in the main text.

TS Oxalic acid decomposition

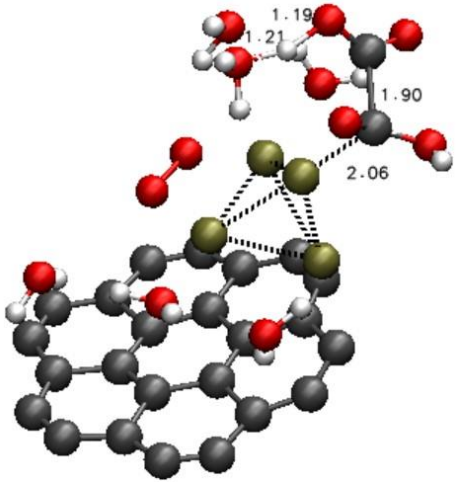
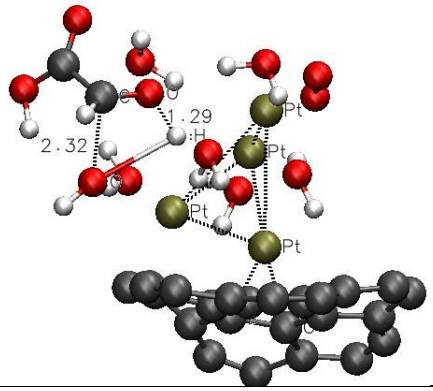


Figure S13. Molecular structures corresponding to the FESs of **Figure 7B** in the main text.

TS Glyoxylic acid to Glyoxylic acid hydrate



Glyoxylic acid hydrate

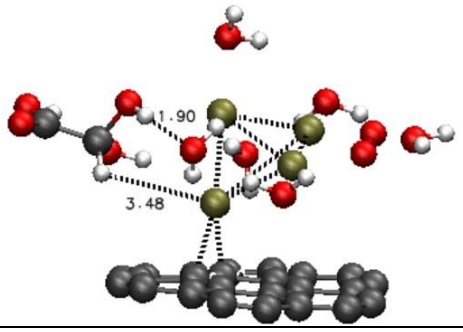


Figure S14. Molecular structures corresponding to the FESs of **Figure 8A** in the main text.

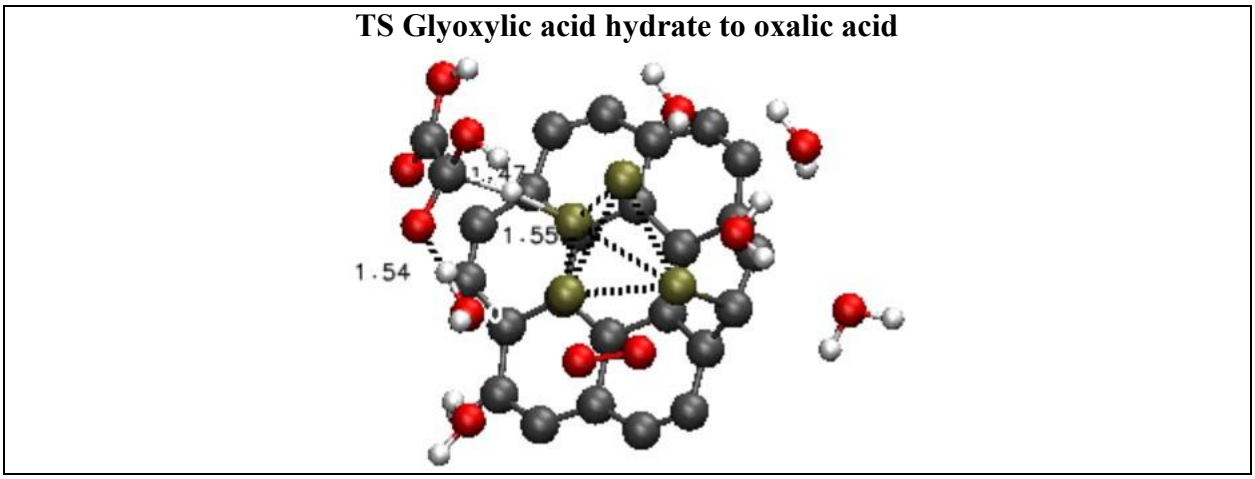


Figure S15. Molecular structures corresponding to the FESs of **Figure 8B** in the main text.

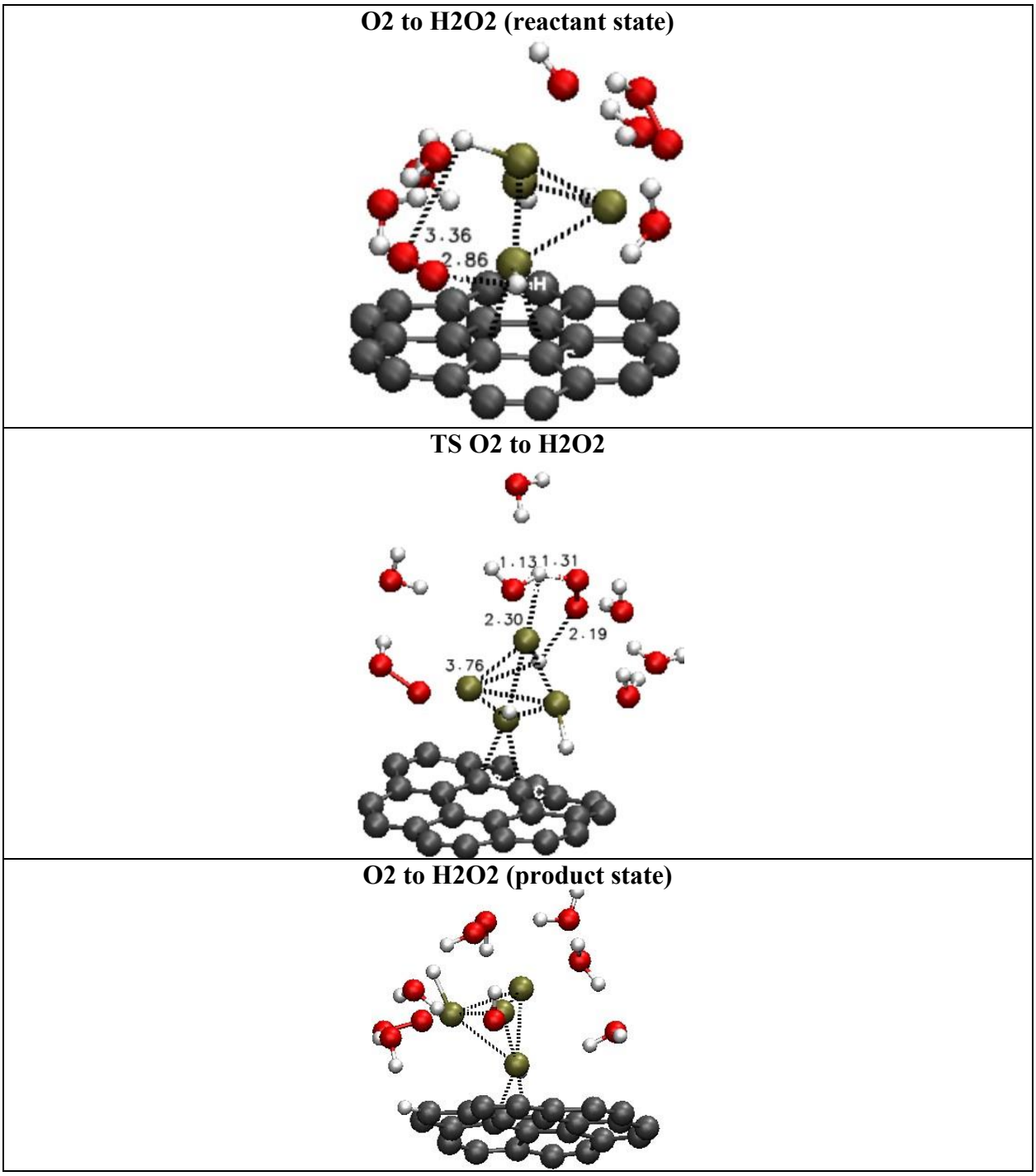


Figure S16. Molecular structures corresponding to the FESs of **Figure 13A** in the main text.

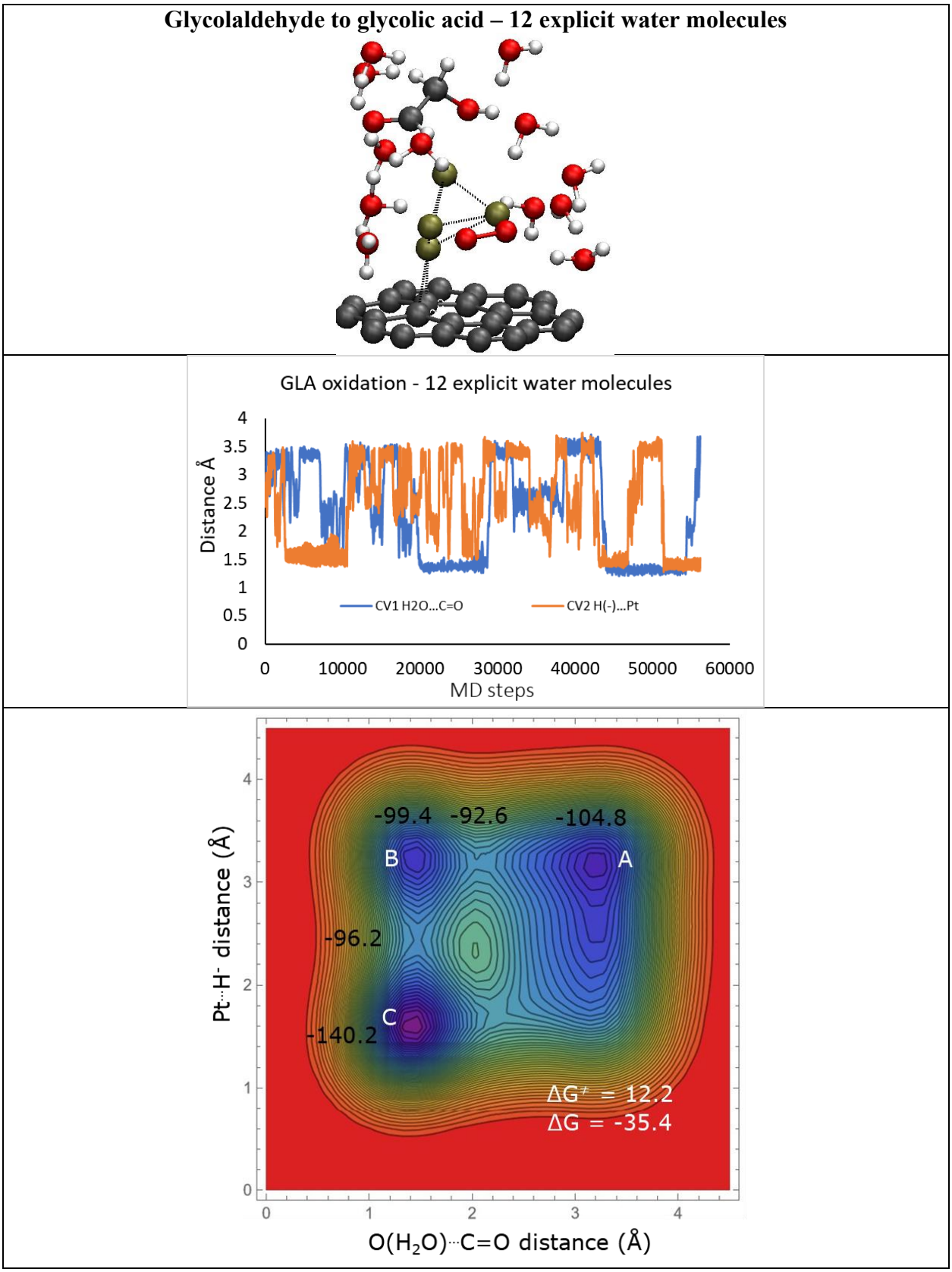


Figure S17. Glycolaldehyde oxidation to glycolic acid including 12 explicit water molecules.

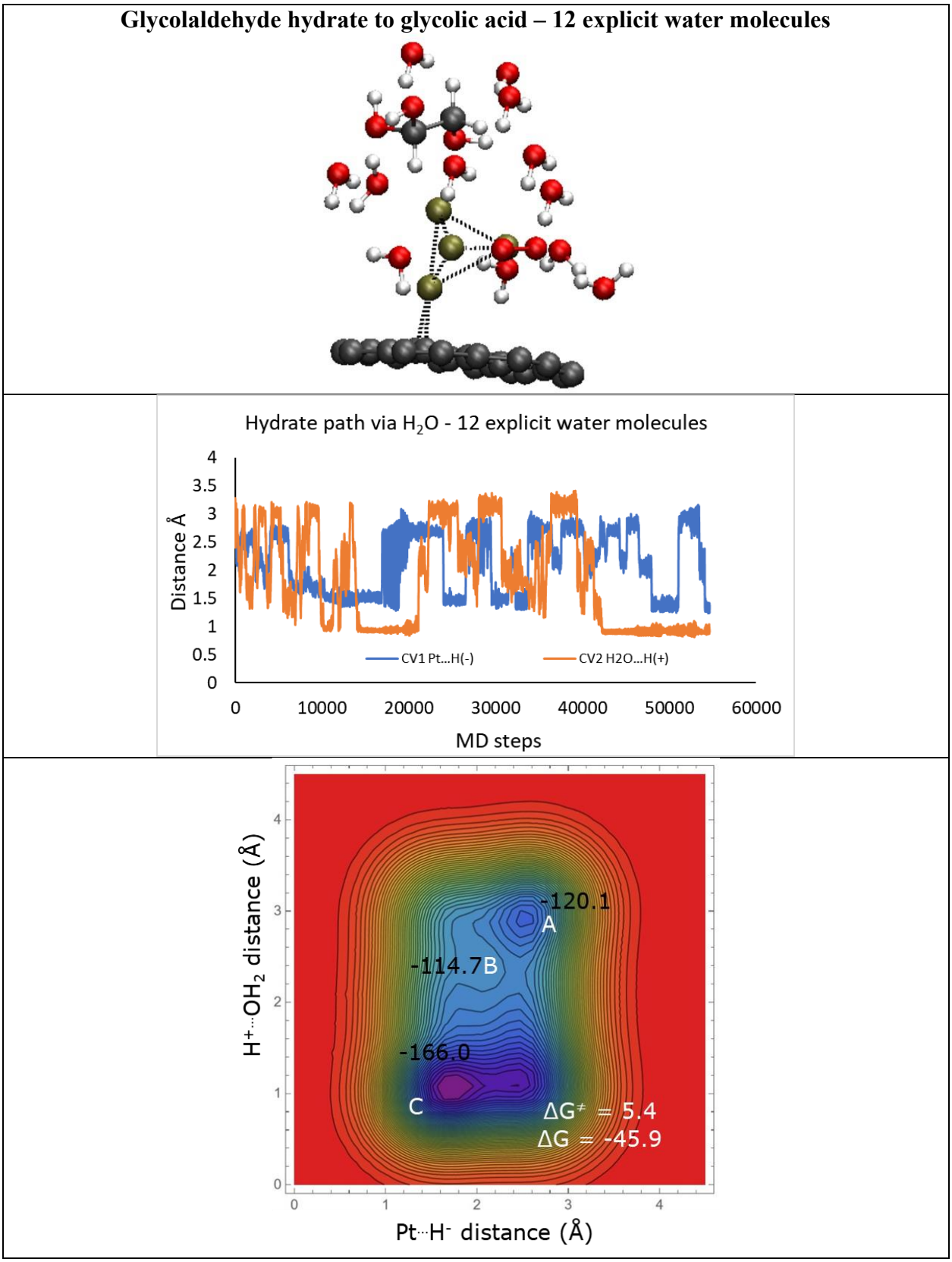


Figure S18. Glycolaldehyde hydrate oxidation to glycolic acid including 12 explicit water molecules.

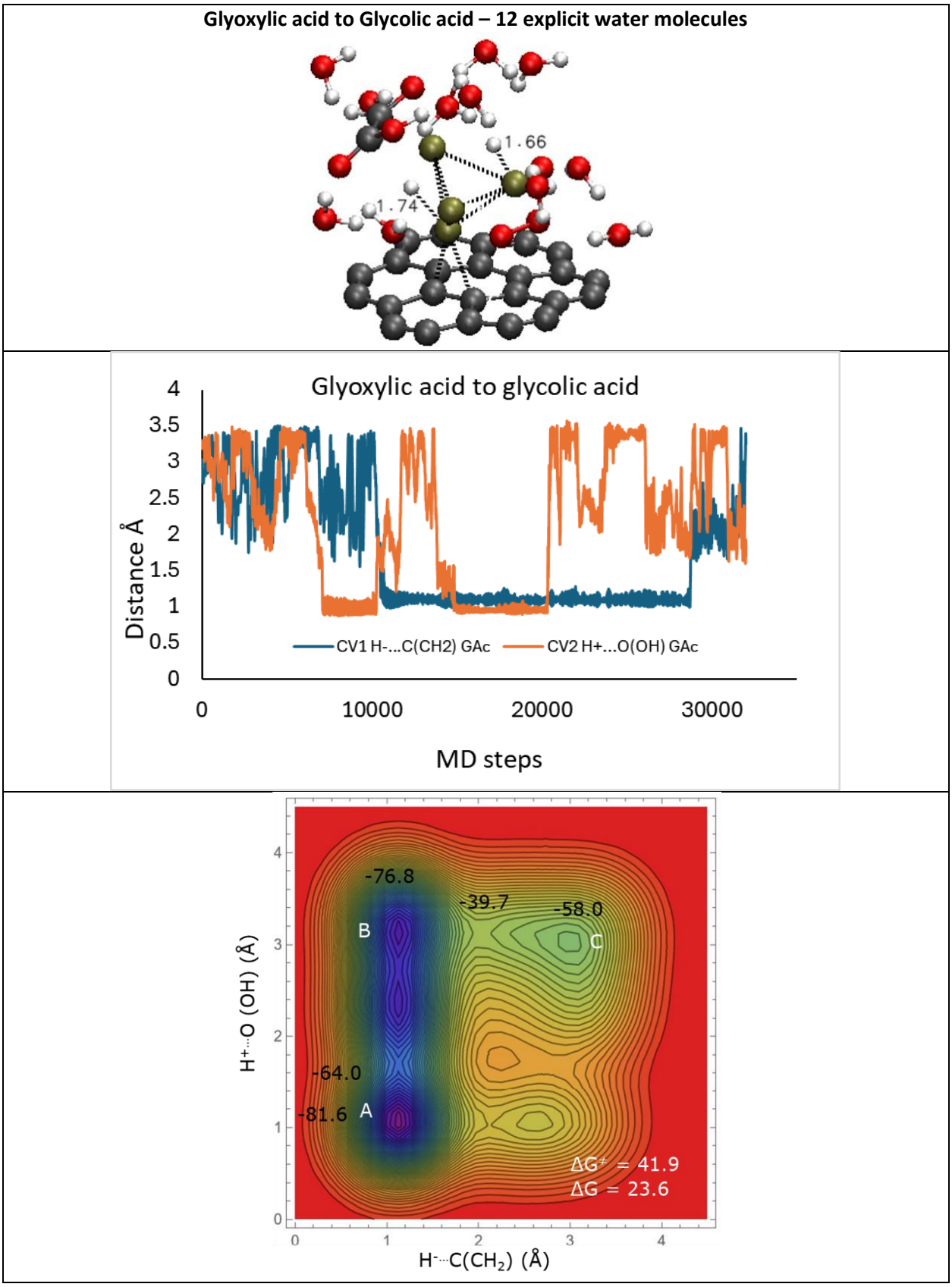


Figure S19. Glyoxylic oxidation to glycolic acid including 12 explicit water molecules.

References

1. G. te Velde, F. M. Bickelhaupt, E. J. Baerends, C. F. Guerra, S. J. A. van Gisbergen, J. G. Sijders, T. Ziegler, Chemistry with ADF. J. Comput. Chem. 2001, 22, 931– 967, DOI: 10.1002/jcc.1056,

2. E. J. Baerends, T. Ziegler, ADF 2021, Theoretical Chemistry; Vrije Universiteit Amsterdam: The Netherlands, 2021.

Cartesian coordinates of the optimized molecular structures

Glycolaldehyde monomer

C	-1.7223376948	0.9846066683	1.2571077223
C	-0.8882797368	-0.1091128434	1.3138746586
C	-0.8946360475	-1.3931597507	1.8243313158
C	-1.5097209709	2.1157015120	0.7693937363
C	-0.3703701449	2.5939262036	0.1630799588
C	0.7302203329	1.5365936282	0.1012068218
C	0.4758239598	0.1955577135	0.6685561158
C	0.0280889747	-2.2292895077	1.8613555040
C	1.3406555483	-2.0882609336	1.4354785749
C	1.5965215823	-0.7470723921	0.8199323072
C	0.0662949180	3.7849088836	-0.4055290862
C	1.2009464745	4.0404241956	-0.8562499220
C	2.3400500050	3.2458262468	-0.9052319074
C	2.0913445280	1.8981270264	-0.3118301238
C	3.1671126155	0.9431145905	-0.1875883727
C	2.9272454445	-0.3709171606	0.3913687620
C	2.4935738625	-2.8593855340	1.4552295962
C	3.6364461629	-2.5604595785	1.0584725504
C	4.0514804841	-1.3539462061	0.5053957408
C	3.6448085368	3.3870507579	-1.3404096682
C	4.5714344678	2.5602235635	-1.2603269523
C	4.5330837561	1.2954479499	-0.6987340177
C	5.4296314042	0.2617455551	-0.5030323779
C	5.2455611266	-0.8616773312	-0.0016706619
Pt	0.2047910181	0.0125191704	-1.4732636003
Pt	-0.0698063626	-1.2657933704	-3.6342671188
Pt	2.3087047446	-0.2942408154	-3.6326080023
Pt	0.6736252095	1.4836271126	-3.5661489555
O	-0.7789722174	3.2896190643	-3.4163053344
H	-0.5071840865	3.9732161940	-4.0555433720
H	-0.5361172691	3.6502804243	-2.5325477854
O	2.2617760036	-1.8684768419	-6.3828973347
H	2.9821664027	-2.4626167315	-6.1013071736
H	2.2953002330	-1.1574411893	-5.6682597206
O	3.9474958627	-1.8130922588	-3.7234181677
H	4.7575312476	-1.2782608664	-3.5029763435
H	3.6820342693	-2.4018612669	-2.9542445524
O	-2.3937770433	-1.6195329126	-3.3721881300
H	-2.4640878311	-1.0824171006	-2.5587517684
H	-2.7236392755	-1.0308519206	-4.1021123559
O	5.7523072950	0.2504858423	-3.5815934556
H	6.3644000756	0.3010095100	-4.3350351613
H	5.0396943923	0.8999730044	-3.7902481284
O	2.2946965007	2.3704191147	-4.3398416881
O	3.2690133894	1.3437442770	-4.4152238862
O	2.5087001672	-3.2510136938	-2.0055644345
H	2.5921386136	-3.1605086343	-1.0368515134
H	1.7335251570	-2.6854836070	-2.2418141759
O	-2.4002308417	-0.0599181993	-5.6312789793
C	-1.2903991469	-0.5341107962	-5.9308245423
C	-1.1151595041	-2.0150196896	-6.2790311874
O	-0.0778390535	-2.6110324248	-5.4653005537
H	-0.8691284172	-2.1265462492	-7.3502599506
H	-2.0509418424	-2.5500825620	-6.0664911913
H	0.8328285243	-2.4257289309	-5.8856444433
H	-0.4132516503	0.1212149442	-6.1097694254

TS Glycolaldehyde monomer to Glycolic acid

C	2.22536400	2.10017600	1.30848700
C	3.26741400	1.42240100	0.68848600
C	4.38875200	0.71966300	1.14304700
C	1.34039900	2.80621800	0.76984300
C	1.06790600	3.06990700	-0.55716700
C	2.03609200	2.31391300	-1.34945900
C	3.22952100	1.65840700	-0.76402200
C	5.45144700	0.54762500	0.48888400

C	5.63303900	0.84207000	-0.89063400
C	4.42282200	1.39609300	-1.61698500
C	0.10489900	3.78651100	-1.20762300
C	-0.13985000	3.75549300	-2.53217400
C	0.89441800	3.21435500	-3.46502100
C	2.08732800	2.60732400	-2.81708400
C	3.23508800	2.25740400	-3.66902200
C	4.41603800	1.70748600	-3.00802200
C	6.67462400	0.75741700	-1.75109200
C	6.68704100	0.92291800	-2.98706800
C	5.67584800	1.42412400	-3.78056800
C	1.02489000	3.23783800	-4.81114400
C	2.00571800	2.99093700	-5.55265800
C	3.21905000	2.49283100	-5.11101600
C	4.49915700	2.23864800	-5.65749700
C	5.49721800	1.68807900	-5.16762900
Pt	1.89381500	0.11403700	-1.69800400
Pt	0.46758100	-1.88368900	-2.29145200
Pt	0.10298300	-0.50151500	-4.58551100
Pt	-0.59070900	0.51347200	-2.42221600
O	-1.23046800	0.93642400	-0.52268700
H	-0.72101900	0.14866000	0.02213000
H	-2.14850800	0.68997800	-0.45499600
O	-3.58240300	-0.33190500	-0.27670300
H	-4.06390700	-0.55929100	-1.07972600
H	-3.07988400	-1.07990100	0.05232400
O	1.95931200	-0.61679400	-5.24413800
H	-0.80524800	4.56178400	-3.03025600
H	2.72249200	-1.03098300	-4.77616200
O	0.32673100	-0.58782000	0.93624500
H	1.02382300	-0.59264800	0.22420100
H	0.54178300	-0.02317500	1.74595100
O	3.93553800	-1.41358300	-3.40621400
H	3.16556500	-2.02103600	-3.16066700
H	4.79190800	-1.88935600	-3.26642000
O	-2.32621400	0.26301600	-3.40645700
O	-1.90934300	-0.45745300	-4.57984900
O	1.70627000	0.58220600	-8.04979300
H	2.20682000	0.18394000	-8.74148700
H	1.80034900	-0.00809600	-7.22133400
O	-0.85617300	-3.13367300	-0.27736600
C	0.32835300	-2.82104300	-0.59656400
C	1.51650400	-3.17335900	0.30974600
O	2.75684600	-2.72587300	-0.12462100
H	1.62303800	-4.26184400	0.62673300
H	1.08534700	-2.77536800	1.22625000
H	2.53910300	-1.81696200	-0.59188400
H	1.83666100	-3.49137800	-2.77133800

Glycolaldehyde hydrate

i = 231, E = -814.1471323051

C	-1.3594842067	1.3080072000	1.0781406775
C	-0.6189444554	0.1623636894	1.2519099991
C	-0.7253152831	-1.0568798511	1.8937271100
C	-1.0567518790	2.3690211880	0.4874423881
C	0.1189752607	2.6966976359	-0.1475268304
C	1.1339375040	1.5494742348	-0.0941744576
C	0.7759413712	0.2965777633	0.6057703615
C	0.1362095620	-1.9441907775	2.0465061960
C	1.4676285659	-1.9319864436	1.6547766386
C	1.8297590244	-0.6883012288	0.9045344374
C	0.6452332093	3.7857543703	-0.8344826790
C	1.7989559042	3.8922042290	-1.2990726905
C	2.8796534882	3.0228915810	-1.2374952586
C	2.5273379230	1.7715517793	-0.5039507684
C	3.5359313852	0.7754066945	-0.2302581891
C	3.1941935051	-0.4441833302	0.4877101251
C	2.5667290125	-2.7657156485	1.8019782383
C	3.7391492987	-2.5858692888	1.4181799012
C	4.2487197657	-1.4755238311	0.7547670529
C	4.2003627941	3.0287721629	-1.6463201740
C	5.0716327465	2.1659676995	-1.4329993296
C	4.9362021114	0.9832910209	-0.7265139466
C	5.7623445788	-0.0710498754	-0.3791639181
C	5.4863243226	-1.1120827074	0.2434814937
Pt	0.5128090708	-0.0628395976	-1.4985696197
Pt	-0.0983113576	-1.2281158148	-3.6586635384
Pt	2.3940062620	-0.4893731766	-3.6039293529
Pt	0.8353005734	1.3373617465	-3.7497378491
O	-0.5225081381	3.2471836852	-3.6585932712
H	-0.0791290224	3.6712934467	-2.8856271137
H	-1.3644697903	2.9214851057	-3.2906290447
O	2.1724348875	-2.5546192141	-6.0602184044

H	2.6558642252	-3.2939844040	-5.6511710347
H	2.3113454547	-1.8103344879	-5.3943022692
O	3.9866260394	-2.0349664372	-3.4414698498
H	4.8091911078	-1.4955560952	-3.2911930451
H	3.7012945978	-2.5180017381	-2.6095975366
O	-2.2898362788	-1.8249694983	-3.5030871060
H	-2.6463021776	-1.2713728467	-2.7854657365
H	-2.6396189750	-1.4438142563	-4.3594408012
O	5.8463532090	-0.0350368471	-3.6532173275
H	6.3290202408	-0.1725017558	-4.4856596218
H	5.1227529304	0.5942912764	-3.8948325036
O	2.4692507079	2.0647218820	-4.6544500733
O	3.4089130153	1.0002500816	-4.6235892684
O	2.4871825077	-3.2509392253	-1.6223543295
H	1.7598718326	-2.6132991705	-1.8172862699
H	2.6090937896	-3.1971841411	-0.6553654954
O	-1.8712403889	0.5956311556	-7.6175312315
C	-1.6134888400	-0.1632766591	-6.4567468037
C	-0.6282057336	-1.2488439217	-6.8733538699
O	-0.4180625821	-2.1847808502	-5.7951454660
H	0.3179996411	-0.7599855914	-7.1554540469
H	-1.0244421719	-1.7837680582	-7.7535779849
H	0.5289401019	-2.5240988907	-5.9113582254
O	-2.8481553470	-0.7033619001	-5.9127787645
H	-1.1916055698	0.4308652127	-5.6264293763
H	-3.2416476863	-1.2758777176	-6.5996217376
H	-2.3247435429	1.4142773687	-7.3488084373

TS Glycolaldehyde hydrate to Glycolic acid

C	1.48940900	3.75568700	-2.25200000
C	2.55865800	3.25466200	-1.55900900
C	3.10353700	3.14689200	-0.27474200
C	1.15611600	3.70032300	-3.45085400
C	1.88505600	3.04990400	-4.46564900
C	2.88871300	2.05907300	-3.86182200
C	3.29518700	2.22707600	-2.44193100
C	4.11226300	2.59820300	0.20155100
C	4.94711900	1.79215200	-0.55444300
C	4.54594300	1.62741700	-2.00404500
C	1.76645100	2.80273900	-5.81956700
C	2.45467000	2.07420000	-6.56346400
C	3.48216200	1.22034100	-6.22008700
C	3.82054500	1.31944600	-4.82119900
C	5.07128700	0.85452200	-4.31063900
C	5.42699100	0.95463700	-2.89609800
C	6.10427300	1.09029200	-0.25996100
C	6.80264900	0.40489700	-1.03101100
C	6.69759200	0.29523600	-2.39146600
C	4.33975600	0.36248700	-6.91075400
C	5.44730400	-0.05951600	-6.55497500
C	5.99846800	0.06200800	-5.30562100
C	7.11548900	-0.35577600	-4.62214200
C	7.39367200	-0.30427100	-3.38716300
Pt	1.96274500	0.60636000	-2.53591800
Pt	0.69569000	-0.85081900	-0.89686000
Pt	0.46021200	-1.70629300	-3.21052500
Pt	-0.61334700	0.46417100	-2.81784800
O	-1.72261900	2.63583200	-2.18769600
H	-1.97932300	3.17451300	-3.06841100
H	-2.54424000	2.42549600	-1.76745600
O	2.29584600	-3.04279700	-0.60705000
H	1.29407700	-2.89468800	-0.53647200
H	2.59515400	-2.11731300	-0.74717000
O	1.61472800	-3.56642200	-3.56128700
H	2.21233100	-3.26407500	-4.27983200
H	2.12654600	-3.52948200	-2.74460700
O	-2.68165300	-0.63617200	0.88621800
H	-1.76262300	-1.01438900	0.84403000
H	-3.23985800	-1.38350900	1.15610200
O	2.58564700	-2.22189700	-5.73454100
H	3.54207500	-2.05875300	-5.56538600
H	2.17626200	-1.35107000	-5.62953600
O	-0.56369400	0.12424500	-4.98740100
O	-0.06405600	-1.17480100	-5.00329600
O	4.10831600	-1.96730700	-2.86342200
H	4.99903700	-1.51854600	-2.83013800
H	3.56432100	-1.17012600	-3.00721400
O	-3.95105500	0.88898000	-3.33353700
C	-3.50355700	-0.03472200	-2.39302300
C	-4.10231500	-1.38850400	-2.56422800
O	-3.20472800	-2.48231100	-2.13689200
H	-4.42709100	-1.52640600	-3.64955700
H	-5.02303000	-1.46582700	-1.94056400

H	-2.35738900	-2.48930900	-2.61211400
O	-3.79481600	0.55890800	-1.04639500
H	-2.19549600	-0.15487500	-2.44481500
H	-3.30651900	0.07471100	-0.16406800
H	-4.39442200	1.45449700	-2.64697800

Glycolic acid

i = 234, E = -812.9674610383

C	-1.3490148808	1.3274654857	1.3127432976
C	-0.5017682369	0.2586531148	1.4919362466
C	-0.4768835767	-0.9442969705	2.1715503953
C	-1.1618059457	2.3886220861	0.6774251279
C	-0.0482338267	2.7944959191	-0.0190330020
C	1.0636845084	1.7419744398	0.0250915663
C	0.8454286436	0.4870361733	0.7775873676
C	0.4602606643	-1.7543054810	2.3036193223
C	1.7632541417	-1.6538000624	1.8371298935
C	1.9859978347	-0.4061527592	1.0402194675
C	0.3562292574	3.8988655807	-0.7592790927
C	1.4765838263	4.0960150396	-1.2717885840
C	2.6269087247	3.3181715981	-1.2386996516
C	2.4125314609	2.0627731766	-0.4596345614
C	3.5092933479	1.1553863512	-0.2159224308
C	3.3027605629	-0.0701174956	0.5428063155
C	2.9284462192	-2.3995612556	1.9391222872
C	4.0593885957	-2.1402316719	1.4840524248
C	4.4466306295	-1.0107421923	0.7717708485
C	3.9229716369	3.4208207695	-1.7096058431
C	4.8670644167	2.6316921134	-1.5232929898
C	4.8622370315	1.4592995741	-0.7876437169
C	5.7825250006	0.4797038075	-0.4636260136
C	5.6252506911	-0.5674171402	0.1889159561
Pt	0.5145840027	0.0373201877	-1.3069907928
Pt	-0.0501869100	-1.3335043908	-3.3440561013
Pt	2.3813495821	-0.4420826855	-3.5062896786
Pt	0.7184768468	1.3025308718	-3.6104403626
O	-0.7673149714	3.0956156937	-3.5795632620
H	-0.6206732506	3.6622272851	-4.3583908209
H	-0.4194106805	3.6023261332	-2.8103620109
O	1.6151138238	-1.2519411880	-6.4415151383
H	2.4185084411	-1.3696438645	-6.9768862397
H	1.9378038800	-0.9345243660	-5.5148098582
O	4.0673466373	-1.8790187633	-3.4267550807
H	4.8629785811	-1.2973830446	-3.2945484588
H	3.8501355801	-2.3812861222	-2.5861133673
O	-2.3864120458	-1.4725272632	-3.0723933664
H	-2.4273576327	-0.8544019511	-2.3174686449
H	-2.7387582331	-0.9643370517	-3.8494374445
O	5.8255973632	0.2346880073	-3.5909011884
H	6.4130683561	0.2083090100	-4.3644420911
H	5.0825137038	0.8294658033	-3.8540418228
O	2.3124582264	2.1366986557	-4.4991567719
O	3.3113457093	1.1226803796	-4.4870823148
O	2.7461372523	-3.1131463213	-1.4628631642
H	2.9063026567	-2.9458434162	-0.5147198016
H	1.9626716728	-2.5572539130	-1.6853058751
O	-2.7592793840	-0.3100947015	-5.6059699241
C	-1.7019794300	-0.7713152924	-6.0349604196
C	-1.4330447699	-2.2865635447	-6.0179164866
O	-0.2829148473	-2.6765964149	-5.2374864509
H	-1.3257574446	-2.6496922532	-7.0546915448
H	-2.3030144590	-2.7694274384	-5.5561579348
H	0.5380197915	-2.4257229412	-5.7437093023
O	-0.7860662037	0.0295068507	-6.6024298696
H	0.0982630701	-0.4239023450	-6.7121798805

TS Glycolic acid to Glyoxylic acid

C	4.05355100	3.48800900	0.94150100
C	4.68320000	3.27363300	-0.24659300
C	5.90743000	2.81328400	-0.68740000
C	2.99892800	4.12522200	1.23094100
C	2.12355100	4.67491000	0.26546200
C	2.40847700	4.16426100	-1.11657400
C	3.78851200	3.63020400	-1.39142500
C	6.33399700	2.65624400	-1.85143300
C	5.66572300	3.04877500	-3.00110200
C	4.26670700	3.51476900	-2.73552200
C	1.03241000	5.56875200	0.28266200
C	0.26198600	5.83532900	-0.66970600
C	0.33183700	5.42872000	-1.97274000
C	1.61859200	4.61995200	-2.26611800
C	2.08690500	4.35172400	-3.63487000
C	3.39576100	3.84030900	-3.88626600
C	5.88356600	2.90514600	-4.34551000

C	5.16255300	3.17858900	-5.30191200
C	3.83837900	3.55267000	-5.25180600
C	-0.45021600	5.44898500	-3.19219900
C	0.01232800	5.04657400	-4.28382900
C	1.20626500	4.51782600	-4.75641100
C	1.68810000	4.12705200	-6.00320600
C	2.87533000	3.81215900	-6.23283600
Pt	0.83823400	2.69878000	-1.61457900
Pt	0.79019500	0.23901100	-1.11019500
Pt	0.73746700	0.87294100	-3.64225800
Pt	-1.30340300	1.30072900	-2.00135400
O	-2.40614300	2.37156200	-0.26320700
H	-1.94818900	2.69484700	0.58802300
H	-3.33710800	2.73451300	-0.17576300
O	-2.87119700	2.48616700	-3.60006800
H	-1.97967100	2.55113900	-4.00358800
H	-3.08397600	3.46458400	-3.36642100
O	2.76683500	0.58407200	-4.28987700
H	3.26328400	1.27120500	-4.69546800
H	2.83123500	-0.31319400	-4.77948000
O	3.08239300	-1.79852400	-5.30109200
H	2.16596900	-2.11679400	-5.07544000
H	3.61276500	-2.27915600	-4.64657700
O	0.80881800	-3.48103400	-0.22428900
H	0.03631700	-3.54844600	0.28583400
H	0.55309700	-3.05860700	-1.12188600
O	-0.86773800	2.33302100	-5.55355200
O	0.31269900	1.92968500	-5.53905400
O	1.26322100	-5.48276400	-2.79339600
H	0.75208300	-4.75939000	-2.28503300
H	1.18403600	-5.24468100	-3.74069500
O	-0.55364600	-3.20560600	-2.49350000
C	-0.20498300	-2.75766400	-3.67188800
C	-1.24243700	-1.94996200	-4.29619600
O	-2.05595600	-1.31294500	-3.44019300
H	-2.09316900	-1.96101400	-2.70397400
H	-1.48167600	-1.61504200	-5.36387100
O	0.96142100	-2.83051300	-4.15808100
H	-1.27118100	-0.00704500	-2.86487200
H	0.07956100	-0.30976000	-4.46995900

Glyoxylic acid

i = 74, E = -811.7672240626

C	-1.6871396542	0.9900335296	1.2518955085
C	-0.8490963491	-0.0993166302	1.3440215738
C	-0.8651741759	-1.3781246736	1.8669495288
C	-1.4717081019	2.1089610410	0.7405139892
C	-0.3241173940	2.5774260936	0.1388075870
C	0.7793285614	1.5278748312	0.1235587190
C	0.5174779564	0.1981189424	0.7082732302
C	0.0550728016	-2.2159279231	1.9102640514
C	1.3656742880	-2.0912708212	1.4771338891
C	1.6292824528	-0.7538021924	0.8535063942
C	0.1087304796	3.7602911348	-0.4503404009
C	1.2512187752	4.0092203255	-0.8816475858
C	2.3953360262	3.2228211417	-0.8980592674
C	2.1390660385	1.8808242625	-0.2938242142
C	3.2090976016	0.9198597168	-0.1674478164
C	2.9597913566	-0.3914135801	0.4118964063
C	2.5105808010	-2.8738977713	1.4931911690
C	3.6511810962	-2.5799480221	1.0883743896
C	4.0764978960	-1.3838452906	0.5229901982
C	3.7054784629	3.3627764303	-1.3154023143
C	4.6274471999	2.5324508750	-1.2238060969
C	4.5795704341	1.2638141942	-0.6730422292
C	5.4671840714	0.2215655833	-0.4840315679
C	5.2727638284	-0.9015554004	0.0137576447
Pt	0.2438863719	-0.0715562990	-1.4459209900
Pt	-0.0443468887	-1.3737273543	-3.5930746660
Pt	2.3239752412	-0.3423567295	-3.5276204584
Pt	0.6668689174	1.4279517496	-3.5151473625
O	-0.8709718824	3.1693032499	-3.4152290661
H	-0.7803253008	3.7820981938	-4.1679240309
H	-0.5727432751	3.6665871554	-2.6217826387
O	2.0063090896	-1.0022259287	-6.8202138943
H	1.7727857174	-1.7867566651	-6.2635589572
H	2.3842271923	-0.3847523758	-6.1560518372
O	3.9523644556	-1.8179375816	-3.6527394228
H	4.7828882951	-1.3077629740	-3.4543899086
H	3.7286069160	-2.4566918849	-2.9149183313
O	-2.4204661732	-1.1950089799	-3.2630822984
H	-2.3974199590	-0.3854523117	-2.7163120999
H	-2.6689464191	-0.8998063684	-4.1916946326

O	5.8226629930	0.1820561064	-3.5663905756
H	6.4126689781	0.1815054872	-4.3396239807
H	5.1332934804	0.8529366870	-3.7734140243
O	2.3151367034	2.3174838545	-4.2195862512
O	3.2904006516	1.2952930129	-4.2742993466
O	2.5766879475	-3.3875928867	-1.9788403179
H	2.6055883392	-3.2478049209	-1.0134079094
H	1.7758184827	-2.8936269109	-2.2732116085
O	-2.4703056804	-0.6067733993	-5.9131489357
C	-1.3039479564	-0.9751672842	-6.1343388995
C	-0.8231178649	-2.2151609482	-5.3915840196
O	0.3949459507	-2.6693565586	-5.3493541250
H	0.4773971725	-0.6301491640	-6.9351568960
H	-1.6556385660	-2.8892084573	-5.1193826828
O	-0.5084923693	-0.3218587843	-6.9649267965

TS Glyoxylic acid to Oxalic acid

C	-0.49843738	0.19201611	-5.75945085
C	0.55711495	0.86777140	-5.19028541
C	1.11184751	2.14203061	-5.29572629
C	-0.73932993	-1.03466643	-5.92196103
C	0.20912343	-2.01025950	-5.53326421
C	1.40689860	-1.53548842	-4.76120181
C	1.54750692	-0.09382607	-4.48356842
C	2.08414624	2.65601862	-4.69697716
C	3.05775380	1.89850985	-4.10278138
C	2.79882103	0.42859663	-3.91641662
C	0.22244087	-3.36845791	-5.58913185
C	1.09555782	-4.18403808	-5.23092471
C	2.27109826	-3.87120477	-4.57760000
C	2.42149263	-2.40541533	-4.33289811
C	3.64132080	-1.89793599	-3.73502924
C	3.80123311	-0.52310625	-3.41600392
C	4.26595819	2.17726110	-3.44710218
C	5.06773311	1.44007778	-2.91285554
C	5.04215496	0.05108622	-2.84583157
C	3.34281801	-4.64534674	-4.07461932
C	4.24672366	-4.08859961	-3.42505939
C	4.73945806	-2.82730614	-3.27192449
C	5.83392671	-2.20118117	-2.68010374
C	5.94821298	-0.96436144	-2.56466182
C	-3.48999378	0.51465842	-2.70667353
C	-1.99190872	0.50885406	-2.15564021
Pt	1.38338390	0.33227720	-2.33373029
Pt	0.25782725	0.41010374	-0.06176013
Pt	2.77452778	-0.43228656	0.06747943
Pt	1.16269031	-1.87358131	-1.00446667
O	0.02279939	-3.46607573	-2.20153818
O	0.30755719	1.03006042	2.36098547
O	4.62227627	0.85376668	0.37231726
O	-2.77996047	-2.69566843	-1.65228093
O	6.66683171	-0.97530583	1.41330853
O	2.61091694	-3.13036466	-0.69526268
O	3.69019311	-2.32413664	-0.03178724
O	0.01461663	3.73553310	-0.14835347
O	-4.37973865	0.53669533	-1.89206719
O	-1.76870387	0.82963387	-0.96051524
O	-3.74677174	0.66433439	-4.04211282
O	-1.44296737	2.46896908	-3.05162488
H	-0.94698450	-3.35672726	-1.87620693
H	0.00871976	-3.22490444	-3.15227540
H	0.39801617	0.03663601	2.41903299
H	1.26490828	1.22112510	2.30705654
H	5.46609592	0.42468189	0.73737379
H	4.85400650	0.93116656	-0.59803031
H	-3.34977195	-2.16693316	-2.21686289
H	-2.93091753	-2.47562669	-0.66675286
H	7.29500988	-1.18688729	2.11890671
H	5.96677820	-1.65059310	1.35103931
H	0.13196088	3.08957641	-0.86713303
H	-0.27577477	3.26634247	0.66262012
H	-2.86360172	0.52251608	-4.52938270
H	-1.21773024	-0.23470927	-2.62048546
H	-1.44315353	2.49037948	-3.97414975
H	-0.46202236	2.15346804	-2.91719939

TS Glyoxylic acid to Glyoxylic acid hydrate

C	1.36756500	-0.24192800	0.12324000
C	2.73054100	-0.72568800	0.25774800
C	3.54309200	-1.71208300	0.70283100
C	1.03969000	1.00862100	0.34114000
C	1.73831700	2.09403700	-0.09298400
C	3.05393200	1.67771300	-0.68151600
C	3.49107000	0.29560100	-0.59593800

C	4.70057800	-2.07380400	0.33472500
C	5.39255800	-1.56083000	-0.78103400
C	4.72551300	-0.25570500	-1.22163700
C	1.56603800	3.43861600	-0.18830700
C	2.27381400	4.32309300	-0.67454700
C	3.48404200	4.06077000	-1.35735400
C	3.79491000	2.61256100	-1.42049800
C	4.85326500	2.10179500	-2.25310300
C	5.31786900	0.71456700	-2.13968700
C	6.52493000	-1.78285800	-1.56737800
C	6.83885000	-0.99978500	-2.45028900
C	6.45837400	0.26249900	-2.96396300
C	4.38485400	4.79600600	-2.10106400
C	5.31142500	4.40139200	-2.83306000
C	5.57448100	3.09566800	-3.19882200
C	6.43382200	2.34530900	-3.99251800
C	6.77371200	1.14195800	-4.00832100
C	-3.87488200	-0.92480100	-2.86327700
C	-2.56239900	-0.20538400	-2.89985200
Pt	3.00522300	-0.82077200	-2.43260200
Pt	0.59467200	-1.00352500	-1.64594700
Pt	1.14876700	-2.00265000	-3.96871900
Pt	0.98085800	0.13479500	-5.27720900
O	0.39700300	2.29781800	-6.41589700
O	2.77089800	2.63141400	-4.74798900
O	1.38129800	-3.89441800	-2.82354400
O	0.57381500	1.33789300	-3.61499100
O	-1.01589800	-4.18601100	-1.24419500
O	1.36477200	-1.28614500	-6.63268900
O	1.54744900	-2.50322800	-6.05473700
O	-2.67222000	-4.77400800	-3.75852400
O	-4.31786900	-1.22873800	-3.95202800
O	-1.70169500	-0.74096000	-3.67107100
O	-4.32261900	-1.38879900	-1.70176100
O	-1.46227100	-0.92578600	-0.98749400
H	-0.33847000	2.40532900	-5.76331400
H	1.17545800	2.74891500	-6.01505500
H	2.48933100	1.66741800	-4.89950300
H	3.63997600	2.60427900	-4.32052900
H	0.55831700	-4.44950600	-2.55113100
H	1.62673900	-3.47963500	-1.92302500
H	1.28973200	1.96029700	-3.33120400
H	0.71675600	0.56893900	-2.88349800
H	-1.23574900	-3.30292400	-0.91699600
H	-1.91942400	-4.58939300	-1.49514500
H	-1.69209000	-4.81080500	-3.89709400
H	-2.93629500	-3.94868200	-4.27929200
H	-3.57083400	-1.08021300	-1.02794500
H	-2.53591900	0.79019900	-2.39375100
H	-1.64151900	-0.51876000	-0.09270700
H	-0.50440200	-0.95076000	-3.23339500

Glyoxylic acid hydrate

i = 179, E = -828.9790484655

C	-2.3044957010	0.2679334741	-0.1914952913
C	-1.3173822582	-0.6989929188	-0.1275316787
C	-1.2173760128	-2.0572264231	0.0626704704
C	-2.1709588180	1.5051628279	-0.2473644665
C	-1.0062303720	2.2619290769	-0.2255446661
C	0.2175842025	1.4032594961	-0.2225063721
C	0.0700453147	-0.0558280836	-0.2844022030
C	-0.1938878193	-2.7766290055	0.0976326630
C	1.1271949607	-2.4255174451	-0.0408085687
C	1.2745446883	-0.9063845038	-0.2565430309
C	-0.6926391505	3.6112912893	-0.1657179514
C	0.4424977388	4.1183582019	-0.1101021435
C	1.6730998369	3.4855427188	-0.1126948525
C	1.5336771835	1.9916636465	-0.1644316829
C	2.7230377224	1.1532752436	-0.2149460875
C	2.6079739627	-0.2831253342	-0.2335595945
C	2.3740095195	-3.0270930172	-0.0595517290
C	3.4965816259	-2.5027731599	-0.1942144407
C	3.8199928767	-1.1503050681	-0.2813958737
C	2.9999231566	3.8799224302	-0.1328663310
C	4.0130426800	3.1628746477	-0.2134541975
C	4.0867716214	1.7820258040	-0.2778616268
C	5.0884249958	0.8342317134	-0.3835172592
C	4.9828241871	-0.4063561668	-0.3849911426
C	-3.8463406976	-2.2722726388	-4.2332329867
C	-2.4747193374	-1.6611132887	-3.8658321451
Pt	0.7612140620	-0.6293740313	-2.3546836179
Pt	1.0880218662	-1.3900229453	-4.7503799789
Pt	3.5677492905	-0.9511631915	-4.4085718154

Pt	2.2800485402	0.9795249749	-3.6898971674
O	1.1860214848	2.9609750679	-3.1528023595
O	1.5598886863	-2.4672031183	-6.7491887582
O	4.8103853682	-2.7178633055	-4.9519012810
O	-0.9782571838	1.4577204085	-4.1218044918
O	7.1168666728	-1.7055642894	-4.1066118511
O	4.0675743836	1.7224730192	-4.1701420440
O	4.8216564463	0.5858635306	-4.5736450763
O	3.0501394422	-3.9478607645	-3.2574223947
O	-4.8649564132	-1.6018638342	-4.3128039737
O	-1.9184624209	-1.0534791483	-5.0307159075
O	-3.8244938338	-3.5961920820	-4.4872975061
O	-1.6640641518	-2.7319355010	-3.4286094719
H	0.2543629646	2.7730651508	-3.4330677607
H	1.5057496343	3.6656269586	-3.7445460386
H	2.5354113511	-2.5185127689	-6.6562605696
H	1.4081843128	-1.8265723366	-7.4692939637
H	5.7544484754	-2.4925279734	-4.6761178507
H	4.4240332837	-3.3491779422	-4.2815434543
H	-0.6725367067	0.8805388508	-3.3545984288
H	-0.2439242081	1.2551858193	-4.7471293773
H	8.0838717792	-1.7925755381	-4.2854066200
H	6.9302132383	-0.7497148578	-4.0908552171
H	3.1657661849	-3.7010694786	-2.3175326059
H	2.3410097522	-3.3275837836	-3.5600425607
H	-2.9015273271	-3.8924054064	-4.2848857387
H	-2.6294152239	-0.9068599530	-3.0757944128
H	-0.7466037297	-2.3654762831	-3.2814934102
H	-1.8191838311	-0.0892741881	-4.8308677681

TS Glyoxylic acid hydrate to oxalic acid

C	-2.61994000	-1.95988400	-0.85334200
C	-1.79232100	-2.76920000	-1.57259800
C	-1.90440200	-3.80318500	-2.51648200
C	-2.36418800	-1.12702800	0.01220700
C	-1.08694100	-0.73460500	0.47092800
C	-0.03162800	-1.38907500	-0.32045100
C	-0.34013700	-2.46023800	-1.28991700
C	-0.95727500	-4.49645600	-2.91127400
C	0.41072900	-4.27626000	-2.94858600
C	0.70939900	-3.18890500	-1.99535300
C	-0.70443200	0.14024700	1.60738000
C	0.59774100	0.50622100	1.64807700
C	1.68064900	-0.07391900	1.02767900
C	1.33408800	-1.10825500	-0.00900200
C	2.42125000	-1.80389800	-0.66802200
C	2.10598200	-2.80689500	-1.67331500
C	1.60631700	-4.68679000	-3.53183100
C	2.75087800	-4.25136200	-3.42901400
C	3.24931300	-3.26737100	-2.55796300
C	3.00670100	0.13357300	1.02741900
C	3.97310300	-0.31271900	0.38088900
C	3.78812600	-1.22122800	-0.65511600
C	4.43239300	-1.40415500	-1.91722300
C	4.30061600	-2.42146300	-2.71706600
C	-2.86668300	-0.51567600	-4.00482600
C	-1.77731700	0.39324800	-4.16457500
Pt	0.47167500	-1.08405400	-2.81592300
Pt	2.00048600	-0.82058300	-4.79848900
Pt	3.91813500	-0.02151800	-3.21653400
Pt	1.78494200	1.12824500	-2.83743000
O	0.19835500	2.60219300	-2.59625100
O	2.98820000	-1.52343600	-6.58708200
O	5.39545300	-0.17990300	-5.18312600
O	0.28176946	2.76061095	0.17484653
O	8.07777000	-0.50688500	-4.00349400
O	3.14145100	2.64960700	-2.58909500
O	4.31243600	2.05873300	-2.92930700
O	5.29513000	-2.94447400	-5.70552900
O	-3.44261000	-0.49026500	-2.97233700
O	-1.80047000	1.50920000	-3.44970800
O	-3.07557900	-1.38958700	-5.03558500
O	-1.22588700	0.40179200	-5.45520800
H	-0.51284300	2.33046200	-3.24914600
H	0.55408000	3.39307300	-3.06793900
H	3.48337400	-0.80117200	-7.00254400
H	2.25177300	-1.64980700	-7.24845700
H	6.26653800	0.09791400	-5.06399500
H	5.41127200	-1.07417600	-5.47485400
H	-0.50019154	2.18747095	0.37361653
H	-1.43206800	0.68199000	2.08075100
H	7.94876300	0.05676200	-3.24132900
H	9.00464700	-0.80565300	-3.97195300

H	5.08956700	-3.30875300	-4.81371200
H	4.52526200	-3.04855200	-6.28640300
H	-2.36558900	-1.28501600	-5.67997600
H	-0.63943200	-0.36914700	-3.62491300
H	-0.28088400	0.63095500	-5.35602600
H	-0.00400454	3.47010695	0.76992753

Oxalic acid

i = 227, E = -827.7938689194

C	-1.4715887563	1.0273821554	1.4371234658
C	-0.5648725534	0.0046901422	1.6068440160
C	-0.4666220594	-1.1873442023	2.2985232986
C	-1.3493773194	2.0858637220	0.7847255312
C	-0.2704677470	2.5384384497	0.0589613806
C	0.8902817598	1.5441365194	0.0878446676
C	0.7459728692	0.2892029364	0.8536097913
C	0.5092138824	-1.9533442444	2.4078122118
C	1.7892733921	-1.8028151678	1.8952428415
C	1.9294105973	-0.5569817567	1.0761579271
C	0.0742873048	3.6654291569	-0.6715144923
C	1.1610567511	3.9233813115	-1.2243295053
C	2.3445124833	3.1923198933	-1.2158019659
C	2.2063111383	1.9245294914	-0.4397440386
C	3.3383340437	1.0492556357	-0.2566948982
C	3.2082120913	-0.1790306077	0.5146771417
C	2.9877492033	-2.4984860519	1.9645095611
C	4.0855862360	-2.1959166139	1.4590944138
C	4.3967880338	-1.0727189337	0.7019725849
C	3.6143923491	3.3388378551	-1.7430982558
C	4.5893056944	2.5773967255	-1.6085243736
C	4.6541163864	1.3969851471	-0.8902396567
C	5.6169207203	0.4456771374	-0.6124727988
C	5.5290025585	-0.6006528897	0.0543452960
Pt	0.3531559282	-0.2134135331	-1.2330963219
Pt	-0.0885325519	-1.5049913557	-3.3701726840
Pt	2.3178090148	-0.5523590886	-3.3499025511
Pt	0.6136592828	1.1628382763	-3.4719170522
O	-0.9644914602	2.8683219142	-3.5846379118
H	-1.0070000114	3.2276229291	-4.4897688449
H	-0.6000551851	3.5774003686	-3.0152828428
O	1.7081237761	-0.5393202177	-6.7494759449
H	1.6825177846	-1.3922434744	-6.2626313315
H	2.2332274690	0.0468256144	-6.1498606964
O	4.0112193403	-1.9686480942	-3.3593312017
H	4.8113639037	-1.3827834536	-3.2922427374
H	3.8680351766	-2.4929367157	-2.5206310929
O	-2.3550045309	-1.6896934473	-2.9158852713
H	-2.3888272977	-1.0061589768	-2.2176713660
H	-2.7287732308	-1.2517711319	-3.7404496025
O	5.6817244616	0.1817726132	-3.7392811233
H	6.2707170853	0.1026460748	-4.5087151007
H	4.9142276531	0.7141454647	-4.0577935393
O	2.0521890067	1.9286847186	-4.5912580999
O	3.0722832809	0.9002504807	-4.6346911791
O	2.7829102340	-3.3106100707	-1.3888812487
H	2.9488598359	-3.1587773260	-0.4389289624
H	1.9809439517	-2.7768929899	-1.5865949590
O	-2.6507250259	-0.4581735254	-5.3230447531
C	-1.5242364648	-0.7645443832	-5.7346546696
C	-0.9761695885	-2.1712156574	-5.4326750476
O	0.2328582228	-2.5435879064	-5.4682918926
H	0.2243423038	-0.2395778425	-6.5769645753
O	-1.9901453190	-3.0850370551	-5.3760713865
O	-0.7741929952	0.0524398174	-6.4487863001
H	-1.5600913080	-3.9502819013	-5.2118612250

TS Oxalic acid decomposition

C	0.66170900	2.71541200	-1.05162600
C	1.77434300	1.99700700	-0.67946800
C	2.03831500	1.06298700	0.49941000
C	0.40242900	3.51879900	-1.96121400
C	1.31252800	3.87829900	-2.94696900
C	2.62185300	3.17102700	-2.79674600
C	2.83686800	2.32180600	-1.57769300
C	3.29776100	0.79704800	0.69166700
C	4.38469800	0.96838500	-0.11021100
C	4.09560800	1.70056300	-1.39933000
C	1.35979300	4.68120800	-4.05637100
C	2.25042500	4.82903700	-4.92930500
C	3.48430800	4.16236600	-4.96986400
C	3.71516000	3.40586800	-3.71938500
C	4.94020100	2.65750300	-3.58088400
C	5.14728500	1.77858200	-2.44953700
C	5.69975100	0.50781500	-0.13217300

C	6.52879200	0.43095200	-1.04791300
C	6.46622300	1.09109700	-2.23214400
C	4.47687100	3.99776800	-5.91739300
C	5.45231600	3.30322000	-5.75964400
C	5.93244700	2.55975600	-4.70064000
C	7.06874400	1.77510100	-4.38654000
C	7.28021800	1.10619800	-3.36332900
Pt	0.76560700	0.00725500	-0.74975200
Pt	-0.20960300	-2.10562700	-1.83786500
Pt	1.84347500	-0.62468800	-3.04639600
Pt	-0.46517400	0.15590400	-3.22376300
O	-2.71311900	0.97324300	-3.38281900
H	-3.35151300	0.88362200	-2.68143700
H	-2.93390200	0.32950400	-4.13608000
O	-1.23409000	-3.75714000	-4.26037600
H	-0.94322700	-4.70418500	-4.27566800
H	-0.46758900	-3.35454600	-3.63715200
O	3.86249400	-1.33495300	-2.86140400
H	4.26182300	-1.58725400	-3.72046600
H	4.06259500	-2.14778200	-2.35110800
O	-2.28086900	-0.91833400	-5.48455500
H	-1.94685800	-1.81928900	-5.57635900
H	-1.40496900	-0.42614300	-5.60857600
O	4.85335400	-0.70818800	-5.59719900
H	4.51294200	0.19489000	-5.45591700
H	5.82010000	-0.63011800	-5.57116800
O	0.34445200	0.91264400	-4.91161200
O	1.59717200	0.34091100	-4.90783200
O	3.26846100	-2.24621500	-0.29859600
H	2.30452200	-2.26576200	-0.01084700
H	3.50936600	-1.29653200	-0.24393700
O	-4.27912400	-1.79314400	-1.88518000
C	-3.36176700	-2.48733000	-2.22659300
C	-1.94333700	-2.84058800	-1.01163300
O	-1.47715200	-4.00858400	-1.36678200
H	-2.15351400	-3.57699700	-3.52767100
O	-2.41017700	-2.43677500	0.19505000
O	-3.29898200	-3.36547600	-3.19473400
H	-2.14336000	-3.19480400	0.79089900

Reactant O2 to H2O2

i = 337, E = -785.4809026581

C	-0.6005100678	0.4507883659	1.3259202355
C	0.4812419568	-0.4011678517	1.3298136804
C	0.8294380047	-1.6187246227	1.8811372143
C	-0.7324872628	1.5480728110	0.7468770128
C	0.1728636962	2.2107309506	-0.0569241652
C	1.4821930155	1.4520672856	-0.1691755506
C	1.6344728550	0.1560584801	0.4962845438
C	1.9197623580	-2.2195043368	1.8410003842
C	3.1101325716	-1.7869353186	1.2686106275
C	2.9525179719	-0.4777497087	0.5584232550
C	0.2051795830	3.3747354549	-0.8059425641
C	1.1575590011	3.8261907869	-1.4682600468
C	2.4452070142	3.3321780758	-1.5968728179
C	2.6290619377	2.0547138036	-0.8363495586
C	3.9148232545	1.3992497602	-0.8012731087
C	4.0832653618	0.1467917223	-0.0865864809
C	4.4087985947	-2.2608524238	1.1920413126
C	5.3852949413	-1.7290910661	0.6331240105
C	5.4203871386	-0.5289480504	-0.0564403262
C	3.6097708302	3.7164840704	-2.2368116541
C	4.7207236675	3.1570558783	-2.2197569208
C	5.0691684590	1.9990859384	-1.5490219442
C	6.2100949177	1.2345136758	-1.3907109051
C	6.3885196935	0.1625700227	-0.7812951996
Pt	1.0423133566	-0.3606582839	-1.7517018838
Pt	0.5708108615	-1.4923040996	-3.9850413015
Pt	3.1211872541	-0.8996266216	-3.4553806218
Pt	1.4049723597	1.0003844196	-4.0196038892
O	-0.5367618755	1.8820163022	-4.2111108129
H	-0.9782556148	1.6471998693	-3.3719993066
H	-0.9923142781	1.2932280318	-4.9468004556
O	0.2715234887	-1.5317892472	-6.0423823946
H	0.2890652609	-2.4188947051	-6.4384683729
H	1.4896814235	-0.2805407418	-6.6473586182
O	3.7990786713	-2.8312503295	-2.9820787424
H	4.7366929388	-2.8151521115	-2.6357002937
H	3.1625450831	-3.2122890354	-2.2851130378
O	-1.5648327271	0.3405769867	-6.0096924725
H	-2.4334545608	-0.0368620805	-5.7954628802
H	-0.9336654710	-0.4556184426	-6.1108888418
O	6.4128590314	-2.6024160412	-2.3563874558

H	6.9172277321	-2.7354419066	-3.1779448731
H	6.5070965824	-1.6493638965	-2.1480262020
O	1.5591856245	1.4970020636	-5.9498513374
O	2.1801791355	0.4504374874	-6.6892309659
O	1.8290048940	-3.6677704888	-1.4728971443
H	1.2001551112	-3.1316512460	-2.0243403860
H	1.7570346058	-3.2701901064	-0.5845305292
H	3.0992639322	0.7306564974	-3.9216455743
H	4.5482820587	-0.3425201824	-3.1218746573
H	0.1985957578	-2.9963228166	-3.7486982180
H	-0.4748925497	-0.2950611359	-1.4180733443
O	-2.2656274669	-2.4049008621	-0.7080119995
O	-1.2383916385	-3.0811624067	-0.7148888744

TS O2 to H2O2

C	2.77476300	0.91851300	1.51009800
C	3.58158900	0.02320200	0.91454500
C	4.07555400	-1.24347500	1.04025900
C	1.97407700	1.82087800	1.13679800
C	2.12832000	2.48679100	-0.04456200
C	3.23515900	1.82919100	-0.93520900
C	3.80111400	0.55779400	-0.55537000
C	4.84225200	-1.86357800	0.26861000
C	5.35820900	-1.50573600	-0.91402200
C	4.90361000	-0.07253600	-1.24757200
C	1.72459600	3.62305200	-0.64890300
C	2.22424700	4.36218900	-1.49643600
C	3.39144600	3.98777200	-2.22495400
C	3.85227300	2.57940100	-2.01163400
C	4.99448500	2.01519100	-2.69042300
C	5.49764200	0.66889700	-2.37167100
C	6.35167600	-1.82844800	-1.84527000
C	6.82160300	-1.18959800	-2.79808800
C	6.55801300	0.09336400	-3.22256900
C	4.18213500	4.55456900	-3.20651200
C	5.20151400	4.14792100	-3.81948300
C	5.66836000	2.83105700	-3.74104500
C	6.61230200	2.09610600	-4.45067500
C	6.96550800	0.94040300	-4.22674100
Pt	1.67493200	0.38199100	-1.58131600
Pt	-0.30835800	-0.97964200	-2.57366800
Pt	2.16160900	-1.88419900	-2.64215700
Pt	1.57802300	0.41037400	-4.18290900
O	-1.68706700	1.80539000	-6.41554900
H	-1.55657500	1.14348500	-5.68117800
H	-1.75327000	-1.18410300	-5.25393200
O	-4.98347500	-1.72548000	-3.99306900
H	-3.97359700	-1.71713500	-3.81949900
H	0.30752000	2.25546500	-6.35388100
O	2.41491600	-4.23433000	-2.35299400
H	1.62494700	-4.35274000	-1.76579900
H	2.07809800	-4.52049400	-3.22044200
O	-1.19454200	-1.53309000	-4.51381500
H	-2.22672200	1.22013000	-7.01501600
H	-5.30413200	-2.26984500	-3.23251800
O	0.55040300	-4.39292500	-0.34913500
H	0.20438400	-5.02313800	0.29009700
H	-0.13693400	-3.70551700	-0.40650800
O	2.05962700	1.43011700	-5.79064600
O	1.23769100	2.26531800	-6.69529100
O	0.15803100	-4.88625200	-3.74410800
H	-0.35378800	-5.19452000	-4.47499700
H	-0.43098300	-4.19423100	-3.32865200
H	2.66950600	-0.82166400	-3.98351200
H	3.70987200	-2.07845900	-2.64129300
H	-0.22520700	-0.67695400	-1.06613300
H	-1.83100200	-2.15841100	-3.82592400
O	-1.76515900	-3.03115700	-2.85093600
O	-1.41927000	-2.40104800	-1.68214800

Product O2 to H2O2

C	1.7225745031	1.9449053364	2.0066748617
C	2.8813868578	1.2134860929	2.1287672607
C	3.5719670543	0.4963994863	3.0857230370
C	1.2816633876	2.5145250784	0.9865741736
C	1.8160678623	2.6435259350	-0.2797037576
C	3.1207235447	1.8928072558	-0.3704771384
C	3.6378509902	1.1472780660	0.7911097673
C	4.6665004298	-0.0900569326	2.9819055169
C	5.5394367600	-0.1479144312	1.9044160497
C	5.0035115722	0.6034815408	0.7283904785
C	1.4190213022	3.3506824554	-1.4079180038
C	2.1563156330	3.5831527739	-2.5229414095
C	3.4750617176	3.0371865186	-2.5643316775

C	3.9998414094	2.1929578424	-1.4971734688
C	5.3257510503	1.6336055492	-1.5410983162
C	5.8156517329	0.8128266735	-0.4459200458
C	6.7985705533	-0.6663726735	1.6510652321
C	7.4896138671	-0.5192542327	0.6265582160
C	7.1865615803	0.1992503771	-0.5185208582
C	4.4196145102	3.1912530009	-3.5702237561
C	5.5658038598	2.7212741433	-3.6541072120
C	6.1920966885	1.8936206199	-2.7368470788
C	7.4072423211	1.2384361771	-2.6266785775
C	7.8310020226	0.5214489025	-1.7018909262
Pt	2.6386199743	-0.3116945773	-0.5698339470
Pt	0.3652950946	-0.3791878682	-2.0973531465
Pt	1.7624123965	-2.4295345185	-1.7041574730
Pt	2.6450501812	-0.5636037966	-3.2352027493
O	3.4552152599	0.5513242779	-4.6309053218
H	1.7936467360	4.1627841911	-3.3728990925
H	3.3445581272	-0.0053232580	-5.4385235871
O	0.8148529391	1.1308841383	-5.6260277888
H	0.0937295301	1.1567887336	-4.9726584159
H	1.6397843760	1.1535063415	-5.0820920656
O	3.0853237367	-4.1348185249	-1.8502510686
H	3.2859410873	-4.1394520520	-2.8439519857
H	3.9239087795	-3.8049800478	-1.4001030645
O	-0.6761859691	1.5780018974	-2.6966720907
H	-1.4381374825	1.4084642458	-2.0287814823
H	-0.1159303965	2.2925356474	-2.3102207226
O	3.4616009567	-4.0345838474	-4.5073809672
H	3.3950980780	-4.8693342886	-5.0008686256
H	2.8522526207	-3.4043035870	-4.9818487299
O	1.9914085114	-1.2398379264	-6.5022673373
O	1.5218996990	-2.2684482528	-5.5561715830
O	5.0577144608	-2.8138900341	-0.5693043190
H	4.4140699299	-2.0896474458	-0.3816429979
H	5.6822209531	-2.4075716613	-1.1971469412
H	1.3097240076	-0.5219550619	-6.3615613366
H	1.6081575737	-1.7873186915	-4.6668850851
H	-0.5046594550	-1.0376283827	-3.1962010613
H	2.0540260172	-0.8220104223	0.7749722621
O	-2.1550555902	0.5355764759	-0.9071946636
O	-1.2681547059	-0.4281922450	-0.7788499961

Reactant Glycolaldehyde to ethylene glycol

i = 130, E = -798.1168189208

C	-1.6205568950	0.8098824530	1.4827100587
C	-0.7174143563	-0.2272105695	1.5490392095
C	-0.6286993666	-1.4849356754	2.1121390833
C	-1.5096498522	1.9323119862	0.9447740319
C	-0.4389635048	2.4529709313	0.2529863234
C	0.7213010046	1.4465618077	0.1881898945
C	0.5925986084	0.1272299615	0.8437428421
C	0.3544081181	-2.2466314859	2.1853358645
C	1.6526481477	-2.0120842702	1.7567745011
C	1.7857724868	-0.7052254208	1.0383756045
C	-0.0867899203	3.6166094248	-0.4068729730
C	0.9809754496	3.8971144844	-0.9944516093
C	2.1483737082	3.1487845471	-1.0876355572
C	2.0274894691	1.8378132462	-0.3637907992
C	3.1862769961	0.9808568309	-0.1946891924
C	3.0758722735	-0.2652976664	0.5434447572
C	2.8734666974	-2.6641178633	1.8469434868
C	3.9850042791	-2.3002525816	1.4173017805
C	4.2855846241	-1.1274880479	0.7319106351
C	3.4052186978	3.3039897984	-1.6385640211
C	4.3914518955	2.5468791448	-1.5502874996
C	4.4874749943	1.3720642476	-0.8208556461
C	5.4798047682	0.4509576012	-0.5338369488
C	5.4171896760	-0.6054185125	0.1201582806
Pt	0.3810590689	0.0924618029	-1.4272344816
Pt	-0.3307530493	-1.3307091561	-3.6491739797
Pt	2.2938023234	-0.6167752205	-3.8155985933
Pt	0.6740944835	1.2114971312	-3.7890903256
O	-0.6824008981	3.0941642795	-3.5919050067
H	-0.3799524436	3.7724755754	-4.2229587948
H	-0.4211648409	3.4313812941	-2.7028563251
O	2.4629632128	-1.6074498940	-6.8479026815
H	3.1448830414	-2.2705913419	-6.6419233378
H	2.3085015003	-1.1711454902	-5.9558250752
O	4.0519006782	-1.9769132764	-3.7263755079
H	4.8173374723	-1.3507535631	-3.5744244213
H	3.8484948988	-2.4538691006	-2.8694500173
O	-2.4903344456	-1.1942298130	-4.0522681387
H	-2.8509308544	-0.4991626085	-3.4719328507

H	-2.5290707411	-0.8249680846	-5.0127411234
O	5.8024175472	0.1113618658	-3.6524105299
H	6.3690763588	0.1283269932	-4.4423170831
H	5.0771540849	0.7548807095	-3.8507366176
O	2.3503032760	2.0807252095	-4.4149162023
O	3.3400407042	1.0635125450	-4.3470041783
O	2.8415724088	-3.1084309139	-1.5898467232
H	3.1667548032	-3.1030508505	-0.6695359871
H	2.1114529816	-2.4535435338	-1.5980257162
O	-2.3173101417	-0.3294263229	-6.4976125834
C	-1.4636663795	-0.9462775320	-7.1566309168
C	-0.8211398947	-2.2230305589	-6.7039860766
O	0.1309629998	-2.7506038284	-7.5760077037
H	-1.6124185778	-2.9679374462	-6.5003184601
H	-0.3931426955	-1.9965612202	-5.6459639516
H	1.0181750721	-2.3350214451	-7.3651924166
H	-1.1191189489	-0.5472487731	-8.1312956841
H	-0.6910836158	-1.0995952008	-1.8897709338
H	1.2873477308	-2.0036071405	-3.6957107411

TS Glycolaldehyde to ethylene glycol

C	-1.64432500	3.30920700	-2.17339500
C	-1.89900400	2.57025300	-1.04102100
C	-2.97810200	2.16432800	-0.26728900
C	-0.65949800	3.57031000	-2.88849900
C	0.66700100	3.26787500	-2.59555700
C	0.70938500	2.55001900	-1.28593000
C	-0.47418000	2.13200800	-0.53910200
C	-2.89803100	1.70745300	0.87693900
C	-1.70939900	1.57998300	1.65286500
C	-0.42960900	1.84159400	0.93446600
C	1.84450700	3.06912500	-3.31264000
C	2.98438300	2.65120700	-2.80739000
C	3.19143900	2.43425800	-1.43478800
C	1.99287500	2.24498800	-0.59881500
C	2.06440100	2.12088800	0.84562300
C	0.87177900	1.91773700	1.59150600
C	-1.43978000	1.66813900	3.01581900
C	-0.34727300	1.73193200	3.63638300
C	0.95027400	1.70759200	3.12580000
C	4.31005900	2.35795700	-0.62967100
C	4.33362100	2.29265100	0.59865700
C	3.38607400	2.07727500	1.55890600
C	3.28925200	1.58822700	2.83577200
C	2.25557200	1.44399700	3.51541400
Pt	0.81044300	0.44394400	-1.62340600
Pt	0.58934200	-1.40344500	-3.62905800
Pt	2.11127500	-0.82427000	-5.68160500
Pt	1.96939500	0.99516500	-3.87856200
O	-3.04757900	-0.37795700	-3.26602100
H	-2.35589900	-0.73443800	-3.89291300
H	-2.60560800	-0.58650000	-2.42477200
O	-8.93636100	-1.00937500	-2.53757500
H	-9.29879100	-0.14919900	-2.81894500
H	-7.99006700	-0.82924300	-2.66162700
O	2.80604400	-2.09370800	-7.33270000
H	3.62121700	-1.77770000	-7.81608600
H	3.14002000	-2.96544800	-6.98331300
O	1.53679900	-10.60310600	17.51786000
H	2.19975100	-11.16643000	17.08266400
H	1.92669000	-10.36315000	18.39248500
O	3.24451600	-3.42151000	-2.72320000
H	2.38858500	-3.15548600	-2.33598800
H	3.49949600	-2.52884000	-3.07610400
O	3.06240200	1.62064400	-5.65461400
O	3.02421400	0.59619600	-6.55662600
O	3.80569200	-4.03864700	-5.79846000
H	3.35356700	-4.91292800	-5.99344900
H	3.24888300	-3.62223600	-5.08608600
O	-0.13783500	-2.95587100	-2.24271500
C	-0.54050100	-3.24379000	-3.52823600
C	0.24077300	-4.39931500	-4.20392200
O	0.64771900	-4.13898100	-5.65555000
H	-0.30124200	-5.32031300	-4.10781400
H	1.11344700	-4.50654800	-3.60374200
H	-0.05515900	-3.65159500	-6.08254600
H	-1.62281800	-3.16090200	-3.72790700
H	0.46596900	-1.22610000	-1.43464700
H	0.18174600	-2.06770200	-4.82392800