Supplementary information II– Computational Studies

A Stereoselective Organocascade and Multicomponent Approach for the Preparation of Tetrahydropyridines and Chimeric Derivatives

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A. Computational Details

All DFT calculations were performed with Gaussian 09 suit of programs using a ultrafine grid.[1] Full optimizations were conducted using M06-2X/def2-tzvp or B3LYP/def2-svp level of theory. The IEF-PCM [TFE] was used for inclusion of the solvent effect for all optimizations. All Cartesian coordinates are supplied in this ESI. Visualizations were done with the beta version of CYLview.[2] Frequency calculations at 295.15 K (1 atm) ensured that the stationary points represent either minima (no imaginary frequency) or transition states (single imaginary frequency) on the potential-energy surface, furnishing also the zero-point vibrational energies, from which the ZPE corrected electronic energies were determined. The IRC calculations were done ensuring that each transition state connects reagents and products. The Non Covalent Interaction (NCI) analysis was carried out with the NCIplot 3.0 software,[3] with VMD[4] as visual interface.

The conformational searches were done in gas phase using the Monte Carlo (MCMM) method as implemented as implemented in Macromodel (Version 9.9).[5] The energy minimization was carried out using the Polak-Ribiere Conjugate Gradient (PRCG), and the MMFF force field, using dielectric constant-dependent electrostatics (e=1) and normal cut-off points to model the non-bonded interactions. All heavy atoms and hydrogens at heteroatoms were included in the test for redundant conformers, using the default cutoff (maximum atom deviation) of 0.5 Å. All rotatable single bonds were included in the conformational search. The energy window for saving new structures was 5 kcal/mol relative to the current global minimum, using a maximum number of steps of 30000 and 1000 steps per rotable bond. Each search was continued until the global energy minima were found at least 10-20 times, thus giving confidence that all the relevant conformers had been found.

To refine the electronic energy, single-point calculations were performed using the M06-2X/def2-tzvp [IEF-PCM] geometries (except for **TS-1**, **TS-5.** and **TS-7** in which we use B3LYP/def2-svp [IEF-PCM]). The Grime D3[6] empirical dispersion was used for B3LYP and B97 functionals. In addition, the functional WB97XD was explored. The basis set 6-311+G(d,p) and def2-TZVP were also used in this study.

B. Discussion of Computational Results

Computational studies were initiated in order to investigate the reaction energy profile for the I-MCR. The relative energies and geometries for intermediates and transition states were calculated at **M06-2X/def2-tzvp/IEF-PCM** and **M062X/def2-tzvp/IEF-PCM//B3LYP/def2-svp/IEF-PCM**, although some transition states were not found in both cases. In the Scheme S1, it is shown the summary of all investigated intermediates and transition states and relative ZPE corrected electronic energies. In Figure S1, we represent the geometries of founded Transition States for both theories. In Tables S1 and S2 are the absolute electronic energy, zero-point corrections and the imaginary frequency for transition states at **M06-2X/def2-tzvp/IEF-PCM** and **M062X/def2-tzvp/IEF-PCM//B3LYP/def2-svp/IEF-PCM**. In Figures S2-S8 are the IRC analyses for the founded transition states.

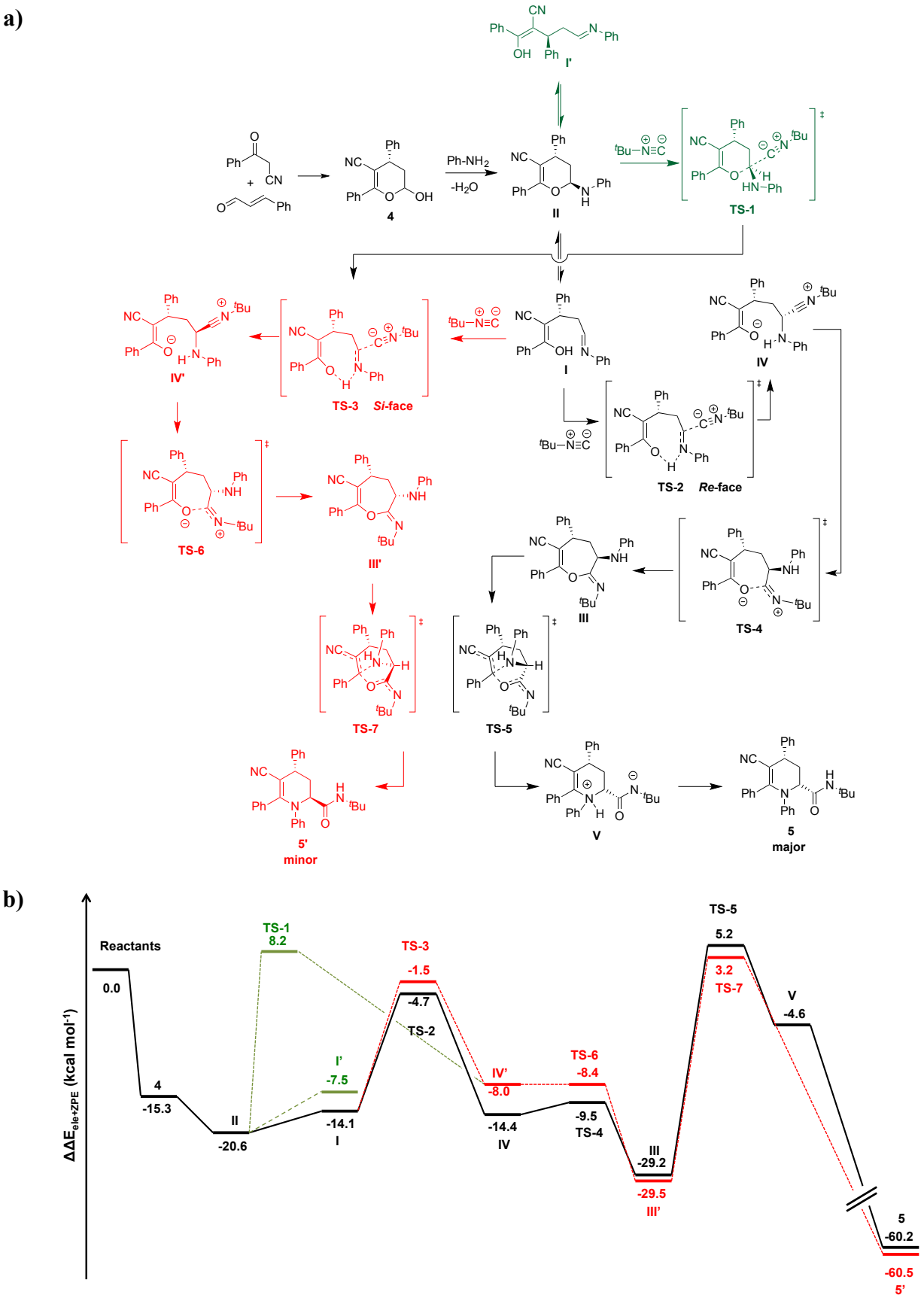
The results provided a full description of the reaction path for the stereoselective I-MCR, starting from the hemicetal derivative **4**. The addition of the aniline leads to the formation of the species **I**, **I'** and **II**, which can likely be in equilibrium. The lower energy intermediate **II** would lead to the minor diastereoisomer in the final process, via the transition state **TS-1** in a S_N2 mechanism, which presents a high asynchronous character, as observed by the IRC in Figure S7.

From our theoretical results, we concluded that the stereoselectivity of these reactions are based on kinetic control, closely related to the conformation of the starting imine **I**, and determined by the attack of the isocyanide to the formed iminium ion. An interesting point was the energetic preference for the highly substituted cyclic intermediate **I** over the acyclic intermediate **I'**. These findings are based on extensive conformational search, as indicated in Table S6. This conformation is the key for understanding the found experimental diastereoselectivity. The isocyanide can approach via the *Re* or *Si* face of the imine, but it has a clear preference for the face via **TS-2** that leads to the formation of the favored diastereoisomer, which is lower in energy than **TS-1**. Therefore, the H-bonding activates the imine for the isocyanide attack, and it is also responsible for the orientation of the enol and isocyanide **π**-systems, reducing the energy of **TS-2** by a stabilizing non-covalent interaction, as revealed by NCI analysis (Figure S9). Finally, a curious aspect of both **TS-2** and **TS-3** transition states are their concerted and asynchronous characters. The first step involves a proton transfer to the imine, followed by formation of the C-C bond. This aspect is evidenced by the shoulder presented in the start of both IRC calculations curves (Figures S2 and S3 for **TS-2** and **TS-3**, respectively). The α-adduct **III** is readily formed from the alkoxy attack to the nitrilium-ion in **IV** via **TS-4** ($\Delta\Delta E^{\ddagger}$ = 4.9 kcal mol^{-1}). These steps are not reversible, as the α-adduct **III** is 15.1

kcal mol^{-1} more stable than **I**, and the reverse reactions involves a total energy barrier of 24.5 kcal mol^{-1}. It is worth mentioning that in contrast to the classic mechanistic view of Ugi reaction, involving a sequence of equilibrium reactions before ending with the irreversible Mumm rearrangement and forming the thermodynamic product, in our case the stereochemistry is setted before this event. This scenario is even more evident analyzing the energies of intermediates **III**/**III'**, and products **5**/**5'** (see full conformational analysis in Table S7 and S8, respectively), in which both pairs showed essentially the same energy, with a slight preference in energy for the minoritary diastereoisomer pathway, discarding a scenario of thermodynamic control. Assuming a kinetic control, the diastereoselectivity can be determinated by the energy difference between **TS-2** and **TS-3** ($\Delta\Delta E_{ele+ZPE}$ = 3.1 kcal mol^{-1}), delivering a theoretical diastereoselectivity of >99:1 after Boltzmann analysis at 70 ºC, in excellent agreement with experimental results.

Finally, we also could find the **TS-5** responsible for the concerted migration of the exocyclic amine to the nitrile conjugate position and cleavage of C-O bond. The high-energy barrier for this step can be understood considering the crowd geometry of **TS-5**.

In order to check the reliability of these computational results, we describe in Tables S3-S4 the single point energies and ZPE corrected electronic energies for the other investigated levels of theory. Finally, in Table S5 the relative reaction free energy profile and barriers for all investigated levels of theory are represented. The B3LYP presents an endothermic reaction for the formation of hemiketal **4**, differing drastically from others functionals. Not surprisingly, the WB97XD is the functional that is more closed in energy with M06-2X, and both are very well documented in literature as appropriate to describe reaction mechanisms. A similar increase in energy of hemiketal **4**, compared to M06-2X, is related to the second group of DFTs (B97D3, B3LYP-D3), and is also observed for other intermediates and transition states of the reaction energy profile. Despite these trends, the reaction energy barriers of reaction energy profile for all employed levels of theory are similar and consistent in favor of major diastereoisomer, except for the B3LYP without the empirical dispersion, which predict the opposite diastereoselectivity. This result reinforces our conclusions that the non-covalent interactions presented in **TS-2** are responsible for the decrease in the reaction energy by this reaction path. A final analysis comparing the Aldrich's (def2-TZVP) and Pople (6-311+G(d,p)) basis sets showed consistent results which is not dependent of the employed basis set.



Scheme 1. (a) Summary of all investigated intermediates and transition states. **(b)** Reaction energy profile for M06-2X/def2-TZVP level of theory.

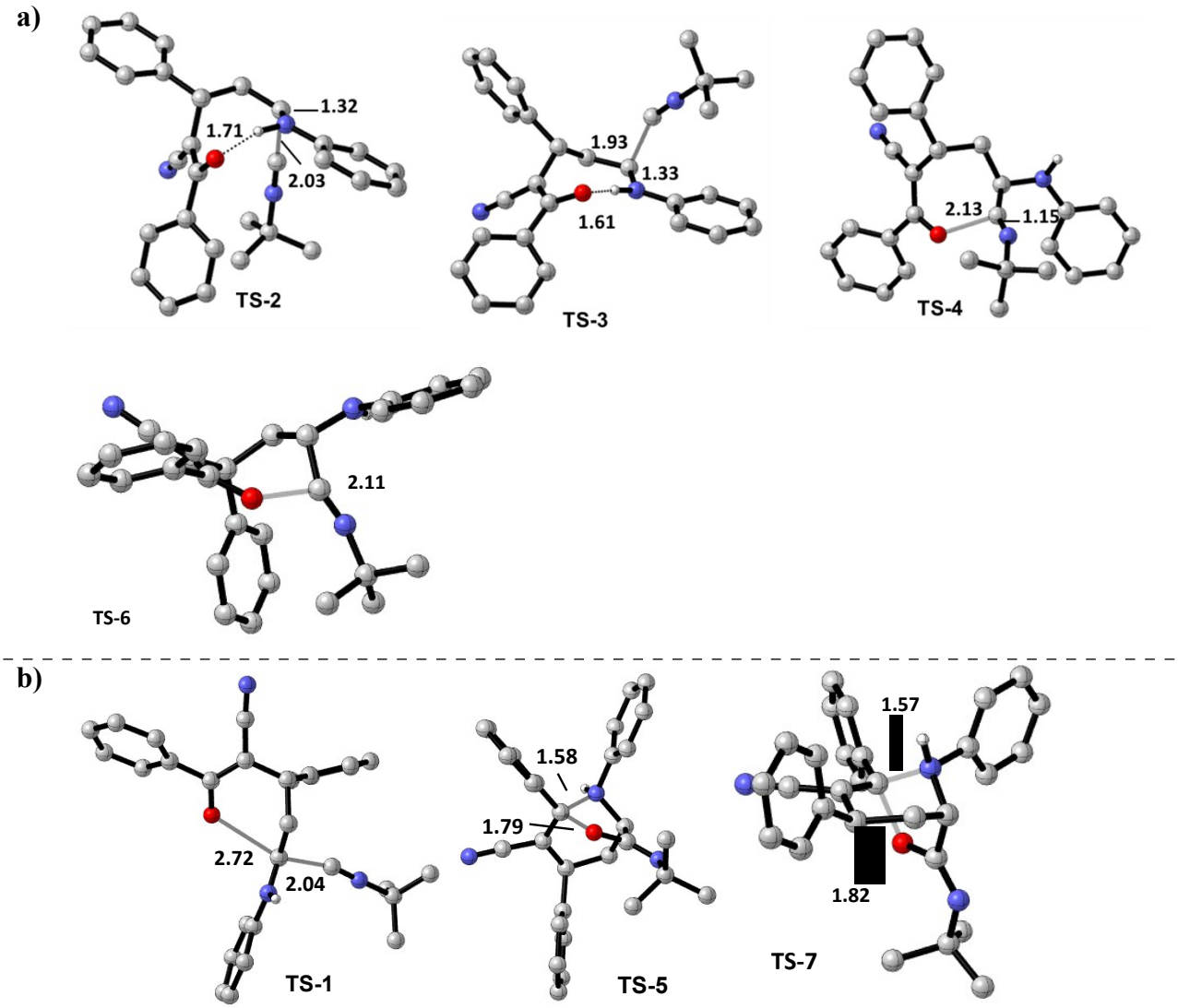


Figure S1. Calculated structures of founded Transition States for: **a)** M06-2X/def2-tzvp/IEF-PCM; **b)** M062X/def2-tzvp/IEF-PCM//B3LYP/def2-svp/IEF-PCM. Distances in angstrom.

Table S1: Energies (in Hartree) at **M062X/def2-TZVP/IEFPCM**.

Name	ΔE_{ele}	ZPE correction	Imaginary Frequency (cm^{-1})	$\Delta E_{ele+ZPE}$
water	-76.43341074	0.021402	-	-76.41200874
3-phenyl-3-oxo propanenitrile	-477.1263456	0.138301	-	-476.9880446
cinnamaldehyde	-422.9576492	0.144454	-	-422.8131952
aniline	-287.5916219	0.117904	-	-287.4737179
^{t}Bu-isocyanide	-250.6494782	0.130704	-	-250.5187742
4	-900.115726	0.290101	-	-899.825625
II	-1111.279826	0.384018	-	-1110.895808
I	-1111.266442	0.381046	-	-1110.885396
I'	-1111.255607	0.380696	-	-1110.874911
TS-1		*not founded*		
TS-2	-1361.903344	0.514194	-269.41	-1361.38915
TS-3	-1361.897728	0.513553	-351.42	-1361.384175
IV	-1361.921234	0.516565	-	-1361.404669
IV'	-1361.910179	0.515759	-	-1361.39442
TS-4	-1361.912440	0.515605	-192.26	-1361.396835
TS-6	-1361.911171	0.516080	-148.92	-1361.395091
III	-1361.946795	0.518546	-	-1361.428249
III'	-1361.946979	0.518222	-	-1361.428757
TS-5		*not founded*		
TS-7		*not founded*		
V	-1361.908283	0.519184	-	-1361.389099
5	-1361.997102	0.519408	-	-1361.477694
5'	-1361.997043	0.518833	-	-1361.47821

Table S2: Energies (in Hartree) at **M062X/def2-tzvp/IEF-PCM//B3LYP/def2-svp/IEF-PCM**.

	B3LYP/def2-svp/IEF-PCM			M062X/def2-tzvp/IEF-PCM//B3LYP/def2-svp/IEF-PCM	
Name	**ΔE_{ele}**	**ZPE correction**	**Imaginary Frequency (cm^{-1})**	**ΔE_{ele}**	**$\Delta E_{ele+ZPE}$ ***
TS-1	-1360.966607	0.509264	-254.37	-1361.877915	-1361.368651
TS-5	-1360.967406	0.513634	-248.67	-1361.887018	-1361.373384
TS-7	-1360.972683	0.513751	-252.28	-1361.890323	-1361.376572

* Obtained from the sum of ΔE_{ele} at **M062X/def2-tzvp/IEF-PCM//B3LYP/def2-svp/IEF-PCM** and **ZPE correction** at **B3LYP/def2-svp/IEF-PCM**.

Table S3: Single point Electronic Energies (in Hartree) at different levels of theory for **M062X/def2-tzvp/IEF-PCM** geometries.

Name	B97D3/ def2-TZVP	B3LYP-D3/ def2-TZVP	B3LYP/ def2-TZVP	WB97XD/ def2-TZVP	M06-2X/ 6-311+G(d,p)
water	-76.430052	-76.470149	-76.470141	-76.444965	-76.428591
3-phenyl-3-oxo propanenitrile	-477.009336	-477.338092	-477.325144	-477.150599	-477.074052
cinnamaldehyde	-422.869352	-423.160199	-423.148993	-422.989738	-422.910960
aniline	-287.530828	-287.731936	-287.724753	-287.618055	-287.560770
^{t}Bu-isocyanide	-250.605155	-250.782440	-250.771218	-250.684153	-250.625041
4	-899.890840	-900.512180	-900.475097	-900.167276	-900.018192
II	-1110.999931	-1111.780252	-1111.728987	-1111.347449	-1111.158733
TS-1*	-1361.577387	-1362.523338	-1362.452716	-1361.983144	-1361.736573
I	-1110.995641	-1111.772593	-1111.722334	-1111.333731	-1111.146367
I'	-1110.983538	-1111.760548	-1111.713006	-1111.323035	-1111.135137
TS-2	-1361.595437	-1362.544774	-1362.465048	-1362.008465	-1361.759549
TS-3	-1361.590094	-1362.539706	-1362.464898	-1362.003189	-1361.753675
IV	-1361.609643	-1362.559759	-1362.477428	-1362.028228	-1361.777885
IV'	-1361.598921	-1362.550446	-1362.479411	-1362.017897	-1361.765462
TS-4	-1361.603454	-1362.553243	-1362.480668	-1362.019201	-1361.767817
TS-6	-1361.602960	-1362.552385	-1362.473418	-1362.019173	-1361.767347
III	-1361.626468	-1362.580498	-1362.505326	-1362.053203	-1361.802218
III'	-1361.627948	-1362.580588	-1362.497669	-1362.053799	-1361.803472
TS-5*	-1361.581851	-1362.525345	-1362.443553	-1361.997081	-1361.748151
TS-7*	-1361.584865	-1362.528392	-1362.449535	-1361.999540	-1361.751225
V	-1361.594804	-1362.544176	-1362.458550	-1362.017878	-1361.766616
5	-1361.679679	-1362.631488	-1362.546743	-1362.108468	-1361.854622
5'	-1361.679431	-1362.631581	-1362.553171	-1362.107823	-1361.853927

* Geometry at **B3LYP/def2-svp/IEF-PCM.**

Table S4: ZPE corrected Electronic Energies** (in Hartree) at different levels of theory for **M062X/def2-tzvp/IEF-PCM** geometries.

Name	B97D3/ def2-TZVP	B3LYP-D3/ def2-TZVP	B3LYP/ def2-TZVP	WB97XD/ def2-TZVP	M06-2X/ 6-311+G(d,p)
water	-76.40865017	-76.44874727	-76.44873897	-76.42356272	-76.40718889
3-phenyl-3-oxo propanenitrile	-476.8710352	-477.1997905	-477.186843	-477.0122982	-476.9357513
cinnamaldehyde	-422.7248978	-423.0157445	-423.0045389	-422.8452839	-422.7665064
aniline	-287.4129238	-287.6140322	-287.6068493	-287.5001509	-287.442866
^{t}Bu-isocyanide	-250.474451	-250.6517356	-250.6405137	-250.5534488	-250.4943366
4	-899.6007393	-900.2220791	-900.1849957	-899.8771748	-899.7280907
II	-1110.615913	-1111.396234	-1111.344969	-1110.963431	-1110.774715
TS-1*	-1361.068123	-1362.014074	-1361.943452	-1361.47388	-1361.227309
I	-1110.614595	-1111.391547	-1111.341288	-1110.952685	-1110.765321
I'	-1110.602842	-1111.379852	-1111.33231	-1110.942339	-1110.754441
TS-2	-1361.081243	-1362.03058	-1361.950854	-1361.494271	-1361.245355
TS-3	-1361.076541	-1362.026153	-1361.951345	-1361.489636	-1361.240122
IV	-1361.093078	-1362.043194	-1361.960863	-1361.511663	-1361.26132
IV'	-1361.083162	-1362.034687	-1361.963652	-1361.502138	-1361.249703
TS-4	-1361.087849	-1362.037638	-1361.965063	-1361.503596	-1361.252212
TS-5	-1361.08688	-1362.036305	-1361.957338	-1361.503093	-1361.251267
III	-1361.107922	-1362.061952	-1361.98678	-1361.534657	-1361.283672
III'	-1361.109726	-1362.062366	-1361.979447	-1361.535577	-1361.28525
TS-5*	-1361.068217	-1362.011711	-1361.929919	-1361.483447	-1361.234517
TS-7*	-1361.071114	-1362.014641	-1361.935784	-1361.485789	-1361.237474
V	-1361.07562	-1362.024992	-1361.939366	-1361.498694	-1361.247432
5	-1361.160271	-1362.11208	-1362.027335	-1361.58906	-1361.335214
5'	-1361.160598	-1362.112748	-1362.034338	-1361.58899	-1361.335094

* Geometry and ZPE correction at **B3LYP/def2-svp/IEF-PCM. ** ** Obtained from the sum of ΔE_{ele} at **M062X/def2-tzvp/IEF-PCM** and **ZPE correction** at **M062X/def2-tzvp/IEF-PCM**.

Table S5. ZPE corrected energy profiles for all investigated levels of theory**.** Energies** (in kcal mol^{-1}) for studied compounds at different levels of theory for **M062X/def2-tzvp/IEF-PCM** geometries. Reaction barrier in bracket.

	B97D3/ def2-TZVP	**B3LYP-D3/ def2-TZVP**	**B3LYP/ def2-TZVP**	**WB97XD/ def2-TZVP**	**M06-2X/ 6-311+G(d,p)**	**M062X/ def2-TZVP**
Reactant	0.0	0.0	0.0	0.0	0.0	0.0
4	-3.0	-4.1	4.0	-12.3	-16.2	-15.3
II	-9.9	-9.7	2.8	-18.4	-23.1	-20.6
I	-9.0	-6.7	5.1	-11.6	-17.2	-14.1
I'	-1.7	0.6	10.8	-5.1	-10.4	-7.5
TS-1*	4.1 [14.0]	11.6 [21.3]	29.2 [26.4]	8.6 [27.0]	3.1 [26.2]	8.2 [28.8]
TS-2	-4.1 [4.9]	1.2 [8.0]	24.6 [19.4]	-4.2 [7.4]	-8.2 [9.0]	-4.7 [9.4]
TS-3	-1.2 [7.8]	4.0 [10.7]	24.3 [19.1]	-1.3 [10.4]	-4.9 [12.3]	-1.5 [12.5]
IV	-11.6	-6.7	18.3	-15.1	-18.2	-14.4
IV'	-5.3	-1.3	16.5	-9.1	-10.9	-8.0
TS-4	-8.3 [3.3]	-3.2 [3.5]	15.7 [-2.6]	-10.0 [5.1]	-12.5 [5.7]	-9.5 [4.9]
TS-6	-7.7 [-2.3]	-2.4 [-1.0]	20.5 [4.0]	-9.7 [-0.6]	-11.9 [-1.0]	-8.4 [-0.4]
III	-20.9	-18.4	2.0	-29.5	-32.3	-29.2
III'	-22.0	-18.7	6.6	-30.1	-33.2	-29.5
TS-5*	4.0 [24.9]	13.1 [31.5]	37.7 [35.7]	2.6 [32.1]	-1.4 [30.8]	5.2 [34.4]
TS-7*	2.2 [24.2]	11.2 [29.9]	34.0 [27.4]	1.1 [31.2]	-3.3 [30.0]	3.2 [32.7]
V	-0.6	4.7	31.8	-6.9	-9.5	-4.6
5	-53.7	-49.9	-23.4	-63.7	-64.6	-60.2
5'	-53.9	-50.3	-27.8	-63.6	-64.5	-60.5

* Geometry and ZPE correction at **B3LYP/def2-svp/IEF-PCM. ** ** Obtained from the sum of ΔE_{ele} at **M062X/def2-tzvp/IEF-PCM** and **ZPE correction** at **M062X/def2-tzvp/IEF-PCM**.

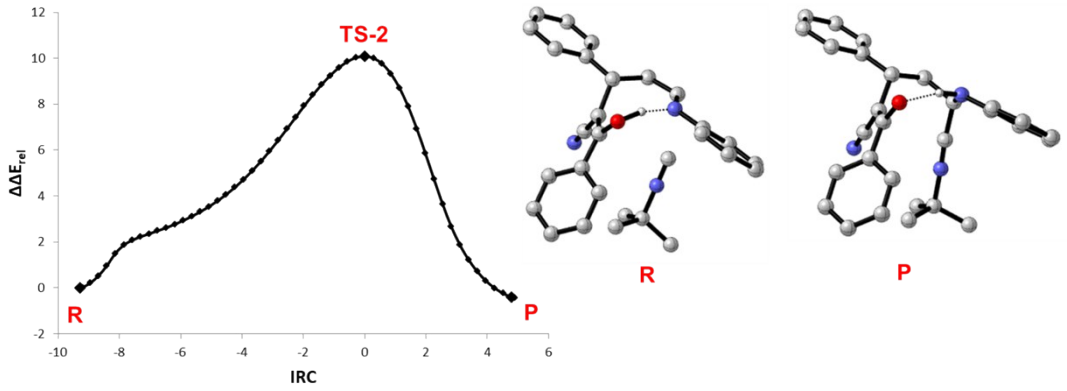


Figure S2. IRC for **TS-2** at **M062X/def2-tzvp/IEF-PCM**.

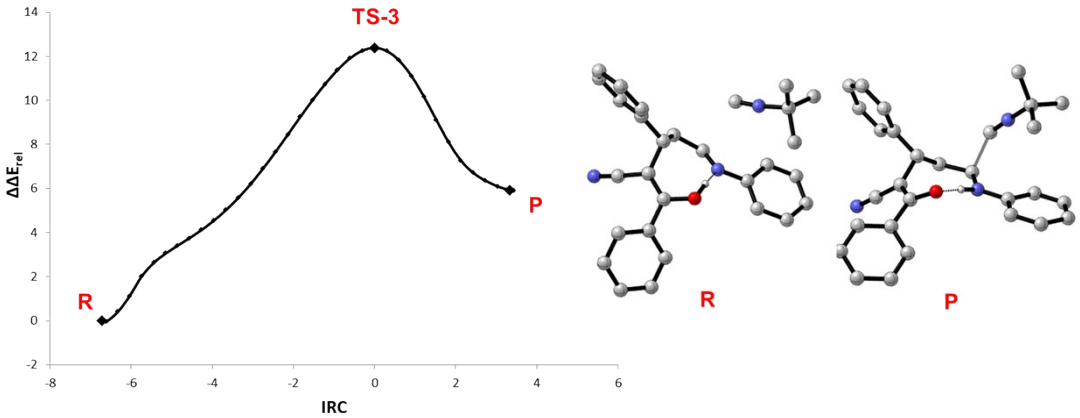


Figure S3. IRC for **TS-3** at **M062X/def2-tzvp/IEF-PCM**.

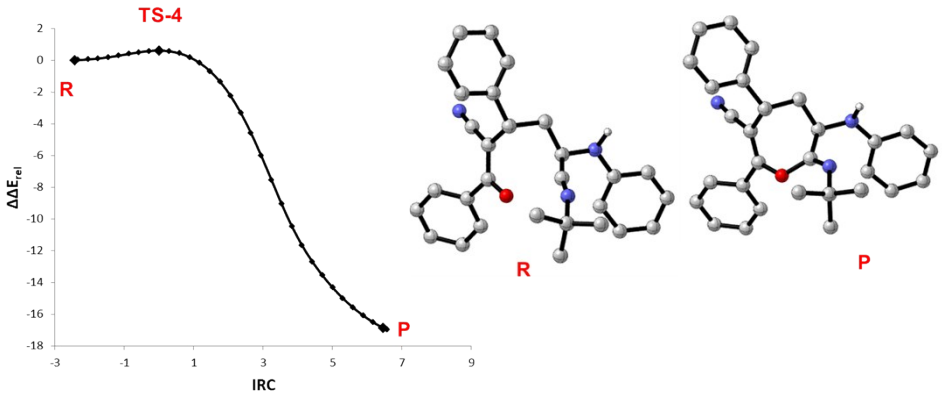


Figure S4. IRC for **TS-4** at **M062X/def2-tzvp/IEF-PCM**.

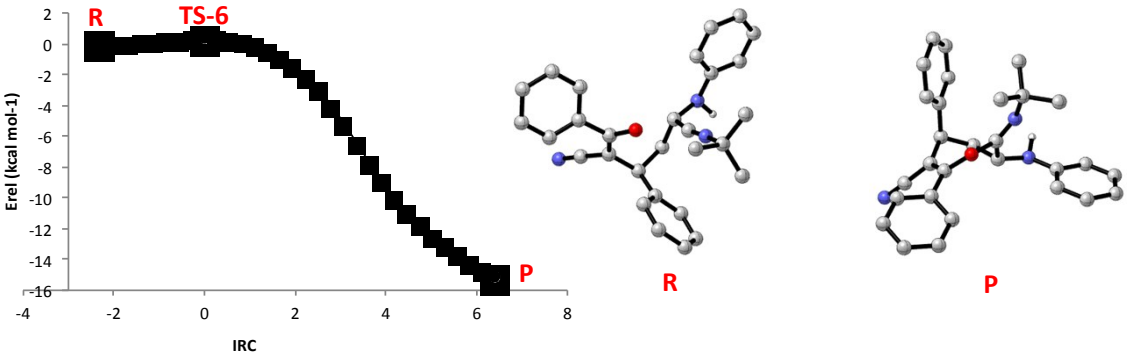


Figure S5. IRC for **TS-6** at **M062X/def2-tzvp/IEF-PCM**.

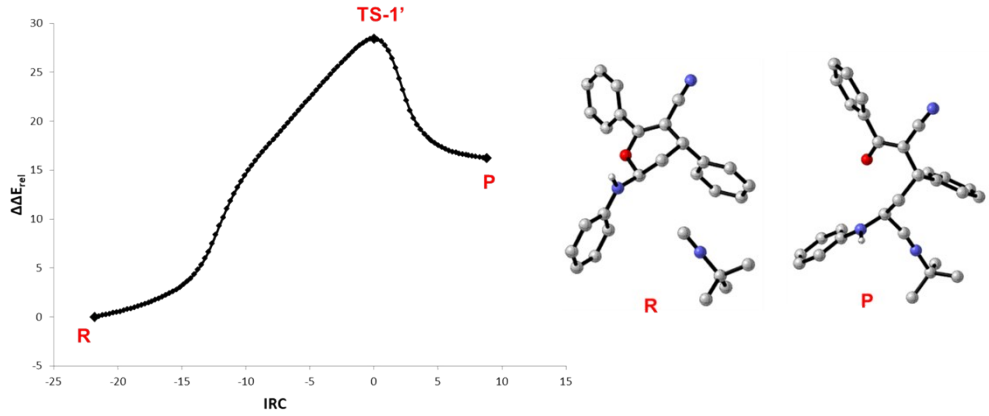


Figure S6. IRC for **TS-1** at **B3LYP/def2-svp/IEF-PCM**.

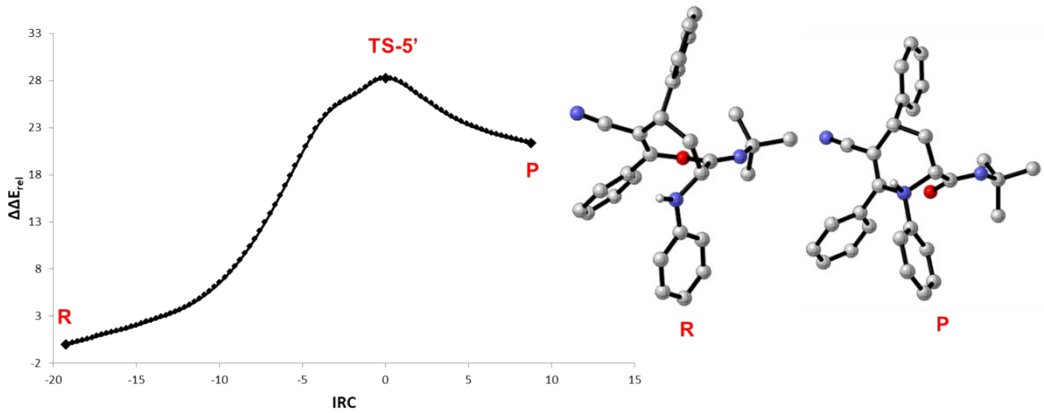


Figure S7. IRC for **TS-5** at **B3LYP/def2-svp/IEF-PCM**.

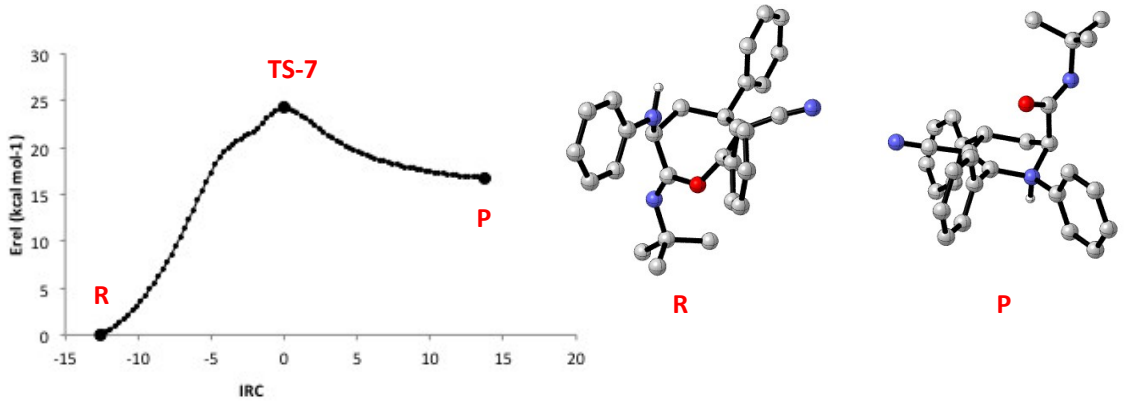
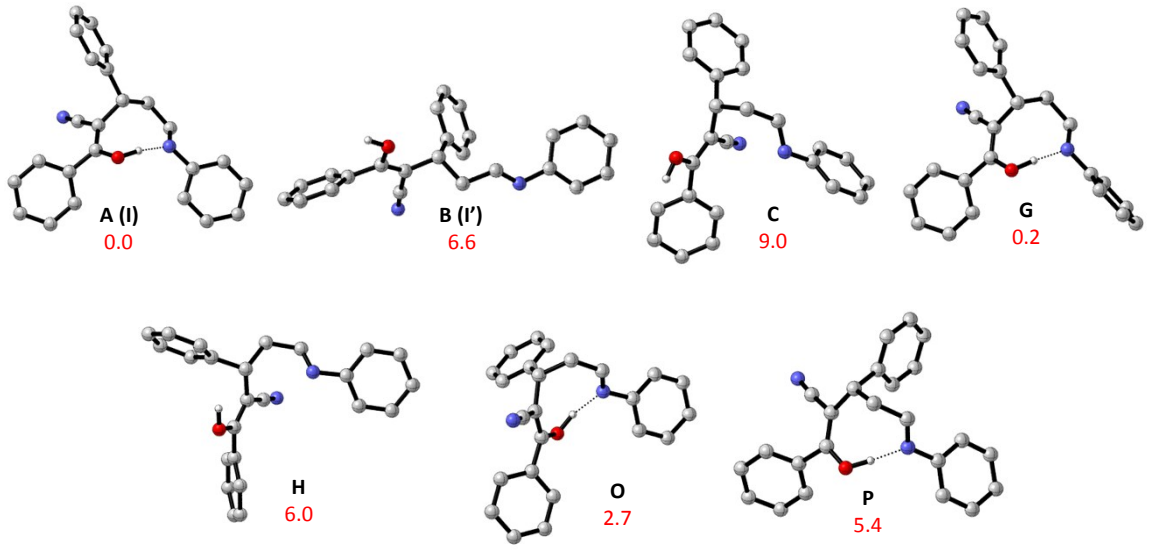


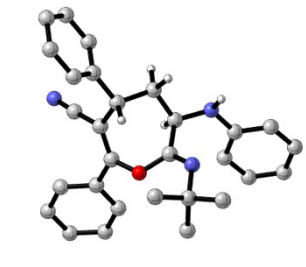
Figure S8. IRC for **TS-7** at **B3LYP/def2-svp/IEF-PCM**.

Table S6: Energies (in Hartree) for conformers of structures **I** and **I'** at **M062X/def2-tzvp/IEFPCM.**

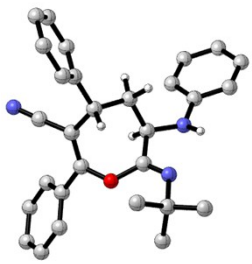


Conformer	ΔE_{ele}	ZPE correction	$\Delta E_{ele+ZPE}$	$\Delta\Delta E_{ele+ZPE}$
A (I)	***-1111.266442***	0.381802	-1110.88464	0.0
B (I')	***-1111.255607***	0.381488	-1110.874119	6.6
C	-1111.252058	0.381735	-1110.870323	9.0
D	-1111.251581	0.382040	-1110.869541	9.5
E	-1111.252695	0.381827	-1110.870868	8.6
F	-1111.257135	0.381705	-1110.87543	5.8
G	-1111.266171	0.381883	-1110.884288	0.2
H	-1111.256225	0.381218	-1110.875007	6.0
I	-1111.255845	0.381901	-1110.873944	6.7
J	-1111.254184	0.382027	-1110.872157	7.8
K	-1111.252682	0.381841	-1110.870841	8.7
L	-1111.252941	0.382134	-1110.870807	8.7
M	-1111.252621	0.382260	-1110.870361	9.0
N	-1111.253105	0.381672	-1110.871433	8.3
O	-1111.262177	0.381916	-1110.880261	2.7
P	-1111.257719	0.381606	-1110.876113	5.4
Q	-1111.254855	0.381521	-1110.873334	7.1
R	-1111.25557	0.381478	-1110.874092	6.6
S	-1111.254855	0.381522	-1110.873333	7.1
T	-1111.255164	0.381541	-1110.873623	6.9
U	-1111.255508	0.381488	-1110.87402	6.7
V	-1111.25071	0.381681	-1110.869029	9.8
W	-1111.253391	0.381863	-1110.871528	8.2
X	-1111.253665	0.381612	-1110.872053	7.9

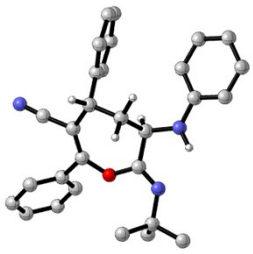
Table S7: Energies (in Hartree) for conformers of structures **III** and **III'** at **M062X/def2-tzvp/IEFPCM.**



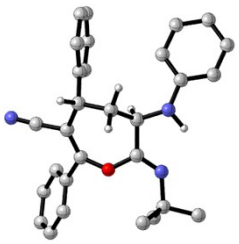
III
0.3



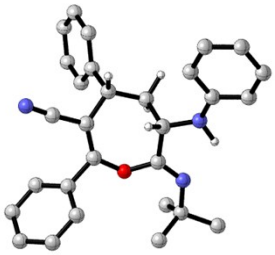
III-b
2.4



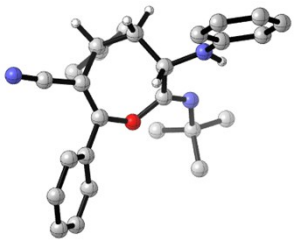
III-c
2.5



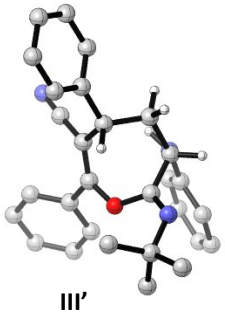
III-d
2.4



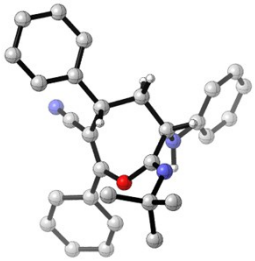
III'-b
2.6



III'-c
3.4



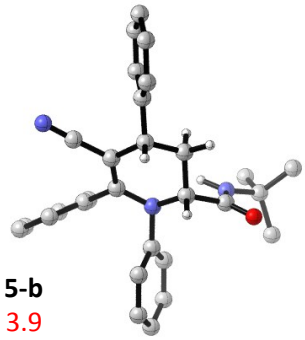
III'
0.0



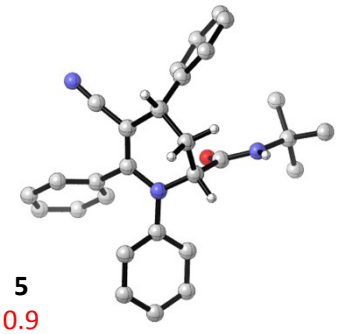
III'-d
4.4

M062X/def2-tzvp/IEFPCM				
Name	**ΔE_{ele}**	**ZPE correction**	**$\Delta E_{ele+ZPE}$**	**$\Delta\Delta E_{ele+ZPE}$**
III	***-1361.946795***	0.518546	-1361.428249	0.3
III-b	-1361.94301	0.518156	-1361.424854	2.4
III-c	-1361.94267	0.518007	-1361.424663	2.5
III-d	-1361.942642	0.517855	-1361.424787	2.4
III'-b	-1361.942809	0.518217	-1361.424592	2.6
III'-c	-1361.941546	0.518330	-1361.423216	3.4
III'	***-1361.946979***	0.518306	-1361.428673	0.0
III'-d	-1361.939755	0.518159	-1361.421596	4.4

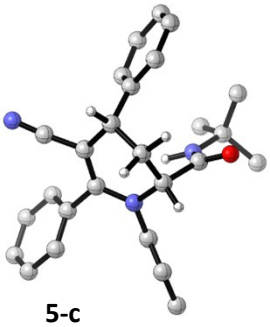
Table S8: Energies (in Hartree) for conformers of structures **5** and **5'** at **M062X/def2-tzvp/IEFPCM.**



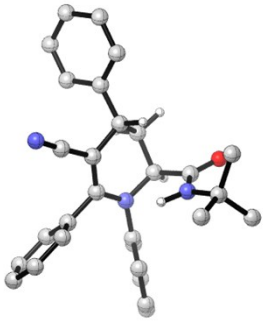
5-b
3.9



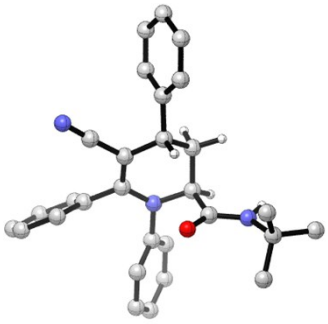
5
0.9



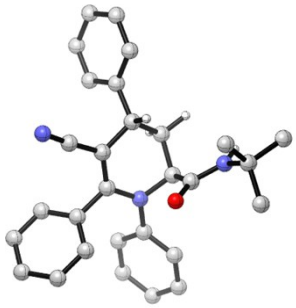
5-c
1.9



5'-b
1.6

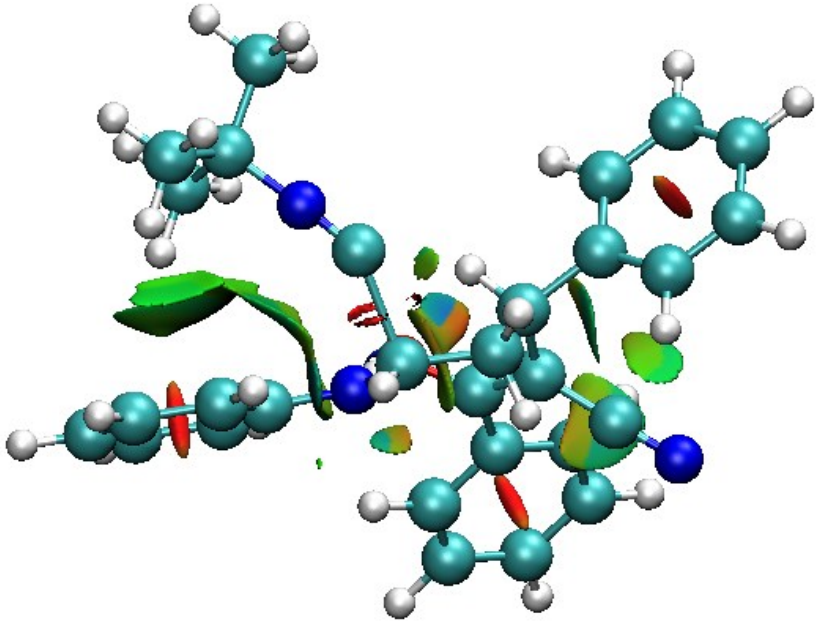


5'-c
1.4

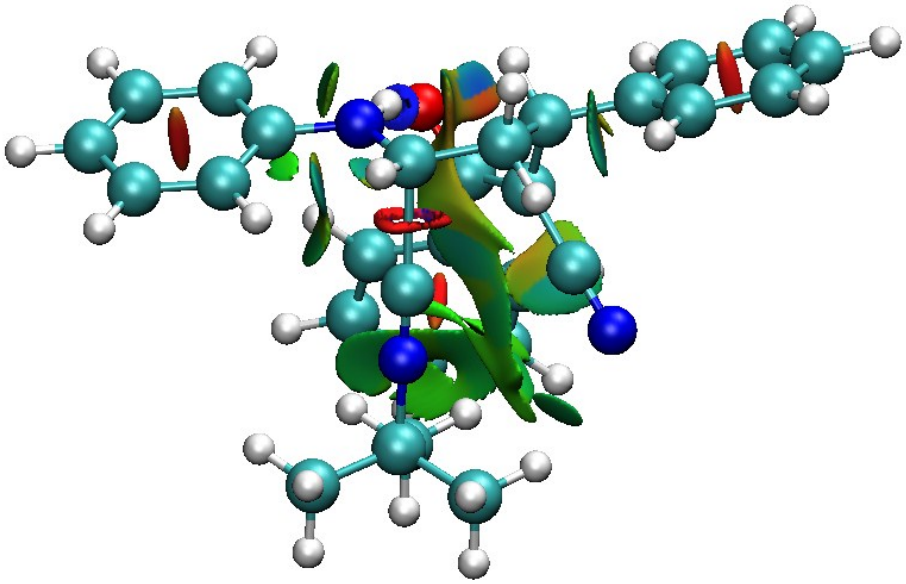


5'
0.0

M062X/def2-tzvp/IEFPCM				
Name	**ΔE_{ele}**	**ZPE correction**	**$\Delta E_{ele+ZPE}$**	**$\Delta\Delta E_{ele+ZPE}$**
5-b	-1361.991711	0.518858	-1361.472853	3.9
5	***-1361.997102***	0.519408	-1361.477694	0.9
5-c	-1361.995712	0.519702	-1361.47601	1.9
5'-b	-1361.995644	0.519041	-1361.476603	1.6
5'-c	-1361.99538	0.518489	-1361.476891	1.4
5'	***-1361.997043***	0.517929	-1361.479114	0.0



TS-3



TS-2

Figure S9. NCI analysis for **TS-2** and **TS-3** at M06-2X/def2-TZVP.

C. Cartesian Coordinates

M062X/def2-tzvp/IEFPCM

3-phenyl-3-oxo-propanenitrile

C	1.85783	-0.81459	-0.00012
H	1.66513	-1.43257	-0.87926
H	1.66525	-1.43333	0.87845
C	0.92292	0.39567	0.00033
C	3.25692	-0.41107	-0.00001
O	1.37063	1.51523	0.00038
N	4.35919	-0.10049	-0.00032
C	-0.53983	0.12355	0.00003
C	-1.05639	-1.17115	0.00010
C	-1.40882	1.21549	-0.00007
C	-2.42947	-1.37003	0.00016
H	-0.40221	-2.03284	0.00052
C	-2.77758	1.01447	-0.00028
H	-0.99379	2.21438	-0.00010
C	-3.28864	-0.27967	-0.00014
H	-2.82728	-2.37583	0.00029
H	-3.44882	1.86286	-0.00043
H	-4.35939	-0.43709	-0.00025

aniline

C	1.87247	-0.00001	0.00694
C	1.16569	-1.19677	0.00347
C	-0.22062	-1.20239	-0.00471
C	-0.93364	0.00002	-0.00894
C	-0.22058	1.20239	-0.00470
C	1.16572	1.19676	0.00332
H	2.95403	-0.00012	0.01422
H	1.69787	-2.13991	0.00888
H	-0.76244	-2.14085	-0.00828
H	-0.76244	2.14084	-0.00820
H	1.69784	2.13994	0.00866
N	-2.32338	0.00008	-0.07643
H	-2.76778	-0.83570	0.27288
H	-2.76767	0.83521	0.27462

cinnamaldehyde

C	-0.93470	-0.58493	0.00000
H	-1.14963	-1.65133	0.00001
C	-1.97833	0.25339	-0.00001
H	-1.88047	1.33224	-0.00002
C	-3.33351	-0.28916	-0.00001
H	-3.39910	-1.39252	0.00001
C	0.48534	-0.23810	0.00000
C	1.42585	-1.27085	0.00000
C	0.93829	1.08562	0.00000
C	2.78489	-0.99355	0.00000
H	1.08256	-2.29846	0.00000
C	2.29396	1.36214	0.00000
H	0.22943	1.90314	0.00000
C	3.22127	0.32390	0.00000
H	3.50125	-1.80441	-0.00000
H	2.63269	2.38981	0.00000
H	4.28065	0.54494	0.00000
O	-4.33946	0.38572	0.00001

5

C	0.22307	0.92160	-1.18448
C	0.83809	-0.08956	-2.15537
C	0.92916	-1.49534	-1.55433
C	-0.34253	-1.79251	-0.79554
C	-1.27402	-0.85096	-0.47253
H	0.08579	1.86151	-1.72068
H	1.82251	0.24763	-2.47807
H	0.19584	-0.11809	-3.03630
H	0.97764	-2.18943	-2.39917
N	-1.09173	0.47097	-0.76828
C	-4.71899	-1.89936	1.81687
C	-4.49893	-2.51014	0.58955
C	-3.38256	-2.17439	-0.16435
C	-2.48814	-1.21885	0.30391
C	-2.71130	-0.60459	1.53475
C	-3.82091	-0.94944	2.29064
H	-5.58886	-2.16249	2.40447
H	-5.19724	-3.24757	0.21620
H	-3.21006	-2.64459	-1.12465
H	-2.00802	0.13952	1.88956
H	-3.98653	-0.47638	3.24971
C	-4.14306	3.36181	-0.59404
C	-2.89761	3.62081	-0.03815
C	-1.89481	2.66219	-0.08343
C	-2.13212	1.43610	-0.69882
C	-3.37296	1.18468	-1.27965
C	-4.37528	2.14026	-1.21443
H	-4.92516	4.10796	-0.55033
H	-2.70481	4.56930	0.44597
H	-0.93465	2.85736	0.37795
H	-3.54543	0.24345	-1.78457
H	-5.33724	1.93359	-1.66518
C	4.58684	-2.31340	0.60194
C	4.59990	-2.07523	-0.76846
C	3.41681	-1.79416	-1.43387
C	2.20166	-1.73684	-0.74848
C	2.20399	-1.95505	0.62469

C	3.38755	-2.24768	1.29396
H	5.50685	-2.54362	1.12359
H	5.53027	-2.12205	-1.31999
H	3.43039	-1.63588	-2.50716
H	1.27704	-1.89453	1.18053
H	3.36798	-2.41920	2.36279
C	1.10764	1.22480	0.04288
O	0.76605	0.90930	1.17085
H	2.37945	2.13518	-1.22986
N	2.23265	1.89238	-0.26164
C	3.24673	2.36770	0.69768
C	3.84594	1.18110	1.44690
H	3.08773	0.67432	2.04092
H	4.26483	0.46252	0.74053
H	4.64070	1.53029	2.10839
C	4.32731	3.05578	-0.13006
H	4.78094	2.35334	-0.83235
H	3.91267	3.89666	-0.68988
H	5.10827	3.43525	0.52812
C	2.61587	3.36689	1.66691
H	3.37646	3.73865	2.35507
H	2.19938	4.21472	1.12038
H	1.82305	2.89412	2.24415
C	-0.52165	-3.13800	-0.37862
N	-0.59697	-4.24699	-0.07199

I

C	-1.00742	0.16765	0.29203
C	-0.29609	1.13424	-0.34305
C	-1.88711	0.50276	1.35989
C	-0.93536	-1.31407	-0.05972
C	-0.13005	-2.12685	0.95310
C	1.34809	-1.94600	0.86949
N	1.91791	-1.20225	0.01546
N	-2.58892	0.69202	2.25355
H	-0.43105	-1.38473	-1.02524
H	-0.32022	-3.19704	0.81635
H	-0.44018	-1.90563	1.97968
C	-0.87575	5.33509	0.10024
C	0.40549	4.80935	-0.01544
C	0.58404	3.44308	-0.16518
C	-0.51770	2.58727	-0.18032
C	-1.80115	3.12182	-0.07848
C	-1.97772	4.49028	0.06148
H	-1.01544	6.40259	0.21061
H	1.26581	5.46523	0.00767
H	1.57820	3.02867	-0.26488
H	-2.66279	2.46937	-0.13218
H	-2.97755	4.89794	0.13080

C	6.10604	-0.96327	-0.18445
C	5.49911	-2.20043	-0.01252
C	4.11680	-2.29910	0.06048
C	3.33515	-1.15045	-0.03620
C	3.94069	0.08738	-0.23535
C	5.32263	0.17924	-0.29702
H	7.18390	-0.89076	-0.24277
H	6.10222	-3.09636	0.05629
H	3.64204	-3.26637	0.16563
H	3.32085	0.97011	-0.32931
H	5.78876	1.14543	-0.43913
C	-4.96360	-2.71864	-0.71533
C	-4.29300	-1.98988	-1.69134
C	-2.99572	-1.55716	-1.46405
C	-2.34392	-1.84736	-0.26620
C	-3.02404	-2.57317	0.70614
C	-4.32637	-3.00682	0.48241
H	-5.97602	-3.05906	-0.88936
H	-4.78065	-1.76116	-2.63020
H	-2.47479	-0.98549	-2.22449
H	-2.54703	-2.80546	1.64989
H	-4.84139	-3.57097	1.24929
O	0.68937	0.83313	-1.18950
H	1.12767	-0.02491	-0.88951
H	1.94152	-2.51454	1.59013

I'

C	1.69485	-0.19741	0.08337
C	2.69634	-0.64282	-0.70250
C	1.96220	0.21337	1.42089
C	0.24154	-0.16016	-0.35338
C	-0.57416	-1.22199	0.40353
C	-2.01033	-1.19689	-0.00833
N	-2.95685	-1.18307	0.83001
N	2.09711	0.54479	2.51496
H	0.23095	-0.42245	-1.41155
H	-0.50201	-1.09484	1.48454
H	-0.15200	-2.20059	0.15719
C	6.83749	-0.70757	0.29189
C	6.08437	0.43028	0.55292
C	4.73434	0.45958	0.23901
C	4.12901	-0.65411	-0.34057
C	4.89187	-1.79083	-0.61340
C	6.24017	-1.81739	-0.29187
H	7.89071	-0.72778	0.53923
H	6.55062	1.30070	0.99495
H	4.15202	1.35246	0.42487
H	4.42535	-2.66349	-1.05473
H	6.82295	-2.70612	-0.49386

C	-6.92770	-0.91300	-0.51011
C	-5.96649	-0.05790	-1.03235
C	-4.64737	-0.14236	-0.60734
C	-4.28206	-1.08812	0.35054
C	-5.25363	-1.92602	0.89527
C	-6.56558	-1.84686	0.45498
H	-7.95501	-0.84486	-0.84277
H	-6.24353	0.68401	-1.77037
H	-3.89889	0.53889	-0.99456
H	-4.96334	-2.64004	1.65542
H	-7.31116	-2.51126	0.87254
C	-1.24150	3.88078	-0.05210
C	-0.55783	3.45655	-1.18556
C	-0.09735	2.15094	-1.26888
C	-0.31205	1.24893	-0.22793
C	-0.99652	1.68304	0.90403
C	-1.45808	2.99147	0.99099
H	-1.60516	4.89786	0.01531
H	-0.38654	4.14198	-2.00562
H	0.43714	1.82126	-2.15319
H	-1.18392	1.00033	1.72329
H	-1.99121	3.31297	1.87645
O	2.37591	-1.15222	-1.90766
H	3.17149	-1.27591	-2.44102
H	-2.20677	-1.18660	-1.08825

II

C	0.46734	-1.41518	-1.16730
C	-1.02802	-1.64780	-1.10540
C	-1.63025	-1.01637	0.15508
C	-0.98729	0.33829	0.38526
C	0.07928	0.78160	-0.31899
O	0.71320	0.01839	-1.22057
H	0.87849	-1.76282	-2.11327
N	1.15138	-2.02507	-0.08696
H	-1.24517	-2.71449	-1.13756
H	-1.47035	-1.18424	-1.98798
H	-1.41796	-1.65148	1.02112
C	1.93906	4.59306	0.04933
C	0.55280	4.50619	0.03987
C	-0.06659	3.27066	-0.07773
C	0.70200	2.11397	-0.18788
C	2.09435	2.20616	-0.19909
C	2.70865	3.44194	-0.07148
H	2.41979	5.55808	0.14322
H	-0.04838	5.40247	0.11629
H	-1.14663	3.20649	-0.10512
H	2.68525	1.30383	-0.29881
H	3.78867	3.50795	-0.06813
C	-5.91662	-0.83482	-0.23974
C	-5.32879	-1.80555	0.55886
C	-3.94645	-1.85096	0.69650
C	-3.13944	-0.93154	0.03606
C	-3.73690	0.04105	-0.76312
C	-5.11624	0.09026	-0.90040
H	-6.99297	-0.79506	-0.34474
H	-5.94479	-2.52695	1.08005
H	-3.49068	-2.60723	1.32514
H	-3.11671	0.76817	-1.27651
H	-5.56808	0.85282	-1.52160
C	-1.53525	1.12531	1.43726
N	-2.01818	1.69802	2.31119
H	0.64209	-2.12045	0.77826
C	5.32457	-1.98784	0.35888
C	4.74720	-1.50508	-0.80624
C	3.36756	-1.48856	-0.96927
C	2.53844	-1.97666	0.04367
C	3.12257	-2.45838	1.22000
C	4.49786	-2.46102	1.37269
H	6.39927	-1.99094	0.47982
H	5.37307	-1.12353	-1.60313
H	2.94558	-1.07933	-1.87659
H	2.48540	-2.83534	2.01131
H	4.92722	-2.83808	2.29222

4

C	1.02202	0.42881	0.16529
C	0.05735	-0.23627	0.83902
O	0.83347	1.66050	-0.33065
O	-0.38727	3.56571	-0.49185
H	-0.10683	3.77245	-1.39100
C	-1.20922	1.88147	0.94668
H	-2.20194	2.32877	0.92859
H	-0.63913	2.32629	1.76450
C	-1.30214	0.36185	1.12476
H	-1.53327	0.16844	2.17453
C	-0.50409	2.20005	-0.34518
H	-1.00850	1.74015	-1.20158
C	0.30293	-1.52716	1.38327
N	0.42577	-2.56868	1.85787
C	2.39529	-0.06097	-0.08348
C	3.46507	0.82011	0.07604
C	2.63572	-1.36856	-0.49852
C	4.76195	0.38622	-0.14758
H	3.27456	1.84024	0.38202
C	3.93540	-1.79548	-0.73153
H	1.80856	-2.04669	-0.66153
C	4.99960	-0.92270	-0.55016

H	5.58850	1.07074	-0.00973
H	4.11423	-2.80993	-1.06243
H	6.01244	-1.25893	-0.72953
C	-2.42330	-0.24595	0.29671
C	-2.19778	-0.89345	-0.91353
C	-3.73462	-0.11957	0.75529
C	-3.26119	-1.39837	-1.65477
H	-1.18601	-1.01287	-1.28285
C	-4.79613	-0.62149	0.01894
H	-3.92152	0.37593	1.70179
C	-4.56145	-1.26315	-1.19245
H	-3.06821	-1.90046	-2.59406
H	-5.80707	-0.51696	0.39135
H	-5.38826	-1.65852	-1.76795

IV

C	-0.67050	-0.03548	0.57270
C	0.08320	0.92560	-0.12012
C	-1.21792	0.17415	1.84906
C	-0.86673	-1.41804	-0.01917
C	-0.06030	-2.48432	0.73343
N	2.07429	-1.58096	-0.16121
N	-1.66521	0.25128	2.91564
H	-0.46865	-1.35257	-1.03449
H	-0.03780	-3.41718	0.16810
H	-0.51718	-2.69958	1.70260
C	0.91844	4.78761	1.55265
C	1.89876	4.07032	0.87594
C	1.59893	2.82923	0.33489
C	0.32397	2.28143	0.47909
C	-0.65750	3.01254	1.14294
C	-0.36074	4.26071	1.67585
H	1.14829	5.75787	1.97392
H	2.89573	4.47914	0.77166
H	2.35057	2.26158	-0.20030
H	-1.65988	2.61510	1.23442
H	-1.13237	4.82469	2.18404
C	6.10597	-0.40391	-0.03243
C	5.61289	-1.26674	0.93287
C	4.28001	-1.66432	0.92244
C	3.41967	-1.19899	-0.07300
C	3.91844	-0.32178	-1.04350
C	5.24552	0.06616	-1.02116
H	7.14302	-0.09748	-0.01647
H	6.26532	-1.64029	1.71185
H	3.93392	-2.34298	1.69095
H	3.24430	0.05185	-1.80491
H	5.61152	0.74583	-1.78019
C	-5.06251	-2.34015	-0.52121
C	-4.50777	-1.17842	-1.05139
C	-3.16289	-0.90629	-0.86913
C	-2.33683	-1.78347	-0.16151
C	-2.90068	-2.94301	0.35948
C	-4.25521	-3.21796	0.18257
H	-6.11446	-2.55449	-0.65798
H	-5.12734	-0.48515	-1.60601
H	-2.73325	0.00295	-1.27503
H	-2.29726	-3.65363	0.90818
H	-4.67362	-4.12503	0.59994
O	0.64174	0.68170	-1.22203
H	1.52208	-0.90706	-0.69696
C	1.39704	-2.08854	0.99330
H	1.91308	-2.96902	1.38672
C	1.47871	-1.10814	2.12525
N	1.65106	-0.42206	3.01796
C	1.88616	0.41472	4.19301
C	1.36961	1.81541	3.88322
H	1.88545	2.24403	3.02448
H	0.29975	1.79313	3.68355
H	1.55940	2.43883	4.75675
C	3.39289	0.40138	4.43493
H	3.59969	1.01080	5.31378
H	3.74840	-0.61226	4.61698
H	3.92385	0.82220	3.58142
C	1.11115	-0.22736	5.34015
H	0.04761	-0.25589	5.10553
H	1.47175	-1.23617	5.53684
H	1.26422	0.38153	6.23045

IV'

C	-0.81714	-0.17787	0.22414
C	0.01877	0.50485	-0.65846
C	-1.77016	0.48695	1.01790
C	-0.66922	-1.67428	0.45602
C	0.00960	-2.01650	1.80198
N	2.21157	-1.08181	1.11060
N	-2.55349	0.97035	1.72102
H	-0.02958	-2.02592	-0.35904
H	-0.38942	-2.94524	2.21248
H	-0.17085	-1.23158	2.53776
C	-0.56449	4.66176	-1.55785
C	0.70671	4.16075	-1.30043
C	0.87623	2.81484	-1.01178
C	-0.22170	1.95822	-0.95227
C	-1.49132	2.46635	-1.21590
C	-1.66127	3.81050	-1.52205
H	-0.69808	5.71021	-1.79157
H	1.56527	4.81953	-1.32956

H	1.86386	2.41169	-0.82593
H	-2.34788	1.80449	-1.19600
H	-2.65122	4.19220	-1.73677
C	6.39662	-0.95581	0.77177
C	5.80978	-1.83348	1.66842
C	4.42610	-1.90778	1.79547
C	3.60864	-1.08584	1.01817
C	4.20412	-0.20455	0.10687
C	5.57993	-0.14221	-0.01005
H	7.47283	-0.90531	0.67759
H	6.42771	-2.47609	2.28254
H	4.00742	-2.60304	2.51102
H	3.56340	0.41826	-0.50636
H	6.02101	0.54527	-0.72061
C	-4.49358	-3.60524	-0.07366
C	-3.61545	-3.46822	-1.14183
C	-2.38372	-2.85639	-0.95518
C	-2.00479	-2.37666	0.29714
C	-2.89320	-2.51790	1.36087
C	-4.12887	-3.12627	1.17744
H	-5.45433	-4.08287	-0.21554
H	-3.88876	-3.84044	-2.12101
H	-1.70272	-2.74717	-1.79208
H	-2.62506	-2.14511	2.34251
H	-4.80726	-3.22578	2.01521
O	1.01758	-0.03592	-1.21831
H	1.76330	-0.72584	0.25436
C	1.52983	-2.18750	1.70810
H	1.91624	-2.39726	2.70667
C	1.81796	-3.41456	0.89737
N	2.05947	-4.26800	0.18465
C	2.38914	-5.33677	-0.75597
C	1.07005	-5.97046	-1.18664
H	0.54584	-6.39456	-0.33137
H	0.43040	-5.23752	-1.67667
H	1.29552	-6.76868	-1.89253
C	3.11418	-4.67314	-1.92388
H	4.03072	-4.19104	-1.58576
H	3.36773	-5.44789	-2.64626
H	2.47472	-3.93572	-2.40722
C	3.28539	-6.32296	-0.01376
H	4.19753	-5.83487	0.32705
H	2.76432	-6.75544	0.83905
H	3.55117	-7.12126	-0.70538

III

C	1.82758	-0.95547	0.01381
C	0.81039	-1.76649	-0.79961
C	-0.56517	-1.08996	-0.79885
C	-0.85729	-0.50888	0.58095
O	-0.29340	0.73600	0.84639
C	0.71600	1.28523	0.11472
C	1.73651	0.52758	-0.33696
H	1.52593	-1.02133	1.06316
H	1.12844	-1.89364	-1.83412
H	0.72703	-2.75912	-0.34987
H	-0.53058	-0.25813	-1.50595
N	-1.56648	-2.02300	-1.23779
N	-1.58587	-1.08958	1.40894
C	-1.90468	-0.58022	2.75307
C	-0.63542	-0.42809	3.59490
H	0.01210	0.35768	3.20993
H	-0.90812	-0.17739	4.62127
H	-0.08000	-1.36788	3.61007
C	-2.80925	-1.63078	3.39563
H	-2.29192	-2.58949	3.45516
H	-3.09553	-1.32458	4.40277
H	-3.71322	-1.76432	2.79920
C	-2.66716	0.74386	2.65568
H	-3.02884	1.02784	3.64523
H	-2.03560	1.54458	2.27515
H	-3.52907	0.63065	1.99506
C	0.15758	5.48023	-0.35420
C	1.43843	4.97414	-0.17288
C	1.63383	3.61059	-0.01806
C	0.54444	2.74002	-0.04681
C	-0.74342	3.25678	-0.20191
C	-0.93314	4.61963	-0.36483
H	0.00844	6.54516	-0.47517
H	2.28782	5.64335	-0.14107
H	2.63066	3.22707	0.15102
H	-1.59442	2.58818	-0.19630
H	-1.93330	5.01067	-0.49580
C	2.70204	1.08409	-1.22385
N	3.49325	1.48049	-1.95873
C	5.85590	-2.47717	-0.14799
C	5.28349	-2.11981	1.06500
C	3.98292	-1.63467	1.10263
C	3.23666	-1.50109	-0.06534
C	3.82114	-1.85993	-1.27822
C	5.12113	-2.34460	-1.31935
H	6.86846	-2.85767	-0.18139
H	5.84689	-2.22026	1.98363
H	3.53884	-1.35831	2.05206
H	3.26825	-1.75497	-2.20338
H	5.56068	-2.61891	-2.26958
H	-1.50007	-2.91463	-0.76590
C	-5.56257	-0.89194	-1.88022

C	-4.56733	0.07261	-1.83894
C	-3.24193	-0.27539	-1.60783
C	-2.88713	-1.61329	-1.42055
C	-3.89609	-2.58312	-1.45901
C	-5.21285	-2.22493	-1.68549
H	-6.59260	-0.61342	-2.05656
H	-4.81776	1.11628	-1.98248
H	-2.49272	0.50391	-1.57796
H	-3.63230	-3.62375	-1.31040
H	-5.97413	-2.99455	-1.70869

III'

C	-2.08498	0.89763	1.65857
C	-3.54033	1.11247	1.21577
C	-4.41776	1.67812	2.34849
C	-3.94401	1.10868	3.68296
O	-2.84625	1.70562	4.28124
C	-1.91368	2.44671	3.62510
C	-1.52899	2.13108	2.36983
H	-2.09712	0.10950	2.41733
H	-3.60456	1.79071	0.36325
H	-3.94143	0.15060	0.89606
H	-5.43155	1.29103	2.23647
N	-4.44376	3.12192	2.29067
N	-4.55302	0.16364	4.22777
C	-4.14032	-0.47549	5.48975
C	-2.73440	-1.06946	5.37236
H	-1.97529	-0.29689	5.26226
H	-2.50819	-1.64717	6.26999
H	-2.68188	-1.74199	4.51354
C	-5.14008	-1.60468	5.73312
H	-5.11256	-2.31786	4.90779
H	-4.90381	-2.13171	6.65862
H	-6.15173	-1.20295	5.80706
C	-4.22506	0.52784	6.64322
H	-4.04745	0.01111	7.58790
H	-3.48846	1.32245	6.53766
H	-5.22076	0.97450	6.67990
C	-0.47374	5.57554	6.13133
C	0.39707	4.94424	5.25222
C	-0.05963	3.92603	4.43022
C	-1.39766	3.53261	4.47924
H	1.43813	5.23667	5.21399
H	0.63246	3.41976	3.77123
C	-0.67057	3.00665	1.64681
N	-0.00292	3.69426	1.00999
C	0.49811	-0.55275	-1.47097
C	0.51093	-1.14157	-0.21420
C	-0.32805	-0.66482	0.78424
C	-1.19023	0.40157	0.54366
C	-1.19276	0.98833	-0.71984
C	-0.35501	0.51457	-1.72010
H	-3.70004	3.55465	1.76686
C	-6.00716	5.57640	5.30550
C	-6.34508	4.23218	5.25910
C	-5.85332	3.40089	4.25924
C	-4.99121	3.91466	3.28510
C	-4.67248	5.27945	3.31977
C	-5.17295	6.09369	4.31755
H	-6.38981	6.21403	6.09077
H	-7.00246	3.81313	6.01099
H	-4.00541	5.68497	2.56733
H	-4.89994	7.14165	4.33172
H	-0.11422	6.37024	6.77213
H	-6.13411	2.35628	4.24902
H	-0.31635	-1.12945	1.76379
H	-0.37014	0.98117	-2.69673
H	-1.84378	1.82772	-0.93132
H	1.17125	-1.97447	-0.00936
H	1.14877	-0.92312	-2.25253
C	-2.26298	4.15223	5.38446
H	-3.29959	3.84296	5.44018
C	-1.80204	5.17498	6.19816
H	-2.48332	5.65758	6.88686

isocyanide

C	-0.26131	0.00000	-0.00001
C	-0.72941	1.45226	0.06132
H	-0.36723	2.00806	-0.80311
H	-1.81906	1.47424	0.06202
H	-0.36760	1.93303	0.96978
C	-0.72991	-0.67298	-1.28819
H	-0.36824	-1.69968	-1.33726
H	-1.81958	-0.68281	-1.30736
H	-0.36803	-0.12693	-2.15894
C	-0.72958	-0.77909	1.22704
H	-1.81923	-0.79083	1.24548
H	-0.36763	-1.80618	1.18944
H	-0.36772	-0.30819	2.14062
C	2.34480	-0.00016	-0.00016
N	1.18525	-0.00013	-0.00010

5'

C	-0.50597	0.22784	-4.29165
C	-1.02427	-0.04683	-2.87891
C	0.09254	-0.61114	-2.00133
C	0.82347	-1.69001	-2.77429
C	0.70816	-1.85977	-4.12218

H	-1.32365	0.60928	-4.90358
H	-1.83703	-0.77195	-2.95392
H	-1.42826	0.85924	-2.42853
H	0.80115	0.19730	-1.78397
N	-0.05176	-1.01654	-4.88578
C	3.01933	-4.81936	-6.14403
C	3.14301	-3.47713	-6.48510
C	2.37947	-2.52186	-5.83279
C	1.49606	-2.90512	-4.82587
C	1.38160	-4.24602	-4.47835
C	2.13929	-5.20228	-5.14078
H	3.60941	-5.56581	-6.65985
H	3.83338	-3.17516	-7.26197
H	2.46234	-1.47269	-6.09178
H	0.69029	-4.53929	-3.69723
H	2.03959	-6.24636	-4.87425
C	-1.09625	-1.75947	-8.89051
C	-0.60925	-0.51606	-8.51056
C	-0.25371	-0.27509	-7.19093
C	-0.39629	-1.27955	-6.23749
C	-0.90652	-2.51989	-6.61240
C	-1.24176	-2.75900	-7.93616
H	-1.36489	-1.94785	-9.92153
H	-0.49057	0.26922	-9.24579
H	0.15571	0.68583	-6.90337
H	-1.04125	-3.29047	-5.86466
H	-1.63261	-3.72776	-8.21946
C	-1.58252	-1.92834	1.74221
C	-0.93011	-0.70601	1.65907
C	-0.37578	-0.29347	0.45335
C	-0.46840	-1.09364	-0.68036
C	-1.12431	-2.31956	-0.58783
C	-1.67771	-2.73512	0.61430
H	-2.01016	-2.25465	2.68151
H	-0.84835	-0.07339	2.53383
H	0.13788	0.65963	0.39196
H	-1.19289	-2.95516	-1.46447
H	-2.18101	-3.69184	0.67349
C	0.63248	1.26930	-4.29040
O	1.77194	0.96567	-4.60473
H	-0.72953	2.64066	-3.70507
N	0.24878	2.49742	-3.90544
C	1.13652	3.66592	-3.74873
C	2.20072	3.36436	-2.69449
H	1.72877	3.13220	-1.73794
H	2.81716	2.51985	-2.99829
H	2.84184	4.23700	-2.56125
C	1.78036	4.01865	-5.08885
H	2.41329	3.20568	-5.43931
H	1.01139	4.21692	-5.83734
H	2.39131	4.91539	-4.97468
C	0.25153	4.81574	-3.28036
H	0.85596	5.71218	-3.14455
H	-0.52327	5.03228	-4.01860
H	-0.22560	4.57549	-2.32811
C	1.75851	-2.46675	-2.04161
N	2.50122	-3.05697	-1.38618

TS-2

C	-0.61091	-0.13515	0.42708
C	0.14859	0.83645	-0.22418
C	-1.19973	0.06406	1.68902
C	-0.78407	-1.51257	-0.18705
C	0.05005	-2.58975	0.51280
N	2.12010	-1.57817	-0.31866
N	-1.69439	0.14408	2.73333
H	-0.41666	-1.41928	-1.21204
H	-0.02566	-3.53406	-0.03750
H	-0.31747	-2.78516	1.52099
C	0.64846	4.77379	1.40097
C	1.71652	4.09811	0.82205
C	1.52884	2.83117	0.29044
C	0.27935	2.21543	0.34962
C	-0.79111	2.90617	0.91288
C	-0.60699	4.17984	1.43478
H	0.79154	5.76418	1.81380
H	2.69514	4.55975	0.78655
H	2.35094	2.29691	-0.16983
H	-1.77381	2.45312	0.93412
H	-1.44663	4.71108	1.86436
C	6.22799	-0.77492	-0.53107
C	5.74233	-1.56335	0.50117
C	4.38575	-1.84835	0.59883
C	3.51028	-1.34347	-0.35820
C	3.99226	-0.54018	-1.39143
C	5.34513	-0.26133	-1.47517
H	7.28530	-0.55689	-0.59832
H	6.41916	-1.96023	1.24629
H	4.03322	-2.45501	1.42135
H	3.29410	-0.13782	-2.11473
H	5.71197	0.36097	-2.28077
C	-4.98495	-2.45850	-0.58025
C	-4.42802	-1.35279	-1.21745
C	-3.07985	-1.07544	-1.07189
C	-2.25313	-1.89251	-0.29656
C	-2.81920	-2.99532	0.33292
C	-4.17711	-3.27517	0.19312
H	-6.03928	-2.67726	-0.68884

H	-5.04822	-0.70816	-1.82726
H	-2.64783	-0.20909	-1.56101
H	-2.21537	-3.65601	0.94044
H	-4.59783	-4.13755	0.69441
O	0.79676	0.59259	-1.28745
H	1.56061	-0.87256	-0.84217
C	1.52026	-2.30305	0.60973
H	2.10785	-3.09374	1.05743
C	1.62243	-1.21336	2.32369
N	1.70845	-0.47497	3.20027
C	1.79127	0.45286	4.31578
C	1.47025	1.84474	3.77846
H	2.19862	2.14710	3.02683
H	0.47525	1.86431	3.33283
H	1.50531	2.55093	4.60807
C	3.21333	0.37769	4.86491
H	3.29840	1.06988	5.70217
H	3.43845	-0.62855	5.21701
H	3.93700	0.66027	4.10075
C	0.76333	0.00572	5.35162
H	-0.23652	0.02549	4.91974
H	0.98683	-1.00021	5.70621
H	0.80402	0.69280	6.19647

TS-3

C	-0.99105	0.00848	0.35937
C	-0.09756	0.62045	-0.51123
C	-1.91968	0.74981	1.11766
C	-0.94749	-1.49107	0.62224
C	-0.24576	-1.85584	1.94663
N	1.96974	-1.26543	1.05962
N	-2.68493	1.29665	1.79211
H	-0.36524	-1.92007	-0.19833
H	-0.65976	-2.76777	2.37487
H	-0.38738	-1.06183	2.68643
C	-0.39344	4.76552	-1.57472
C	0.84033	4.18903	-1.29451
C	0.91702	2.84727	-0.95245
C	-0.23770	2.07133	-0.86247
C	-1.46938	2.65405	-1.15134
C	-1.54615	3.99367	-1.50960
H	-0.45474	5.81059	-1.84997
H	1.74212	4.78548	-1.34782
H	1.87445	2.38476	-0.74813
H	-2.36914	2.05342	-1.11257
H	-2.50728	4.43335	-1.74325
C	6.12199	-1.51217	0.53821
C	5.51154	-2.29778	1.50490
C	4.13971	-2.22941	1.71314
C	3.37035	-1.35665	0.94618
C	3.98166	-0.56343	-0.02604
C	5.34902	-0.64367	-0.22517
H	7.18983	-1.57640	0.37866
H	6.10164	-2.97996	2.10291
H	3.69301	-2.86565	2.46487
H	3.36538	0.09591	-0.62531
H	5.81319	-0.02799	-0.98438
C	-4.93037	-3.11814	0.28101
C	-4.09961	-3.03690	-0.83008
C	-2.81671	-2.52372	-0.70254
C	-2.33908	-2.08832	0.53211
C	-3.18032	-2.17220	1.63871
C	-4.46693	-2.68235	1.51492
H	-5.93109	-3.51900	0.18532
H	-4.45005	-3.37646	-1.79646
H	-2.17223	-2.45819	-1.57216
H	-2.83592	-1.83091	2.60782
H	-5.10749	-2.73852	2.38580
O	0.88892	0.00116	-1.02512
H	1.50796	-0.79257	0.23603
C	1.23594	-2.06512	1.83120
H	1.70928	-2.41892	2.74004
C	1.41413	-3.76520	0.94406
N	2.04997	-4.37378	0.20426
C	2.89373	-5.08428	-0.74120
C	1.98922	-5.96884	-1.59380
H	1.45880	-6.68970	-0.97281
H	1.26566	-5.36503	-2.14030
H	2.60839	-6.50884	-2.30910
C	3.60526	-4.02559	-1.58297
H	4.24557	-3.40278	-0.95655
H	4.22088	-4.53263	-2.32559
H	2.88260	-3.39199	-2.09705
C	3.88947	-5.90747	0.07097
H	4.49610	-5.25683	0.70134
H	3.37226	-6.63474	0.69551
H	4.54395	-6.43786	-0.62001

TS-4

C	1.63087	-1.11193	-0.02350
C	0.52641	-1.73825	-0.87912
C	-0.78881	-0.96079	-0.80844
C	-1.20417	-0.74345	0.61201
O	0.01819	0.96884	0.96789
C	1.01368	1.30291	0.23980
C	1.84112	0.35879	-0.34705
H	1.28933	-1.13472	1.01767
H	0.80898	-1.74848	-1.93370

H	0.34814	-2.77084	-0.56578
H	-0.62951	0.03452	-1.22469
N	-1.83139	-1.63594	-1.52305
N	-1.83218	-0.91586	1.56162
C	-2.34115	-0.66118	2.90230
C	-1.14600	-0.74290	3.84855
H	-0.39025	-0.01278	3.56097
H	-1.48976	-0.52776	4.86002
H	-0.70876	-1.74092	3.83161
C	-3.39619	-1.71105	3.22501
H	-2.96520	-2.71146	3.20279
H	-3.78609	-1.52023	4.22435
H	-4.21909	-1.66060	2.51221
C	-2.93313	0.74662	2.87109
H	-3.31693	0.98390	3.86299
H	-2.16486	1.46910	2.59727
H	-3.75233	0.80187	2.15398
C	1.52635	5.52388	-0.30089
C	2.64194	4.71953	-0.10724
C	2.49364	3.34867	0.05664
C	1.22636	2.77062	0.03568
C	0.10957	3.58755	-0.13560
C	0.25809	4.95469	-0.31482
H	1.64367	6.59177	-0.43299
H	3.63010	5.16024	-0.07852
H	3.36510	2.72749	0.21878
H	-0.87502	3.13698	-0.12780
H	-0.61460	5.57813	-0.46114
C	2.80769	0.69335	-1.31699
N	3.60486	0.90736	-2.12749
C	5.39197	-3.23487	-0.05980
C	5.15605	-2.20058	0.84126
C	3.94003	-1.53870	0.83345
C	2.93237	-1.89135	-0.06698
C	3.17818	-2.92619	-0.96195
C	4.40079	-3.59330	-0.95879
H	6.34164	-3.75387	-0.05797
H	5.92206	-1.91239	1.54988
H	3.75992	-0.72830	1.53145
H	2.42306	-3.22860	-1.67542
H	4.57246	-4.39553	-1.66509
H	-1.81868	-2.64189	-1.42610
C	-5.68730	-0.03348	-1.95164
C	-4.65048	0.77064	-1.50582
C	-3.36822	0.25899	-1.34114
C	-3.10895	-1.08125	-1.63411
C	-4.15806	-1.89269	-2.07903
C	-5.42934	-1.37157	-2.23530
H	-6.68257	0.37127	-2.07439
H	-4.83215	1.81264	-1.27531
H	-2.58400	0.91544	-0.98562
H	-3.96222	-2.93425	-2.30439
H	-6.22687	-2.01660	-2.58130

water

O	0.00000	0.00000	0.11732
H	0.00000	0.76223	-0.46927
H	0.00000	-0.76223	-0.46927

TS-6

C	1.90147	-1.04227	0.19582
C	0.89602	-1.57362	-0.84611
C	-0.46384	-0.87457	-0.88295
C	-1.05680	-0.76642	0.48457
O	-0.02711	1.01382	0.96204
C	1.11413	1.36700	0.51777
C	2.08221	0.46429	0.10641
H	1.31793	-1.44532	-1.84344
H	0.73120	-2.64244	-0.69998
H	-0.32615	0.14956	-1.22694
N	-1.36572	-1.57211	-1.75342
N	-1.78792	-1.03298	1.33045
C	-2.55163	-1.06920	2.56296
C	-2.23572	-2.39852	3.24147
H	-1.16833	-2.47023	3.45271
H	-2.78772	-2.45025	4.17959
H	-2.53429	-3.23505	2.61019
C	-4.02492	-0.96619	2.17806
H	-4.31634	-1.80025	1.53995
H	-4.62433	-0.99119	3.08760
H	-4.22006	-0.03104	1.65332
C	-2.10434	0.11397	3.41695
H	-2.65888	0.09371	4.35525
H	-1.03728	0.04511	3.62697
H	-2.30190	1.05406	2.90386
C	1.71402	5.61135	0.41745
C	2.71241	4.79203	0.92768
C	2.54071	3.41391	0.94905
C	1.36404	2.84475	0.46928
C	0.35648	3.67469	-0.01953
C	0.53453	5.04942	-0.05806
H	1.85099	6.68483	0.39616
H	3.62587	5.22583	1.31365
H	3.31827	2.77845	1.35380
H	-0.56594	3.22953	-0.37113
H	-0.24783	5.68432	-0.45371
C	3.27187	0.90560	-0.51189
N	4.25853	1.20264	-1.03787

H	-1.29547	-2.57908	-1.70186
C	-5.26168	-0.21248	-2.52590
C	-4.33494	0.63860	-1.94475
C	-3.04320	0.20713	-1.66596
C	-2.66099	-1.09886	-1.97919
C	-3.59904	-1.95755	-2.56207
C	-4.88176	-1.51629	-2.83105
H	-6.26566	0.13004	-2.73623
H	-4.61275	1.65484	-1.69575
H	-2.34734	0.89671	-1.20499
H	-3.30809	-2.97276	-2.80441
H	-5.59204	-2.19739	-3.28214
H	2.85428	-1.47891	-0.11432
C	1.67075	-1.59843	1.60434
C	1.57178	-2.98203	1.77527
C	1.65956	-0.80072	2.74550
C	1.46269	-3.54887	3.03705
H	1.61199	-3.63778	0.91385
C	1.54630	-1.36414	4.01187
H	1.74929	0.27201	2.65130
C	1.44845	-2.73941	4.16576
H	1.39816	-4.62486	3.13726
H	1.53941	-0.71946	4.88199
H	1.36410	-3.17640	5.15234

B3LYP/def2-svp/IEFPCM

TS-1

C	0.58834	0.60714	-0.85149
C	-0.11816	-0.33304	-1.80147
C	-0.92217	-1.52051	-1.19472
C	-2.36590	-1.16697	-0.80776
C	-2.69880	0.00804	-0.09591
O	-1.83387	0.81029	0.35957
H	0.29238	0.56798	0.19277
N	0.93152	1.81300	-1.32330
H	0.61821	-0.72316	-2.52060
H	-0.81871	0.28410	-2.38688
H	-1.01377	-2.21657	-2.04254
C	-6.77749	1.19078	0.78783
C	-6.48529	0.62252	-0.45615
C	-5.18191	0.21067	-0.75594
C	-4.14590	0.36504	0.18102
C	-4.44918	0.96343	1.41789
C	-5.75182	1.36033	1.72603
H	-7.79705	1.50804	1.02252
H	-7.27549	0.50372	-1.20257
H	-4.96935	-0.22010	-1.73571
H	-3.63891	1.11680	2.13358
H	-5.96888	1.80990	2.69898
C	1.30946	-3.75861	1.80741
C	1.37776	-4.11416	0.45637
C	0.65772	-3.38636	-0.49737
C	-0.14390	-2.29354	-0.12616
C	-0.21108	-1.95298	1.23720
C	0.51096	-2.67519	2.19268
H	1.86576	-4.32807	2.55652
H	1.98601	-4.96718	0.14336
H	0.71254	-3.67818	-1.55067
H	-0.83907	-1.11430	1.54380
H	0.44418	-2.39378	3.24722
C	-3.31801	-2.15012	-1.14990
N	-4.05081	-3.01391	-1.45533
H	0.97769	1.92290	-2.33405
C	2.43793	5.11600	0.82679
C	2.11041	3.93886	1.50604
C	1.61372	2.82891	0.81685
C	1.43662	2.89812	-0.57427
C	1.76942	4.07825	-1.26007
C	2.26538	5.17856	-0.56054
H	2.82656	5.97789	1.37366
H	2.24314	3.87587	2.58877
H	1.36969	1.92243	1.37119
H	1.63451	4.13140	-2.34360
H	2.51831	6.09084	-1.10606
C	2.33921	-0.36317	-0.46949
N	3.44652	-0.64777	-0.26299
C	4.82475	-1.02852	0.00355
C	4.94798	-1.28931	1.51439
H	5.98240	-1.58450	1.74249
H	4.70758	-0.38399	2.09096
H	4.27398	-2.09960	1.82831
C	5.11987	-2.30070	-0.80868
H	5.00381	-2.11521	-1.88662
H	6.15660	-2.61334	-0.61764
H	4.44665	-3.11875	-0.51395
C	5.72312	0.13889	-0.43815
H	5.60585	0.34120	-1.51293
H	5.48459	1.05357	0.12415
H	6.77294	-0.12571	-0.24563

TS-5

C	-0.50613	-0.92982	-0.08645
C	0.59310	-1.71945	-0.45433
C	0.08643	0.82699	-1.62843
C	1.65729	-1.26151	-1.46125
C	1.22956	0.02168	-2.24991
H	-0.26730	1.59764	-2.32245

H	1.75473	-2.05254	-2.22285
H	0.92249	-0.25766	-3.27099
H	2.08168	0.70632	-2.36159
C	0.85540	-2.91130	0.25648
N	1.11337	-3.91454	0.80098
C	-1.56948	-1.50024	0.80601
C	-2.37220	-2.54897	0.32185
C	-1.76148	-1.04745	2.12084
C	-3.35421	-3.12373	1.13173
H	-2.22518	-2.92653	-0.69276
C	-2.73841	-1.63243	2.93197
H	-1.13950	-0.24038	2.50350
C	-3.53966	-2.66714	2.44072
H	-3.97133	-3.93554	0.73933
H	-2.87222	-1.27471	3.95586
H	-4.30459	-3.11957	3.07674
O	-0.01699	0.59719	0.70128
C	0.37165	1.42782	-0.25007
N	0.88993	2.58959	-0.18420
C	1.17555	3.29531	1.07851
N	-1.04848	-0.13231	-1.33396
H	-1.06900	-0.83132	-2.08229
C	3.05918	-1.11583	-0.85840
C	3.27289	-0.69753	0.46315
C	4.18032	-1.39586	-1.65846
C	4.57015	-0.55583	0.96856
H	2.41362	-0.48307	1.10071
C	5.47781	-1.25404	-1.15791
H	4.03492	-1.73664	-2.68826
C	5.67791	-0.83232	0.16110
H	4.71445	-0.22980	2.00213
H	6.33474	-1.48158	-1.79763
H	6.69066	-0.72599	0.55838
C	-2.39572	0.46807	-1.30435
C	-2.79758	1.35410	-0.30091
C	-3.25485	0.13417	-2.35633
C	-4.07877	1.90932	-0.36556
H	-2.13408	1.59744	0.52494
C	-4.53262	0.69644	-2.40855
H	-2.93377	-0.55984	-3.13754
C	-4.94635	1.58593	-1.41318
H	-4.39843	2.59976	0.41800
H	-5.20194	0.43432	-3.23060
H	-5.94554	2.02537	-1.45229
C	-0.13486	3.57802	1.84162
H	-0.60307	2.64346	2.18373
H	0.06030	4.20621	2.72578
H	-0.85101	4.11099	1.19585
C	1.82499	4.63298	0.67844
H	2.75772	4.45469	0.11989
H	1.14851	5.20872	0.02699
H	2.06135	5.24435	1.56402
C	2.14970	2.51166	1.97853
H	1.70196	1.56893	2.32233
H	3.07725	2.27489	1.43455
H	2.41720	3.11095	2.86399

TS-7

C	-0.35038	-0.13449	0.59215
C	0.27450	-1.33881	0.94103
C	1.14558	0.23027	-1.27541
C	1.61053	-1.74424	0.29785
C	1.76640	-1.15954	-1.12909
H	1.26300	0.62344	-2.29169
H	1.30861	-1.83092	-1.87466
H	2.83265	-1.08398	-1.38634
C	-0.04792	-1.93359	2.18337
N	-0.28518	-2.47282	3.19376
C	-1.61848	0.28735	1.27020
C	-2.76555	-0.51177	1.11245
C	-1.69110	1.43187	2.08003
C	-3.96279	-0.16737	1.74388
H	-2.71975	-1.41277	0.49678
C	-2.88915	1.76802	2.71710
H	-0.80433	2.04900	2.21154
C	-4.02760	0.97422	2.54916
H	-4.84545	-0.79729	1.60956
H	-2.93032	2.65775	3.35023
H	-4.96285	1.24230	3.04695
O	0.79992	1.25704	0.80511
C	1.63203	1.22401	-0.21609
N	2.72730	1.84526	-0.42082
C	3.31847	2.76561	0.56757
N	-0.32944	0.09353	-0.96234
H	-0.64702	-0.80062	-1.34968
C	-1.20874	1.12015	-1.55491
C	-1.09101	2.47805	-1.24403
C	-2.15822	0.67388	-2.47895
C	-1.93838	3.39025	-1.87936
H	-0.36663	2.82415	-0.51085
C	-3.00005	1.59601	-3.10550
H	-2.24305	-0.38967	-2.71639
C	-2.89016	2.95677	-2.80737
H	-1.85114	4.45204	-1.63890
H	-3.74001	1.24449	-3.82749
H	-3.54677	3.67957	-3.29669
C	2.37706	3.95380	0.85281
H	1.45339	3.61962	1.34644

H	2.87081	4.69061	1.50696
H	2.10464	4.46196	-0.08648
C	4.61873	3.29510	-0.06376
H	5.30131	2.46138	-0.29321
H	4.40159	3.82061	-1.00749
H	5.13711	3.99370	0.61254
C	3.65579	2.02493	1.87754
H	2.74559	1.63880	2.35757
H	4.32862	1.17548	1.67639
H	4.16393	2.69984	2.58541
H	2.41325	-1.29188	0.90839
C	1.86709	-3.24609	0.28553
C	3.10206	-3.75525	0.71419
C	0.90055	-4.14916	-0.18877
C	3.36960	-5.12832	0.66938
H	3.86451	-3.06760	1.09169
C	1.16315	-5.52080	-0.23523
H	-0.07284	-3.77371	-0.51674
C	2.40041	-6.01613	0.19370
H	4.33767	-5.50387	1.01121
H	0.39709	-6.20767	-0.60482
H	2.60500	-7.08932	0.16047

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