Supporting Information

The Challenge of Reproducing with Calculations Raw Experimental Kinetic Data for an Organic Reaction

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1. Computational Details

All the DFT calculations were carried out with Gaussian09[1] (Revision D.01) with a grid of 75 radial shells and 302 angular points per shell ("Finegrid" in Gaussian). Most of the work was done using B3LYP-D3[2,3,4] (where D3 stands for GD3[5] empirical dispersion) with RRHO approximations for the free energy corrections, implicit SMD[6] solvation for dichloromethane (DCM) and reference state corrections[7] for liquid phase at 1M and 298.15K. The basis set used for all atoms was cc-pVTZ[8]. Per each optimized structure a frequency calculation was performed to ensure the minima/transition state nature of the obtained structure. In all the optimizations the symmetry was disabled with the keyword nosymm. Quasi-harmonic corrections[9] were obtained with a threshold of 100cm^{-1}, using the GoodVibes software.[10] Microkinetic simulations were carried out with a script developed in-house, the details are discussed in Section 5 and an example script is provided in Section 8.
DFT calculations of Section 3 were carried out using the 6-31+g(d,p)[11] for all atoms unless specified otherwise. The DFT functionals used were BP86-D3, PBEPBE-D3 (generally known as PBE0-D3), PBE1PBE-D3, M06-D3, M06-2X-D3 and ωB97X-D.[12,13,14,15,16] From those PBEPBE-D3 and M06-2X-D3 were chosen to run kinetic simulations and therefore reoptimized with cc-pVTZ basis set for all atoms (Section 6). Single-point DLPNO-CCSD(T)[17] calculations with the cc-pVTZ basis set were performed in ORCA4.0[18] always with the autoaux[19] option enabled to include matching auxiliary basis functions. Default NormalPNO[20] options and TightSCF cutoff were employed. When the implicit solvation was included the SMD method for dichloromethane as implemented in ORCA4.0 was included.

2. Data extraction from experiment

As the experimental results were reported in a graphic we had to interpolate the experimental values from the graph. To obtain the numerical values we measured the relative position of the center of the data markers/axes ticks by visual inspection with an error of ±1 pixel. When in doubt the mid value between the two pixel relative positions was considered.
First the ticks of the X and Y axes were measured. With the value that was indicated per each tick we calculated a conversion factor to convert pixel distances in times and concentrations this is summarized in Table S2. Next the factors obtained per each axis were averaged obtaining 27.3 ± 0.9 s/pixel for the X axis and 0.357 ± 0.009 mM/pixel for the Y axis. Finally the coordinates of each of the data points were measured and translated with the conversion factors to time-concentration pairs. Table S1 summarizes this final step and includes the values used as reference in the work.

Table S1: Pixel measurements on the Data points and estimated time-concentration values

	Relative Position				**Final Values**	
Point Id	**X**	**Y**	**X-O$_x$**	**Y-O$_y$**	**Time**	**Concentration**
	(pixel)	**(pixel)**	**(pixel)**	**(pixel)**	**(s)**	**(mM)**
Origin	43.0	177.0	0.0	0.0	0.0	0.000
1	49.5	167.5	6.5	9.5	177.2	3.391
2	60.0	144.5	17.0	32.5	463.4	11.600
3	70.5	127.0	27.5	50.0	749.7	17.846
4	81.5	112.5	38.5	64.5	1049.5	23.021
5	92.0	102.0	49.0	75.0	1335.7	26.769
6	113.0	84.5	70.0	92.5	1908.2	33.015
7	134.5	72.0	91.5	105.0	2494.3	37.477
8	155.5	62.0	112.5	115.0	3066.8	41.046
9	198.0	48.0	155.0	129.0	4225.3	46.043

Table S2: Marker pixel measurements and values for the selection of a conversion factor from pixels to time and concentrations.

Y Axis					X Axis				
X Coord	**Y Coord**	**Value**	**Y-O_y**	**Conv. Factor**	**X Coord**	**Y Coord**	**Value**	**X-O_x**	**Conv. Factor**
(pixel)	**(pixel)**	**(mM)**	**(pixel)**	**(mM/pixel)**	**(pixel)**	**(pixel)**	**(s)**	**(pixel)**	**(s/pixel)**
	177.0	0	0.0	---	41.0		0	0.0	---
	172.0	2	5.0	0.4000	61.0		500	20.0	25.00
	166.0	4	11.0	0.3636	78.5		1000	37.5	26.67
	160.0	6	17.0	0.3529	96.0	177.0	1500	55.0	27.27
	155.0	8	22.0	0.3636	114.0		2000	73.0	27.40
	149.0	10	28.0	0.3571	131.5		2500	90.5	27.62
	143.0	12	34.0	0.3529	149.0		3000	108.0	27.78
	138.0	14	39.0	0.3590	167.0		3500	126.0	27.78
	132.0	16	45.0	0.3556	184.5		4000	143.5	27.87
	126.5	18	50.5	0.3564	202.0		4500	161.0	27.95
	121.0	20	56.0	0.3571					
	115.0	22	62.0	0.3548					
	109.0	24	68.0	0.3529					
	104.0	26	73.0	0.3562					
	98.0	28	79.0	0.3544					
41.0	92.5	30	84.5	0.3550					
	87.0	32	90.0	0.3556					
	81.0	34	96.0	0.3542					
	75.0	36	102.0	0.3529					
	70.0	38	107.0	0.3551					
	64.0	40	113.0	0.3540					
	58.0	42	119.0	0.3529					
	53.0	44	124.0	0.3548					
	47.0	46	130.0	0.3538					
	42.5	48	134.5	0.3569					
	36.0	50	141.0	0.3546					
	30.0	52	147.0	0.3537					
	24.5	54	152.5	0.3541					
	19.0	56	158.0	0.3544					
	13.0	58	164.0	0.3537					
	8.0	60	169.0	0.3550					

3. Benchmark with DFT and DLPNO-CCSD(T)

In order to decide an appropriate theory level (method, functional, basis set, solvation model etc…) a small set of relevant structures were calculated. Initially only single point (SP) calculations over the structures optimized with B3LYP-D3/6-31+g(d,p) and SMD implicit solvation for dichloromethane. For some cases we did optimize the structure with the new theory level. The set of structures included the Aldehyde, Amine, Water, Hemiaminal, Imine and the Transition states for the dehydration of the hemiaminal (TS2, TS2W, TS2N, TS2NW and TS2WW) see Figure 1 of the main text. Table S3 compiles the relative free energies of the transition states, intermediates and products referred to the appropriate free molecules of reactants. For SP calculations the free energy of each structure was obtained $G_{SP} = U_{SP} + G^{ref} - U^{ref}$ where *ref* corresponds to B3LYP-D3/6-31+g(d,p) with SMD for that structure.

Entries 1, 2 and 5 show the effect of changing the basis set within the Pople Basis set family. The most significant difference is between entries 1 and 2 that switch the reaction from endergonic to exergonic. This clearly indicates the importance of polarization functions in the basis set for this system.

Entries 2, 3 and 4 show the effect of changing the solvation model as well as the reaction in vacuum. No significant difference was found between pcm and smd for this system. There is a significant difference for the transition state catalyzed by two waters in vacuum which is likely due to the lack of interactions of the Hydrogen's of the water and the solvent.

Entries 2, 7, 8, 9, 10, 11 and 12 show the effect of changing the DFT functional. In all of them GD3 empirical dispersion was added except for the ωB97X-D functional. The two pure functionals, BP86-D3 and PBEPBE-D3 (Entries 8 and 9), predict more stable structures than B3LYP-D3 overall. PBE1PBE-D3 functional gives similar results to B3LYP for the Transition states. PBE1PBE-D3 and M06-2X-D3 substantially stabilize the Hemiaminal. The Minnesota family (Entries 10 and 11) and ωB97X-D (Entry 12) predict slightly higher barriers.

Entries 13-16 show the effect of increasing the basis function for the DLPNO-CCSD(T) method. As the basis set is larger the predicted stabilities increase. However the large difference between Entry 6 and Entry 14 motivated the test done in the section 4 "DLPNO-CCSD(T) Solvation Effect". In Entry 16, the TS2NW was not included because the computational cost was high and, with the other results in sight, it was unlikely to provide any new insights.

Finally as B3LYP-D3 seems to have an intermediate behavior between the tested functionals we decided to move on with it and increased the basis set.

Table S3: DFT and DLPNO-CCSD(T) benchmark results.

Free Energies with 1M as reference state (kcal mol^{-1})				**Optimized relative energies (SP relative energies)**					
Entry	**Method**	**Basis Set**	**Solvation Model**	**TS2**	**TS2W**	**TS2WW**	**TS2NW**	**Hemiaminal**	**Imine + Water**
1▲	B3LYP-D3	6-31+g(d)	smd	43.1 (43.3)	30.7 (30.8)	24.4 (24.4)	28.2 (27.0)	10.1 (10.2)	0.8 (0.9)
2*▲	B3LYP-D3	6-31+g(d,p)	smd	41.1 (41.1)	28.3 (28.3)	22.1 (22.1)	24.3 (24.3)	8.8 (8.8)	-2.1 (-2.1)
3▲	B3LYP-D3	6-31+g(d,p)	pcm	41.7 (42.5)	27.4 (28.2)	20.7 (21.2)	24.2 (22.8)	8.2 (8.9)	-1.6 (-1.4)
4▲	B3LYP-D3	6-31+g(d,p)	---	47.0 (53.0)	25.8 (31.1)	16.0 (16.8)	21.5 (22.2)	5.5 (6.4)	-1.0 (-0.9)
5▲	B3LYP-D3	6-311++g(d,p)	smd	41.2 (41.3)	29.4 (29.3)	23.3 (23.6)	26.4 (25.6)	9.7 (9.5)	-2.3 (-2.4)
6▲□	B3LYP-D3	cc-pVTZ	smd	47.7 (------)	32.5 (------)	22.4 (------)	23.1 (------)	9.2 (------)	-1.1 (-----)
7▲	PBE1PBE-D3	6-31+g(d,p)	smd	42.8 (42.8)	27.8 (28.7)	21.3 (21.3)	23.6 (23.8)	3.0 (3.4)	-3.0 (-3.1)
8▲	PBEPBE-D3	6-31+g(d,p)	smd	37.0 (38.2)	22.2 (23.7)	15.9 (16.0)	18.6 (18.7)	6.6 (6.7)	-2.8 (-2.9)
9▲	BP86-D3	6-31+g(d,p)	smd	36.6 (37.8)	20.7 (22.8)	14.8 (15.5)	18.0 (17.5)	6.6 (6.7)	-2.7 (-2.8)
10▲	M06-D3	6-31+g(d,p)	smd	44.8 (44.5)	32.0 (32.7)	28.1 (26.9)	31.2 (27.9)	5.5 (6.2)	-2.0 (-2.7)
11▲	M06-2X-D3	6-31+g(d,p)	smd	44.5 (44.5)	29.6 (30.8)	25.4 (24.9)	27.3 (27.3)	2.6 (2.5)	-3.6 (-4.4)
12	ωB97X-D	6-31+g(d,p)	smd	43.5 (43.7)	32.3 (31.9)	26.6 (26.2)	29.5 (27.4)	5.3 (5.1)	-1.9 (-2.5)
13	DLPNO	cc-pVDZ	smd	------ (72.6)	------ (47.8)	------ (37.5)	------ (44.2)	------ (7.3)	----- (-1.0)
14	DLPNO	cc-pVTZ	smd	------ (56.8)	------ (39.4)	------ (33.8)	------ (38.0)	------ (6.1)	----- (-3.5)
15	DLPNO	cc-pVQZ	smd	------ (50.3)	------ (37.2)	------ (33.5)	------ (36.7)	------ (6.0)	----- (-4.2)
16	DLPNO	cc-pV5Z	smd	------ (46.5)	------ (36.4)	------ (33.7)	------ (------)	------ (6.0)	----- (-4.6)

* The geometries optimized with this theory level were used for the single point (SP) calculations. ▲ Empirical dispersion GD3 included. □ Manuscript structures. Energies referred to the free reactants (and free water for the TSs with water molecules as catalysts).

4. DLPNO-CCSD(T) Solvation effect

The effect of the solvation on the DLPNO-CCSD(T) energy was checked to discard that the increase in the barriers was due to an incorrect coupling between the DLPNO-CCSD(T) methodology and the SMD implicit solvation. First the geometries of each compound were optimized in B3LYP-D3/cc-pVTZ with implicit solvation for dichloromethane with SMD. Over those geometries a SP calculation was run in vacuum maintaining the theory level. Finally two SP calculations per structure were done with DLPNO-CCSD(T)/cc-pVTZ, one with SMD solvation and the other without it.

Table S4: Single point calculations on structures optimized in B3LYP-D3/cc-pVTZ with implicit solvation

Structure Name	**B3LYP-D3/cc-pVTZ**		**DLPNO-CCSD(T)/cc-pVTZ**		**B3LYP-D3**	**DLPNO**
	U_{vac}	**U_{sol}**	**U_{vac}**	**U_{sol}**	**$U_{sol} - U_{vac}$**	
	hartree		**hartree**		**kcal mol^{-1}**	
Benzaldehyde	-345.706974	-345.719632	-344.959042	-344.966951	-7.9	-5.0
NButylamine	-213.895670	-213.904198	-213.416621	-213.423305	-5.4	-4.2
Water	-76.459829	-76.466651	-76.331990	-76.338910	-4.3	-4.3
Hemiaminal	-559.611741	-559.630035	-558.389832	-558.401077	-11.5	-7.1
Imine	-483.142477	-483.158753	-482.047899	-482.056414	-10.2	-5.3
TS2	-559.534063	-559.563968	-558.292421	-558.318276	-18.8	-16.2
TS2W	-636.029384	-636.067008	-634.660364	-634.691998	-23.6	-19.9
TS2N	-773.472516	-773.501454	-771.760086	-771.779235	-18.2	-12.0
TS2NW	-849.966431	-849.998025	-848.115925	-848.138254	-19.8	-14.0
TS2WW	-712.539097	-712.566653	-711.039192	-711.060149	-17.3	-13.2

As can be seen in Table S4 the difference in the solvation effect between one and the other theory level depends on the compound that we compare. It is generally smaller in the reactants and for the transition states, intermediates and products increases as the number of molecules within the calculation increase. In all cases the inclusion of implicit solvation implies a decrease in potential energy. As the main interest is discerning if the high barrier is due to the solvation, relative energies in vacuum and in solution need to be calculated and compared. This is what is reported in the Table 1 of the main text.

5. Microkinetic Study

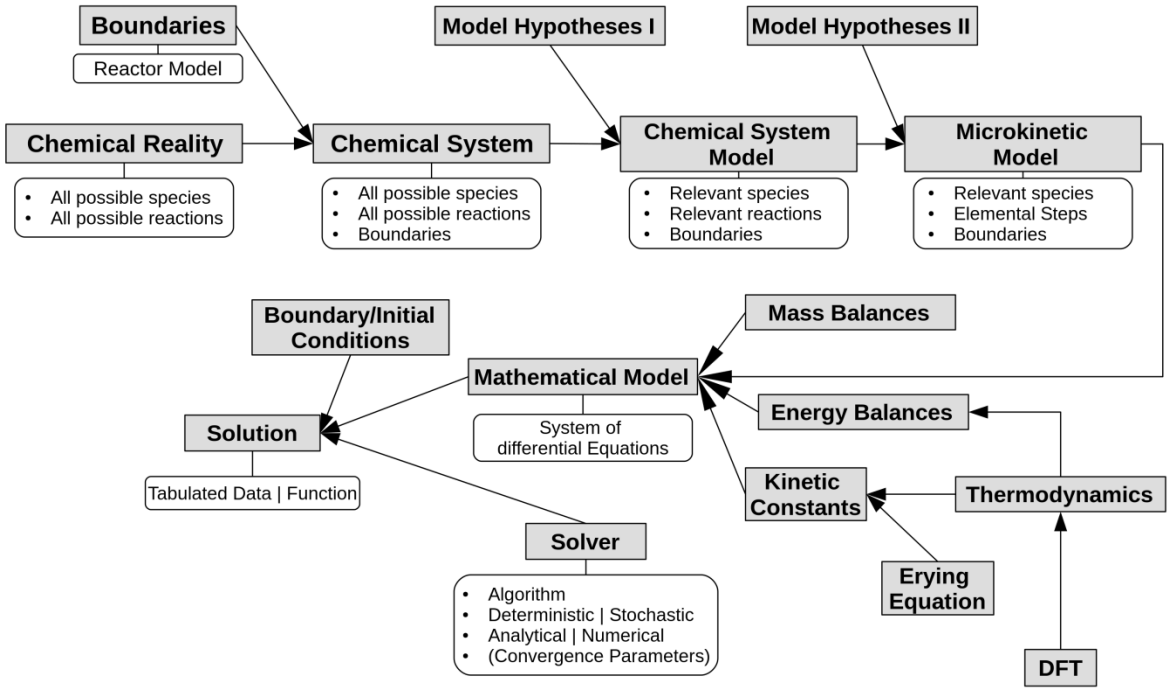

Chart S1: Summary of the terms related to microkinetic simulations

As the usage of the term microkinetic modeling is relatively broad Chart S1 summarizes the different concepts related to microkinetic simulations as used for the following sections.

Boundaries: Isothermal (T=cte) liquid phase (V=cte) batch reactor model (Closed System) thus rendering the Energy Balances unnecessary for the simulations. Therefore temperature is only included in Thermodynamic and Kinetic Constant calculations.

Thermodynamics: Values are at 298.15K and 1 atm (default for Gaussian09 calculations). Since the reactions were in liquid phase free energies were corrected for a 1M reference state.

Kinetic Constants: The constants were calculated within the standard Transition State Theory with the Erying Equation: $k = \alpha_T \frac{k_b T}{h} e^{\frac{-\Delta G^{\ddagger}}{RT}}$ using $\alpha_T = 1$. The constants were always used in the same format as Table S12, this is important due to the numeric nature of the solver and intrinsic limitations of computers, since in some of the simulations the usage of less decimal places led to numerical instability of the differential system. In this case the increase of the decimal places avoids the need of reducing the tolerance of the solver and therefore the time needed for the calculation.

Solver: The Solver employed was a deterministic numerical algorithm, the LSODA from the ODEPACK package[21] as used by the python Scipy library (version 1.3.0).[22] The relative tolerance (rtol) was set up to 10^{-6} and the absolute tolerance (atol) was set up to 10^{-11} as a tradeoff between performance and accuracy. The remaining parameters were the default values of the scipy.integrate.odeint function. The concentrations obtained were saved at intervals of 0.1s.

Initial Conditions: The initial conditions concentration of all species was zero except the benzaldehyde, 0.06M, n-butylamine 0.06M and the water 0.001M (Compounds C00, C01 and C02 in Table S5 respectively) unless specified otherwise.

5.1 Microkinetic Model

To explain the modeling criteria for the elemental steps used we will use the profile of the target reaction catalyzed by a single water molecule (red energy profile in Figure 1 of the manuscript). As the hemiaminal formation and dehydration cannot be modeled as bimolecular reversible elemental steps:

$$C_5H_5CHO + C_4H_9NH_2 + H_2O \leftrightarrows C_{10}H_{17}ON + H_2O \leftrightarrows C_{10}H_{15}N + H_2O + H_2O$$

The first hypothesis considered is that every bond-forming and bond-breaking reaction which involve a calculated TS are unimolecular, meaning that first the molecules form an adduct, and is this adduct the one that proceeds through the TS. Therefore for the hemiaminal formation (and similarly for the dehydration) is represented by the steps:

Step 1) $C_5H_5CHO + C_4H_9NH_2 + H_2O \leftrightarrows [C_5H_5CHO + C_4H_9NH_2 + H_2O]$
Step 2) $[C_5H_5CHO + C_4H_9NH_2 + H_2O] \leftrightarrows [C_{10}H_{17}ON + H_2O]$
Step 3) $[C_{10}H_{17}ON + H_2O] \leftrightarrows C_{10}H_{17}ON + H_2O$

The second hypothesis considered is relative to steps 1) and 3). In order to form the adducts all the different combinations of 2 were considered, for step 1) those would be:

Step 1a) $C_5H_5CHO + C_4H_9NH_2 \leftrightarrows [C_5H_5CHO + C_4H_9NH_2]$
Step 1b) $C_5H_5CHO + H_2O \leftrightarrows [C_5H_5CHO + H_2O]$
Step 1c) $C_4H_9NH_2 + H_2O \leftrightarrows [C_4H_9NH_2 + H_2O]$
Step 1d) $[C_5H_5CHO + C_4H_9NH_2] + H_2O \leftrightarrows [C_5H_5CHO + C_4H_9NH_2 + H_2O]$
Step 1e) $[C_5H_5CHO + H_2O] + C_4H_9NH_2 \leftrightarrows [C_5H_5CHO + C_4H_9NH_2 + H_2O]$
Step 1f) $C_5H_5CHO + [C_4H_9NH_2 + H_2O] \leftrightarrows [C_5H_5CHO + C_4H_9NH_2 + H_2O]$

Any of these different adducts formations were all considered to be fast, diffusion-controlled elemental steps. By fast we refer to including a "fictional" barrier of 2 kcal mol^{-1} in the endergonic direction of the reversible step.

Therefore, we modeled each bond-forming bond breaking event as a set of soft, diffusion-controlled, bimolecular collisions with fast diffusions that have apparent barriers of 2 kcal mol^{-1}. Only the barriers of the unimolecular bond breaking/formation steps (as step 2 of the example) were calculated using the energies of the corresponding transition state structures. Tables from S5 to S12 include all the information about the Microkinetic model as well as the thermodynamics derived from B3LYP-D3/cc-pVTZ. Section 8 shows an example of the python code used.

Table S5: List of Species/Compounds considered in the Microkinetic Model.

Compound ID	**Model Label**	**Structure Name**	$\mathbf{G_{1atm,\ 298.15K}}$ **(hartree)**	$\mathbf{\Delta G_{1M,\ 298.15K}}$ **(**kcal mol^{-1}**)**
C00	A	Benzaldehyde	-345.640471	0.0
C01	B	NButylamine	-213.785156	0.0
C02	W	Water	-76.463950	0.0
C03	[A+B]	A_N	-559.415509	4.5
C04	[A+W]	A_W	-422.097795	2.3
C05	[B+W]	N_W	-290.246742	-0.4
C06	[W+W]	W_W	-152.923000	1.2
C07	[B+B]	N_N	-427.560866	4.0
C08	[A+B+W]	A_N_W	-635.872800	6.7
C09	[A+B+B]	A_N_N	-773.193472	7.1
C10	[A+W+W]	A_W_W	-498.555875	4.1
C11	[B+W+W]	N_W_W	-366.706991	0.0
C12	[B+B+W]	N_N_W	-504.023772	2.8
C13	[W+W+W]	W_W_W	-229.382056	2.4
C14	[A+B+B+W]	A_N_N_W	-849.654737	6.9
C15	[A+B+W+W]	A_N_W_W	-712.337684	4.3
C16	Hemi	Hemiaminal	-559.408007	9.2
C17	[Hemi+W]	Int_W	-635.869928	8.5
C18	[Hemi+B]	Int_N	-773.187317	10.9
C19	[Hemi+B+W]	Int_N_W	-849.649184	10.4
C20	[Hemi+W+W]	Int_W_W	-712.332717	7.4
C21	I	Imine	-482.963413	-1.1
C22	[I+W]	I_W	-559.423021	-0.3
C23	[I+B]	I_N	-696.739874	2.5
C24	[I+W+W]	I_W_W	-635.882776	0.5
C25	[I+B+W]	I_N_W	-773.200786	2.5
C26	[I+B+W+W]	I_N_W_W	-849.662415	2.1
C27	[I+W+W+W]	I_W_W_W	-712.341547	1.8

Model Label corresponds to the encoding used in the reaction listing. The Structure Name corresponds to the name of the entry in the IOChemBD data collection. The energy values correspond to the structures optimized in B3LYP-D3/cc-pVTZ

Table S6: List of Transition State Structures considered for the microkinetic model.

Model Label	Structure Name	$G_{1atm, 298.15K}$ (hartree)	$\Delta G_{1M, 298.15K}$ (kcal mol^{-1})
TS1	TS1	-559.364154	36.7
TS2	TS2	-559.346617	47.7
TS1W	TS1W	-635.849649	21.3
TS2W	TS2W	-635.831806	32.5
TS1N	TS1N	-773.160610	27.7
TS2N	TS2N	-773.146697	36.4
TS1WW	TS1WW	-712.316303	17.7
TS2WW	TS2WW	-712.308845	22.4
TS1NW	TS1NW	-849.632365	20.9
TS2NW	TS2NW	-849.628951	23.1

Table S7: List of reactions considered for the microkinetic model to describe the aggregation of the reactants.

Event ID	Chemical Event	TS Label	Reaction ID		Barriers (kcal mol^{-1})	
			Direct	Reverse	Direct	Reverse
E01	A + B ⇆ [A+B]	---	R000	R001	6.5	2.0
E02	A + W ⇆ [A+W]	---	R002	R003	4.3	2.0
E03	B + W ⇆ [B+W]	---	R004	R005	2.0	2.4
E04	B + B ⇆ [B+B]	---	R006	R007	6.0	2.0
E05	W + W ⇆ [W+W]	---	R008	R009	3.2	2.0
E06	A + [B+W] ⇆ [A+B+W]	---	R010	R011	9.1	2.0
E07	A + [B+B] ⇆ [A+B+B]	---	R012	R013	5.0	2.0
E08	A + [W+W] ⇆ [A+W+W]	---	R014	R015	4.9	2.0
E09	B + [A+B] ⇆ [A+B+B]	---	R016	R017	4.6	2.0
E10	B + [A+W] ⇆ [A+B+W]	---	R018	R019	6.5	2.0
E11	B + [B+W] ⇆ [B+B+W]	---	R020	R021	5.2	2.0
E12	B + [W+W] ⇆ [B+W+W]	---	R022	R023	2.0	3.2
E13	W + [A+B] ⇆ [A+B+W]	---	R024	R025	4.3	2.0
E14	W + [A+W] ⇆ [A+W+W]	---	R026	R027	3.8	2.0
E15	W + [B+W] ⇆ [B+W+W]	---	R028	R029	2.4	2.0
E16	W + [B+B] ⇆ [B+B+W]	---	R030	R031	2.0	3.2
E17	W + [W+W] ⇆ [W+W+W]	---	R032	R033	3.2	2.0
E18	[A+B] + [B+W] ⇆ [A+B+B+W]	---	R034	R035	4.8	2.0

E19	[A+B] + [W+W] ⇆ [A+B+W+W]	---	R036	R037	2.0	3.4
E20	[A+W] + [B+W] ⇆ [A+B+W+W]	---	R038	R039	4.4	2.0
E21	[A+W] + [B+B] ⇆ [A+B+B+W]	---	R040	R041	2.6	2.0

Table S8: List of reactions considered for the microkinetic model to describe the Hemiaminal formation.

Event ID	Chemical Event	TS Label	Reaction ID		Barriers (kcal mol^{-1})	
			Direct	Reverse	Direct	Reverse
E22	[A+B] ⇆ Hemi	TS1	R042	R043	32.2	27.5
E23	[A+B+W] ⇆ [Hemi+W]	TS1W	R044	R045	14.6	12.8
E24	[A+B+B] ⇆ [Hemi+B]	TS1N	R046	R047	20.6	16.8
E25	[A+B+W+W] ⇆ [Hemi+W+W]	TS1WW	R048	R049	13.4	10.3
E26	[A+B+B+W] ⇆ [Hemi+B+W]	TS1NW	R050	R051	14.0	10.6

Table S9: List of reactions considered for the microkinetic model to describe the diffusion of the Hemiaminal-catalyst adducts.

Event ID	Chemical Event	TS Label	Reaction ID		Barriers (kcal mol^{-1})	
			Direct	Reverse	Direct	Reverse
E27	[Hemi+W] ⇆ Hemi + W	---	R052	R053	2.6	2.0
E28	[Hemi+B] ⇆ Hemi + B	---	R054	R055	2.0	3.8
E29	[Hemi+B+W] ⇆ Hemi + [B+W]	---	R056	R057	2.0	3.6
E30	[Hemi+B+W] ⇆ [Hemi+B] + W	---	R058	R059	2.6	2.0
E31	[Hemi+B+W] ⇆ [Hemi+W] + B	---	R060	R061	2.0	3.8
E32	[Hemi+W+W] ⇆ Hemi + [W+W]	---	R062	R063	5.0	2.0
E33	[Hemi+W+W] ⇆ [Hemi+W] + W	---	R064	R065	3.2	2.0

Table S10: List of reactions considered for the microkinetic model to describe the dehydration of the Hemiaminal.

Event ID	Chemical Event	TS Label	Reaction ID		Barriers (kcal mol^{-1})	
			Direct	Reverse	Direct	Reverse
E34	Hemi ⇆ [I+W]	TS2	R066	R067	38.5	47.9
E35	[Hemi+W] ⇆ [I+W+W]	TS2W	R068	R069	23.9	32.0
E36	[Hemi+B] ⇆ [I+B+W]	TS2N	R070	R071	25.5	33.9
E37	[Hemi+W+W] ⇆ [I+W+W+W]	TS2WW	R072	R073	15.0	20.5
E38	[Hemi+B+W] ⇆ [I+B+W+W]	TS2NW	R074	R075	12.7	21.0

Table S11: List of reactions considered for the microkinetic model to describe the diffusion of the products.

Event ID	Chemical Event	TS Label	Reaction ID		Barriers (kcal mol^{-1})	
			Direct	Reverse	Direct	Reverse
E39	[I+W] ⇆ I + W	---	R076	R077	2.0	2.8
E40	[I+W+W] ⇆ I + [W+W]	---	R078	R079	2.0	2.4
E41	[I+W+W] ⇆ [I+W] + W	---	R080	R081	2.0	2.7
E42	[I+B+W] ⇆ I + [B+W]	---	R082	R083	2.0	6.0
E43	[I+B+W] ⇆ [I+B] + W	---	R084	R085	2.0	2.0
E44	[I+B+W] ⇆ [I+W] + B	---	R086	R087	2.0	4.7
E45	[I+B+W+W] ⇆ I + [B+W+W]	---	R088	R089	2.0	5.1
E46	[I+B+W+W] ⇆ [I+B] + [W+W]	---	R090	R091	3.6	2.0
E47	[I+B+W+W] ⇆ [I+W] + [B+W]	---	R092	R093	2.0	4.7
E48	[I+B+W+W] ⇆ [I+W+W] + B	---	R094	R095	2.0	3.6
E49	[I+B+W+W] ⇆ [I+B+W] + W	---	R096	R097	2.4	2.0
E50	[I+W+W+W] ⇆ I + [W+W+W]	---	R098	R099	2.0	2.6
E51	[I+W+W+W] ⇆ [I+W] + [W+W]	---	R100	R101	2.0	2.9
E52	[I+W+W+W] ⇆ [I+W+W] + W	---	R102	R103	2.0	3.4

Table S12: List of kinetic constants at 298.15K in s^{-1} for the unimolecular steps and $M^{-1}s^{-1}$ for the bimolecular steps for the B3LYP-D3/cc-pVTZ calculated energies.

Event ID	Direct Constant	Reverse Constant
E01	1.1520016141E+08	2.1243982518E+11
E02	4.6522262685E+09	2.1243982518E+11
E03	2.1243982518E+11	1.0627425113E+11
E04	2.3472075016E+08	2.1243982518E+11
E05	2.8944452758E+10	2.1243982518E+11
E06	1.2474135377E+06	2.1243982518E+11
E07	1.2524507574E+09	2.1243982518E+11
E08	1.6652981977E+09	2.1243982518E+11
E09	2.5518729986E+09	2.1243982518E+11
E10	1.1386583655E+08	2.1243982518E+11
E11	9.4996816172E+08	2.1243982518E+11
E12	2.1243982518E+11	2.9848780886E+10
E13	4.5983410911E+09	2.1243982518E+11
E14	1.0360877187E+10	2.1243982518E+11
E15	1.0305446152E+11	2.1243982518E+11
E16	2.1243982518E+11	2.6258534710E+10
E17	2.9128971462E+10	2.1243982518E+11
E18	1.8163911446E+09	2.1243982518E+11

E19	2.1243982518E+11	2.0822723299E+10
E20	3.6580372751E+09	2.1243982518E+11
E21	8.1375555674E+10	2.1243982518E+11
E22	1.4846115923E-11	4.1907492732E-08
E23	1.3627835178E+02	2.9212843905E+03
E24	4.7620982072E-03	3.2277543932E+00
E25	9.0926246695E+02	1.7512558087E+05
E26	3.1831794500E+02	1.1404141794E+05
E27	7.4531321673E+10	2.1243982518E+11
E28	2.1243982518E+11	1.0627613561E+10
E29	2.1243982518E+11	1.4311551605E+10
E30	7.8918184665E+10	2.1243982518E+11
E31	2.1243982518E+11	1.0036851306E+10
E32	1.4207544383E+09	2.1243982518E+11
E33	2.9722595183E+10	2.1243982518E+11
E34	3.5961305166E-16	4.4655823739E-23
E35	1.8128732564E-05	2.2320322775E-11
E36	1.2863754590E-06	8.2046628228E-13
E37	6.4999399338E+01	5.6414819627E-03
E38	3.0671312390E+03	2.5170839485E-03
E39	2.1243982518E+11	5.2266979709E+10
E40	2.1243982518E+11	1.1028202726E+11
E41	2.1243982518E+11	6.1072075449E+10
E42	2.1243982518E+11	2.5466485201E+08
E43	2.1243982518E+11	2.0798187287E+11
E44	2.1243982518E+11	2.0691187767E+09
E45	2.1243982518E+11	1.0983092618E+09
E46	1.4131533551E+10	2.1243982518E+11
E47	2.1243982518E+11	2.1655291772E+09
E48	2.1243982518E+11	1.5057926667E+10
E49	1.0154287036E+11	2.1243982518E+11
E50	2.1243982518E+11	8.1548110537E+10
E51	2.1243982518E+11	4.5447672655E+10
E52	2.1243982518E+11	2.1539435241E+10

5.2 Hypotheses Tested

Figure 2 of the manuscript contains the total concentration of imine which was calculated as the sum of the concentrations of compounds C21 to C27. The direct simulation of the microkinetic model with the constants of Table S12 (purple line) yielded an unexpected result: the reaction can't proceed with those conditions. Two main hypotheses were introduced in order to introduce changes in the Mathematical Model and see if it improved or not the agreement with experiment.

The first hypothesis (see H1 in Chart S2) considered that only the TSs' energies were overestimated by DFT. Testing the mentioned hypothesis is straight forward, it just involves reducing the barriers for both direct and reverse reactions for the Hemiaminal formations and Hemiaminal Dehydrations. This in the mathematical model translates as only recalculating the barriers for those 20 reactions. Although simple, it gives a lot of information, since it has the same effect over the Mathematical Model as finding a lower-energy TS for the same reaction or even the impact on the kinetics of

Tunneling effects. Consistent with the hypothesis, we applied a correction to the TSs of the indicated reactions systematically and simultaneously. When at any of those reactions, the energy of any TS reached either the energy of its reactant or product we stopped decreasing the energy of that TS while we continued with the rest of TSs. The correction values used went from 0.00 to 8.00 kcal mol^{-1} in steps of 0.25 kcal mol^{-1} and therefore simulating a total of 33 free energy profiles. As can be clearly seen in the main text Figure 2 (top) this hypothesis was refuted.

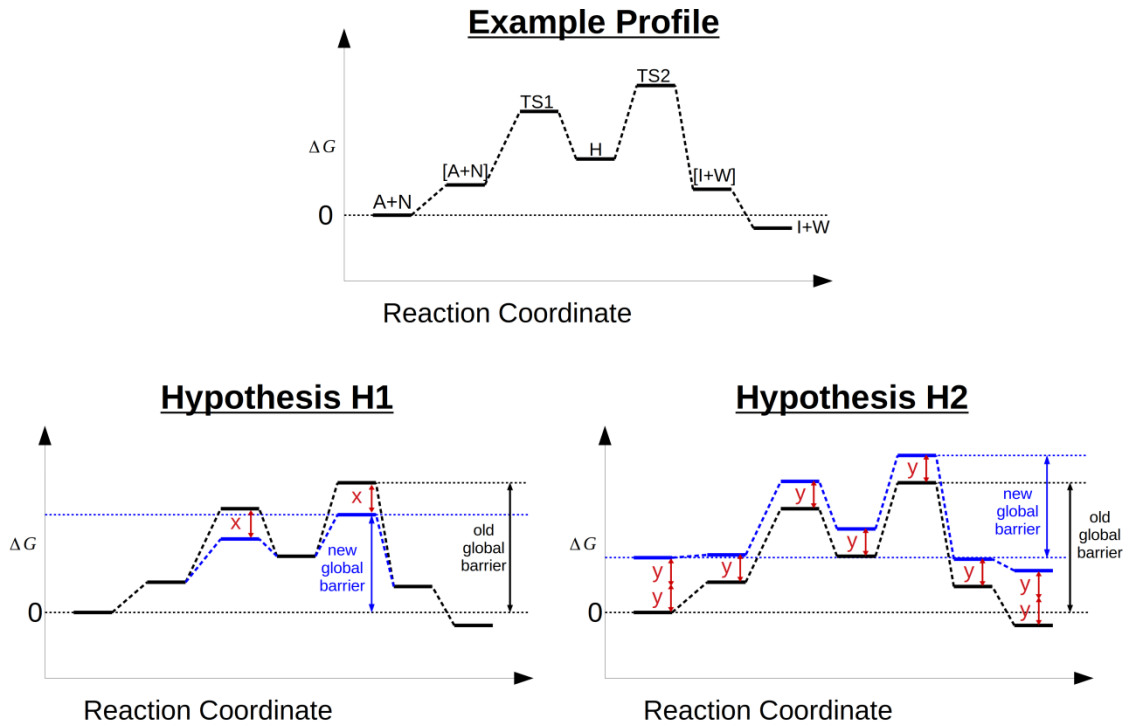

Chart S2: Visual explanation of Hypotheses H1 and H2 and their effects on the free energy profile

The second hypothesis (see H2 in Chart S2), the systematic error, consists on assuming that every DFT calculation has an error that, at least for this system, can be considered constant. This hypothesis has no effect for unimolecular reactions but the system of study corresponds to a system with a big amount of bimolecular aggregations. The overall effect on the whole free energy profile of this hypothesis is that the compounds that require more reactants to be obtained will be more affected. But for the Hemiaminal formations and dehydrations, since we have modeled them as unimolecular reactions, the relative barrier will remain unchanged, but the stability of its reactants and products will change. This raises the effects of the concentration of each species. For the mathematical model, we are only changing the values of the kinetic constants. The correction values used went from 0 to 4 kcal mol^{-1} and the steps considered were of 0.1 kcal mol^{-1}. Figure 2 (bottom) contains these results although the models with correction values in the interval (0,2.3] were not represented for clarity reasons. The best fitting model corresponds to the correction of 3.2 kcal mol^{-1}.

5.3 Inspecting the microkinetic simulation results.

Assuming that the systematic correction is the way to proceed we do analyze in detail the results of the microkinetic simulation to get some chemical insight. Figure S1 has the time evolution of the concentration of different concentrations described by the equations 1-5:

1) $[R+W]_{total} = [C04] + [C05] + [C08] + 2\,[C10] + 2\,[C11] + [C12] + [C14] + 2\,[C15]$
2) $[P+W]_{total} = [C22] + 2\,[C24] + [C25] + 2\,[C26] + 3\,[C27]$
3) $[Free\,W]_{total} = [C02] + 2\,[C06] + 3\,[C13]$
4) $[Aldehyde]_{total} = [C00] + [C03] + [C04] + [C08] + [C09] + [C10] + [C14] + [C15]$
5) $[Imine]_{total} = [C21] + [C22] + [C23] + [C24] + [C25] + [C26] + [C27]$

The concentration of the Hemiaminal species remains around 10^{-6} and 10^{-7} M and was not included in the plot for that reason. Looking at the dotted lines we can see how the water moves. Initially, due to the high concentration of reactants the water aggregates with them. In the first ca 1000s all the water produced with the imine formed is directly stolen by the reactants, as would be the case for any subproduct-catalyzed reaction. At that point the concentration of reactants has decreased significantly and the concentration of imine risen. As consequence of the further consumption of reactants the water is freed from them, and has two main sinks, either the black dotted lines (alone or forming water dimers or trimers) or the blue dotted line (forming adducts with the Imine).

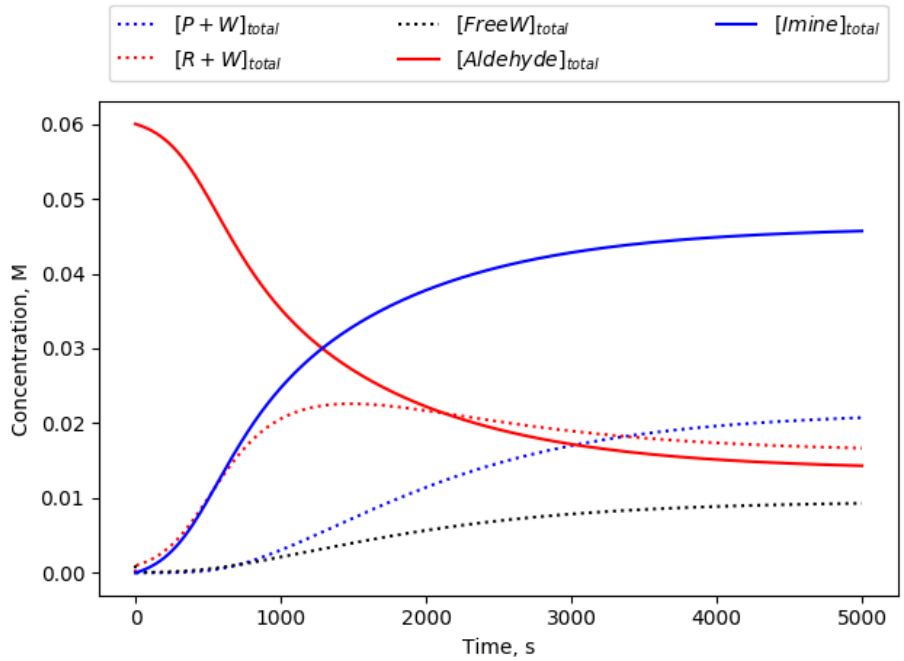

Figure S1: Time Evolution of Water adducts, Aldehyde and Imine for the model corrected with a systematic correction of 3.2 kcal mol^{-1}

This provides some insight in how the water is moving in the system, clearly preferring to be with the reactants and products and pushed aside as the reactants disappear. However, this does not provide insight into which one is the preferential pathway and the rate limiting step. To do so we inspected the values of the rates of all the hemiaminal formation and dehydration step. However a simpler and more illustrative procedure is what we ended up with. This consists on simulating the same model, but "disabling" certain pathways. "Disabling" a pathway can be done in several manners. In order to keep the microkinetic model constant, to disable a certain reaction all what is needed is to set up its kinetic constant to 0. If it is a reversible reaction setting up both kinetic constants to 0 is all it takes. Figure S2 shows the results of removing either the reversible reaction E37 (TS2WW) or E38 (TS2NW).

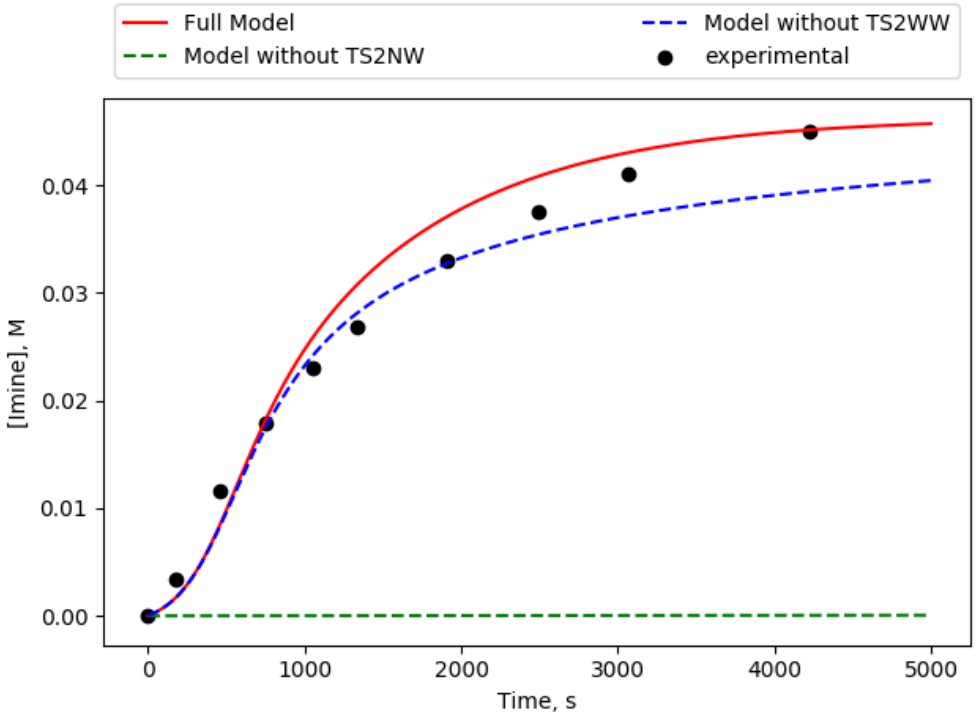

Figure S2: Time evolution of the Total Imine concentration for the Full model and its versions.

When we move from the full model to the model without E38 (green) we see that the reaction does not happen. For the model without E37 (blue) we see an initial overlap that starts to diverge after ca 500s. Comparing Figure S1 with Figure S2 gives us the key to understand it. Initially the amount of water is so low that forming a dimer that can catalyze the reaction is very unlikely, on the other hand the amine is in high concentration, so initially the reaction proceeds through the amine-water catalyzed pathways. As water build up and amine is abundant the water forms adducts with the reactants. We can see in Figure S1 a crossing point between the red dotted line and the solid blue line more or less at the time where the two curves of Figure S2 start to diverge. Approximately at that point, the water concentration is enough for the Water-dimer-catalyzed pathway to start working. Around time 1000s is when we start seeing the water moving out of the reactants due their consumption which accentuates the divergence seen in Figure S2.

5.4 Effect of the Initial Water Content

Until now the initial water concentration was considered to be 1mM based on Sigma Aldrich datasheets.[23] The effects of this estimate on the imine concentration evolution are inspected in this section. To do so the previously analyzed model (Section 5.3) was simulated at different initial water concentrations. To explore different orders of magnitude the concentration was sampled from 10^{-6} to 10^{-2} in exponential steps of 0.5. Figure S3 summarizes the results from these simulations.

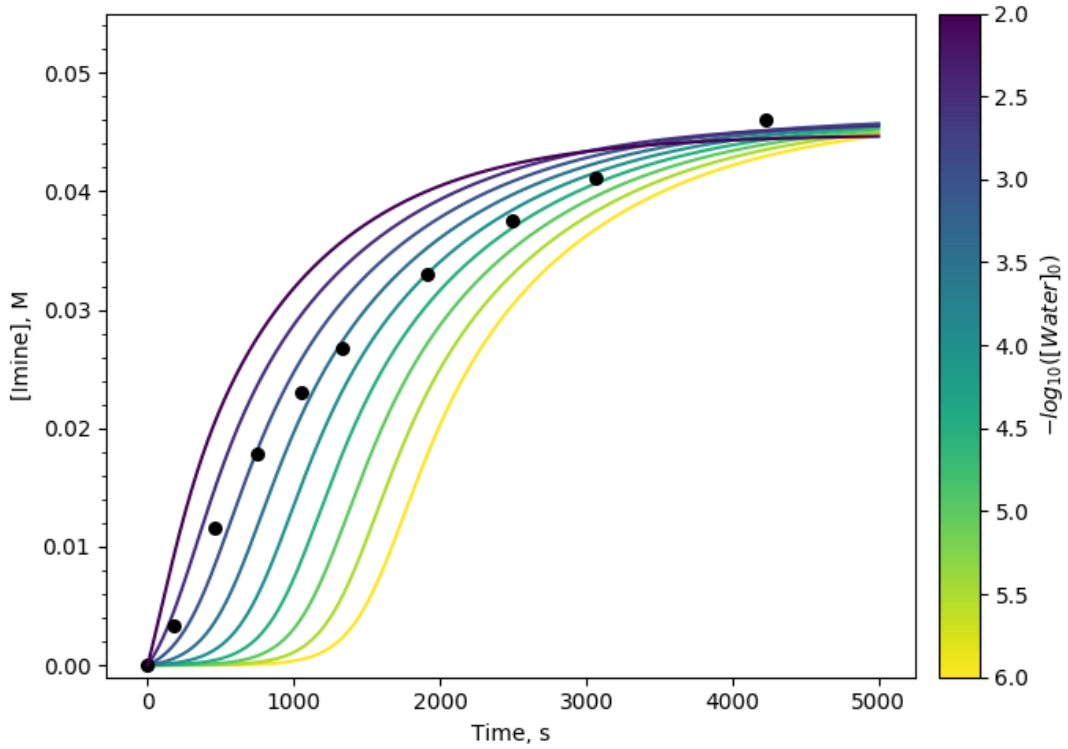

Figure S3: Simulations For the Model Corrected with 3.2 kcal mol^{-1} at different initial water concentrations.

Reducing the initial water concentration does not change the shape of the profile significantly but shifts it to the right, introducing an initial delay period in which the water necessary to start the catalysis via the TS2NW builds up. As increasing the correction shifts the curve towards the left in a similar fashion we can conclude that if the experimental initial water concentration was different we would have found a different value for the correction that would fit similarly since the shape of the predicted concentration evolution does not change significantly.

6. Revisiting the Benchmark

From the DFT methods attempted in Table S3 we selected two that displayed significantly different behaviors compared to B3LYP-D3. PBEPBE-D3 had a general stabilization of all species and M06-2X-D3 had a significant stabilization of the intermediate which were the reasons for their selection.

Per each of the newly selected functionals we re-optimized and re-calculated the frequencies for all the structures included in Table S5 and Table S6. The cc-pVTZ basis set was employed for these new calculations. Table S13 and Table S14 are the equivalents of Table S6 and Table S5 respectively. As the systematic error hypothesis approach gave good agreement with the experimental values, we also applied it to M06-2X-D3 and PBEPBE-D3.

Table S13: Free Energies of structures corresponding to transition states.

		PBEPBE-D3	M06-2X-D3
Model Label	**Structure Name**	**$G_{1atm, 298.15K}$ (hartree)**	**$G_{1atm, 298.15K}$ (hartree)**
TS1	TS1	-558.628144	-559.084080
TS2	TS2	-558.607151	-559.054667
TS1W	TS1W	-635.027706	-635.533698
TS2W	TS2W	-635.002556	-635.506067
TS1N	TS1N	-772.115648	-772.749151
TS2N	TS2N	-772.102271	-772.726823
TS1WW	TS1WW	-711.410713	-711.965147
TS2WW	TS2WW	-711.399978	-711.946752
TS1NW	TS1NW	-848.503461	-849.186971
TS2NW	TS2NW	-848.487403	-849.167306

Table S14: Free Energies of the structures corresponding to minima

			PBEPBE-D3	M06-2X-D3
Compound ID	**Model Label**	**Structure Name**	**$G_{1atm, 298.15K}$ (hartree)**	**$G_{1atm, 298.15K}$ (hartree)**
C00	A	Benzaldehyde	-345.204216	-345.482549
C01	B	NButylamine	-213.473811	-213.655803
C02	W	Water	-76.377566	-76.429318
C03	[A+B]	A_N	-558.669245	-559.128296
C04	[A+W]	A_W	-421.575321	-421.904397
C05	[B+W]	N_W	-289.850805	-290.081831
C06	[W+W]	W_W	-152.751291	-152.852759
C07	[B+B]	N_N	-426.939508	-427.299347
C08	[A+B+W]	A_N_W	-635.039977	-635.550808
C09	[A+B+B]	A_N_N	-772.135506	-772.772138
C10	[A+W+W]	A_W_W	-497.948640	-498.325321
C11	[B+W+W]	N_W_W	-366.227140	-366.504631
C12	[B+B+W]	N_N_W	-503.317954	-503.725971
C13	[W+W+W]	W_W_W	-229.125807	-229.275851
C14	[A+B+B+W]	A_N_N_W	-848.512752	-849.198224
C15	[A+B+W+W]	A_N_W_W	-711.420442	-711.975968
C16	Hemi	Hemiaminal	-558.664707	-559.131156

C17	[Hemi+W]	Int_W	-635.042635	-635.556037
C18	[Hemi+B]	Int_N	-772.133501	-772.775743
C19	[Hemi+B+W]	Int_N_W	-848.509617	-849.202810
C20	[Hemi+W+W]	Int_W_W	-711.420803	-711.982975
C21	I	Imine	-482.303116	-482.713941
C22	[I+W]	I_W	-558.677931	-559.137508
C23	[I+B]	I_N	-695.768724	-696.358570
C24	[I+W+W]	I_W_W	-635.052830	-635.561528
C25	[I+B+W]	I_N_W	-772.146455	-772.785180
C26	[I+B+W+W]	I_N_W_W	-848.522175	-849.208152
C27	[I+W+W+W]	I_W_W_W	-711.427680	-711.983994

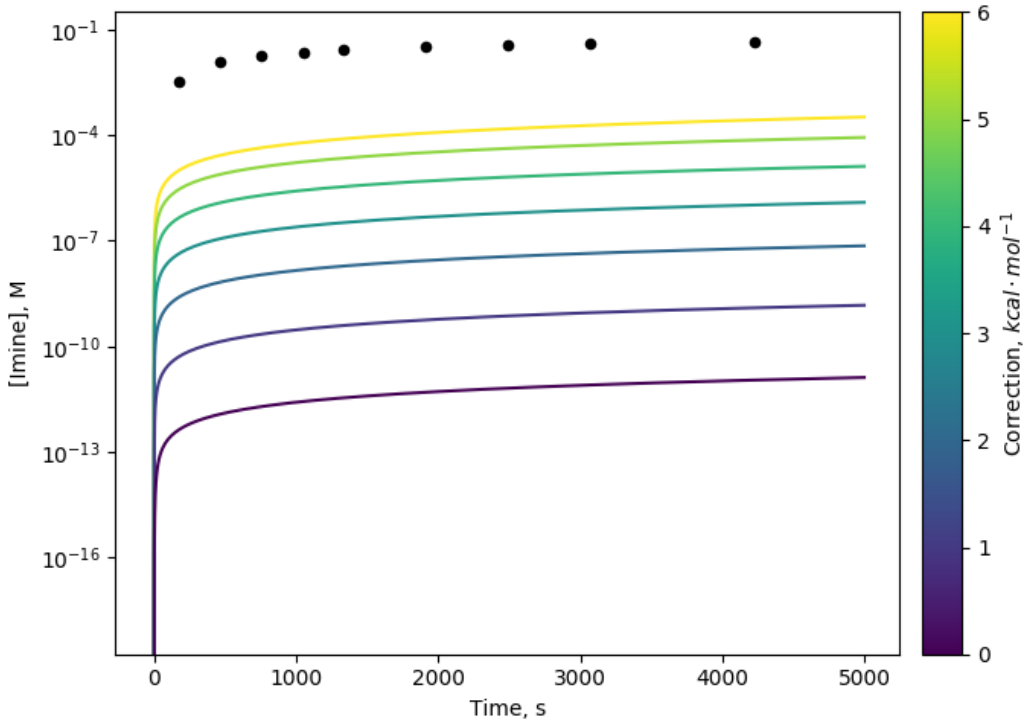

Figure S4: Imine concentration for all the models obtained from systematic corrections to the M06-2X Free energy profile. Y axis is in logarithmic scale for visualization reasons.

As can be seen for M06-2X-D3 (Figure S4) was systematically corrected from 0.0 to 6.0 kcal mol^{-1} at steps of 1.0 kcal mol^{-1}. Even with the correction, the imine is not formed. The main reason for this is likely the reason why we selected M06-2X-D3. The stability of the intermediate coupled with the overall increase of the energy of the transition state structures ends up creating a wall after the hemiaminal is formed in the free energy surface which cannot be surpassed at 298.15K even with the proposed catalysts.

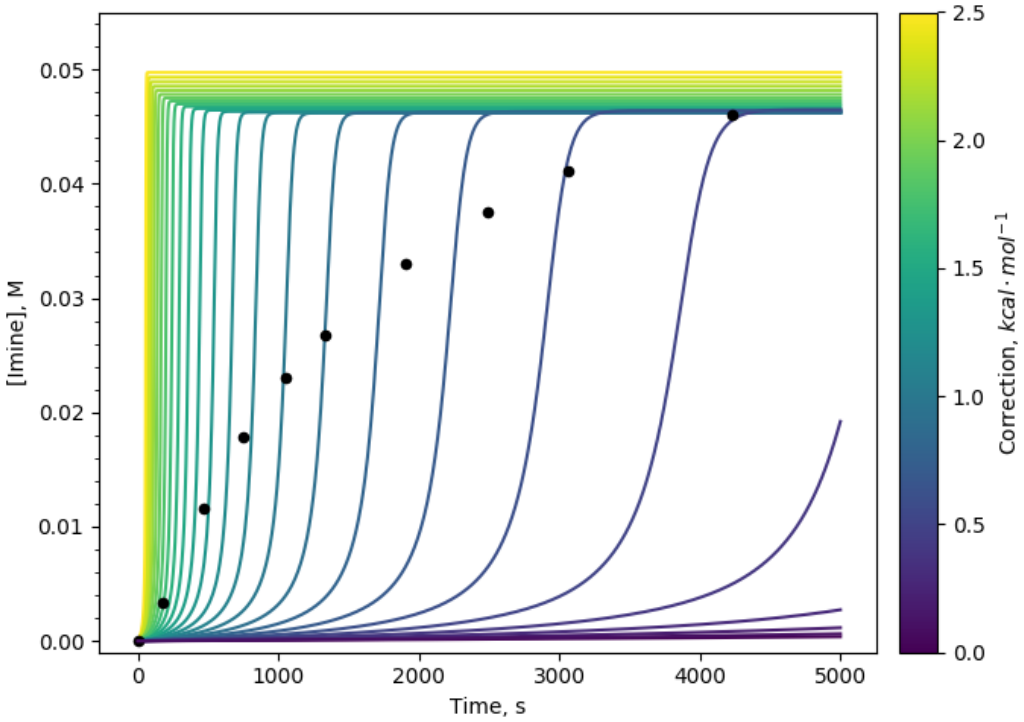

Figure S5: Imine concentration for all the models obtained from systematic corrections to the PBEPBE Free energy profile.

PBEPBE-D3 (Figure S5) was systematically corrected from 0.0 to 2.5 kcal mol^{-1} at steps of 0.1 kcal mol^{-1} and displayed a completely different behavior. Without the correction the barriers are too small and upon the addition of the systematic correction we see that the reaction has an induction period and then proceeds in a very short time window. This indicates that the barriers predicted for the catalyzed pathways relative to the hemiaminal-catalyst adducts are too small. So when the stabilization of the adducts due to the systematic correction occurs and concentration is not limiting the hemiaminal dehydration, it goes too fast.

7. Quasi-harmonic corrected models

In order to refine the results quasi-harmonic corrections to the free energies for frequencies below 100 cm^{-1} using the GoodVibes software as indicated in the section 1. Generally the magnitude of these corrections is not too large and it could be expected that a small improvement in the prediction of the experimental results could be obtained, either in the description of the overall equilibrium or in the shape of the concentration profiles. Table S15 has the values of the corrections obtained for each structure relevant to the Microkinetic Model.

Table S15: Quasi-harmonic corrections for each functional revisited.

	$G_{qh} - G$ (kcal mol^{-1})				$G_{qh} - G$ (kcal mol^{-1})		
Model Label	**B3LYP**	**PBEPBE**	**M06-2X**	**Model Label**	**B3LYP**	**PBEPBE**	**M06-2X**
A	0.1	0.1	0.0	**TS1**	1.6	1.6	1.6
B	0.1	0.1	0.1	**TS2**	1.3	1.4	1.3
W	0.0	0.0	0.0	**TS1W**	1.8	1.6	1.5
[A+B]	1.9	2.3	1.4	**TS2W**	2.1	1.9	1.9
[A+W]	1.0	0.9	1.0	**TS1N**	2.7	3.0	2.8
[B+W]	0.7	0.7	0.9	**TS2N**	3.1	3.1	2.8
[W+W]	0.1	0.2	0.0	**TS1WW**	2.0	2.3	1.9
[B+B]	2.0	2.0	1.4	**TS2WW**	2.2	2.4	2.0
[A+B+W]	2.7	2.6	2.9	**TS1NW**	3.0	3.9	3.2
[A+B+B]	4.7	4.6	3.7	**TS2NW**	7.1	3.5	3.6
[A+W+W]	1.9	2.0	1.7				
[B+W+W]	1.3	1.4	1.0				
[B+B+W]	3.2	3.3	2.6				
[W+W+W]	0.0	0.0	0.7				
[A+B+B+W]	4.6	4.6	3.5				
[A+B+W+W]	3.8	3.6	3.3				
Hemi	1.3	1.4	1.5				
[Hemi+W]	1.9	2.0	1.7				
[Hemi+B]	3.0	3.3	2.0				
[Hemi+B+W]	4.4	4.1	3.8				
[Hemi+W+W]	2.3	2.4	2.3				
I	1.2	1.2	0.9				
[I+W]	1.6	1.7	1.6				
[I+B]	3.2	3.1	2.4				
[I+W+W]	2.5	2.6	2.6				
[I+B+W]	3.7	4.0	3.7				
[I+W+W+W]	2.8	3.3	2.5				
[I+B+W+W]	4.6	4.1	3.6				

As seen in Figure S6, Figure S7 and Figure S8 the model without correction (purple line) remained mostly the same for the results with the different functionals. Therefore the same Systematic Correction applied previously was applied to these new sets of thermodynamic values.

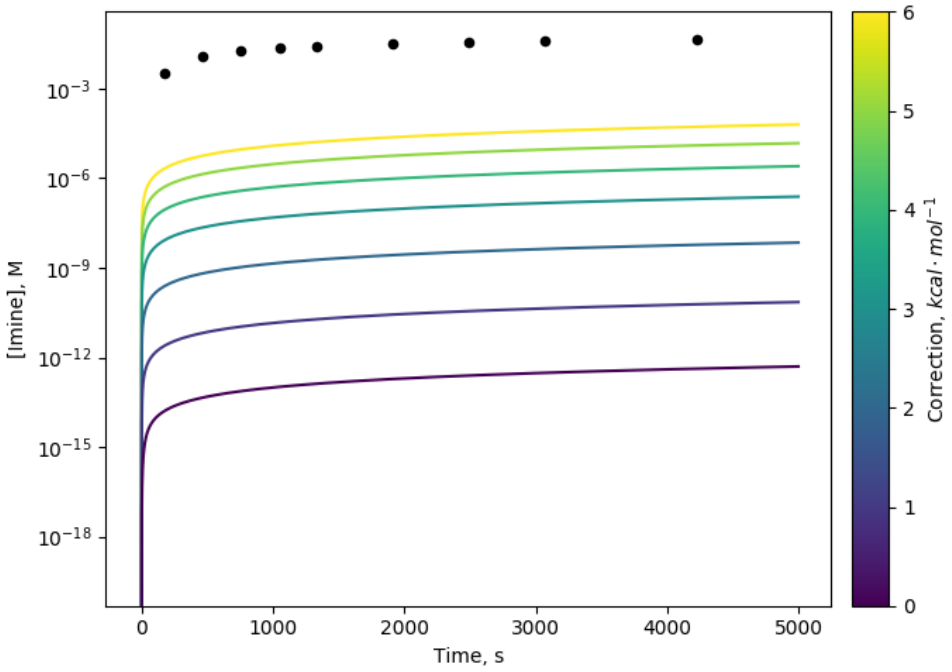

Figure S6: Imine concentration for all the models obtained from systematic corrections to the M06-2X Free energy profile with quasi-harmonic corrections. Systematic correction steps of 1.0 kcal mol^{-1}

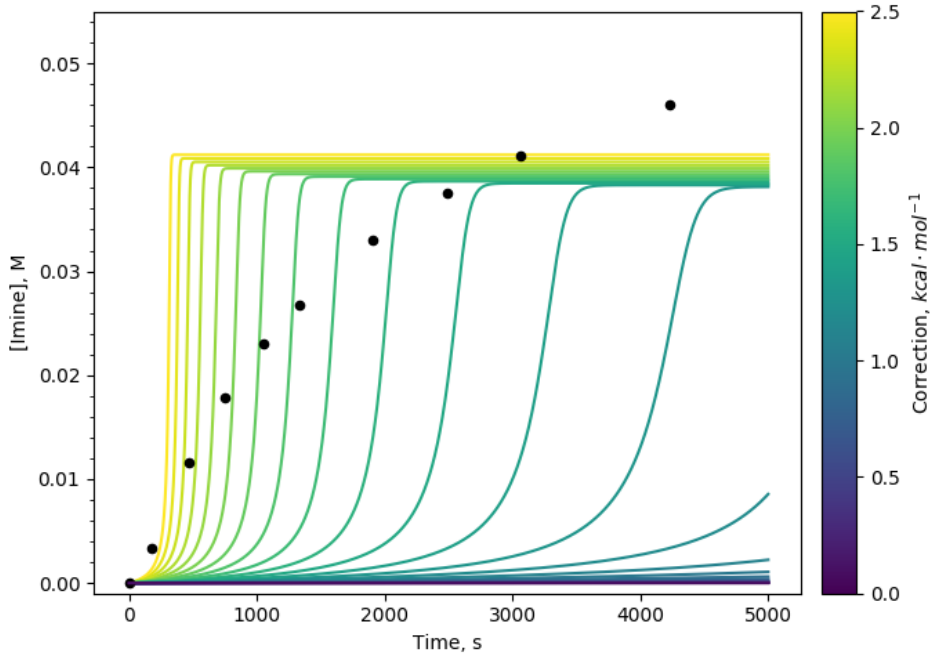

Figure S7: Imine concentration for all the models obtained from systematic corrections to the PBEPBE Free energy profile with quasi-harmonic corrections. Systematic correction steps of 0.1 kcal mol^{-1}

The shape of the curves obtained with M06-2X-D3 (Figure S6) and PBEPBE-D3 (Figure S7) did not improve the prediction of the experimental values. No significant change can be seen with M06-2X-D3 but in the case of PBEPBE-D3 a significant deterioration of the description of the equilibrium can be appreciated. In the case of B3LYP-D3 (Figure S8) not only did not improve, but did exactly the opposite. This is likely due to the large correction over the TS2NW structure of 7.1 kcal mol^{-1} which overall reduces the relative barriers ca 3.0 kcal mol^{-1} with respect to [I+B+W+W] and [Hemi+B+W].

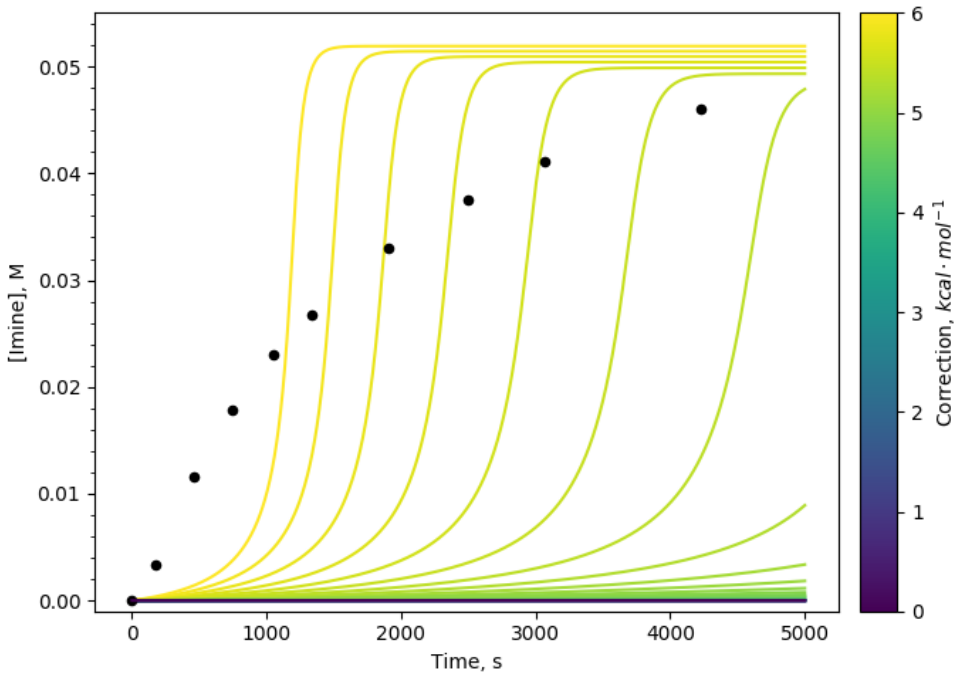

Figure S8: Imine concentration for all the models obtained from systematic corrections to the B3LYP Free energy profile with quasi-harmonic corrections. Systematic correction steps of 0.5 kcal mol^{-1} for the until 4.5 kcal mol^{-1} and of 0.1 kcal mol^{-1} until 6.0 kcal mol^{-1}

8. Python Script example with the values of section 5.1

```
import sys
import numpy as np
import scipy.integrate

OFile = 'Outputs/Scan_000.out'

# alias for ode function
odeint = scipy.integrate.odeint

# Calculations Memory Constraint
MaxMem = 28*1E6

# Parameters
species = 28
dt = 1E-5 # Timestep s
report_t = 1E-1 # s
tfin = 5000 # Final Time
xini = np.zeros(species)
xini[0] = 0.06
xini[1] = 0.06
xini[2] = 0.001
# Model at T=298.15 K
def f(x,t):
        dxdt = np.zeros(28)
```

```
        #Constants
        k00 = 1.1520016141e+08
        k01 = 2.1243982518e+11
        k02 = 4.6522262685e+09
        k03 = 2.1243982518e+11
        k04 = 2.1243982518e+11
        k05 = 1.0627425113e+11
        k06 = 2.3472075016e+08
        k07 = 2.1243982518e+11
        k08 = 2.8944452758e+10
        k09 = 2.1243982518e+11
        k10 = 1.2474135377e+06
        k11 = 2.1243982518e+11
        k12 = 1.2524507574e+09
        k13 = 2.1243982518e+11
        k14 = 1.6652981977e+09
        k15 = 2.1243982518e+11
        k16 = 2.5518729986e+09
        k17 = 2.1243982518e+11
        k18 = 1.1386583655e+08
        k19 = 2.1243982518e+11
        k20 = 9.4996816172e+08
        k21 = 2.1243982518e+11
        k22 = 2.1243982518e+11
        k23 = 2.9848780886e+10
        k24 = 4.5983410911e+09
        k25 = 2.1243982518e+11
        k26 = 1.0360877187e+10
        k27 = 2.1243982518e+11
        k28 = 1.0305446152e+11
        k29 = 2.1243982518e+11
        k30 = 2.1243982518e+11
        k31 = 2.6258534710e+10
        k32 = 2.9128971462e+10
        k33 = 2.1243982518e+11
        k34 = 1.8163911446e+09
        k35 = 2.1243982518e+11
        k36 = 2.1243982518e+11
        k37 = 2.0822723299e+10
        k38 = 3.6580372751e+09
        k39 = 2.1243982518e+11
        k40 = 8.1375555674e+10
        k41 = 2.1243982518e+11
        k42 = 1.4846115923e-11
        k43 = 4.1907492732e-08
        k44 = 1.3627835178e+02
        k45 = 2.9212843905e+03
        k46 = 4.7620982072e-03
        k47 = 3.2277543932e+00
        k48 = 9.0926246695e+02
        k49 = 1.7512558087e+05
        k50 = 3.1831794500e+02
        k51 = 1.1404141794e+05
        k52 = 7.4531321673e+10
        k53 = 2.1243982518e+11
        k54 = 2.1243982518e+11
        k55 = 1.0627613561e+10
        k56 = 2.1243982518e+11
        k57 = 1.4311551605e+10
        k58 = 7.8918184665e+10
        k59 = 2.1243982518e+11
        k60 = 2.1243982518e+11
        k61 = 1.0036851306e+10
        k62 = 1.4207544383e+09
```

```
        k63 = 2.1243982518e+11
        k64 = 2.9722595183e+10
        k65 = 2.1243982518e+11
        k66 = 3.5961305166e-16
        k67 = 4.4655823739e-23
        k68 = 1.8128732564e-05
        k69 = 2.2320322775e-11
        k70 = 1.2863754590e-06
        k71 = 8.2046628228e-13
        k72 = 6.4999399338e+01
        k73 = 5.6414819627e-03
        k74 = 3.0671312390e+03
        k75 = 2.5170839485e-03
        k76 = 2.1243982518e+11
        k77 = 5.2266979709e+10
        k78 = 2.1243982518e+11
        k79 = 1.1028202726e+11
        k80 = 2.1243982518e+11
        k81 = 6.1072075449e+10
        k82 = 2.1243982518e+11
        k83 = 2.5466485201e+08
        k84 = 2.1243982518e+11
        k85 = 2.0798187287e+11
        k86 = 2.1243982518e+11
        k87 = 2.0691187767e+09
        k88 = 2.1243982518e+11
        k89 = 1.0983092618e+09
        k90 = 1.4131533551e+10
        k91 = 2.1243982518e+11
        k92 = 2.1243982518e+11
        k93 = 2.1655291772e+09
        k94 = 2.1243982518e+11
        k95 = 1.5057926667e+10
        k96 = 1.0154287036e+11
        k97 = 2.1243982518e+11
        k98 = 2.1243982518e+11
        k99 = 8.1548110537e+10
       k100 = 2.1243982518e+11
       k101 = 4.5447672655e+10
       k102 = 2.1243982518e+11
       k103 = 2.1539435241e+10
       #Rate laws
       r00 = k00*x[0]*x[1]
       r01 = k01*x[3]
       r02 = k02*x[0]*x[2]
       r03 = k03*x[4]
       r04 = k04*x[1]*x[2]
       r05 = k05*x[5]
       r06 = k06*x[1]*x[1]
       r07 = k07*x[7]
       r08 = k08*x[2]*x[2]
       r09 = k09*x[6]
       r10 = k10*x[0]*x[5]
       r11 = k11*x[8]
       r12 = k12*x[0]*x[7]
       r13 = k13*x[9]
       r14 = k14*x[0]*x[6]
       r15 = k15*x[10]
       r16 = k16*x[1]*x[3]
       r17 = k17*x[9]
       r18 = k18*x[1]*x[4]
       r19 = k19*x[8]
       r20 = k20*x[1]*x[5]
       r21 = k21*x[12]
```

```
        r22 = k22*x[1]*x[6]
        r23 = k23*x[11]
        r24 = k24*x[2]*x[3]
        r25 = k25*x[8]
        r26 = k26*x[2]*x[4]
        r27 = k27*x[10]
        r28 = k28*x[2]*x[5]
        r29 = k29*x[11]
        r30 = k30*x[2]*x[7]
        r31 = k31*x[12]
        r32 = k32*x[2]*x[6]
        r33 = k33*x[13]
        r34 = k34*x[3]*x[5]
        r35 = k35*x[14]
        r36 = k36*x[3]*x[6]
        r37 = k37*x[15]
        r38 = k38*x[4]*x[5]
        r39 = k39*x[15]
        r40 = k40*x[4]*x[7]
        r41 = k41*x[14]
        r42 = k42*x[3]
        r43 = k43*x[16]
        r44 = k44*x[8]
        r45 = k45*x[17]
        r46 = k46*x[9]
        r47 = k47*x[18]
        r48 = k48*x[15]
        r49 = k49*x[20]
        r50 = k50*x[14]
        r51 = k51*x[19]
        r52 = k52*x[17]
        r53 = k53*x[2]*x[16]
        r54 = k54*x[18]
        r55 = k55*x[1]*x[16]
        r56 = k56*x[19]
        r57 = k57*x[5]*x[16]
        r58 = k58*x[19]
        r59 = k59*x[2]*x[18]
        r60 = k60*x[19]
        r61 = k61*x[1]*x[17]
        r62 = k62*x[20]
        r63 = k63*x[6]*x[16]
        r64 = k64*x[20]
        r65 = k65*x[2]*x[17]
        r66 = k66*x[16]
        r67 = k67*x[22]
        r68 = k68*x[17]
        r69 = k69*x[24]
        r70 = k70*x[18]
        r71 = k71*x[25]
        r72 = k72*x[20]
        r73 = k73*x[27]
        r74 = k74*x[19]
        r75 = k75*x[26]
        r76 = k76*x[22]
        r77 = k77*x[2]*x[21]
        r78 = k78*x[24]
        r79 = k79*x[6]*x[21]
        r80 = k80*x[24]
        r81 = k81*x[2]*x[22]
        r82 = k82*x[25]
        r83 = k83*x[5]*x[21]
        r84 = k84*x[25]
        r85 = k85*x[2]*x[23]
```

```
        r86 = k86*x[25]
        r87 = k87*x[1]*x[22]
        r88 = k88*x[26]
        r89 = k89*x[11]*x[21]
        r90 = k90*x[26]
        r91 = k91*x[6]*x[23]
        r92 = k92*x[26]
        r93 = k93*x[5]*x[22]
        r94 = k94*x[26]
        r95 = k95*x[1]*x[24]
        r96 = k96*x[26]
        r97 = k97*x[2]*x[25]
        r98 = k98*x[27]
        r99 = k99*x[13]*x[21]
        r100 = k100*x[27]
        r101 = k101*x[6]*x[22]
        r102 = k102*x[27]
        r103 = k103*x[2]*x[24]
        #MassBalances
        dxdt[0] = -r00+r01-r02+r03-r10+r11-r12+r13-r14+r15
        dxdt[1] = -r00+r01-r04+r05-2.0*r06+2.0*r07-r16+r17-r18+r19-r20+r21-
r22+r23+r54-r55+r60-r61+r86-r87+r94-r95
        dxdt[2] = -r02+r03-r04+r05-2.0*r08+2.0*r09-r24+r25-r26+r27-r28+r29-
r30+r31-r32+r33+r52-r53+r58-r59+r64-r65+r76-r77+r80-r81+r84-r85+r96-r97+r102-
r103
        dxdt[3] = +r00-r01-r16+r17-r24+r25-r34+r35-r36+r37-r42+r43
        dxdt[4] = +r02-r03-r18+r19-r26+r27-r38+r39-r40+r41
        dxdt[5] = +r04-r05-r10+r11-r20+r21-r28+r29-r34+r35-r38+r39+r56-
r57+r82-r83+r92-r93
        dxdt[6] = +r08-r09-r14+r15-r22+r23-r32+r33-r36+r37+r62-r63+r78-
r79+r90-r91+r100-r101
        dxdt[7] = +r06-r07-r12+r13-r30+r31-r40+r41
        dxdt[8] = +r10-r11+r18-r19+r24-r25-r44+r45
        dxdt[9] = +r12-r13+r16-r17-r46+r47
        dxdt[10] = +r14-r15+r26-r27
        dxdt[11] = +r22-r23+r28-r29+r88-r89
        dxdt[12] = +r20-r21+r30-r31
        dxdt[13] = +r32-r33+r98-r99
        dxdt[14] = +r34-r35+r40-r41-r50+r51
        dxdt[15] = +r36-r37+r38-r39-r48+r49
        dxdt[16] = +r42-r43+r52-r53+r54-r55+r56-r57+r62-r63-r66+r67
        dxdt[17] = +r44-r45-r52+r53+r60-r61+r64-r65-r68+r69
        dxdt[18] = +r46-r47-r54+r55+r58-r59-r70+r71
        dxdt[19] = +r50-r51-r56+r57-r58+r59-r60+r61-r74+r75
        dxdt[20] = +r48-r49-r62+r63-r64+r65-r72+r73
        dxdt[21] = +r76-r77+r78-r79+r82-r83+r88-r89+r98-r99
        dxdt[22] = +r66-r67-r76+r77+r80-r81+r86-r87+r92-r93+r100-r101
        dxdt[23] = +r84-r85+r90-r91
        dxdt[24] = +r68-r69-r78+r79-r80+r81+r94-r95+r102-r103
        dxdt[25] = +r70-r71-r82+r83-r84+r85-r86+r87+r96-r97
        dxdt[26] = +r74-r75-r88+r89-r90+r91-r92+r93-r94+r95-r96+r97
        dxdt[27] = +r72-r73-r98+r99-r100+r101-r102+r103
        return dxdt


def Jacobian(x,t):
        Jac = np.zeros(shape=(28,28))
        #Constants
        k00 = 1.1520016141e+08
        k01 = 2.1243982518e+11
        k02 = 4.6522262685e+09
        k03 = 2.1243982518e+11
        k04 = 2.1243982518e+11
        k05 = 1.0627425113e+11
```

```
        k06 = 2.3472075016e+08
        k07 = 2.1243982518e+11
        k08 = 2.8944452758e+10
        k09 = 2.1243982518e+11
        k10 = 1.2474135377e+06
        k11 = 2.1243982518e+11
        k12 = 1.2524507574e+09
        k13 = 2.1243982518e+11
        k14 = 1.6652981977e+09
        k15 = 2.1243982518e+11
        k16 = 2.5518729986e+09
        k17 = 2.1243982518e+11
        k18 = 1.1386583655e+08
        k19 = 2.1243982518e+11
        k20 = 9.4996816172e+08
        k21 = 2.1243982518e+11
        k22 = 2.1243982518e+11
        k23 = 2.9848780886e+10
        k24 = 4.5983410911e+09
        k25 = 2.1243982518e+11
        k26 = 1.0360877187e+10
        k27 = 2.1243982518e+11
        k28 = 1.0305446152e+11
        k29 = 2.1243982518e+11
        k30 = 2.1243982518e+11
        k31 = 2.6258534710e+10
        k32 = 2.9128971462e+10
        k33 = 2.1243982518e+11
        k34 = 1.8163911446e+09
        k35 = 2.1243982518e+11
        k36 = 2.1243982518e+11
        k37 = 2.0822723299e+10
        k38 = 3.6580372751e+09
        k39 = 2.1243982518e+11
        k40 = 8.1375555674e+10
        k41 = 2.1243982518e+11
        k42 = 1.4846115923e-11
        k43 = 4.1907492732e-08
        k44 = 1.3627835178e+02
        k45 = 2.9212843905e+03
        k46 = 4.7620982072e-03
        k47 = 3.2277543932e+00
        k48 = 9.0926246695e+02
        k49 = 1.7512558087e+05
        k50 = 3.1831794500e+02
        k51 = 1.1404141794e+05
        k52 = 7.4531321673e+10
        k53 = 2.1243982518e+11
        k54 = 2.1243982518e+11
        k55 = 1.0627613561e+10
        k56 = 2.1243982518e+11
        k57 = 1.4311551605e+10
        k58 = 7.8918184665e+10
        k59 = 2.1243982518e+11
        k60 = 2.1243982518e+11
        k61 = 1.0036851306e+10
        k62 = 1.4207544383e+09
        k63 = 2.1243982518e+11
        k64 = 2.9722595183e+10
        k65 = 2.1243982518e+11
        k66 = 3.5961305166e-16
        k67 = 4.4655823739e-23
        k68 = 1.8128732564e-05
        k69 = 2.2320322775e-11
```

```
        k70 = 1.2863754590e-06
        k71 = 8.2046628228e-13
        k72 = 6.4999399338e+01
        k73 = 5.6414819627e-03
        k74 = 3.0671312390e+03
        k75 = 2.5170839485e-03
        k76 = 2.1243982518e+11
        k77 = 5.2266979709e+10
        k78 = 2.1243982518e+11
        k79 = 1.1028202726e+11
        k80 = 2.1243982518e+11
        k81 = 6.1072075449e+10
        k82 = 2.1243982518e+11
        k83 = 2.5466485201e+08
        k84 = 2.1243982518e+11
        k85 = 2.0798187287e+11
        k86 = 2.1243982518e+11
        k87 = 2.0691187767e+09
        k88 = 2.1243982518e+11
        k89 = 1.0983092618e+09
        k90 = 1.4131533551e+10
        k91 = 2.1243982518e+11
        k92 = 2.1243982518e+11
        k93 = 2.1655291772e+09
        k94 = 2.1243982518e+11
        k95 = 1.5057926667e+10
        k96 = 1.0154287036e+11
        k97 = 2.1243982518e+11
        k98 = 2.1243982518e+11
        k99 = 8.1548110537e+10
        k100 = 2.1243982518e+11
        k101 = 4.5447672655e+10
        k102 = 2.1243982518e+11
        k103 = 2.1539435241e+10
        # Partial Derivatives
        Jac[0,0] = -k00*x[1]-k02*x[2]-k10*x[5]-k12*x[7]-k14*x[6]
        Jac[0,1] = -k00*x[0]
        Jac[0,2] = -k02*x[0]
        Jac[0,3] = +k01
        Jac[0,4] = +k03
        Jac[0,5] = -k10*x[0]
        Jac[0,6] = -k14*x[0]
        Jac[0,7] = -k12*x[0]
        Jac[0,8] = +k11
        Jac[0,9] = +k13
        Jac[0,10] = +k15
        Jac[1,0] = -k00*x[1]
        Jac[1,1] = -k00*x[0]-k04*x[2]-2.0*k06*2.0*x[1]-k16*x[3]-k18*x[4]-
k20*x[5]-k22*x[6]-k55*x[16]-k61*x[17]-k87*x[22]-k95*x[24]
        Jac[1,2] = -k04*x[1]
        Jac[1,3] = +k01-k16*x[1]
        Jac[1,4] = -k18*x[1]
        Jac[1,5] = +k05-k20*x[1]
        Jac[1,6] = -k22*x[1]
        Jac[1,7] = +2.0*k07
        Jac[1,8] = +k19
        Jac[1,9] = +k17
        Jac[1,11] = +k23
        Jac[1,12] = +k21
        Jac[1,16] = -k55*x[1]
        Jac[1,17] = -k61*x[1]
        Jac[1,18] = +k54
        Jac[1,19] = +k60
        Jac[1,22] = -k87*x[1]
```

```
403         Jac[1,24] = -k95*x[1]
404         Jac[1,25] = +k86
405         Jac[1,26] = +k94
406         Jac[2,0] = -k02*x[2]
407         Jac[2,1] = -k04*x[2]
408         Jac[2,2] = -k02*x[0]-k04*x[1]-2.0*k08*2.0*x[2]-k24*x[3]-k26*x[4]-
k28*x[5]-k30*x[7]-k32*x[6]-k53*x[16]-k59*x[18]-k65*x[17]-k77*x[21]-k81*x[22]-
k85*x[23]-k97*x[25]-k103*x[24]
409         Jac[2,3] = -k24*x[2]
410         Jac[2,4] = +k03-k26*x[2]
411         Jac[2,5] = +k05-k28*x[2]
412         Jac[2,6] = +2.0*k09-k32*x[2]
413         Jac[2,7] = -k30*x[2]
414         Jac[2,8] = +k25
415         Jac[2,10] = +k27
416         Jac[2,11] = +k29
417         Jac[2,12] = +k31
418         Jac[2,13] = +k33
419         Jac[2,16] = -k53*x[2]
420         Jac[2,17] = +k52-k65*x[2]
421         Jac[2,18] = -k59*x[2]
422         Jac[2,19] = +k58
423         Jac[2,20] = +k64
424         Jac[2,21] = -k77*x[2]
425         Jac[2,22] = +k76-k81*x[2]
426         Jac[2,23] = -k85*x[2]
427         Jac[2,24] = +k80-k103*x[2]
428         Jac[2,25] = +k84-k97*x[2]
429         Jac[2,26] = +k96
430         Jac[2,27] = +k102
431         Jac[3,0] = +k00*x[1]
432         Jac[3,1] = +k00*x[0]-k16*x[3]
433         Jac[3,2] = -k24*x[3]
434         Jac[3,3] = -k01-k16*x[1]-k24*x[2]-k34*x[5]-k36*x[6]-k42
435         Jac[3,5] = -k34*x[3]
436         Jac[3,6] = -k36*x[3]
437         Jac[3,8] = +k25
438         Jac[3,9] = +k17
439         Jac[3,14] = +k35
440         Jac[3,15] = +k37
441         Jac[3,16] = +k43
442         Jac[4,0] = +k02*x[2]
443         Jac[4,1] = -k18*x[4]
444         Jac[4,2] = +k02*x[0]-k26*x[4]
445         Jac[4,4] = -k03-k18*x[1]-k26*x[2]-k38*x[5]-k40*x[7]
446         Jac[4,5] = -k38*x[4]
447         Jac[4,7] = -k40*x[4]
448         Jac[4,8] = +k19
449         Jac[4,10] = +k27
450         Jac[4,14] = +k41
451         Jac[4,15] = +k39
452         Jac[5,0] = -k10*x[5]
453         Jac[5,1] = +k04*x[2]-k20*x[5]
454         Jac[5,2] = +k04*x[1]-k28*x[5]
455         Jac[5,3] = -k34*x[5]
456         Jac[5,4] = -k38*x[5]
457         Jac[5,5] = -k05-k10*x[0]-k20*x[1]-k28*x[2]-k34*x[3]-k38*x[4]-
k57*x[16]-k83*x[21]-k93*x[22]
458         Jac[5,8] = +k11
459         Jac[5,11] = +k29
460         Jac[5,12] = +k21
461         Jac[5,14] = +k35
462         Jac[5,15] = +k39
463         Jac[5,16] = -k57*x[5]
```

```
464         Jac[5,19] = +k56
465         Jac[5,21] = -k83*x[5]
466         Jac[5,22] = -k93*x[5]
467         Jac[5,25] = +k82
468         Jac[5,26] = +k92
469         Jac[6,0] = -k14*x[6]
470         Jac[6,1] = -k22*x[6]
471         Jac[6,2] = +k08*2.0*x[2]-k32*x[6]
472         Jac[6,3] = -k36*x[6]
473         Jac[6,6] = -k09-k14*x[0]-k22*x[1]-k32*x[2]-k36*x[3]-k63*x[16]-
k79*x[21]-k91*x[23]-k101*x[22]
474         Jac[6,10] = +k15
475         Jac[6,11] = +k23
476         Jac[6,13] = +k33
477         Jac[6,15] = +k37
478         Jac[6,16] = -k63*x[6]
479         Jac[6,20] = +k62
480         Jac[6,21] = -k79*x[6]
481         Jac[6,22] = -k101*x[6]
482         Jac[6,23] = -k91*x[6]
483         Jac[6,24] = +k78
484         Jac[6,26] = +k90
485         Jac[6,27] = +k100
486         Jac[7,0] = -k12*x[7]
487         Jac[7,1] = +k06*2.0*x[1]
488         Jac[7,2] = -k30*x[7]
489         Jac[7,4] = -k40*x[7]
490         Jac[7,7] = -k07-k12*x[0]-k30*x[2]-k40*x[4]
491         Jac[7,9] = +k13
492         Jac[7,12] = +k31
493         Jac[7,14] = +k41
494         Jac[8,0] = +k10*x[5]
495         Jac[8,1] = +k18*x[4]
496         Jac[8,2] = +k24*x[3]
497         Jac[8,3] = +k24*x[2]
498         Jac[8,4] = +k18*x[1]
499         Jac[8,5] = +k10*x[0]
500         Jac[8,8] = -k11-k19-k25-k44
501         Jac[8,17] = +k45
502         Jac[9,0] = +k12*x[7]
503         Jac[9,1] = +k16*x[3]
504         Jac[9,3] = +k16*x[1]
505         Jac[9,7] = +k12*x[0]
506         Jac[9,9] = -k13-k17-k46
507         Jac[9,18] = +k47
508         Jac[10,0] = +k14*x[6]
509         Jac[10,2] = +k26*x[4]
510         Jac[10,4] = +k26*x[2]
511         Jac[10,6] = +k14*x[0]
512         Jac[10,10] = -k15-k27
513         Jac[11,1] = +k22*x[6]
514         Jac[11,2] = +k28*x[5]
515         Jac[11,5] = +k28*x[2]
516         Jac[11,6] = +k22*x[1]
517         Jac[11,11] = -k23-k29-k89*x[21]
518         Jac[11,21] = -k89*x[11]
519         Jac[11,26] = +k88
520         Jac[12,1] = +k20*x[5]
521         Jac[12,2] = +k30*x[7]
522         Jac[12,5] = +k20*x[1]
523         Jac[12,7] = +k30*x[2]
524         Jac[12,12] = -k21-k31
525         Jac[13,2] = +k32*x[6]
526         Jac[13,6] = +k32*x[2]
```

```
        Jac[13,13] = -k33-k99*x[21]
        Jac[13,21] = -k99*x[13]
        Jac[13,27] = +k98
        Jac[14,3] = +k34*x[5]
        Jac[14,4] = +k40*x[7]
        Jac[14,5] = +k34*x[3]
        Jac[14,7] = +k40*x[4]
        Jac[14,14] = -k35-k41-k50
        Jac[14,19] = +k51
        Jac[15,3] = +k36*x[6]
        Jac[15,4] = +k38*x[5]
        Jac[15,5] = +k38*x[4]
        Jac[15,6] = +k36*x[3]
        Jac[15,15] = -k37-k39-k48
        Jac[15,20] = +k49
        Jac[16,1] = -k55*x[16]
        Jac[16,2] = -k53*x[16]
        Jac[16,3] = +k42
        Jac[16,5] = -k57*x[16]
        Jac[16,6] = -k63*x[16]
        Jac[16,16] = -k43-k53*x[2]-k55*x[1]-k57*x[5]-k63*x[6]-k66
        Jac[16,17] = +k52
        Jac[16,18] = +k54
        Jac[16,19] = +k56
        Jac[16,20] = +k62
        Jac[16,22] = +k67
        Jac[17,1] = -k61*x[17]
        Jac[17,2] = +k53*x[16]-k65*x[17]
        Jac[17,8] = +k44
        Jac[17,16] = +k53*x[2]
        Jac[17,17] = -k45-k52-k61*x[1]-k65*x[2]-k68
        Jac[17,19] = +k60
        Jac[17,20] = +k64
        Jac[17,24] = +k69
        Jac[18,1] = +k55*x[16]
        Jac[18,2] = -k59*x[18]
        Jac[18,9] = +k46
        Jac[18,16] = +k55*x[1]
        Jac[18,18] = -k47-k54-k59*x[2]-k70
        Jac[18,19] = +k58
        Jac[18,25] = +k71
        Jac[19,1] = +k61*x[17]
        Jac[19,2] = +k59*x[18]
        Jac[19,5] = +k57*x[16]
        Jac[19,14] = +k50
        Jac[19,16] = +k57*x[5]
        Jac[19,17] = +k61*x[1]
        Jac[19,18] = +k59*x[2]
        Jac[19,19] = -k51-k56-k58-k60-k74
        Jac[19,26] = +k75
        Jac[20,2] = +k65*x[17]
        Jac[20,6] = +k63*x[16]
        Jac[20,15] = +k48
        Jac[20,16] = +k63*x[6]
        Jac[20,17] = +k65*x[2]
        Jac[20,20] = -k49-k62-k64-k72
        Jac[20,27] = +k73
        Jac[21,2] = -k77*x[21]
        Jac[21,5] = -k83*x[21]
        Jac[21,6] = -k79*x[21]
        Jac[21,11] = -k89*x[21]
        Jac[21,13] = -k99*x[21]
        Jac[21,21] = -k77*x[2]-k79*x[6]-k83*x[5]-k89*x[11]-k99*x[13]
        Jac[21,22] = +k76
```

```
        Jac[21,24] = +k78
        Jac[21,25] = +k82
        Jac[21,26] = +k88
        Jac[21,27] = +k98
        Jac[22,1] = -k87*x[22]
        Jac[22,2] = +k77*x[21]-k81*x[22]
        Jac[22,5] = -k93*x[22]
        Jac[22,6] = -k101*x[22]
        Jac[22,16] = +k66
        Jac[22,21] = +k77*x[2]
        Jac[22,22] = -k67-k76-k81*x[2]-k87*x[1]-k93*x[5]-k101*x[6]
        Jac[22,24] = +k80
        Jac[22,25] = +k86
        Jac[22,26] = +k92
        Jac[22,27] = +k100
        Jac[23,2] = -k85*x[23]
        Jac[23,6] = -k91*x[23]
        Jac[23,23] = -k85*x[2]-k91*x[6]
        Jac[23,25] = +k84
        Jac[23,26] = +k90
        Jac[24,1] = -k95*x[24]
        Jac[24,2] = +k81*x[22]-k103*x[24]
        Jac[24,6] = +k79*x[21]
        Jac[24,17] = +k68
        Jac[24,21] = +k79*x[6]
        Jac[24,22] = +k81*x[2]
        Jac[24,24] = -k69-k78-k80-k95*x[1]-k103*x[2]
        Jac[24,26] = +k94
        Jac[24,27] = +k102
        Jac[25,1] = +k87*x[22]
        Jac[25,2] = +k85*x[23]-k97*x[25]
        Jac[25,5] = +k83*x[21]
        Jac[25,18] = +k70
        Jac[25,21] = +k83*x[5]
        Jac[25,22] = +k87*x[1]
        Jac[25,23] = +k85*x[2]
        Jac[25,25] = -k71-k82-k84-k86-k97*x[2]
        Jac[25,26] = +k96
        Jac[26,1] = +k95*x[24]
        Jac[26,2] = +k97*x[25]
        Jac[26,5] = +k93*x[22]
        Jac[26,6] = +k91*x[23]
        Jac[26,11] = +k89*x[21]
        Jac[26,19] = +k74
        Jac[26,21] = +k89*x[11]
        Jac[26,22] = +k93*x[5]
        Jac[26,23] = +k91*x[6]
        Jac[26,24] = +k95*x[1]
        Jac[26,25] = +k97*x[2]
        Jac[26,26] = -k75-k88-k90-k92-k94-k96
        Jac[27,2] = +k103*x[24]
        Jac[27,6] = +k101*x[22]
        Jac[27,13] = +k99*x[21]
        Jac[27,20] = +k72
        Jac[27,21] = +k99*x[13]
        Jac[27,22] = +k101*x[6]
        Jac[27,24] = +k103*x[2]
        Jac[27,27] = -k73-k98-k100-k102
        return Jac


# Calculation handling a maximum matrix size
if species*tfin/dt > MaxMem:
        tfin2 = MaxMem*dt/species
```

```
        ti = 0
else:
        tfin2 = tfin
        ti = 0
t = np.arange(0,tfin2+dt,dt)
xini2 = xini
# Time indexes and Out predefinition
Out_index = []
t_old = -(report_t+1.0)
for i in range(len(t)):
        if t[i] - t_old >= report_t:
                Out_index.append(i)
                t_old = t[i]
Out = ['' for i in Out_index]
while ti+tfin2 <= tfin:
        #print('Current interval: [{},{}] s'.format(ti,ti+tfin2))
        x = odeint(f,xini2,t,Dfun=Jacobian,rtol=1E-6,atol=1E-11)
        # Output Writing
        for j,i in enumerate(Out_index):
                Row = '\t'.join(map(str,x[i,:].tolist()))
                Out[j] = '{}\t{}'.format(ti+t[i],Row)
                t_old = t[i]
        with open('{}.txt'.format(OFile),'a') as F:
                F.write('\n'.join(Out))
                F.write('\n')
        xini2 = x[-1,:]
        ti += tfin2


```

9. Geometries

Benzaldehyde
Energy (POTENTIAL) = -345.719632320 Eh
Number of Imaginary Frequencies = 0

	Atom	X	Y	Z
1	C	-1.6968	0.0685	-0.0001
2	C	-0.3000	0.0615	0.0004
3	C	0.4033	1.2594	-0.0001
4	C	-0.2894	2.4662	-0.0010
5	C	-1.6850	2.4790	-0.0014
6	C	-2.3877	1.2855	-0.0010
7	H	0.2288	-0.8840	0.0011
8	H	1.4850	1.2543	0.0003
9	H	0.2566	3.4005	-0.0013
10	H	-2.2163	3.4213	-0.0022
11	H	-3.4693	1.2754	-0.0014
12	C	-2.4231	-1.2136	0.0004
13	O	-3.6322	-1.3279	0.0006
14	H	-1.7754	-2.1108	0.0016

NButylamine
Energy (POTENTIAL) = -213.904198497 Eh
Number of Imaginary Frequencies = 0

	Atom	X	Y	Z
1	C	-3.5451	-1.0834	-0.0000
2	H	-3.2750	-2.1440	0.0064
3	H	-3.0914	-0.6563	-0.8997
4	C	-2.9526	-0.4069	1.2354
5	H	-3.2206	0.6558	1.2297
6	H	-3.3960	-0.8337	2.1401
7	C	-1.4365	-0.5351	1.3223
8	H	-0.9910	-0.1276	0.4038
9	H	-1.1656	-1.5937	1.3588
10	N	-0.9238	0.1047	2.5431
11	H	0.0838	-0.0023	2.5908
12	H	-1.0928	1.1046	2.4948
13	C	-5.0638	-0.9454	-0.0816
14	H	-5.3616	0.1054	-0.1187
15	H	-5.4630	-1.4356	-0.9718
16	H	-5.5467	-1.3941	0.7898

Water
Energy (POTENTIAL) = -76.4666514750 Eh
Number of Imaginary Frequencies = 0

	Atom	X	Y	Z
1	O	0.8096	0.1311	0.0000
2	H	1.7728	0.1775	0.0000
3	H	0.5317	1.0546	0.0000

Hemiaminal
Energy (POTENTIAL) = -559.630034705 Eh
Number of Imaginary Frequencies = 0

	Atom	X	Y	Z
1	C	2.1965	1.1709	-0.0648
2	C	0.8511	1.1909	0.2798
3	C	0.1160	0.0068	0.3443
4	C	0.7492	-1.1993	0.0556
5	C	2.0969	-1.2217	-0.2961
6	C	2.8242	-0.0384	-0.3556
7	H	0.3626	2.1325	0.4990
8	H	0.1857	-2.1202	0.1132
9	H	3.8726	-0.0562	-0.6235
10	N	-2.1182	0.4044	-0.4763
11	C	-3.5300	0.7523	-0.3133
12	H	-3.6005	1.4408	0.5333
13	H	-3.8300	1.3208	-1.1987
14	H	-1.9765	-0.2783	-1.2117
15	H	-1.3334	-1.3423	2.0752
16	C	-1.3654	0.0656	0.6888
17	H	-1.5275	0.8603	1.4247
18	O	-1.8256	-1.1818	1.2592
19	C	-4.5133	-0.4064	-0.1186
20	H	-4.2576	-0.9486	0.7923
21	H	-4.3932	-1.1132	-0.9470
22	H	2.7563	2.0964	-0.1057
23	H	2.5782	-2.1652	-0.5198
24	C	-5.9652	0.0669	-0.0588
25	H	-6.2104	0.6077	-0.9786
26	H	-6.0753	0.7879	0.7576
27	C	-6.9576	-1.0769	0.1386
28	H	-6.7584	-1.6146	1.0688
29	H	-7.9864	-0.7131	0.1793
30	H	-6.8937	-1.7996	-0.6786

Imine
Energy (POTENTIAL) = -483.158752526 Eh
Number of Imaginary Frequencies = 0

	Atom	X	Y	Z
1	C	-8.8986	1.6627	2.8139
2	C	-9.6353	2.7188	3.3382
3	C	-9.0674	3.9849	3.4242
4	C	-7.7575	4.2095	2.9912
5	C	-7.0242	3.1393	2.4636
6	C	-7.5916	1.8776	2.3766
7	H	-9.3379	0.6763	2.7444
8	H	-9.6407	4.8087	3.8315
9	H	-6.0112	3.3109	2.1270
10	C	-7.1935	5.5638	3.1051
11	H	-7.8801	6.3226	3.5023
12	N	-6.0045	5.8587	2.7778
13	C	-5.5585	7.2299	2.9558
14	C	-4.4166	7.3067	3.9707
15	H	-4.7796	6.9432	4.9370
16	H	-3.6184	6.6271	3.6599
17	H	-5.1962	7.5897	1.9881
18	H	-6.3791	7.8901	3.2695
19	C	-3.8615	8.7217	4.1288
20	H	-3.4892	9.0733	3.1617
21	H	-4.6727	9.3996	4.4109
22	H	-7.0177	1.0566	1.9673
23	H	-10.6500	2.5580	3.6778
24	C	-2.7452	8.8055	5.1670
25	H	-1.9073	8.1579	4.8979
26	H	-2.3617	9.8236	5.2589
27	H	-3.0998	8.4937	6.1523

W_W
Energy (POTENTIAL) = -152.942640477 Eh
Number of Imaginary Frequencies = 0

	Atom	X	Y	Z
1	O	-1.1223	1.1696	0.1090
2	H	-0.2446	1.4768	-0.1757
3	H	-1.6951	1.3662	-0.6400
4	O	1.4317	2.0847	-0.7691
5	H	2.1060	1.4100	-0.6180
6	H	1.7188	2.8403	-0.2406

A_W
Energy (POTENTIAL) = -422.195334037 Eh
Number of Imaginary Frequencies = 0

	Atom	X	Y	Z
1	C	-2.0892	-1.0248	-0.0772
2	C	-0.7263	-0.7732	0.0464
3	C	-0.2784	0.5332	0.1900
4	C	-1.1939	1.5892	0.2097
5	C	-2.5643	1.3298	0.0852
6	C	-3.0076	0.0262	-0.0577
7	H	-2.4403	-2.0423	-0.1895
8	H	0.7797	0.7428	0.2874
9	H	-3.2612	2.1566	0.1017
10	C	-0.6940	2.9585	0.3616
11	H	0.4020	3.0547	0.4446
12	O	-1.3982	3.9552	0.3985
13	O	0.4603	6.0529	0.8034
14	H	0.5981	6.0141	1.7561
15	H	-0.2708	5.4310	0.6438
16	H	-0.0189	-1.5912	0.0306
17	H	-4.0652	-0.1796	-0.1543

N_W
Energy (POTENTIAL) = -290.385672764 Eh
Number of Imaginary Frequencies = 0

	Atom	X	Y	Z
1	C	1.5520	-1.8817	-3.9961
2	C	2.2446	-1.2857	-2.7766
3	H	2.0260	-0.2166	-2.7189
4	H	3.3314	-1.3845	-2.8877
5	H	0.4708	-1.7755	-3.8743
6	H	1.7569	-2.9575	-4.0319
7	H	3.0773	-1.3492	-5.4216
8	N	1.7505	-1.9096	-1.5360
9	O	-1.0339	-1.3887	-1.5239
10	H	-1.0643	-0.4583	-1.7705
11	H	-0.0702	-1.5965	-1.4782
12	C	1.9944	-1.2385	-5.3093
13	H	1.7982	-0.1626	-5.2670
14	H	2.2199	-1.5117	-0.7295
15	H	1.9727	-2.9002	-1.5355
16	C	1.2919	-1.8361	-6.5263
17	H	1.6219	-1.3607	-7.4520
18	H	1.4949	-2.9063	-6.6112
19	H	0.2089	-1.7104	-6.4553

N_N
Energy (POTENTIAL) = -427.816638070 Eh
Number of Imaginary Frequencies = 0

	Atom	X	Y	Z
1	C	-3.0518	-0.6019	-0.8374
2	H	-2.1847	-0.8659	-1.4509
3	H	-3.3351	0.4144	-1.1273
4	C	-2.6470	-0.6165	0.6355
5	H	-3.5088	-0.3378	1.2523
6	H	-2.3724	-1.6323	0.9290
7	C	-1.4866	0.3190	0.9512
8	H	-1.7520	1.3393	0.6426
9	H	-0.6147	0.0268	0.3603
10	N	-1.1148	0.2334	2.3714
11	H	-0.3523	0.8703	2.5751
12	H	-1.8941	0.5290	2.9505
13	H	-0.3541	-1.7705	2.8251
14	C	-3.3606	-4.5695	2.7887
15	H	-2.9793	-5.5939	2.8461
16	H	-3.5614	-4.3762	1.7305
17	C	-2.2868	-3.6020	3.2836
18	H	-2.6678	-2.5775	3.2222
19	H	-2.0762	-3.7897	4.3409
20	C	-0.9830	-3.6919	2.4983
21	H	-1.2064	-3.5700	1.4280
22	H	-0.5610	-4.6945	2.6133
23	N	-0.0052	-2.7152	2.9951
24	H	0.8579	-2.7983	2.4687
25	C	-4.6640	-4.4658	3.5775
26	H	-5.0878	-3.4611	3.5052
27	H	-5.4133	-5.1689	3.2081
28	H	-4.5018	-4.6795	4.6368
29	C	-4.2009	-1.5604	-1.1427
30	H	-4.4743	-1.5349	-2.1994
31	H	-3.9298	-2.5894	-0.8943
32	H	-5.0910	-1.3052	-0.5625

W_W_W
Energy (POTENTIAL) = -229.424938835 Eh
Number of Imaginary Frequencies = 0

	Atom	X	Y	Z
1	O	-3.9675	2.9517	-1.8093
2	H	-3.2529	3.5904	-1.9169
3	O	-6.0171	3.2425	-3.7022
4	H	-4.4581	2.9700	-2.6536
5	H	-5.9509	4.0363	-4.2463
6	O	-6.4731	3.9166	-1.0186
7	H	-6.4430	3.5369	-2.8738
8	H	-5.5385	3.6329	-1.0095
9	H	-6.9444	3.2446	-0.5117

A_N

Energy (POTENTIAL) = -559.632335083 Eh

Number of Imaginary Frequencies = 0

	Atom	X	Y	Z
1	C	-1.1655	-0.7841	0.9657
2	C	0.0611	-0.1948	0.6563
3	C	0.0968	1.0902	0.1079
4	C	-1.0847	1.7730	-0.1329
5	C	-2.3083	1.1777	0.1736
6	C	-2.3494	-0.0991	0.7260
7	H	-1.1859	-1.7847	1.3794
8	H	1.0541	1.5328	-0.1307
9	H	-3.2294	1.7110	-0.0215
10	C	1.3041	-0.9553	0.8808
11	H	1.1579	-1.9633	1.3071
12	O	2.4211	-0.5393	0.6438
13	N	1.0308	-2.4692	-1.7336
14	H	1.9923	-2.7089	-1.5193
15	C	-0.4493	-0.8763	-2.9018
16	C	0.9873	-1.2652	-2.5746
17	H	1.4621	-0.4552	-2.0163
18	H	1.5529	-1.3778	-3.5100
19	H	-1.0074	-0.7712	-1.9685
20	H	-0.9243	-1.6904	-3.4612
21	H	0.6454	-3.2585	-2.2420
22	C	-0.5508	0.4190	-3.7053
23	H	-0.0651	1.2234	-3.1452
24	H	0.0075	0.3144	-4.6407
25	H	-1.0600	2.7643	-0.5651
26	H	-3.3000	-0.5589	0.9608
27	C	-1.9931	0.8137	-4.0132
28	H	-2.0420	1.7452	-4.5808
29	H	-2.4963	0.0407	-4.5992
30	H	-2.5648	0.9542	-3.0930

A_W_W

Energy (POTENTIAL) = -498.672725819 Eh

Number of Imaginary Frequencies = 0

	Atom	X	Y	Z
1	C	-0.6293	0.5136	-0.8906
2	C	-1.4201	1.5976	-0.4947
3	C	-2.5849	1.3841	0.2293
4	C	-2.9612	0.0864	0.5618
5	C	-2.1752	-0.9990	0.1722
6	C	-1.0137	-0.7906	-0.5518
7	C	0.5897	0.7864	-1.6578
8	H	-1.1168	2.6033	-0.7585
9	H	-0.4010	-1.6279	-0.8551
10	H	-3.8683	-0.0830	1.1270
11	O	1.3642	-0.0500	-2.0947
12	O	1.3752	-2.8320	-2.1385
13	H	1.3805	-1.8550	-2.1369
14	H	0.8937	-3.0811	-2.9362
15	O	3.9736	-3.9136	-1.9369
16	H	3.0795	-3.5411	-2.0413
17	H	4.0096	-4.1807	-1.0123
18	H	0.7938	1.8554	-1.8383
19	H	-3.1966	2.2223	0.5339
20	H	-2.4737	-2.0044	0.4369

N_W_W
Energy (POTENTIAL) = -366.866983514 Eh
Number of Imaginary Frequencies = 0

	Atom	X	Y	Z
1	N	0.0780	-1.8566	-2.4095
2	C	1.1139	-1.9652	-3.4538
3	C	2.1930	-0.9080	-3.2588
4	H	2.5855	-0.9859	-2.2424
5	H	1.7421	0.0863	-3.3486
6	H	1.5571	-2.9609	-3.3734
7	H	0.6948	-1.8819	-4.4632
8	H	-0.6552	-2.5403	-2.5656
9	H	-0.3664	-0.9449	-2.4560
10	O	3.9011	-3.1801	-1.1917
11	H	3.0471	-2.9378	-0.7806
12	H	3.6930	-3.2972	-2.1241
13	O	1.4396	-2.4293	-0.0633
14	H	1.5667	-1.6048	0.4201
15	H	0.8885	-2.1837	-0.8568
16	C	3.3426	-1.0378	-4.2565
17	H	3.7648	-2.0453	-4.1880
18	H	2.9561	-0.9365	-5.2751
19	C	4.4476	-0.0119	-4.0192
20	H	4.8827	-0.1326	-3.0245
21	H	5.2522	-0.1154	-4.7499
22	H	4.0615	1.0077	-4.0924

N_N_W
Energy (POTENTIAL) = -504.298154258 Eh
Number of Imaginary Frequencies = 0

	Atom	X	Y	Z
1	O	-6.4830	2.9667	-3.5701
2	H	-4.3507	2.6624	-3.6094
3	H	-6.5667	3.8216	-4.0063
4	H	-6.5730	3.1655	-2.6028
5	H	-5.8689	3.3299	-0.3420
6	H	-7.4378	2.9145	-0.4254
7	H	-3.0599	1.8314	-3.0758
8	C	-3.1585	3.7407	-2.3588
9	H	-3.7112	3.5027	-1.4384
10	H	-3.5620	4.6906	-2.7181
11	C	-1.6855	3.9192	-2.0143
12	H	-1.1362	4.1807	-2.9239
13	H	-1.2789	2.9607	-1.6716
14	C	-1.4465	4.9819	-0.9420
15	H	-2.0129	4.7223	-0.0422
16	H	-1.8472	5.9393	-1.2896
17	C	0.0286	5.1467	-0.5829
18	H	0.1724	5.9150	0.1794
19	H	0.4456	4.2133	-0.1967
20	H	0.6168	5.4328	-1.4582
21	N	-3.3546	2.7413	-3.4166
22	C	-7.1158	4.9391	-0.6190
23	H	-7.2820	5.1706	0.4399
24	H	-8.0636	5.1076	-1.1359
25	C	-6.0521	5.8729	-1.1809
26	H	-5.8914	5.6365	-2.2364
27	H	-5.1013	5.6764	-0.6750
28	C	-6.4065	7.3513	-1.0348
29	H	-7.3514	7.5490	-1.5500
30	H	-6.5777	7.5815	0.0211
31	C	-5.3207	8.2715	-1.5886

32	H	-5.1487	8.0812	-2.6507
33	H	-5.5923	9.3231	-1.4789
34	H	-4.3720	8.1169	-1.0689
35	N	-6.7381	3.5294	-0.8271

A_N_W
Energy (POTENTIAL) = -636.108992967 Eh
Number of Imaginary Frequencies = 0

	Atom	X	Y	Z
1	C	0.4664	1.5702	-1.8626
2	C	-0.1796	1.3625	-0.6517
3	C	0.3580	0.4811	0.2893
4	C	1.5514	-0.1926	0.0097
5	C	2.1943	0.0147	-1.2000
6	C	1.6529	0.8955	-2.1363
7	H	-1.1063	1.8771	-0.4297
8	H	1.9643	-0.8722	0.7416
9	H	2.1589	1.0555	-3.0794
10	N	-2.1984	-1.6968	0.5148
11	H	-1.3583	-2.2562	0.4097
12	C	-2.8896	-2.0696	1.7534
13	H	-3.2084	-3.1217	1.7647
14	H	-2.1785	-1.9473	2.5735
15	H	-2.7881	-1.8860	-0.2885
16	H	0.1463	-3.6919	2.1704
17	H	0.4575	-2.2089	1.9414
18	C	-0.3471	0.2867	1.5650
19	H	-1.2404	0.9151	1.7036
20	O	0.0145	-0.4656	2.4567
21	C	-4.1004	-1.1780	2.0017
22	H	-3.7703	-0.1350	2.0297
23	H	-4.7899	-1.2623	1.1541
24	O	0.5244	-3.0851	1.5242
25	C	-4.8415	-1.5185	3.2936
26	H	-5.1801	-2.5583	3.2538
27	H	-4.1441	-1.4549	4.1346
28	H	3.1168	-0.5063	-1.4185
29	H	0.0493	2.2525	-2.5909
30	C	-6.0360	-0.6031	3.5537
31	H	-6.5502	-0.8681	4.4796
32	H	-5.7210	0.4400	3.6354
33	H	-6.7639	-0.6644	2.7409

A_N_N
Energy (POTENTIAL) = -773.545187223 Eh
Number of Imaginary Frequencies = 0

	Atom	X	Y	Z
1	C	0.6180	1.9599	-1.6191
2	C	0.1379	1.5084	-0.3970
3	C	0.8163	0.5039	0.2958
4	C	1.9838	-0.0454	-0.2426
5	C	2.4628	0.4061	-1.4622
6	C	1.7799	1.4083	-2.1512
7	H	-0.7703	1.9230	0.0220
8	H	2.5059	-0.8173	0.3064
9	H	2.1560	1.7593	-3.1033
10	N	-2.0774	-1.4633	0.5412
11	H	-1.3578	-2.1218	0.2476
12	C	-2.5938	-1.8380	1.8614
13	H	-3.0502	-2.8383	1.8755
14	H	-1.7450	-1.8736	2.5485
15	H	-2.8213	-1.5049	-0.1474

16	H	0.9058	-2.5903	0.7699
17	C	0.2867	0.0416	1.5917
18	H	-0.5885	0.5994	1.9616
19	O	0.7662	-0.8632	2.2503
20	C	-3.6113	-0.8220	2.3679
21	H	-3.1466	0.1689	2.3770
22	H	-4.4450	-0.7654	1.6586
23	C	-4.1509	-1.1511	3.7590
24	H	-4.6172	-2.1409	3.7416
25	H	-3.3143	-1.2191	4.4612
26	H	3.3671	-0.0163	-1.8798
27	H	0.0902	2.7363	-2.1565
28	H	1.0786	-3.6948	-0.4130
29	C	0.2378	-4.4455	1.3002
30	H	-0.2596	-5.2785	0.7957
31	H	-0.4648	-4.0730	2.0497
32	C	1.5011	-4.9498	1.9992
33	H	2.2003	-5.3259	1.2442
34	H	1.9942	-4.1019	2.4860
35	C	1.2247	-6.0417	3.0322
36	H	0.7277	-6.8846	2.5420
37	H	0.5185	-5.6603	3.7761
38	N	0.4502	-3.3763	0.3171
39	C	2.4880	-6.5343	3.7349
40	H	2.2616	-7.3118	4.4674
41	H	3.2000	-6.9508	3.0182
42	H	2.9889	-5.7177	4.2606
43	C	-5.1587	-0.1227	4.2673
44	H	-5.5324	-0.3846	5.2592
45	H	-4.7078	0.8704	4.3341
46	H	-6.0188	-0.0493	3.5972

A_N_W_W
Energy (POTENTIAL) = -712.593621195 Eh
Number of Imaginary Frequencies = 0

	Atom	X	Y	Z
1	C	0.0341	-0.8077	-0.8500
2	C	0.4696	0.5176	-0.7737
3	C	-0.3865	1.5524	-1.1248
4	C	-1.6795	1.2640	-1.5512
5	C	-2.1198	-0.0579	-1.6274
6	C	-1.2672	-1.0921	-1.2779
7	C	0.9621	-1.8839	-0.4836
8	H	1.4762	0.7292	-0.4360
9	H	-1.5905	-2.1226	-1.3321
10	H	-2.3480	2.0698	-1.8247
11	H	1.6916	-1.9942	2.5932
12	O	0.6838	-3.0738	-0.5241
13	H	2.0289	-4.1874	-0.0549
14	H	3.4970	-4.5441	-0.3515
15	H	3.0793	-3.7344	2.0543
16	H	3.1494	-3.5661	3.6789
17	H	1.9673	-1.5584	-0.1836
18	H	0.1775	-2.0059	2.2749
19	H	-0.0509	2.5789	-1.0654
20	H	-3.1266	-0.2737	-1.9588
21	N	3.1617	-3.0509	2.8056
22	C	4.4278	-2.3126	2.6658
23	H	4.5441	-1.6660	3.5388
24	H	5.2973	-2.9826	2.6467
25	C	4.4186	-1.4622	1.4009
26	H	4.2405	-2.1132	0.5383

27	H	3.5730	-0.7710	1.4478
28	C	5.7110	-0.6784	1.1839
29	H	5.8973	-0.0412	2.0539
30	H	6.5535	-1.3741	1.1260
31	C	5.6710	0.1809	-0.0780
32	H	4.8593	0.9111	-0.0307
33	H	6.6037	0.7305	-0.2188
34	H	5.5103	-0.4338	-0.9672
35	O	0.9137	-1.4032	2.4240
36	O	2.7759	-4.7359	0.2584

A_N_N_W
Energy (POTENTIAL) = -850.030454675 Eh
Number of Imaginary Frequencies = 0

	Atom	X	Y	Z
1	C	-0.5867	-0.0720	-1.3738
2	C	-1.1793	1.0386	-0.7702
3	C	-2.5502	1.0635	-0.5497
4	C	-3.3315	-0.0223	-0.9350
5	C	-2.7442	-1.1330	-1.5408
6	C	-1.3765	-1.1592	-1.7589
7	C	0.8714	-0.0855	-1.5848
8	H	-0.5601	1.8748	-0.4699
9	H	-0.9022	-2.0138	-2.2207
10	H	-4.3994	-0.0064	-0.7612
11	N	1.6903	0.0838	1.4051
12	C	2.8561	0.9488	1.1887
13	H	1.9655	-0.7226	1.9602
14	C	3.9495	0.2057	0.4274
15	H	3.2790	1.3396	2.1257
16	H	2.5356	1.8181	0.6062
17	H	3.5376	-0.1701	-0.5130
18	H	4.2466	-0.6719	1.0090
19	O	1.4887	-1.0167	-2.0683
20	N	2.3793	-3.3017	0.0383
21	H	2.3112	-2.4167	-0.4558
22	H	3.0745	-3.8492	-0.4570
23	O	3.0825	-2.4709	2.6108
24	H	2.8646	-2.8353	1.7122
25	H	2.6501	-3.0646	3.2335
26	H	1.3911	0.8402	-1.2923
27	H	0.9747	0.5755	1.9280
28	H	-3.0095	1.9222	-0.0787
29	H	-3.3565	-1.9755	-1.8332
30	C	5.1784	1.0671	0.1437
31	H	4.8806	1.9438	-0.4403
32	H	5.5806	1.4489	1.0872
33	C	1.0723	-3.9816	-0.0001
34	H	0.6869	-4.0657	-1.0235
35	H	1.2100	-4.9993	0.3729
36	C	0.0522	-3.2506	0.8650
37	H	0.3990	-3.2482	1.9021
38	H	0.0096	-2.2040	0.5544
39	C	-1.3462	-3.8586	0.7910
40	H	-1.6890	-3.8462	-0.2476
41	H	-1.3045	-4.9111	1.0890
42	C	6.2718	0.3066	-0.6037
43	H	7.1407	0.9389	-0.7976
44	H	6.6111	-0.5578	-0.0277
45	H	5.9066	-0.0615	-1.5656
46	C	-2.3535	-3.1173	1.6668
47	H	-3.3536	-3.5469	1.5812

48	H	-2.0628	-3.1570	2.7195
49	H	-2.4176	-2.0652	1.3815

Int_W
Energy (POTENTIAL) = -636.113822802 Eh
Number of Imaginary Frequencies = 0

	Atom	X	Y	Z
1	C	0.4143	1.6704	-1.9171
2	C	-0.2317	1.3735	-0.7202
3	C	0.2544	0.3736	0.1193
4	C	1.4012	-0.3284	-0.2543
5	C	2.0477	-0.0334	-1.4485
6	C	1.5560	0.9665	-2.2838
7	H	-1.1178	1.9268	-0.4336
8	H	1.7926	-1.1070	0.3862
9	H	2.0628	1.1963	-3.2119
10	N	-1.1761	-1.2401	1.2497
11	H	0.1603	-2.4669	1.6470
12	C	-2.2472	-1.4890	2.2281
13	H	-2.4567	-2.5615	2.2242
14	H	-1.8458	-1.2507	3.2142
15	H	-1.5328	-1.3247	0.3049
16	H	0.7575	-3.3380	2.7867
17	H	0.8514	-0.8600	2.5133
18	C	-0.4783	0.0429	1.4063
19	H	-1.1734	0.8575	1.6269
20	O	0.3723	-0.0145	2.5412
21	C	-3.5458	-0.7205	1.9833
22	H	-3.3448	0.3541	1.9699
23	H	-3.9284	-0.9810	0.9908
24	O	1.0090	-2.8018	2.0258
25	C	-4.6105	-1.0220	3.0378
26	H	-4.7916	-2.1009	3.0691
27	H	-4.2260	-0.7464	4.0244
28	H	0.0287	2.4521	-2.5587
29	H	2.9369	-0.5839	-1.7273
30	C	-5.9275	-0.2931	2.7809
31	H	-6.3508	-0.5768	1.8144
32	H	-6.6681	-0.5245	3.5489
33	H	-5.7834	0.7900	2.7740

Int_N
Energy (POTENTIAL) = -773.548127632 Eh
Number of Imaginary Frequencies = 0

	Atom	X	Y	Z
1	C	2.6975	2.2083	0.3520
2	C	1.5170	1.8910	1.0161
3	C	0.8931	0.6634	0.8030
4	C	1.4682	-0.2492	-0.0826
5	C	2.6458	0.0695	-0.7501
6	C	3.2640	1.2978	-0.5347
7	H	1.0755	2.6015	1.7041
8	H	0.9951	-1.2081	-0.2484
9	H	4.1825	1.5423	-1.0522
10	N	-1.5168	0.5618	0.6068
11	H	-0.9001	-2.4756	0.3874
12	C	-2.8485	0.3403	1.1768
13	H	-2.9686	-0.6809	1.5565
14	H	-2.9606	1.0115	2.0331
15	H	-1.3918	0.0105	-0.2354
16	N	-0.8230	-3.0457	-0.4500
17	H	0.3390	-1.1707	2.5281

18	C	-1.9285	-2.7662	-1.3709
19	H	-1.7660	-3.3477	-2.2832
20	H	-1.8646	-1.7148	-1.6660
21	C	-0.4172	0.3460	1.4972
22	H	-0.5455	1.0123	2.3559
23	O	-0.4426	-1.0219	1.9809
24	H	-0.8637	-4.0133	-0.1473
25	C	-3.9318	0.6291	0.1463
26	H	-3.7589	0.0027	-0.7343
27	H	-3.8433	1.6667	-0.1881
28	C	-3.3316	-3.0557	-0.8340
29	H	-3.3779	-4.1028	-0.5156
30	H	-3.5031	-2.4510	0.0619
31	C	-5.3419	0.3702	0.6736
32	H	-5.4120	-0.6654	1.0185
33	H	-5.5230	0.9986	1.5511
34	C	-4.4356	-2.7846	-1.8553
35	H	-4.2489	-3.3812	-2.7536
36	H	-4.3863	-1.7379	-2.1693
37	C	-5.8329	-3.0920	-1.3219
38	H	-6.6032	-2.8741	-2.0643
39	H	-5.9242	-4.1460	-1.0485
40	H	-6.0538	-2.5000	-0.4314
41	C	-6.4212	0.6317	-0.3742
42	H	-7.4187	0.4250	0.0184
43	H	-6.4029	1.6727	-0.7056
44	H	-6.2741	0.0024	-1.2545
45	H	3.0823	-0.6437	-1.4374
46	H	3.1758	3.1631	0.5282

Int_W_W
Energy (POTENTIAL) = -712.598744597 Eh
Number of Imaginary Frequencies = 0

	Atom	X	Y	Z
1	C	-0.4082	0.3686	-0.5850
2	C	-1.2350	1.4749	-0.3884
3	C	-2.5664	1.3111	-0.0229
4	C	-3.0882	0.0319	0.1455
5	C	-2.2714	-1.0759	-0.0564
6	C	-0.9382	-0.9090	-0.4197
7	C	1.0578	0.5915	-0.9290
8	H	-0.8330	2.4720	-0.5261
9	H	-0.3169	-1.7786	-0.5798
10	H	-4.1251	-0.1000	0.4257
11	N	1.7861	0.8706	0.3248
12	C	3.1794	1.3313	0.1430
13	H	1.6459	-0.4842	1.4932
14	C	4.2036	0.2027	0.2306
15	H	3.3868	2.0595	0.9294
16	H	3.2862	1.8543	-0.8150
17	H	3.9929	-0.5366	-0.5435
18	H	4.0897	-0.3046	1.1928
19	O	1.6570	-0.4564	-1.6402
20	O	1.9634	-2.7987	-0.1432
21	H	1.7391	-1.2589	-1.0846
22	H	2.8788	-3.0975	-0.1940
23	O	1.5925	-1.2900	2.0773
24	H	1.8649	-2.3964	0.7503
25	H	0.6742	-1.3309	2.3699
26	H	1.1270	1.4573	-1.5991
27	H	1.2669	1.5833	0.8249
28	C	5.6391	0.7047	0.0836

29	H	5.8382	1.4626	0.8479
30	H	5.7504	1.2064	-0.8827
31	H	-2.6720	-2.0740	0.0654
32	H	-3.1963	2.1788	0.1243
33	C	6.6694	-0.4166	0.1980
34	H	7.6881	-0.0373	0.0968
35	H	6.5958	-0.9195	1.1653
36	H	6.5175	-1.1708	-0.5781

Int_N_W
Energy (POTENTIAL) = -850.028529639 Eh
Number of Imaginary Frequencies = 0

	Atom	X	Y	Z
1	C	0.8612	0.0938	-0.2614
2	C	0.6479	1.1540	0.6153
3	C	1.2500	1.1618	1.8710
4	C	2.0725	0.1102	2.2592
5	C	2.2916	-0.9515	1.3845
6	C	1.6874	-0.9583	0.1337
7	C	0.1731	0.0230	-1.6136
8	H	0.0100	1.9736	0.3168
9	H	1.8509	-1.7880	-0.5427
10	H	2.5425	0.1173	3.2340
11	N	-0.9725	-0.8135	-1.5324
12	C	-1.7298	-0.9993	-2.7673
13	H	-1.5786	-0.5377	-0.7552
14	C	-2.8208	-2.0464	-2.5765
15	H	-1.0364	-1.3236	-3.5497
16	H	-2.1829	-0.0636	-3.1207
17	H	-3.4758	-1.7317	-1.7581
18	H	-2.3597	-2.9861	-2.2591
19	O	-0.2016	1.3529	-2.0932
20	H	0.8630	-0.3924	-2.3554
21	H	0.5969	1.8800	-2.2267
22	O	-2.5788	2.5689	-1.3106
23	H	-1.7479	2.1499	-1.6076
24	H	-3.2547	2.2157	-1.8996
25	H	2.9324	-1.7729	1.6779
26	H	1.0743	1.9905	2.5448
27	C	-3.6590	-2.2781	-3.8325
28	H	-4.1007	-1.3296	-4.1531
29	H	-3.0065	-2.6035	-4.6487
30	N	-2.7961	0.2277	0.7343
31	H	-2.7177	1.1664	0.3524
32	H	-2.3673	0.2366	1.6531
33	C	-4.2069	-0.1574	0.8277
34	H	-4.6223	-0.1438	-0.1840
35	H	-4.2577	-1.1958	1.1670
36	C	-5.0682	0.7193	1.7388
37	H	-5.0073	1.7564	1.3919
38	H	-4.6442	0.7037	2.7489
39	C	-6.5314	0.2800	1.7911
40	H	-6.9482	0.2970	0.7791
41	H	-6.5831	-0.7608	2.1256
42	C	-7.3867	1.1520	2.7078
43	H	-7.3752	2.1949	2.3817
44	H	-8.4267	0.8198	2.7208
45	H	-7.0163	1.1241	3.7355
46	C	-4.7659	-3.3087	-3.6219
47	H	-5.4529	-2.9912	-2.8336
48	H	-5.3506	-3.4606	-4.5313
49	H	-4.3515	-4.2758	-3.3270

I_W
Energy (POTENTIAL) = -559.639118313 Eh
Number of Imaginary Frequencies = 0

	Atom	X	Y	Z
1	C	2.3993	1.3071	0.1528
2	C	1.0348	1.5536	0.0577
3	C	0.1268	0.4999	-0.0921
4	C	0.6136	-0.8134	-0.1417
5	C	1.9748	-1.0566	-0.0447
6	C	2.8721	0.0008	0.1018
7	H	0.6656	2.5709	0.0989
8	H	-0.0745	-1.6391	-0.2544
9	H	3.9336	-0.1959	0.1763
10	N	-2.2216	-0.0380	-0.3634
11	C	-3.6050	0.4069	-0.4292
12	H	-3.6814	1.5004	-0.3824
13	H	-4.0069	0.0857	-1.3949
14	H	-2.1818	-1.8649	-0.6568
15	H	-1.9781	-2.9075	-1.7677
16	C	-1.3036	0.8214	-0.1899
17	H	-1.5472	1.8867	-0.1040
18	O	-2.1982	-2.8321	-0.8327
19	C	-4.4359	-0.2281	0.6867
20	H	-4.0346	0.0919	1.6529
21	H	-4.3204	-1.3142	0.6409
22	C	-5.9167	0.1375	0.5949
23	H	-6.3070	-0.1883	-0.3740
24	H	-6.0246	1.2260	0.6209
25	H	3.0902	2.1317	0.2672
26	H	2.3412	-2.0740	-0.0826
27	C	-6.7464	-0.4844	1.7155
28	H	-7.8005	-0.2136	1.6296
29	H	-6.6802	-1.5748	1.6948
30	H	-6.3965	-0.1510	2.6955

I_N
Energy (POTENTIAL) = -697.073287438 Eh
Number of Imaginary Frequencies = 0

	Atom	X	Y	Z
1	C	2.4227	1.5992	-0.2515
2	C	1.0419	1.7454	-0.3175
3	C	0.2002	0.6337	-0.2133
4	C	0.7689	-0.6351	-0.0375
5	C	2.1461	-0.7784	0.0276
6	C	2.9777	0.3363	-0.0785
7	H	0.6085	2.7291	-0.4509
8	H	0.1289	-1.5025	0.0445
9	H	4.0520	0.2177	-0.0265
10	N	-2.1059	-0.0960	-0.2312
11	C	-3.5185	0.2377	-0.2846
12	H	-3.6822	1.2993	-0.5144
13	H	-3.9658	-0.3486	-1.0926
14	H	-1.9307	-2.2909	-0.5185
15	H	-1.8530	-3.6927	-1.3578
16	C	-1.2539	0.8420	-0.2861
17	H	-1.5701	1.8875	-0.3916
18	C	-4.2147	-0.1257	1.0282
19	H	-3.8150	0.5039	1.8286
20	H	-3.9638	-1.1564	1.2880
21	C	-5.7326	0.0288	0.9518
22	H	-6.1112	-0.5786	0.1245

23	H	-5.9827	1.0664	0.7111
24	H	3.0623	2.4679	-0.3341
25	H	2.5770	-1.7619	0.1625
26	C	-2.9234	-3.8351	0.3835
27	H	-2.7286	-4.8936	0.5800
28	H	-2.8957	-3.3329	1.3543
29	C	-4.3217	-3.6848	-0.2207
30	H	-4.3591	-4.2290	-1.1708
31	H	-4.4918	-2.6314	-0.4608
32	C	-5.4350	-4.1813	0.7010
33	H	-5.3752	-3.6460	1.6536
34	H	-5.2692	-5.2378	0.9335
35	N	-1.8232	-3.2987	-0.4233
36	C	-6.8300	-4.0016	0.1063
37	H	-7.6052	-4.3622	0.7855
38	H	-7.0351	-2.9489	-0.1020
39	H	-6.9301	-4.5497	-0.8338
40	C	-6.4326	-0.3812	2.2450
41	H	-7.5155	-0.2684	2.1664
42	H	-6.2241	-1.4254	2.4888
43	H	-6.0948	0.2283	3.0866

I_W_W
Energy (POTENTIAL) = -636.118279666 Eh
Number of Imaginary Frequencies = 0

	Atom	X	Y	Z
1	C	0.2308	-0.5550	0.3711
2	C	1.3677	-1.3621	0.4792
3	C	2.6305	-0.8463	0.2145
4	C	2.7721	0.4878	-0.1512
5	C	1.6467	1.3057	-0.2435
6	C	0.3854	0.7919	0.0175
7	C	-1.0827	-1.1599	0.6268
8	H	1.2567	-2.4011	0.7637
9	H	-0.4795	1.4351	-0.0468
10	H	3.7540	0.8927	-0.3573
11	N	-2.1874	-0.6138	0.3217
12	C	-3.4326	-1.2963	0.6380
13	H	-2.4957	0.7885	-0.7463
14	C	-4.2936	-0.4411	1.5682
15	H	-3.2513	-2.2809	1.0853
16	H	-3.9707	-1.4513	-0.3021
17	H	-4.4234	0.5483	1.1208
18	H	-3.7558	-0.2910	2.5090
19	O	-0.5451	1.0395	-3.2159
20	H	-1.0611	-2.1488	1.0974
21	H	0.1353	0.6685	-2.6449
22	O	-2.6319	1.5452	-1.3717
23	H	-1.2781	1.2471	-2.6065
24	H	-3.5108	1.4188	-1.7466
25	H	3.5010	-1.4835	0.2941
26	H	1.7538	2.3460	-0.5201
27	C	-5.6595	-1.0658	1.8472
28	H	-6.1879	-1.2121	0.9003
29	H	-5.5221	-2.0613	2.2798
30	C	-6.5141	-0.2154	2.7841
31	H	-6.6884	0.7777	2.3634
32	H	-7.4873	-0.6759	2.9642
33	H	-6.0242	-0.0830	3.7516

I_N_W
Energy (POTENTIAL) = -773.554713027 Eh

Number of Imaginary Frequencies = 0

	Atom	X	Y	Z
1	C	3.0949	2.4337	-0.3142
2	C	1.7819	2.6798	0.0708
3	C	0.8713	1.6287	0.2136
4	C	1.3028	0.3198	-0.0374
5	C	2.6114	0.0756	-0.4224
6	C	3.5125	1.1311	-0.5619
7	H	1.4566	3.6950	0.2625
8	H	0.6056	-0.4980	0.0714
9	H	4.5335	0.9359	-0.8626
10	N	-1.4000	1.0489	0.7960
11	H	-3.5883	-2.1199	1.0878
12	C	-2.7430	1.4608	1.1680
13	H	-3.0078	0.9294	2.0867
14	H	-2.7979	2.5378	1.3761
15	H	-1.5106	-1.0713	0.8426
16	N	-1.8064	-2.0349	0.6875
17	H	-4.7896	-3.0673	1.3063
18	C	-1.6103	-2.3922	-0.7252
19	H	-0.5511	-2.3807	-1.0136
20	H	-2.1067	-1.6284	-1.3281
21	C	-0.5097	1.9340	0.6182
22	H	-0.7319	2.9991	0.7597
23	O	-4.5679	-2.1332	1.2335
24	H	-1.2393	-2.6300	1.2821
25	C	-3.7484	1.0838	0.0782
26	H	-3.6551	0.0180	-0.1366
27	H	-3.4931	1.6216	-0.8400
28	C	-2.2075	-3.7579	-1.0437
29	H	-1.7489	-4.5105	-0.3923
30	H	-3.2732	-3.7399	-0.7988
31	C	-2.0214	-4.1690	-2.5034
32	H	-0.9534	-4.1895	-2.7414
33	H	-2.4658	-3.4066	-3.1508
34	C	-5.1905	1.3913	0.4764
35	H	-5.4272	0.8486	1.3953
36	H	-5.2885	2.4568	0.7064
37	H	2.9340	-0.9390	-0.6165
38	H	3.7895	3.2565	-0.4204
39	C	-2.6398	-5.5289	-2.8201
40	H	-2.4965	-5.8001	-3.8679
41	H	-2.1919	-6.3164	-2.2090
42	H	-3.7143	-5.5274	-2.6209
43	C	-6.1912	1.0061	-0.6105
44	H	-6.1408	-0.0639	-0.8236
45	H	-7.2153	1.2377	-0.3106
46	H	-5.9893	1.5415	-1.5416

I_W_W_W

Energy (POTENTIAL) = -712.599349142 Eh

Number of Imaginary Frequencies = 0

	Atom	X	Y	Z
1	C	0.5308	-0.7831	-0.1426
2	C	0.0903	0.1935	0.7593
3	C	0.9621	0.7232	1.6973
4	C	2.2854	0.2872	1.7529
5	C	2.7307	-0.6887	0.8679
6	C	1.8560	-1.2240	-0.0701
7	C	-0.3329	-1.3492	-1.1853
8	H	-0.9283	0.5467	0.7132
9	H	2.2029	-1.9799	-0.7631

10	H	2.9640	0.7082	2.4829
11	N	-1.4854	-0.9070	-1.4836
12	C	-2.2427	-1.5671	-2.5374
13	H	-2.3284	0.5844	-1.0215
14	C	-3.5841	-2.0757	-2.0093
15	H	-1.6730	-2.3907	-2.9835
16	H	-2.4279	-0.8274	-3.3216
17	H	-4.1290	-1.2397	-1.5619
18	H	-3.4006	-2.7981	-1.2084
19	O	1.4930	2.2060	-1.5910
20	H	0.0893	-2.2022	-1.7271
21	H	1.8192	1.6102	-0.9094
22	O	-0.8523	3.3339	-0.5011
23	H	0.6787	2.5834	-1.2070
24	H	-1.1148	4.0960	-1.0297
25	O	-2.8048	1.4396	-0.8505
26	H	-1.5812	2.6838	-0.6075
27	H	-3.3800	1.2690	-0.0960
28	H	0.6145	1.4852	2.3816
29	H	3.7562	-1.0307	0.9066
30	C	-4.4370	-2.7197	-3.1010
31	H	-4.5987	-1.9950	-3.9046
32	H	-3.8877	-3.5551	-3.5455
33	C	-5.7846	-3.2140	-2.5807
34	H	-6.3680	-2.3923	-2.1586
35	H	-6.3772	-3.6677	-3.3774
36	H	-5.6543	-3.9634	-1.7963

I_N_W_W
Energy (POTENTIAL) = -850.037095890 Eh
Number of Imaginary Frequencies = 0

	Atom	X	Y	Z
1	C	0.6333	-0.7437	-0.2808
2	C	0.2721	-0.0196	0.8623
3	C	1.2442	0.4324	1.7398
4	C	2.5916	0.1698	1.4937
5	C	2.9614	-0.5502	0.3634
6	C	1.9870	-1.0039	-0.5182
7	C	-0.3538	-1.2066	-1.2665
8	H	-0.7696	0.1946	1.0475
9	H	2.2736	-1.5586	-1.4031
10	H	3.3473	0.5289	2.1797
11	N	-1.5994	-0.9844	-1.1817
12	C	-2.4648	-1.4728	-2.2418
13	H	-2.6608	0.6770	-0.2441
14	C	-3.5642	-2.3777	-1.6889
15	H	-1.8996	-2.0002	-3.0216
16	H	-2.9295	-0.5999	-2.7096
17	H	-4.0682	-1.8623	-0.8668
18	H	-3.1080	-3.2754	-1.2609
19	O	0.6495	2.1712	-2.0072
20	H	0.0647	-1.7600	-2.1159
21	H	1.1362	1.4622	-1.5749
22	O	-0.8461	3.2768	0.0739
23	H	0.1390	2.5833	-1.2810
24	H	-1.1715	4.1628	-0.1203
25	H	-1.6557	2.6877	0.0631
26	H	-3.6477	1.6071	0.6805
27	H	0.9558	0.9997	2.6147
28	H	4.0052	-0.7556	0.1663
29	C	-4.5860	-2.7697	-2.7547
30	H	-5.0078	-1.8611	-3.1952

31	H	-4.0787	-3.2978	-3.5676
32	N	-3.0268	1.6209	-0.1221
33	C	-3.7614	2.0237	-1.3313
34	H	-3.0819	1.8977	-2.1773
35	H	-3.9799	3.0930	-1.2634
36	C	-5.0562	1.2533	-1.5802
37	H	-4.8388	0.1827	-1.5797
38	H	-5.7405	1.4303	-0.7433
39	C	-5.7429	1.6294	-2.8924
40	H	-5.0498	1.4559	-3.7212
41	H	-5.9614	2.7017	-2.8954
42	C	-5.7138	-3.6383	-2.2042
43	H	-6.2608	-3.1168	-1.4151
44	H	-6.4295	-3.9043	-2.9845
45	H	-5.3253	-4.5667	-1.7790
46	C	-7.0302	0.8438	-3.1321
47	H	-7.7549	1.0242	-2.3345
48	H	-7.4997	1.1225	-4.0773
49	H	-6.8335	-0.2307	-3.1614

TS1
Energy (POTENTIAL) = -559.581410801 Eh
Number of Imaginary Frequencies = 1

	Atom	X	Y	Z
1	C	-1.5715	-0.6122	-0.3110
2	C	-0.2040	-0.4003	-0.1384
3	C	0.2427	0.8570	0.2634
4	C	-0.6621	1.8917	0.4743
5	C	-2.0256	1.6764	0.2929
6	C	-2.4793	0.4196	-0.0977
7	H	-1.9275	-1.5908	-0.6090
8	H	1.3024	1.0016	0.4237
9	H	-2.7305	2.4799	0.4625
10	C	0.7932	-1.5142	-0.3925
11	H	0.2891	-2.4860	-0.2824
12	O	2.0077	-1.4125	0.2387
13	N	1.3561	-1.4678	-1.8352
14	H	2.3151	-1.4083	-1.0630
15	C	-0.2781	-2.7160	-3.2635
16	C	1.1444	-2.6222	-2.7255
17	H	1.8579	-2.5359	-3.5467
18	H	1.4031	-3.5170	-2.1569
19	H	-0.5126	-1.8009	-3.8165
20	H	-0.9763	-2.7618	-2.4247
21	H	1.1341	-0.5921	-2.3030
22	C	-0.4853	-3.9323	-4.1648
23	H	0.2233	-3.8929	-4.9974
24	H	-0.2493	-4.8402	-3.6017
25	H	-3.5389	0.2423	-0.2297
26	H	-0.3054	2.8644	0.7883
27	C	-1.9096	-4.0241	-4.7076
28	H	-2.0403	-4.9060	-5.3373
29	H	-2.6366	-4.0852	-3.8942
30	H	-2.1594	-3.1461	-5.3080

TS2
Energy (POTENTIAL) = -559.563968031 Eh
Number of Imaginary Frequencies = 1

	Atom	X	Y	Z
1	C	3.3622	1.9710	-0.5566
2	C	1.9990	2.2260	-0.6114
3	C	1.1287	1.3095	-1.2136

4	C	1.6550	0.1494	-1.8009
5	C	3.0158	-0.0951	-1.7534
6	C	3.8733	0.8088	-1.1236
7	H	1.5968	3.1290	-0.1708
8	H	1.0044	-0.5528	-2.3021
9	H	4.9360	0.6089	-1.0868
10	N	-1.2179	0.8862	-1.7184
11	C	-2.6269	1.2651	-1.7801
12	H	-2.7007	2.3187	-1.5098
13	H	-2.9580	1.1633	-2.8159
14	H	-1.0256	-0.1149	-1.6534
15	H	-0.2220	-0.7445	1.1179
16	C	-0.2806	1.6399	-1.2485
17	H	-0.5615	2.6494	-0.9692
18	O	-0.6267	-0.2131	0.4210
19	C	-3.4877	0.4023	-0.8600
20	H	-3.0310	0.3958	0.1305
21	H	-3.4567	-0.6323	-1.2144
22	H	4.0244	2.6794	-0.0773
23	H	3.4166	-0.9915	-2.2075
24	C	-4.9351	0.8882	-0.8177
25	H	-5.3492	0.9001	-1.8309
26	H	-4.9578	1.9233	-0.4634
27	C	-5.8142	0.0230	0.0825
28	H	-6.8438	0.3853	0.1014
29	H	-5.8320	-1.0131	-0.2635
30	H	-5.4416	0.0214	1.1093

TS1W
Energy (POTENTIAL) = -636.091079011 Eh
Number of Imaginary Frequencies = 1

	Atom	X	Y	Z
1	C	1.8080	1.4952	0.0770
2	C	1.2168	1.1828	1.2975
3	C	1.8103	0.2578	2.1545
4	C	3.0046	-0.3553	1.7788
5	C	3.5930	-0.0481	0.5576
6	C	2.9980	0.8783	-0.2953
7	H	0.2932	1.6686	1.5902
8	H	3.4587	-1.0786	2.4412
9	H	3.4621	1.1204	-1.2424
10	N	0.2495	-1.3394	3.2126
11	H	0.9695	-2.1354	3.3128
12	C	-0.8269	-1.5540	4.2180
13	H	-1.1026	-2.6079	4.1737
14	H	-0.3787	-1.3664	5.1925
15	H	-0.1347	-1.3191	2.2706
16	H	2.2018	-3.3085	4.6653
17	H	2.2838	-1.4859	4.3467
18	C	1.1439	-0.0865	3.4787
19	H	0.4520	0.7161	3.7478
20	O	1.9797	-0.3907	4.5055
21	C	-2.0434	-0.6729	3.9806
22	H	-1.7496	0.3792	3.9944
23	H	-2.4469	-0.8772	2.9837
24	O	2.3392	-2.7117	3.9229
25	C	-3.1279	-0.9089	5.0319
26	H	-2.7081	-0.7269	6.0253
27	H	-3.4281	-1.9606	5.0113
28	H	4.5190	-0.5299	0.2717
29	H	1.3445	2.2213	-0.5781
30	C	-4.3515	-0.0205	4.8231

31	H	-5.1106	-0.2051	5.5851
32	H	-4.0814	1.0370	4.8711
33	H	-4.8086	-0.2012	3.8473

TS2W
Energy (POTENTIAL) = -636.067008258 Eh
Number of Imaginary Frequencies = 1

	Atom	X	Y	Z
1	C	-3.5494	1.0050	-0.3293
2	C	-2.5620	0.0325	-0.5329
3	C	-1.2188	0.3681	-0.4495
4	C	-0.8489	1.6801	-0.1717
5	C	-1.8247	2.6566	0.0221
6	C	-3.1675	2.3244	-0.0551
7	C	-4.9304	0.5624	-0.4164
8	H	-2.8595	-0.9823	-0.7610
9	H	-3.9097	3.0989	0.0848
10	H	0.1982	1.9456	-0.1111
11	N	-5.9548	1.2577	-0.0463
12	C	-7.3415	0.8001	-0.1893
13	H	-5.8364	2.2158	0.2609
14	C	-8.1260	0.8373	1.1206
15	H	-7.3077	-0.1990	-0.6212
16	H	-7.8097	1.4633	-0.9190
17	H	-9.1815	0.7743	0.8462
18	H	-7.9919	1.8146	1.5963
19	O	-6.0615	-1.6461	-1.9859
20	H	-5.1296	-0.4680	-0.7016
21	H	-5.7218	-2.4170	-2.4490
22	O	-5.2098	0.4407	-2.8901
23	H	-5.6156	-0.6089	-2.5541
24	H	-4.2887	0.3042	-3.1324
25	C	-7.8148	-0.2797	2.1236
26	H	-8.5825	-0.2493	2.9012
27	H	-7.9244	-1.2458	1.6227
28	H	-1.5348	3.6776	0.2297
29	H	-0.4625	-0.3892	-0.6046
30	C	-6.4409	-0.2039	2.7919
31	H	-5.6303	-0.4102	2.0945
32	H	-6.2662	0.7852	3.2226
33	H	-6.3666	-0.9341	3.6001

TS1N
Energy (POTENTIAL) = -773.519736497 Eh
Number of Imaginary Frequencies = 1

	Atom	X	Y	Z
1	C	1.6550	1.1809	-0.0117
2	C	1.0622	0.8125	1.1912
3	C	1.7910	0.1350	2.1711
4	C	3.1322	-0.1431	1.9305
5	C	3.7336	0.2232	0.7291
6	C	2.9952	0.8825	-0.2486
7	H	0.0224	1.0630	1.3724
8	H	3.6898	-0.6425	2.7111
9	H	3.4599	1.1707	-1.1827
10	N	0.0198	-1.3022	3.1247
11	H	0.7721	-2.4500	3.0356
12	C	-0.9678	-1.5041	4.1974
13	H	-1.4364	-2.4830	4.0567
14	H	-0.4034	-1.5496	5.1304
15	H	-0.4478	-1.0338	2.2647
16	N	1.6812	-3.2522	3.2450

17	H	1.3842	-4.0182	3.8420
18	H	2.2183	-2.5614	3.8074
19	C	2.3826	-3.7345	2.0407
20	H	2.7222	-2.8556	1.4935
21	H	3.2680	-4.3058	2.3273
22	C	1.1537	-0.2783	3.5124
23	H	0.6018	0.6146	3.8789
24	O	1.9697	-0.8118	4.4061
25	C	1.4639	-4.5760	1.1665
26	H	1.1085	-5.4382	1.7402
27	H	0.5801	-3.9852	0.9075
28	C	-2.0504	-0.4309	4.2735
29	H	-1.5875	0.5496	4.4087
30	H	-2.5853	-0.3956	3.3180
31	H	4.7789	-0.0018	0.5576
32	H	1.0762	1.7048	-0.7620
33	C	2.1511	-5.0581	-0.1101
34	H	2.5014	-4.1910	-0.6775
35	H	3.0430	-5.6334	0.1555
36	C	-3.0451	-0.6824	5.4066
37	H	-2.5022	-0.7259	6.3556
38	H	-3.5064	-1.6657	5.2717
39	C	1.2376	-5.9086	-0.9891
40	H	0.3503	-5.3478	-1.2921
41	H	1.7497	-6.2357	-1.8957
42	H	0.8994	-6.8013	-0.4577
43	C	-4.1343	0.3841	5.4908
44	H	-4.8290	0.1809	6.3081
45	H	-3.7029	1.3737	5.6593
46	H	-4.7136	0.4301	4.5654

TS2N
Energy (POTENTIAL) = -773.501454343 Eh
Number of Imaginary Frequencies = 1

	Atom	X	Y	Z
1	C	3.2275	1.0516	0.8225
2	C	1.8833	1.0773	1.1730
3	C	0.8915	0.7418	0.2467
4	C	1.2806	0.3998	-1.0501
5	C	2.6255	0.3645	-1.4013
6	C	3.6051	0.6876	-0.4670
7	H	1.5951	1.3586	2.1788
8	H	0.5244	0.1824	-1.7909
9	H	4.6513	0.6660	-0.7432
10	N	-1.4819	0.6821	-0.2748
11	H	-0.8491	-1.8717	0.2599
12	C	-2.8400	0.9615	0.1753
13	H	-3.2186	0.1466	0.8103
14	H	-2.8611	1.8645	0.8025
15	H	-1.4050	-0.6961	-0.7497
16	N	-1.2617	-1.8613	-0.6959
17	H	0.2112	-0.8179	2.1831
18	C	-2.5223	-2.6288	-0.7696
19	H	-2.9503	-2.4833	-1.7619
20	H	-3.2085	-2.1870	-0.0471
21	C	-0.5422	0.7670	0.6654
22	H	-0.7285	1.4227	1.5170
23	O	-0.6086	-0.7919	1.6778
24	H	-0.5791	-2.1908	-1.3722
25	C	-3.7870	1.1463	-1.0057
26	H	-3.7426	0.2537	-1.6391
27	H	-3.4282	1.9774	-1.6213

28	C	-2.3220	-4.1098	-0.4795
29	H	-1.6015	-4.5212	-1.1938
30	H	-1.8777	-4.2187	0.5145
31	H	3.9799	1.3179	1.5537
32	H	2.9091	0.0947	-2.4107
33	C	-5.2339	1.3997	-0.5877
34	H	-5.5818	0.5664	0.0309
35	H	-5.2752	2.2897	0.0480
36	C	-3.6252	-4.9045	-0.5513
37	H	-4.0680	-4.7825	-1.5445
38	H	-4.3424	-4.4835	0.1593
39	C	-3.4289	-6.3902	-0.2590
40	H	-4.3730	-6.9347	-0.3204
41	H	-2.7362	-6.8436	-0.9720
42	H	-3.0205	-6.5437	0.7426
43	C	-6.1772	1.5798	-1.7751
44	H	-7.2030	1.7635	-1.4490
45	H	-5.8708	2.4245	-2.3971
46	H	-6.1858	0.6902	-2.4101

TS1WW
Energy (POTENTIAL) = -712.579697000 Eh
Number of Imaginary Frequencies = 1

	Atom	X	Y	Z
1	C	-0.5939	0.3945	-0.5285
2	C	-1.4928	1.4409	-0.3229
3	C	-2.8160	1.1811	0.0165
4	C	-3.2521	-0.1335	0.1481
5	C	-2.3596	-1.1805	-0.0614
6	C	-1.0357	-0.9211	-0.3996
7	C	0.8508	0.7205	-0.8785
8	H	-1.1572	2.4653	-0.4361
9	H	-0.3485	-1.7391	-0.5598
10	H	-4.2821	-0.3409	0.4069
11	N	1.5813	1.0049	0.4461
12	C	3.0310	1.3328	0.3191
13	H	1.4962	0.1216	1.0892
14	C	3.3007	2.6373	-0.4127
15	H	3.4972	0.4919	-0.1883
16	H	3.4203	1.3722	1.3363
17	H	2.7349	3.4448	0.0631
18	H	2.9496	2.5657	-1.4443
19	O	1.5351	-0.2171	-1.6019
20	O	1.8677	-2.3396	-0.2423
21	H	1.6702	-1.1010	-1.0816
22	H	2.7592	-2.6913	-0.3251
23	O	1.5697	-1.1856	1.8620
24	H	1.7338	-1.8270	0.8893
25	H	0.7063	-1.4239	2.2149
26	H	0.8691	1.6615	-1.4292
27	H	1.0996	1.7702	0.9170
28	H	-3.5056	2.0011	0.1687
29	H	-2.6953	-2.2049	0.0349
30	C	4.7899	2.9846	-0.4118
31	H	5.3483	2.1659	-0.8746
32	H	5.1438	3.0554	0.6208
33	C	5.0883	4.2885	-1.1469
34	H	4.5660	5.1293	-0.6844
35	H	6.1561	4.5140	-1.1365
36	H	4.7696	4.2334	-2.1903

TS2WW

Energy (POTENTIAL) = -712.566653188 Eh
Number of Imaginary Frequencies = 1

	Atom	X	Y	Z
1	C	-3.5036	1.0547	-0.2586
2	C	-4.0465	1.8041	0.7914
3	C	-3.2761	2.0924	1.9070
4	C	-1.9613	1.6381	1.9903
5	C	-1.4142	0.8974	0.9479
6	C	-2.1803	0.6109	-0.1739
7	C	-4.2619	0.7105	-1.4598
8	H	-5.0581	2.1793	0.7267
9	H	-1.7559	0.0418	-0.9910
10	H	-1.3652	1.8663	2.8639
11	N	-5.5573	0.7174	-1.5218
12	C	-6.3009	0.4052	-2.7399
13	H	-6.1003	1.2442	-0.8276
14	C	-7.5961	-0.3317	-2.4254
15	H	-5.6587	-0.1864	-3.3920
16	H	-6.5121	1.3517	-3.2436
17	H	-8.1925	0.2782	-1.7417
18	H	-7.3622	-1.2634	-1.9026
19	O	-3.7182	2.5174	-2.6784
20	H	-3.7385	0.1822	-2.2408
21	H	-2.9731	2.9144	-2.2155
22	O	-5.6808	3.8296	-2.1052
23	H	-4.6691	3.1812	-2.4108
24	H	-6.1265	4.0800	-2.9196
25	O	-7.2236	2.6485	-0.4294
26	H	-6.6602	3.1995	-1.0814
27	H	-7.3321	3.1810	0.3644
28	C	-8.4068	-0.6320	-3.6853
29	H	-8.6161	0.3051	-4.2094
30	H	-7.8044	-1.2394	-4.3675
31	H	-0.3925	0.5472	1.0068
32	H	-3.6988	2.6768	2.7132
33	C	-9.7184	-1.3516	-3.3817
34	H	-10.2794	-1.5579	-4.2950
35	H	-9.5379	-2.3049	-2.8793
36	H	-10.3546	-0.7490	-2.7294

TS1NW
Energy (POTENTIAL) = -850.013761948 Eh
Number of Imaginary Frequencies = 1

	Atom	X	Y	Z
1	C	-0.4631	0.2587	-0.5582
2	C	-1.2353	1.2664	0.0244
3	C	-2.5483	1.0271	0.4136
4	C	-3.1171	-0.2280	0.2096
5	C	-2.3636	-1.2308	-0.3915
6	C	-1.0470	-0.9860	-0.7729
7	C	0.9998	0.5065	-0.9764
8	H	-0.8125	2.2540	0.1717
9	H	-0.4524	-1.7596	-1.2368
10	H	-4.1393	-0.4177	0.5103
11	N	1.7478	0.9206	0.3216
12	C	3.1429	1.3477	0.0596
13	H	1.6773	-0.1218	1.1889
14	C	4.1586	0.2194	0.2175
15	H	3.3850	2.1560	0.7527
16	H	3.2072	1.7572	-0.9528
17	H	3.8417	-0.6203	-0.4005
18	H	4.1614	-0.1263	1.2559

19	O	1.6093	-0.5010	-1.5885
20	O	1.8977	-2.7314	-0.3959
21	H	1.7787	-1.8310	-0.8932
22	H	2.7831	-3.0362	-0.6185
23	H	1.7495	-1.9128	1.2434
24	H	1.0002	1.4400	-1.5821
25	H	1.2503	1.6964	0.7466
26	H	-3.1291	1.8179	0.8711
27	H	-2.8008	-2.2065	-0.5622
28	C	5.5708	0.6529	-0.1699
29	H	5.8678	1.5165	0.4341
30	H	5.5688	0.9914	-1.2104
31	C	6.5966	-0.4656	-0.0011
32	H	6.3390	-1.3292	-0.6191
33	H	7.5977	-0.1387	-0.2890
34	H	6.6435	-0.8044	1.0368
35	H	2.3799	-1.1393	2.5716
36	C	0.3122	-1.2565	2.6249
37	H	-0.4623	-1.3523	1.8661
38	H	0.3005	-2.1670	3.2277
39	C	0.0456	-0.0362	3.4943
40	H	0.0733	0.8601	2.8687
41	H	0.8476	0.0683	4.2326
42	C	-1.3030	-0.1140	4.2076
43	H	-2.0925	-0.2430	3.4619
44	H	-1.3266	-1.0061	4.8403
45	C	-1.5969	1.1224	5.0529
46	H	-1.6234	2.0235	4.4354
47	H	-2.5606	1.0385	5.5586
48	H	-0.8317	1.2687	5.8192
49	N	1.6049	-1.1408	1.9144

TS2NW
Energy (POTENTIAL) = -849.998025454 Eh
Number of Imaginary Frequencies = 1

	Atom	X	Y	Z
1	C	-3.7194	1.0141	-0.0959
2	C	-4.3166	1.5715	1.0412
3	C	-3.5447	1.8771	2.1526
4	C	-2.1754	1.6245	2.1478
5	C	-1.5763	1.0595	1.0254
6	C	-2.3440	0.7538	-0.0882
7	C	-4.4724	0.6568	-1.2942
8	H	-5.3791	1.7654	1.0625
9	H	-1.8815	0.3258	-0.9674
10	H	-1.5786	1.8627	3.0184
11	N	-5.7316	0.8781	-1.4537
12	C	-6.4670	0.5113	-2.6612
13	H	-6.2183	1.5986	-0.8652
14	C	-7.7812	-0.1804	-2.3175
15	H	-5.8333	-0.1323	-3.2706
16	H	-6.6356	1.4402	-3.2098
17	H	-8.3470	0.4486	-1.6262
18	H	-7.5711	-1.1165	-1.7923
19	O	-3.4837	2.3151	-2.7448
20	H	-3.9802	0.0299	-2.0222
21	H	-2.9419	2.7866	-2.1046
22	O	-5.5704	3.5613	-2.8987
23	H	-4.4809	2.9549	-2.8386
24	H	-5.4350	4.3602	-3.4159
25	H	-6.4636	3.5590	-1.3146
26	H	-6.7320	3.7401	0.3172

27	C	-8.6273	-0.4567	-3.5592
28	H	-8.8184	0.4870	-4.0782
29	H	-8.0584	-1.0810	-4.2545
30	H	-0.5136	0.8579	1.0195
31	H	-4.0127	2.3082	3.0274
32	C	-9.9534	-1.1360	-3.2268
33	H	-10.5398	-1.3256	-4.1277
34	H	-9.7918	-2.0940	-2.7271
35	H	-10.5577	-0.5141	-2.5622
36	C	-8.4321	3.2723	-0.7364
37	H	-8.6328	2.7997	-1.7010
38	H	-8.7879	4.3079	-0.8186
39	C	-9.2205	2.5553	0.3533
40	H	-8.8642	1.5229	0.4251
41	H	-9.0041	3.0244	1.3197
42	C	-10.7288	2.5605	0.1120
43	H	-11.0831	3.5939	0.0514
44	H	-10.9379	2.1080	-0.8623
45	C	-11.5064	1.8168	1.1955
46	H	-11.1933	0.7715	1.2552
47	H	-11.3423	2.2672	2.1775
48	H	-12.5804	1.8306	0.9993
49	N	-6.9865	3.1967	-0.4998

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