Electronic Supplementary Material (ESI) for New Journal of Chemistry.

1. Detailed computational methodology

In the present investigation, an attempt has been made to understand the reaction mechanism with the aid of density functional theory (DFT) calculations. Geometries of all the reactants, TSs, intermediates and products were fully optimized without any geometrical/symmetrical constraints using DFT based B3 exchange and Lee, Yong and Paar (LYP) correlation functional with inclusion empirical dispersion correction (D3) as suggested by Grimme's utilizing 6-31G* basis set.[1-3] The energetics of various reactions were calculated at 298.15 K temperature and 1 atm pressure in gaseous phase.

Catalyst Investigation

Both the forms of catalyst were investigated in order to understand the stability of catalyst. The geometries of both complexes were optimized using B3LYP-D3 employing 6-31+G* level of theory. The H-bond interaction energies (IEs) of various complexes were calculated using following equation.

$$IE = E_{complex} - \sum E_{monomer}$$

where, $E_{complex}$ and $E_{monomer}$ are the energy of complex and the energy of monomeric units, respectively. The energies of the monomers were calculated from the respective monomer geometries in the complexes, or in other words, the energy that results from complexation was taken into account. The calculated IEs were corrected for basis set superposition error using the counterpoise method suggested by Boys and Bernardi.[4]

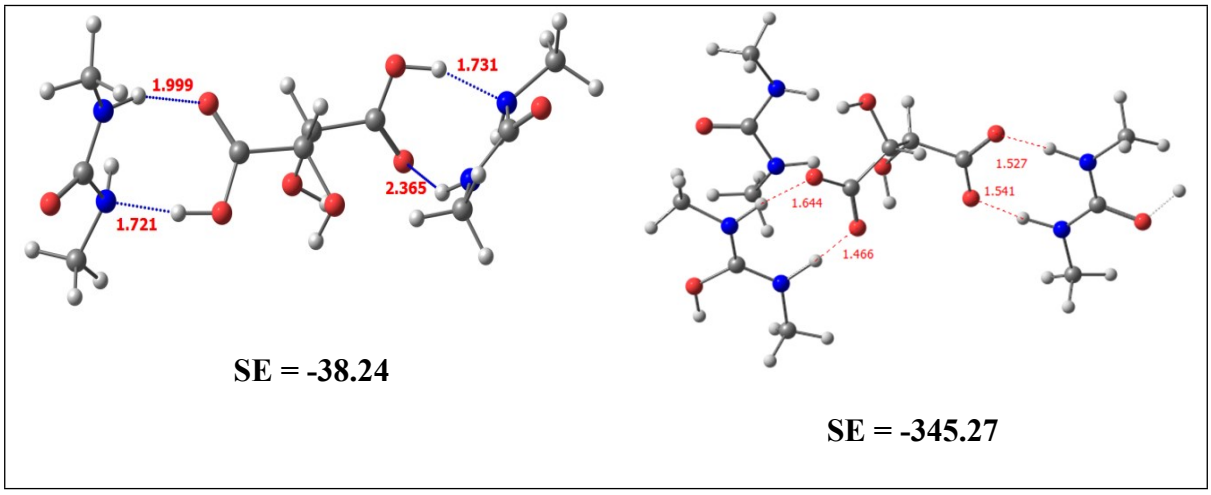


Figure S1. Optimized geometries of both complexes.

It can be noted that the H-bonded complex involved proton from LT to DMU is more stable when compared to non-proton transferred complex. Therefore, in the present investigation proton transferred form of catalyst considered.

Reaction mechanism

To support the results of the present investigation and proposed mechanism, theoretical calculations were performed using density functional theory (DFT) based B3LYP method employing 6-31+G* basis set. For an ease in the calculation the reaction is considered in three stages, which are a) keto-enol tautomerism of the carbonyl compound in the presence of the DES, b) reaction of the enolic form of the ketone with the activated benzophenone compound to give a thermodynamically stable intermediate E and c) reaction of the activated tautomer of stable intermediate with the activated aldehydic compound via aldol condensation to give final products.

a) Reaction mechanism of enolization

Close analysis of geometries of various transition states clearly reveals that the enolization of cyclohexanone undergoes concerted reaction mechanism in the presence of DES as catalyst *via* proton transfer between DES mixture to cyclohexanone. It can be observed from the optimized geometries where DES catalyst also provides the stabilizing environment for various transition states. It is worth to note that the gas-phase conversion of cyclohexanone to cyclohexanol requires 67.7 kcal/mol energy. The same conversion in the presence of DES occurs at 25.65 kcal/mol. The difference in energy clearly indicates the part played by the catalyst in the reaction. Therefore, presence of the catalyst decreases the energy barrier considerably.

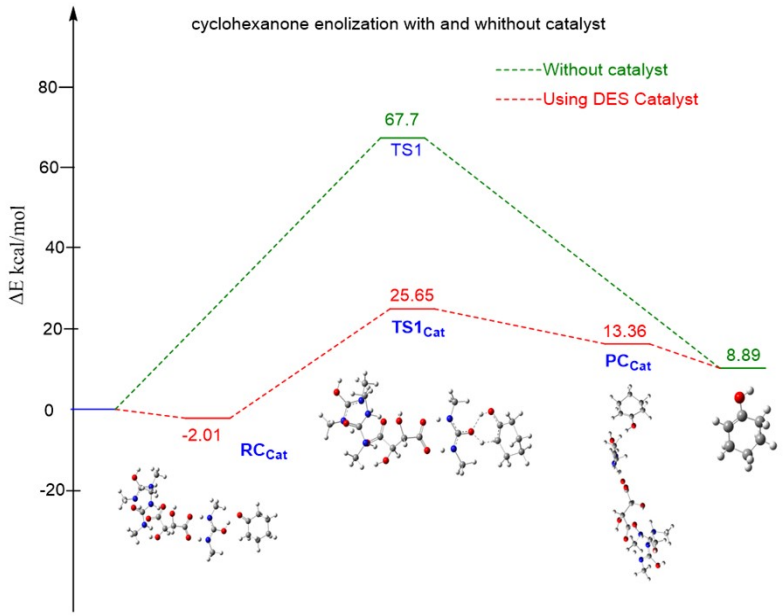


Fig. S2b. Optimized geometries and energetics of enolization of cyclohexanone obtained using B3LYP-D3/6-31+G** level of calculations

b) Mechanism for reaction of activated benzophenone with enolic form

The carbonyl carbon of benzophenone gets activated by proton transfer from DES which reacts with enolic form of the ketone to give intermediate D *via* TS1. D readily loses water molecule to give D1. From the profile it can be observe that the activation energy for this step is 11.97 kcal/mol. Further, D1 is activated by DES and undergoes cyclization *via* proton transfer to give D2 which dehydrates to give the thermodynamically stable intermediate E. The relative free energy for E is -30.67 kcal/mol which highlights its stability.

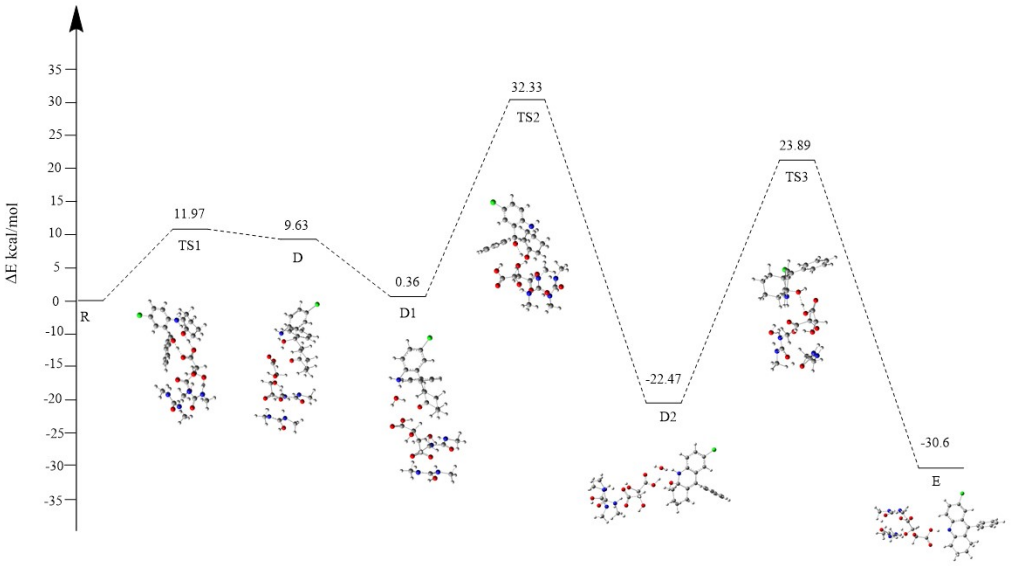


Fig. S2c. Optimized geometries and energetics of reaction between activated benzophenone with enolic form obtained using B3LYP-D3/6-31+G** level of calculations

c) Reaction mechanism of the stable intermediate with activated aldehyde

The tautomeric form of the stable intermediate E obtained from the previous step reacts with the activate aldehydic compound which gives intermediate H *via* TS4. From the profile it can be seen that the relative energy of TS4 was -14.66 kcal/mol which shows that it is a low barrier reaction. Finally, H undergoes dehydration to give the product complex PC via TS5. The energy require for this step is 13.03 kcal/mol. From the profile it can be seen that this reaction is energetically feasible.

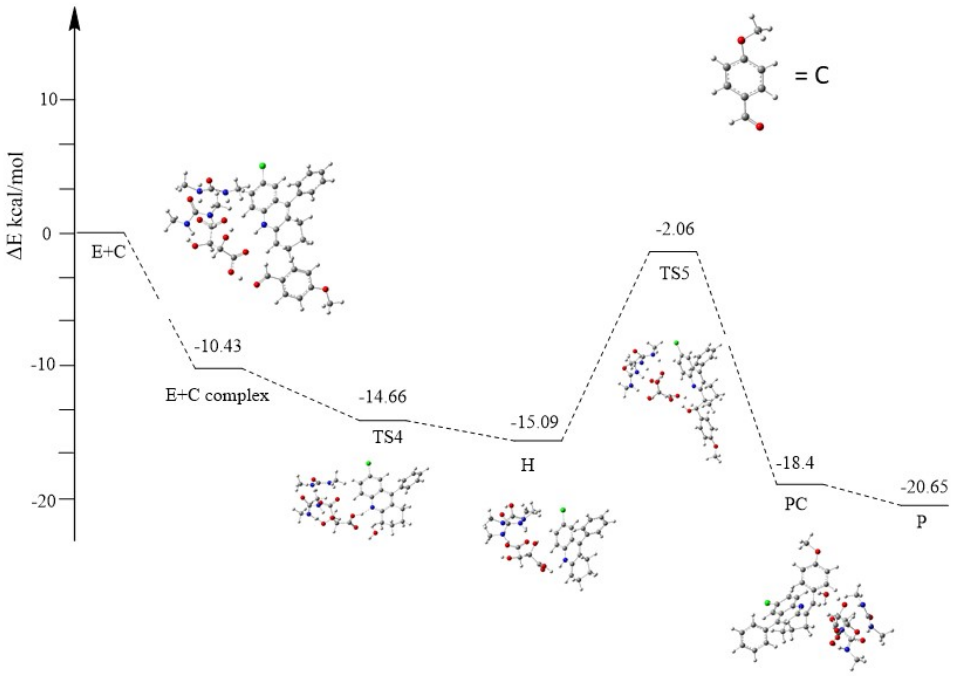
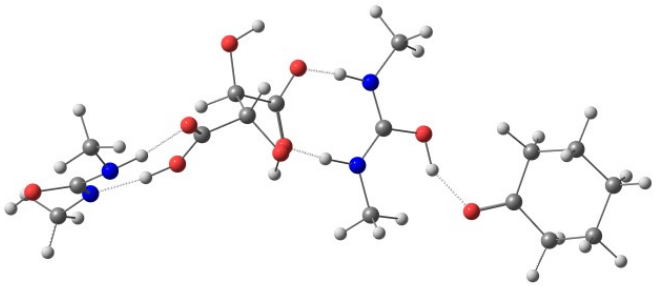


Fig. S2d. Optimized geometries and energetics of reaction between stable intermediate with activated aldehyde obtained using B3LYP-D3/6-31+G** level of calculations

It is also worthy to note that the IMs are found to be very stable throughout the reaction. This is because of the hydrogen bonding by the catalytic mixture with the IMs. Hence, the theoretical calculation compliments the proposed mechanism and shows that the use of DES effectively reduces the activation energy and efficiently catalyses the reaction.

Images and optimized coordinates of the structures obtained in enolization of cyclohexanone

RC



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H	9.73438267	-1.31151520	-2.95722345
H	8.48886002	-3.98759987	-3.88015239
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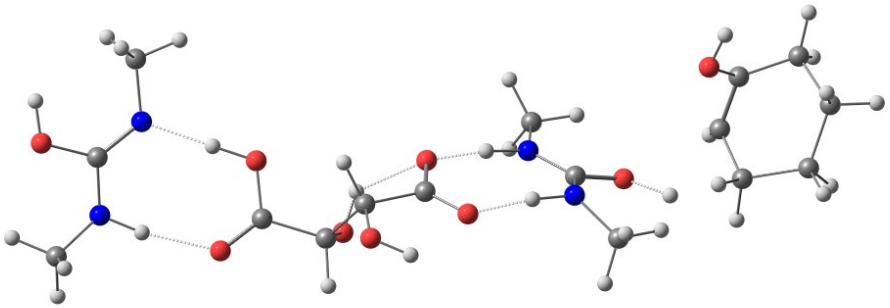
Zero-point corrected energy = **-1828.980791**

PC



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H	-9.09357	-1.68710	0.08720
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H	8.84588	0.28258	1.82577
H	9.13337	-0.85098	-0.98193
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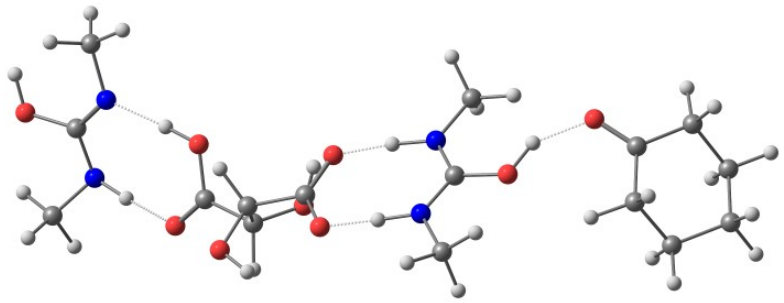
Zero-point corrected energy = **-1828.962695**

TS1



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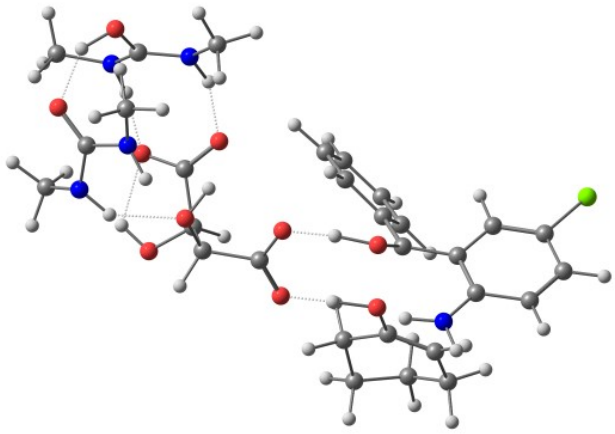
Zero-point corrected energy = **-1828.94311**

Images and optimized coordinates of the structures obtained reaction between reaction of activated benzophenone with enolic form

TS1



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H	4.97200	-2.92836	2.96380
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H	-5.61043	1.01857	0.91702
H	-4.87516	3.33479	-2.03215
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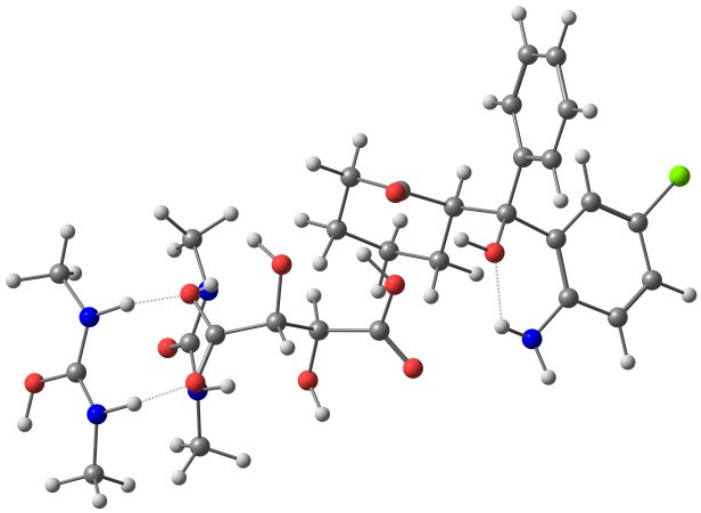
Zero-point corrected energy = **-2616.640276**

D



C	6.36485	-3.04435	0.71164
C	5.27375	-2.91309	1.55579
C	4.34418	-1.84609	1.39125
C	4.57385	-0.86764	0.38093
C	5.67709	-1.02400	-0.46794
C	6.54521	-2.10049	-0.30547
H	7.07086	-3.86607	0.83392
H	5.11578	-3.64148	2.34788
H	5.87454	-0.29574	-1.25857
Cl	7.88866	-2.26951	-1.37840
C	3.68322	0.35162	0.18011
O	3.06511	0.59786	1.44926
C	4.51891	1.59274	-0.15855
C	5.10473	2.29820	0.90358
C	4.72694	2.03088	-1.47257
C	5.87947	3.43318	0.65419
H	4.94567	1.94985	1.92798
C	5.50378	3.16683	-1.72079
H	4.29194	1.49082	-2.31196
C	6.07975	3.87067	-0.65921
H	6.32850	3.97606	1.48434
H	5.66081	3.50213	-2.74408
H	6.68339	4.75486	-0.85376
N	3.17763	-1.88641	2.16089
H	3.20908	-2.40586	3.02555
H	2.60924	-1.03369	2.23631
H	2.43577	1.38193	1.40814
C	-7.16145	0.26503	-0.17126
O	-8.17047	-0.31460	-0.88440
N	-7.07173	0.11274	1.19115
N	-6.40460	1.13007	-0.87522
C	-7.64925	-1.08346	1.83756

H	-8.64852	-1.33457	1.44565
H	-6.98334	-1.97294	1.73646
H	-7.75899	-0.86465	2.91924
C	-6.68142	1.38580	-2.30172
H	-6.33961	0.54108	-2.93288
H	-7.76121	1.52953	-2.49221
H	-6.14762	2.30249	-2.60949
H	-5.46723	1.52158	-0.44442
H	-6.16841	0.49195	1.67298
C	-3.79393	1.32316	1.32226
O	-4.64506	0.86402	2.10129
O	-3.99227	1.66606	0.11621
C	-0.14099	0.34478	2.20152
O	0.27987	-0.54148	2.90365
O	0.57697	1.48929	2.07998
C	-1.46782	0.28856	1.42884
C	-2.34685	1.49910	1.82478
H	-1.27329	0.26898	0.31380
H	-2.33169	1.70600	2.92064
O	-2.12617	-0.94564	1.65401
H	-2.10144	-1.18949	2.61593
O	-1.74526	2.64988	1.23424
H	-2.13220	2.80835	0.32603
H	-8.73914	-0.93322	-0.33547
C	-4.38393	-1.56304	-1.44084
O	-4.90254	-2.31281	-2.25947
N	-3.53619	-0.49741	-1.81315
N	-4.62580	-1.68878	-0.03923
C	-3.43774	-0.17332	-3.25480
H	-2.36210	-0.14179	-3.52815
H	-3.91502	-0.95845	-3.87528
H	-3.89758	0.79412	-3.50170
C	-5.04852	-3.03858	0.41462
H	-5.78533	-2.91250	1.23265
H	-5.53282	-3.59873	-0.40989
H	-4.20818	-3.64819	0.78347
H	-3.93103	-1.26103	0.59895
H	-3.43746	0.31431	-1.18259
C	0.56793	1.01786	-2.14316
C	-0.17149	-0.31511	-1.96661
C	0.80553	-1.48532	-1.80695
C	1.82474	-1.23985	-0.68699
C	2.59444	0.07952	-0.90484
C	1.53823	1.16920	-0.99077
H	0.24017	-2.41473	-1.59221
H	-0.84156	-0.25712	-1.07457

H	-0.85014	-0.49004	-2.83012
H	1.10351	1.04410	-3.11148
H	-0.14275	1.86650	-2.16911
H	1.32741	-1.23018	0.30414
H	2.54173	-2.08588	-0.63991
H	3.12526	0.00599	-1.89029
H	1.33267	-1.67127	-2.76276
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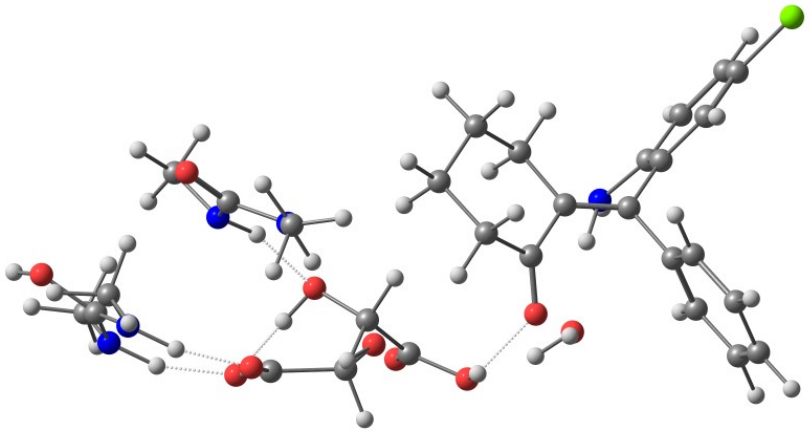
Zero-point corrected energy = **-2616.644012**

D1



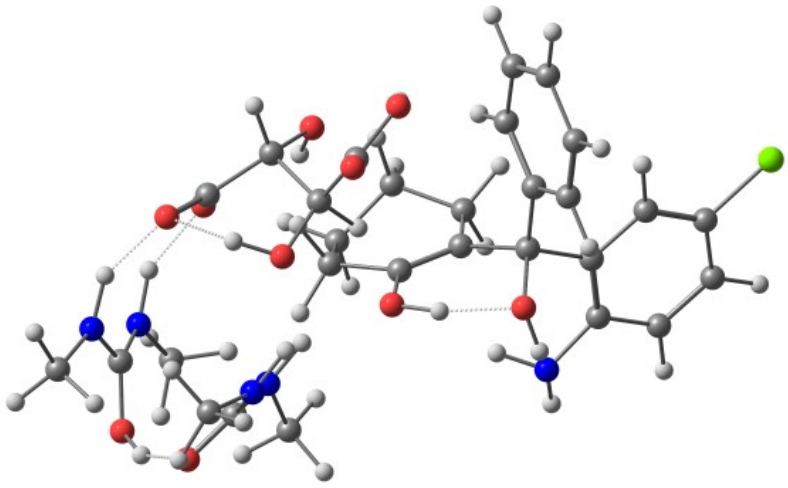
C	6.96130	-2.26028	1.85036
C	6.00544	-1.56331	2.57762
C	4.99791	-0.81502	1.91445
C	4.98635	-0.77297	0.49116
C	5.96252	-1.46910	-0.23083
C	6.92760	-2.20671	0.45208
H	7.73193	-2.84036	2.35969
H	6.02269	-1.59801	3.66469
H	5.96639	-1.42986	-1.32177
Cl	8.11758	-3.07319	-0.44934
C	3.97359	0.01637	-0.24394
O	2.68785	2.29257	1.91707
C	4.51730	1.21212	-0.93827
C	4.90347	2.34045	-0.20067
C	4.66529	1.19802	-2.33357
C	5.43078	3.45301	-0.86154
H	4.78083	2.35466	0.88571
C	5.19836	2.31278	-2.98610
H	4.37107	0.32057	-2.90495
C	5.58051	3.44054	-2.25221
H	5.72446	4.33209	-0.28927
H	5.31601	2.30269	-4.06819

H	5.99357	4.30826	-2.76294
N	3.98381	-0.21063	2.66958
H	4.18702	-0.02277	3.64109
H	3.44377	0.54987	2.23616
H	1.91816	2.62029	2.39800
C	-7.25612	-0.24884	0.28438
O	-8.18093	-1.25244	0.31689
N	-6.90584	0.43029	1.43215
N	-6.88388	0.13185	-0.95193
C	-7.02334	-0.25324	2.73768
H	-8.04882	-0.60819	2.92949
H	-6.31006	-1.10338	2.83558
H	-6.77704	0.48233	3.53100
C	-7.36378	-0.59464	-2.14449
H	-6.77639	-1.53379	-2.29345
H	-8.42805	-0.87614	-2.05936
H	-7.23633	0.04871	-3.03155
H	-6.03600	0.80622	-1.07519
H	-6.04899	1.10247	1.36518
C	-3.99481	1.69100	0.07389
O	-4.50634	1.63574	1.21384
O	-4.57396	1.50620	-1.02590
C	-0.76505	1.99216	1.83139
O	-0.83070	2.07003	3.02860
O	0.19120	2.74779	1.20448
C	-1.63760	1.11654	0.91916
C	-2.47963	1.98079	-0.04087
H	-0.99804	0.38975	0.32989
H	-2.29160	3.07298	0.07598
O	-2.42024	0.25905	1.72661
H	-3.09785	0.79471	2.25824
O	-2.04230	1.59464	-1.35310
H	-2.77899	1.78461	-2.00976
H	-8.56327	-1.41069	1.22823
C	-4.30535	-1.89419	-0.99499
O	-5.10828	-2.67596	-1.49945
N	-3.32729	-1.21496	-1.75689
N	-4.32090	-1.61132	0.39664
C	-3.53131	-1.18993	-3.22582
H	-2.54712	-1.10639	-3.71611
H	-4.00268	-2.13285	-3.56554
H	-4.16741	-0.35210	-3.55313
C	-4.84076	-2.68109	1.28163
H	-5.33964	-2.20842	2.15050
H	-5.58093	-3.30558	0.74321
H	-4.04658	-3.34923	1.65340

H	-3.52410	-1.09013	0.80542
H	-2.93377	-0.33441	-1.38926
C	0.64629	-0.13963	-1.84693
C	0.04804	-1.37033	-1.15493
C	1.14478	-2.30173	-0.62924
C	2.10439	-1.57740	0.32539
C	2.67306	-0.32909	-0.29412
C	1.63202	0.53167	-0.92525
H	0.68846	-3.16684	-0.11023
H	-0.61019	-1.03730	-0.31831
H	-0.61721	-1.91256	-1.85642
H	1.15476	-0.42766	-2.78923
H	-0.15933	0.57291	-2.13983
H	1.58884	-1.31097	1.27359
H	2.91894	-2.26962	0.63048
H	2.43801	2.34142	0.97320
H	1.71676	-2.72609	-1.47812
O	1.52564	1.71742	-0.64534
H	0.23557	2.66824	0.19387

Zero-point corrected energy = **-2616.658786**

TS2



C	6.77032	-2.10320	1.06673
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C	4.34217	-2.27968	1.09566
C	4.21773	-0.93709	0.64845
C	5.38633	-0.20541	0.40494
C	6.63701	-0.78949	0.60978
H	7.75816	-2.53667	1.22989
H	5.70855	-3.87156	1.66303
H	5.33065	0.83177	0.05484

Cl	8.05650	0.13484	0.29401
C	2.85765	-0.27769	0.45589
O	2.17829	-0.24827	1.76148
C	2.94231	1.20832	0.11298
C	2.89631	1.65310	-1.21497
C	3.07612	2.14309	1.15173
C	2.99273	3.01807	-1.50093
H	2.78131	0.94178	-2.03341
C	3.16171	3.50699	0.86350
H	3.10440	1.79634	2.18741
C	3.12389	3.94692	-0.46373
H	2.96564	3.35798	-2.53540
H	3.25266	4.22939	1.67377
H	3.18382	5.01176	-0.68761
N	3.19565	-3.05016	1.44091
H	3.37180	-4.03878	1.57952
H	2.38110	-2.91177	0.84572
H	0.55377	-0.15182	1.36945
C	-5.11197	-1.78760	-0.61099
O	-5.39301	-2.67363	0.36240
N	-5.80976	-0.62398	-0.74175
N	-4.23775	-2.19717	-1.57817
C	-6.95980	-0.32565	0.13240
H	-7.42286	0.62005	-0.20128
H	-7.72309	-1.12245	0.06879
H	-6.67036	-0.21320	1.19815
C	-3.45951	-3.43992	-1.40796
H	-3.92094	-4.12400	-0.67238
H	-3.42213	-3.96324	-2.38156
H	-2.41922	-3.21678	-1.08628
H	-3.81821	-1.46827	-2.24165
H	-5.38615	0.19294	-1.30018
C	-3.03009	0.95615	-1.93344
O	-4.14500	1.30343	-1.47244
O	-2.73947	-0.14203	-2.45573
C	-1.08757	3.63372	-0.02607
O	-1.59361	4.46028	0.68380
O	0.05708	3.98086	-0.69814
C	-1.57312	2.19807	-0.27675
C	-1.88062	1.98132	-1.77922
H	-0.80320	1.45772	0.07616
H	-2.13175	2.92918	-2.30903
O	-2.69423	1.95309	0.55651
H	-3.55511	2.21767	0.08805
O	-0.68214	1.52171	-2.39176
H	-0.74315	0.52246	-2.54562

H	-5.48585	-2.18389	1.33438
C	-4.15997	-0.34120	2.23019
O	-5.13949	-1.10144	2.43082
N	-3.05201	-0.77626	1.47506
N	-4.16115	0.95909	2.70710
C	-2.54391	-2.14328	1.73900
H	-2.24342	-2.29554	2.78935
H	-3.31987	-2.89227	1.49376
H	-1.65642	-2.31497	1.10046
C	-5.40070	1.54730	3.25565
H	-6.08903	0.75586	3.61089
H	-5.14579	2.18693	4.11970
H	-5.92955	2.16148	2.50731
H	-3.42323	1.62475	2.43700
H	-2.31442	-0.08951	1.24063
C	-0.32005	-1.69424	-1.38476
C	0.40190	-2.56276	-2.41916
C	1.69544	-1.88386	-2.88502
C	2.65439	-1.65587	-1.70703
C	1.97440	-1.02679	-0.51880
C	0.62868	-1.08222	-0.40197
H	2.19060	-2.49604	-3.66163
H	0.63122	-3.55660	-1.99048
H	-0.26581	-2.74488	-3.28383
H	-0.88675	-0.86777	-1.90319
H	-1.11843	-2.27136	-0.86174
H	3.11091	-2.62052	-1.40543
H	3.50273	-1.02005	-2.03975
H	2.37940	-1.04644	2.30047
H	1.45699	-0.91561	-3.36894
O	-0.07592	-0.56635	0.65545
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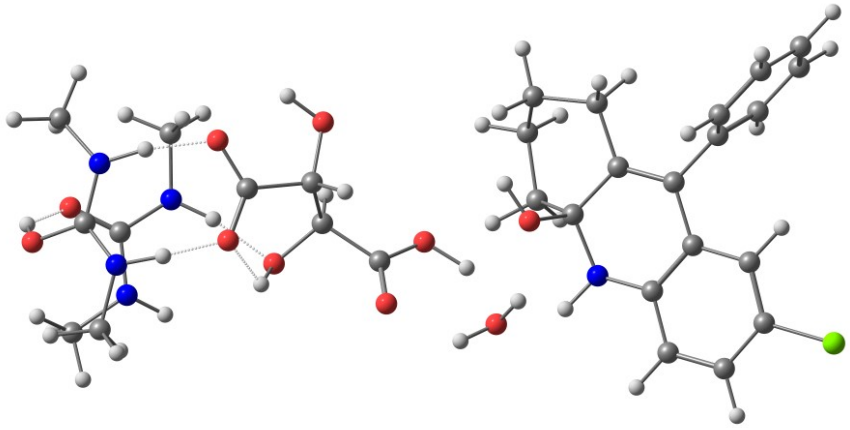
Zero-point corrected energy = **-2616.607838**

D2



C	-6.42297	3.52211	-0.08135
C	-5.21801	3.10437	-0.62766
C	-4.90513	1.72324	-0.67453
C	-5.80373	0.76184	-0.14049
C	-7.02142	1.20239	0.40659
C	-7.31138	2.56179	0.42567
H	-6.67925	4.58163	-0.04292
H	-4.51578	3.83556	-1.02503
H	-7.73260	0.48011	0.81618
Cl	-8.80937	3.09278	1.09979
C	-5.42004	-0.65174	-0.15944
O	-1.37748	2.41902	-0.05988
C	-6.39585	-1.63669	0.37204
C	-7.35202	-2.20509	-0.48261
C	-6.36019	-1.99769	1.72719
C	-8.26752	-3.13341	0.02022
H	-7.38053	-1.91762	-1.53268
C	-7.27932	-2.92651	2.22223
H	-5.62010	-1.54977	2.38895
C	-8.23227	-3.49549	1.37085
H	-9.01160	-3.57374	-0.64184
H	-7.25395	-3.20585	3.27452
H	-8.94742	-4.21786	1.75970
N	-3.73469	1.30939	-1.34365
H	-3.00328	2.02603	-1.46650
H	-0.78852	1.10957	-0.70561
H	-1.83947	1.96682	0.67197
C	7.78180	0.05808	1.47269
O	8.92782	0.41451	0.84237
N	7.13786	1.05094	2.16210
N	7.42351	-1.24758	1.58455
C	7.53066	2.45961	1.94038
H	8.62594	2.56273	1.83674

H	7.05268	2.88218	1.03740
H	7.20913	3.04878	2.81870
C	8.25067	-2.30748	0.97564
H	8.28397	-2.22288	-0.13366
H	9.28577	-2.27768	1.35972
H	7.81706	-3.29025	1.23328
H	6.41293	-1.51713	1.86093
H	6.10868	0.89648	2.39543
C	4.15304	-0.62582	1.39978
O	4.61380	0.52666	1.56693
O	4.78722	-1.70046	1.54507
C	1.17396	0.94793	-0.16141
O	1.08417	1.94470	0.54033
O	0.13145	0.49712	-0.86290
C	2.41461	0.06584	-0.34976
C	2.68637	-0.75889	0.93229
H	2.28277	-0.61612	-1.22931
H	2.00025	-0.48046	1.76684
O	3.49499	0.91443	-0.71402
H	3.83525	1.42037	0.10534
O	2.38712	-2.11394	0.60296
H	3.17084	-2.69602	0.83359
H	8.98883	-0.04185	-0.11531
C	6.86298	0.07861	-1.54628
O	7.96528	-0.48165	-1.36675
N	5.69432	-0.63656	-1.78507
N	6.74965	1.48629	-1.49608
C	5.68587	-2.09466	-1.52987
H	4.91262	-2.55988	-2.16525
H	6.65992	-2.54471	-1.79181
H	5.46069	-2.33035	-0.46910
C	7.97956	2.27626	-1.73953
H	7.77384	3.34047	-1.54023
H	8.78108	1.94571	-1.04959
H	8.36111	2.17496	-2.76990
H	5.89358	1.91582	-1.85805
H	4.77716	-0.16844	-1.64792
C	-2.49102	-0.48163	-2.46905
C	-2.32356	-2.00082	-2.60026
C	-2.40268	-2.70320	-1.24140
C	-3.78231	-2.48548	-0.60955
C	-4.21665	-1.04734	-0.63230
C	-3.21144	-0.05495	-1.17279
H	-2.20098	-3.78482	-1.35263
H	-3.10559	-2.40646	-3.27247
H	-1.35552	-2.22598	-3.08826

H	-1.49252	0.00835	-2.50043
H	-3.04546	-0.09226	-3.34707
H	-4.54061	-3.10188	-1.14142
H	-3.78532	-2.85850	0.43727
H	-0.55076	2.80047	0.33836
H	-1.60533	-2.31611	-0.56847
O	-2.18165	0.13545	-0.13290
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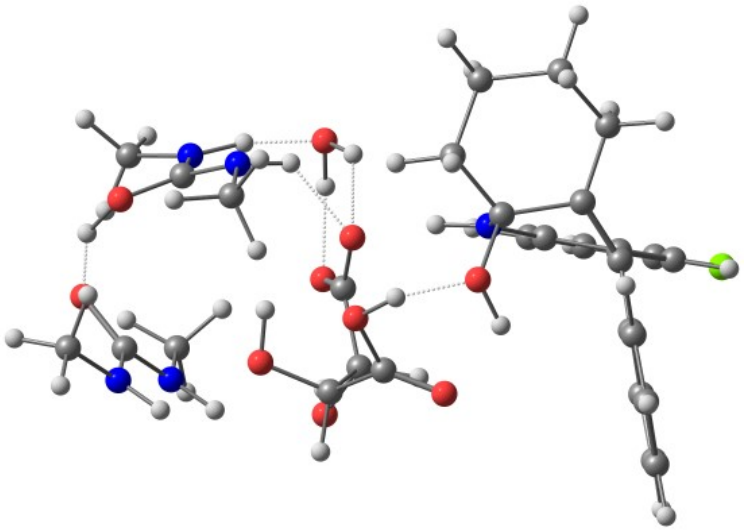
Zero-point corrected energy = **-2616.695182**

TS3



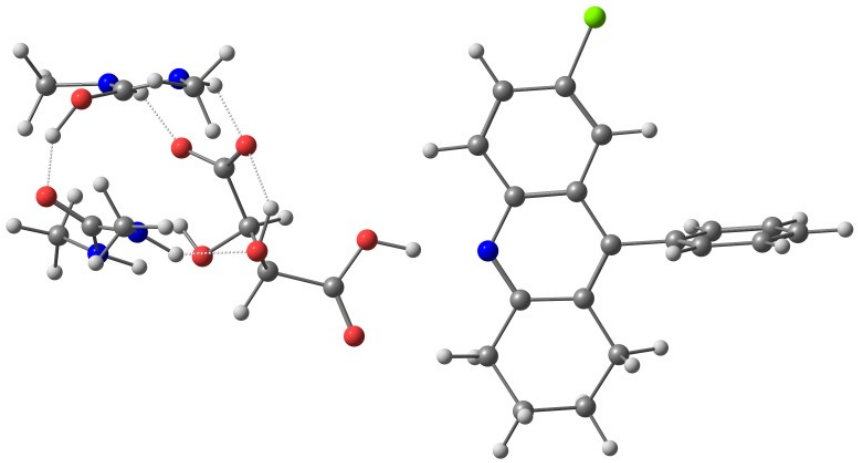
C	4.19475	-0.42252	0.41798
C	3.66651	-0.93870	1.59644
C	4.57494	-1.19923	-0.74983
C	4.05019	-0.40067	2.93743
C	2.23394	-1.37728	1.41944
C	3.77933	0.98616	0.32166
C	5.00402	-2.53074	-0.57344
C	4.57034	-0.64529	-2.04652
C	3.40004	-1.17980	4.08861
H	5.15594	-0.44175	3.03645
H	3.78991	0.67933	3.01669
C	1.51051	-1.98488	2.62598
N	1.60370	-0.08430	0.96065
O	2.01624	-2.36637	0.38281
C	4.49516	2.11361	-0.03928
C	2.34318	1.04571	0.53863
C	5.41463	-3.28953	-1.67180
H	5.01266	-2.96573	0.42680
C	4.98482	-1.40865	-3.13686

H	4.23012	0.38010	-2.19741
C	1.87823	-1.25304	3.92019
H	3.65250	-0.69857	5.05246
H	3.82518	-2.20165	4.13580
H	0.41517	-1.97588	2.47141
H	1.80231	-3.05568	2.69312
H	0.57531	-0.01608	0.95552
H	0.50306	-2.62268	0.07483
C	3.79796	3.31648	-0.21677
H	5.57514	2.06384	-0.18574
C	1.68382	2.26964	0.31444
C	5.40780	-2.73119	-2.95293
H	5.74146	-4.31794	-1.52751
H	4.97393	-0.97664	-4.13662
H	1.45055	-0.23000	3.90941
H	1.42155	-1.76982	4.78515
C	2.41465	3.40075	-0.05527
Cl	4.68108	4.73140	-0.65798
H	0.60582	2.34530	0.45391
H	5.72932	-3.32279	-3.80821
H	1.90077	4.35151	-0.21174
C	-0.09690	-1.52960	-1.50324
C	-1.34357	-0.83629	-2.05609
O	1.03313	-1.46472	-1.93869
O	-0.39297	-2.24816	-0.39845
C	-1.20546	0.68733	-1.88394
H	-1.49646	-1.08310	-3.14019
O	-2.50735	-1.35412	-1.42626
C	-1.62355	1.25231	-0.50721
O	-2.06464	1.24897	-2.88787
H	-0.15964	1.01584	-2.11831
O	-2.30681	2.29913	-0.54512
O	-1.24613	0.69007	0.55272
H	-2.34089	2.17064	-2.59086
N	-2.99177	-0.70608	2.17006
C	-2.72297	-2.12444	1.84374
C	-4.22451	-0.16093	1.83089
H	-2.23650	-2.24098	0.84642
H	-3.64584	-2.73258	1.86388
H	-2.03670	-2.53152	2.60899
N	-4.44582	1.16885	1.95220
O	-5.18002	-1.03373	1.53452
C	-5.80101	1.73783	1.83470
H	-5.96441	-0.62883	0.81029
H	-6.48911	1.31031	2.58557
H	-6.23731	1.56437	0.82410

H	-5.74841	2.82846	2.00011
C	-5.79062	-2.73438	-0.94401
N	-5.16306	-1.66318	-1.74612
H	-6.87307	-2.53673	-0.82122
H	-5.34484	-2.82343	0.06510
H	-5.67865	-3.69639	-1.47119
C	-5.40994	-0.33629	-1.40186
H	-4.30174	-1.91598	-2.24323
N	-4.82865	0.65848	-2.16297
O	-6.25557	-0.04700	-0.49298
C	-5.11043	2.07501	-1.84283
H	-3.95445	0.48508	-2.69082
H	-6.09378	2.18663	-1.35196
H	-4.33063	2.50032	-1.17479
H	-5.13098	2.65526	-2.78131
O	-2.31213	2.75579	1.97523
H	-1.58453	2.10030	1.85503
H	-2.43237	3.11494	1.04715
H	-2.36657	-1.40208	-0.42981
H	2.33194	-2.05316	-0.52735
H	-3.61252	1.87468	2.07835
H	-2.15762	-0.08429	2.08396

Zero-point corrected energy = **-2616.621278**

E



C	2.52058	2.86995	-0.66497
C	2.11545	1.56189	-0.60080
C	3.08272	0.52788	-0.37040
C	4.45611	0.84864	-0.20187
C	4.85482	2.21777	-0.27344
C	3.90106	3.17853	-0.49912
H	1.80782	3.67782	-0.84011

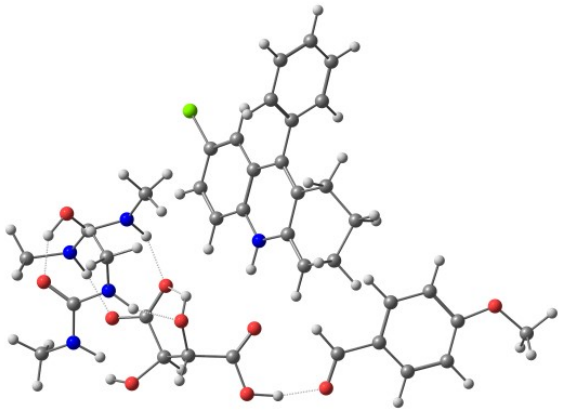
H	1.06293	1.27908	-0.71930
H	5.90836	2.47718	-0.14732
Cl	4.36762	4.83750	-0.58847
C	5.37501	-0.23125	0.03938
C	6.81141	0.08549	0.23094
C	7.31076	0.31592	1.52130
C	7.66635	0.15668	-0.87903
C	8.66434	0.61563	1.69727
H	6.64351	0.26482	2.38063
C	9.01860	0.45638	-0.69407
H	7.27448	-0.01830	-1.88019
C	9.51878	0.68545	0.59205
H	9.05344	0.79678	2.69845
H	9.68364	0.51337	-1.55494
H	10.57270	0.91982	0.73254
N	2.63615	-0.78891	-0.31801
C	-6.12414	2.07564	0.39812
O	-7.09740	1.96483	1.32468
N	-4.92601	2.58772	0.81482
N	-6.39252	1.89306	-0.92750
C	-4.65802	2.76233	2.25806
H	-5.58790	2.92252	2.83380
H	-4.12704	1.89061	2.68106
H	-4.01986	3.65698	2.38341
C	-7.76800	1.58914	-1.36971
H	-8.14252	0.62432	-0.96085
H	-8.46633	2.38715	-1.05943
H	-7.78280	1.52794	-2.47168
H	-5.59773	1.61919	-1.59658
H	-4.06726	2.39837	0.21133
C	-3.51529	0.20657	-1.19510
O	-3.14294	0.98766	-0.28879
O	-4.49083	0.38066	-1.96460
C	-0.76117	-1.99425	-0.06821
O	-0.11313	-0.91360	-0.53689
O	-0.17337	-2.98228	0.31786
C	-2.29092	-1.81220	-0.09850
C	-2.76378	-1.13133	-1.39642
H	-2.77449	-2.81986	0.01262
H	-1.92605	-0.98090	-2.11868
O	-2.66565	-1.11541	1.07882
H	-2.47699	-0.11206	0.96739
O	-3.69466	-2.06754	-1.97063
H	-4.24679	-1.58368	-2.65425
H	-7.62715	1.01780	1.20822
C	-6.44676	-1.08152	0.65259

O	-7.56321	-0.50821	0.74374
N	-6.16000	-1.94172	-0.40768
N	-5.46006	-0.88575	1.61732
C	-7.03692	-1.89713	-1.60050
H	-6.97990	-2.87317	-2.11351
H	-8.08931	-1.73018	-1.30501
H	-6.73467	-1.10276	-2.30680
C	-5.85887	-0.48563	2.98338
H	-4.95709	-0.25296	3.57316
H	-6.50354	0.41444	2.95366
H	-6.41903	-1.28366	3.50246
H	-4.52056	-1.31302	1.52381
H	-5.17434	-2.18546	-0.62495
C	2.93197	-3.17192	-0.09787
C	3.85657	-4.19467	0.56406
C	5.28581	-4.04672	0.03527
C	5.85565	-2.66840	0.38858
C	4.91699	-1.53335	0.09481
C	3.50314	-1.78268	-0.09921
H	5.93484	-4.83861	0.45451
H	3.83966	-4.06497	1.66427
H	3.47622	-5.21711	0.37486
H	2.71712	-3.46977	-1.14874
H	1.92559	-3.18614	0.39890
H	6.11420	-2.63558	1.47075
H	6.81766	-2.51778	-0.14771
H	0.95335	-1.00443	-0.47454
H	5.29925	-4.19203	-1.06282

Zero-point corrected energy = **-2616.70824**

Images and optimized coordinates of the structures obtained reaction between stable intermediate with activated aldehyde

E+C complex



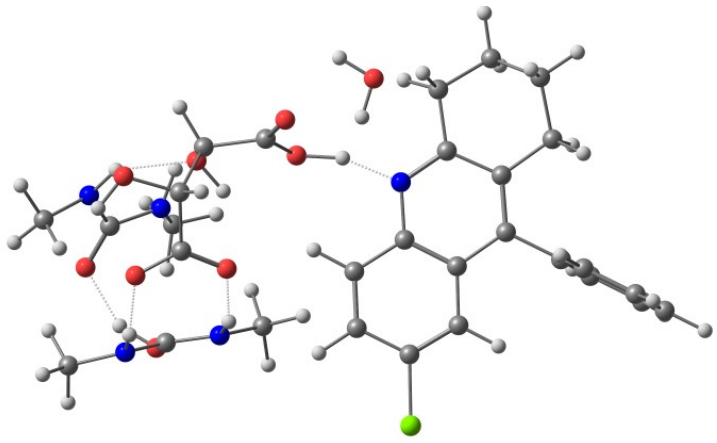
C	1.18150400	2.17895800	2.70931000
C	0.64575800	1.15686400	1.94591900
C	-0.26293000	1.45758100	0.89612600
C	-0.62387500	2.80673500	0.61968600
C	-0.06245400	3.83128400	1.40330200
C	0.82358300	3.50781600	2.42196900
H	1.87252800	1.96254900	3.52555200
H	0.92209200	0.11341500	2.14022100
H	-0.32705400	4.87426000	1.21069200
Cl	1.51140900	4.77342100	3.37344900
C	-1.56780900	3.07029100	-0.46528200
C	-1.91368200	4.48498600	-0.74788500
C	-1.21707300	5.19504000	-1.73717000
C	-2.93746800	5.11352000	-0.02245500
C	-1.54580300	6.52819300	-1.99747900
H	-0.42242300	4.70649900	-2.29739900
C	-3.26090600	6.44623400	-0.28922500
H	-3.47356100	4.56045000	0.74778600
C	-2.56675800	7.15481800	-1.27567300
H	-1.00419300	7.08022200	-2.76394700
H	-4.05454500	6.93449000	0.27448700
H	-2.82001100	8.19328900	-1.47992900
N	-0.78764900	0.41814900	0.12667000
C	4.97228400	0.80386200	0.38500200
O	5.68335000	1.38697500	-0.60403700
N	3.66598100	1.16368100	0.49492300
N	5.59171800	0.05042300	1.34541500
C	3.02590900	2.03821500	-0.50807200
H	3.75839200	2.69181700	-1.01447800
H	2.48944200	1.44715900	-1.27192200

H	2.28895800	2.68402000	0.01318100
C	7.05532600	-0.14253500	1.29622400
H	7.38341700	-0.68859900	0.38408700
H	7.58001900	0.82953700	1.32304600
H	7.36661200	-0.72502900	2.18068800
H	5.03199600	-0.68823100	1.87936000
H	3.01416700	0.58266100	1.09690500
C	3.03558700	-2.12974000	1.24956100
O	2.36525300	-1.09245000	1.03388400
O	4.17945900	-2.18419700	1.75243000
C	0.11800700	-3.48524100	-0.18852800
O	-0.60949100	-2.53776900	0.05244400
O	-0.34751500	-4.74006700	-0.24402300
C	1.62297600	-3.42749300	-0.49126800
C	2.43865400	-3.49298200	0.81433900
H	1.92598800	-4.26096600	-1.17967300
H	1.85549900	-3.94317000	1.65062600
O	1.85075800	-2.24970300	-1.24357300
H	1.68772900	-1.42553900	-0.66014100
O	3.53194200	-4.37640500	0.51426800
H	4.24556300	-4.23843600	1.20516600
H	6.30842700	0.65456900	-1.10174400
C	5.46459300	-1.64277300	-1.61477700
O	6.46940700	-0.89518900	-1.52248900
N	5.48688200	-2.95565900	-1.13805900
N	4.28667200	-1.19526600	-2.21214700
C	6.56408300	-3.33122800	-0.19247900
H	6.71185100	-4.42380100	-0.24571700
H	7.51672000	-2.84645100	-0.47458100
H	6.31550200	-3.05040400	0.84886200
C	4.33688600	-0.05573800	-3.15182400
H	3.31004700	0.25435100	-3.40605300
H	4.85827800	0.80591800	-2.68985900
H	4.86918400	-0.30941700	-4.08563700
H	3.46266600	-1.81174000	-2.28481800
H	4.59299500	-3.45378700	-0.96595000
C	-2.30780900	-0.41060200	-1.53829900
C	-3.30900600	-0.22680900	-2.63284100
C	-4.04363100	1.11640600	-2.50613000
C	-3.05201600	2.27415100	-2.32894300
C	-2.10370000	2.04977900	-1.18262300
C	-1.75581600	0.64341400	-0.89384200
H	-4.67339100	1.29357800	-3.39714600
H	-2.78877700	-0.28386000	-3.61326500
H	-4.04097300	-1.05856000	-2.63230300
H	-2.02432500	-1.43897100	-1.30727900

H	-1.39167700	-4.81364000	-0.06206400
H	-2.45412600	2.40366700	-3.25719200
H	-3.61083700	3.22415600	-2.19679600
H	-0.51284700	-0.55580900	0.33448500
H	-4.73436600	1.08429400	-1.64118300
C	-7.46785100	-2.34266700	0.72123900
C	-6.53021800	-1.32906500	0.40814000
C	-5.21149200	-1.68837200	0.18767500
C	-4.81477100	-3.04241700	0.27226700
C	-5.76441800	-4.03022700	0.58793500
C	-7.09782600	-3.69362000	0.81357700
H	-6.86215800	-0.29422500	0.35175800
H	-4.46880200	-0.91851300	-0.05325100
H	-5.43875600	-5.07426600	0.65395800
H	-7.82013800	-4.46584700	1.05560300
C	-3.41493400	-3.40763800	0.03837900
O	-3.01382200	-4.56712700	0.13222000
H	-2.70998200	-2.58836600	-0.23718700
O	-8.72911400	-1.84951700	0.91206700
C	-9.78895600	-2.78129400	1.24928900
H	-10.65359800	-2.10981600	1.34071400
H	-9.57216400	-3.27339900	2.20182100
H	-9.93406200	-3.50016000	0.43788400

Zero-point corrected energy = **-2786.527853**

TS4



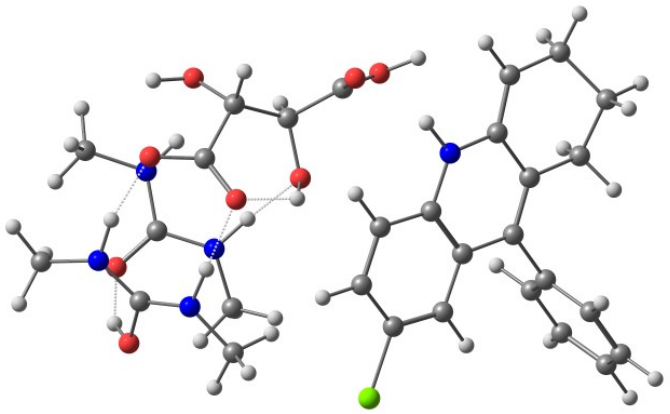
C	-0.84988	2.02981	1.01522
C	-0.84014	0.72106	0.60734
C	-2.05978	0.09969	0.18181
C	-3.27976	0.82683	0.18625
C	-3.26368	2.19126	0.60647
C	-2.07548	2.75413	1.00109

H	0.06372	2.51774	1.36330
H	0.09496	0.13355	0.61748
H	-4.19496	2.76230	0.61030
Cl	-2.04012	4.40303	1.50618
C	-4.47630	0.14683	-0.23256
C	-5.75800	0.89359	-0.23108
C	-6.18215	1.55929	-1.39042
C	-6.54124	0.93341	0.93213
C	-7.38984	2.26259	-1.38262
H	-5.57024	1.53013	-2.29054
C	-7.74767	1.63835	0.93088
H	-6.20678	0.41807	1.83223
C	-8.17307	2.30251	-0.22448
H	-7.72036	2.78191	-2.28128
H	-8.35681	1.67133	1.83366
H	-9.11327	2.85182	-0.22151
N	-2.02301	-1.23230	-0.22940
H	-0.65504	-1.91228	-0.23236
H	-1.72540	-3.28332	2.00036
C	4.21789	2.37286	-0.50349
O	4.74548	2.70792	-1.70439
N	2.86551	2.25320	-0.45052
N	4.98497	2.34058	0.62743
C	2.05429	2.34005	-1.68053
H	1.06478	1.88351	-1.49470
H	1.90831	3.39717	-1.96976
H	2.52860	1.81748	-2.53171
C	6.43785	2.59024	0.54513
H	6.85581	2.58630	1.56742
H	6.96852	1.81406	-0.05012
H	6.64530	3.57735	0.09546
H	4.64558	1.76149	1.46907
H	2.40949	1.79554	0.41132
C	3.09297	-0.26051	1.75863
O	2.14763	0.35231	1.21188
O	4.22142	0.22201	2.02847
C	0.95165	-2.69051	0.81532
O	0.47199	-2.04092	-0.23743
O	0.24576	-3.27012	1.62337
C	2.48120	-2.59676	0.87723
C	2.90819	-1.75561	2.10300
H	2.95401	-3.61015	0.92807
H	2.18597	-1.88433	2.94643
O	2.96715	-2.05332	-0.34974
H	2.44056	-1.22886	-0.57827
O	4.14206	-2.31175	2.55625

H	4.82994	-1.58598	2.63061
H	5.63017	2.14631	-1.89904
C	5.53553	-0.37775	-1.54416
O	6.27068	0.62558	-1.67184
N	5.74417	-1.33392	-0.55498
N	4.43687	-0.57974	-2.40844
C	6.67156	-1.01413	0.55412
H	7.05019	-1.96022	0.97881
H	7.53558	-0.43224	0.18781
H	6.16974	-0.43686	1.35904
C	4.47737	0.07828	-3.73490
H	4.73964	1.14839	-3.62109
H	5.21601	-0.37570	-4.41759
H	3.47971	0.01498	-4.19982
H	3.97632	-1.49739	-2.40246
H	4.96190	-1.96250	-0.28950
C	-3.00570	-3.30205	-0.98697
C	-4.20357	-3.83680	-1.77310
C	-5.51163	-3.42068	-1.09471
C	-5.65785	-1.89523	-1.08750
C	-4.42257	-1.17648	-0.62479
C	-3.14545	-1.85682	-0.61163
H	-6.37670	-3.87895	-1.60946
H	-4.17673	-3.46379	-2.81520
H	-4.14008	-4.94041	-1.84040
H	-2.88007	-3.89318	-0.02998
H	-2.06438	-3.48157	-1.54705
H	-5.91236	-1.53526	-2.10898
H	-6.52466	-1.61163	-0.45108
H	-5.53483	-3.80804	-0.05547
O	-2.05898	-4.16146	1.76536
H	-1.27368	-4.71973	1.76667

Zero-point corrected energy = **-2786.534605**

H



C	0.48342	1.38551	-2.29729
C	0.91791	0.07060	-2.28506
C	2.08511	-0.27810	-1.55647
C	2.79924	0.70378	-0.81414
C	2.33995	2.03258	-0.83854
C	1.20258	2.34838	-1.57063
H	-0.40483	1.66698	-2.86431
H	0.36153	-0.69468	-2.82996
H	2.87618	2.80714	-0.28383
Cl	0.64370	3.98606	-1.59002
C	3.96915	0.28310	-0.04390
C	4.70551	1.32631	0.71103
C	4.38198	1.58144	2.05215
C	5.72341	2.05886	0.08188
C	5.07735	2.56613	2.75888
H	3.58973	1.01253	2.53645
C	6.41434	3.04148	0.79565
H	5.96976	1.86002	-0.96039
C	6.09314	3.29620	2.13307
H	4.82677	2.76503	3.79971
H	7.20423	3.61077	0.30780
H	6.63287	4.06256	2.68605
N	2.53263	-1.60255	-1.57605
C	-4.58823	1.74018	-0.68405
O	-4.85006	2.70867	0.21978
N	-3.44435	1.86803	-1.41531
N	-5.53191	0.80127	-0.99150
C	-2.46274	2.92503	-1.09501
H	-2.89914	3.72991	-0.47580
H	-1.58556	2.51127	-0.56301
H	-2.11502	3.38166	-2.04175
C	-6.84431	0.82461	-0.31481

H	-6.75908	0.66670	0.78316
H	-7.35608	1.78943	-0.48386
H	-7.47607	0.02226	-0.73363
H	-5.23063	-0.12967	-1.42259
H	-3.06234	1.01258	-1.91689
C	-3.08609	-1.51633	-1.09418
O	-2.36995	-0.57775	-1.51500
O	-4.33670	-1.56176	-1.09869
C	0.08608	-3.09384	-0.14689
O	0.36765	-3.32933	-1.30165
O	0.93299	-3.42247	0.86453
C	-1.17502	-2.41766	0.41915
C	-2.39914	-2.75006	-0.45452
H	-1.34383	-2.74623	1.48038
H	-2.16142	-3.49745	-1.24941
O	-0.89682	-1.03476	0.52012
H	-0.97063	-0.57742	-0.40182
O	-3.33434	-3.34667	0.45985
H	-4.25064	-3.29769	0.04953
H	-5.18368	2.27020	1.15489
C	-4.19639	0.15988	2.04456
O	-5.13470	0.98990	2.13687
N	-4.43005	-1.21199	2.15991
N	-2.88388	0.57970	1.82591
C	-5.82747	-1.69238	2.05831
H	-5.90717	-2.65489	2.59339
H	-6.52055	-0.97809	2.54105
H	-6.14231	-1.83781	1.00968
C	-2.48294	1.93743	2.25341
H	-1.49777	2.17848	1.81899
H	-3.21408	2.69071	1.90118
H	-2.41200	2.02379	3.35189
H	-2.11308	-0.10209	1.71951
H	-3.72980	-1.88795	1.80363
C	3.91056	-3.37367	-0.72638
C	5.06735	-3.88374	0.07378
C	6.13169	-2.79410	0.27456
C	5.50820	-1.50254	0.81904
C	4.35144	-1.01988	-0.01285
C	3.61593	-2.05236	-0.77010
H	6.92071	-3.15056	0.96141
H	4.70622	-4.24893	1.05783
H	5.52105	-4.76118	-0.42953
H	3.36351	-4.11423	-1.29962
H	1.82374	-3.76608	0.54267
H	5.14779	-1.66535	1.85836

H	6.28900	-0.71635	0.89320
H	1.99388	-2.30196	-2.10312
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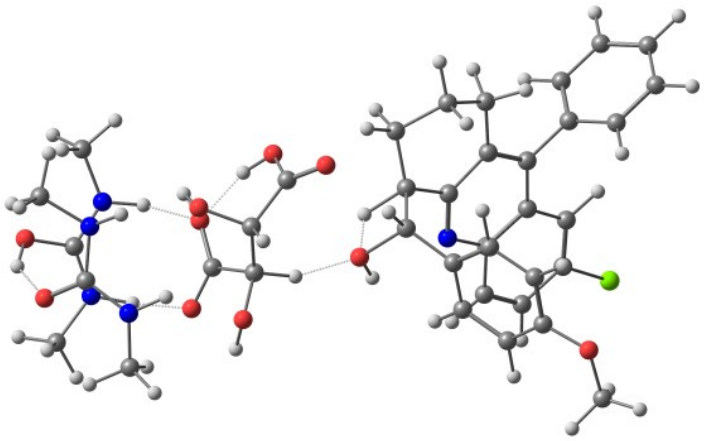
Zero-point corrected energy = **-2786.535293**

TS5



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C	-3.95771	-0.45685	3.06887
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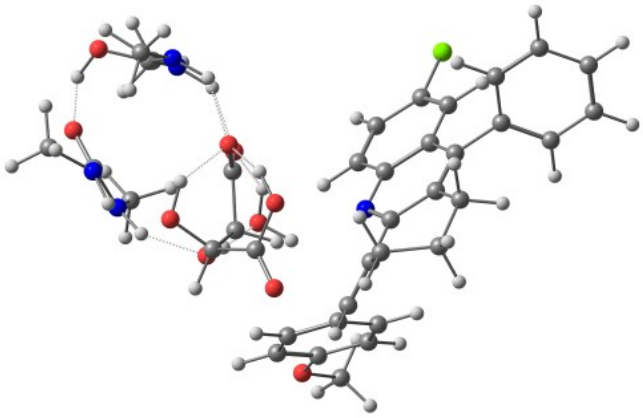
C	-5.04678	0.77142	1.21551
C	-6.26805	0.74440	1.95359
C	-6.28922	0.13731	3.18406
H	-5.21813	-0.93093	4.74800
H	-3.05078	-0.90700	3.47393
H	-7.16225	1.20556	1.52887
Cl	-7.76088	0.09460	4.08939
C	-4.91916	1.39671	-0.07374
C	-6.10717	2.05736	-0.66691
C	-6.36590	3.40935	-0.39695
C	-6.97150	1.32744	-1.49680
C	-7.48698	4.02671	-0.95821
H	-5.69498	3.97218	0.25028
C	-8.09016	1.95223	-2.05403
H	-6.76857	0.27689	-1.70209
C	-8.34909	3.30064	-1.78641
H	-7.68935	5.07590	-0.74840
H	-8.76212	1.38632	-2.69760
H	-9.22151	3.78417	-2.22167
N	-2.67463	0.13862	1.10307
C	6.77104	1.68315	1.83012
O	8.07264	1.93178	1.57872

N	5.87634	2.56100	1.29587
N	6.38822	0.72304	2.72356
C	6.33198	3.61082	0.36208
H	5.48000	3.95671	-0.24906
H	6.73395	4.47246	0.92789
H	7.12918	3.25127	-0.31535
C	7.40498	-0.10008	3.40877
H	7.99184	-0.72598	2.69944
H	8.10975	0.53445	3.97571
H	6.89760	-0.77151	4.12373
H	5.40084	0.31991	2.67465
H	4.84830	2.30494	1.27519
C	3.84342	-0.12473	0.67311
O	3.88233	1.11456	0.38836
O	4.31063	-0.63137	1.70776
C	2.39001	0.35210	-2.30847
O	2.26974	1.54267	-1.67566
O	1.62937	0.09715	-3.21148
C	3.51338	-0.59091	-1.82614
C	3.24212	-1.06847	-0.38921
H	3.61484	-1.46920	-2.51598
H	2.14011	-1.22181	-0.20384
O	4.76468	0.07646	-1.95851
H	4.79250	0.88857	-1.36616
O	3.89452	-2.34205	-0.29494
H	3.94594	-2.60240	0.66467
H	8.60261	1.01902	1.35443
C	7.61600	-0.61905	-0.26570
O	8.45394	-0.43217	0.64947
N	6.78868	-1.73362	-0.27965
N	7.47156	0.31610	-1.30890
C	6.72452	-2.58162	0.93285
H	6.42825	-3.60193	0.63172
H	7.71295	-2.64263	1.42252
H	5.98590	-2.19469	1.66361
C	8.63340	1.17837	-1.62613
H	9.04308	1.62657	-0.70030
H	9.45233	0.62822	-2.12142
H	8.30517	1.99423	-2.29154
H	6.89308	0.05888	-2.12166
H	5.92536	-1.74341	-0.85473
C	-1.26079	0.61889	-0.77400
C	-1.04518	1.69366	-1.81460
C	-2.23281	1.73584	-2.78297
C	-3.53397	2.08418	-2.04900
C	-3.70713	1.37978	-0.73375

C	-2.58683	0.70165	-0.10686
H	-2.04652	2.47258	-3.58621
H	-0.91711	2.67577	-1.31884
H	-0.09602	1.52187	-2.37013
H	-0.31111	0.52441	0.10761
H	-0.27979	-0.90869	0.84666
H	-3.57243	3.18037	-1.86119
H	-4.39980	1.86840	-2.71130
H	2.83963	1.63486	-0.80612
H	-2.33463	0.75477	-3.28651
C	-3.44466	-4.10952	-1.20606
C	-3.13291	-3.43438	-2.40646
C	-2.25316	-2.36220	-2.35735
C	-1.68555	-1.95220	-1.13309
C	-2.01136	-2.63891	0.04124
C	-2.89036	-3.72652	0.02017
H	-3.58342	-3.76474	-3.33925
H	-2.00051	-1.82978	-3.27644
H	-1.58138	-2.31790	0.99358
H	-3.13158	-4.24364	0.94180
C	-0.75803	-0.78360	-1.14816
O	0.22219	-0.76534	0.00552
H	-0.07977	-0.79002	-2.03148
O	-4.32565	-5.15014	-1.39831
C	-4.74494	-5.90560	-0.23634
H	-5.43302	-6.63658	-0.68064
H	-5.26753	-5.25547	0.47141
H	-3.88636	-6.40370	0.22258

Zero-point corrected energy = **-2786.514513**

PC



C	2.57089200	0.19453900	3.50856400
C	1.93491200	0.65175400	2.38370100
C	2.35835200	0.20647000	1.08621000
C	3.44083800	-0.70825700	0.96748900
C	4.08976700	-1.17248800	2.15185900
C	3.65088000	-0.72306200	3.37131400
H	2.26930200	0.52055300	4.50486600
H	1.10634400	1.36484500	2.45086600
H	4.92160700	-1.87560700	2.06729700
Cl	4.42267100	-1.27439300	4.81333800
C	3.82076300	-1.13032900	-0.35197700
C	4.91906500	-2.11631500	-0.49876000
C	6.24316000	-1.67406500	-0.63710400
C	4.63123600	-3.48923400	-0.49732300
C	7.27464100	-2.60666800	-0.77486800
H	6.46399700	-0.60769500	-0.63410400
C	5.66874200	-4.41513200	-0.63565500
H	3.60256400	-3.82963700	-0.38586500
C	6.98948300	-3.97610600	-0.77490300
H	8.30344000	-2.26504700	-0.88134900
H	5.44693800	-5.48161500	-0.63391500
H	7.79547300	-4.70007000	-0.88224100
N	1.69470700	0.70691600	-0.02888800
C	-4.10249300	-2.82952600	1.54516700
O	-5.37003000	-2.94710400	1.96314700
N	-3.74794400	-3.52425900	0.41816000
N	-3.15530700	-2.22753500	2.32500900
C	-4.79318800	-4.16005800	-0.41179400
H	-5.65587600	-4.48518800	0.19955400
H	-5.16201900	-3.47974400	-1.19977800
H	-4.35786800	-5.05600900	-0.89181700
C	-3.51841000	-1.67328700	3.64488400
H	-4.20850500	-0.80377600	3.56264900
H	-4.00669900	-2.43925100	4.27407100
H	-2.59977800	-1.33931100	4.15769100
H	-2.27074100	-1.85093000	1.88053800
H	-2.87159600	-3.23012600	-0.09566600
C	-2.04004100	-0.67721900	-0.46474400
O	-2.35340600	-1.77100900	-1.03363800
O	-1.76767600	-0.57942100	0.74701000
C	-1.97369800	-0.17039300	-3.75735000
O	-1.55698200	-1.45312100	-3.57992000
O	-1.60629600	0.42196700	-4.74116800
C	-2.85306600	0.43276600	-2.63980900
C	-2.00153000	0.58225800	-1.36106500
H	-3.26366500	1.42789300	-2.95194300

H	-0.92971400	0.79710900	-1.61505000
O	-4.01548500	-0.36387200	-2.47593500
H	-3.77171800	-1.27422500	-2.10514600
O	-2.52805400	1.71448900	-0.68458100
H	-1.91303900	1.93866800	0.15349900
H	-5.77713000	-1.95359400	2.26653300
C	-5.36291600	0.09512400	1.07751700
O	-5.75522000	-0.43174300	2.15626400
N	-4.61834800	1.25842600	1.07081900
N	-5.65725900	-0.50295000	-0.16113300
C	-3.99929000	1.74185300	2.32504300
H	-4.02646900	2.84675000	2.32695700
H	-4.55298900	1.38607600	3.21160200
H	-2.94145600	1.42287600	2.40471300
C	-6.91653900	-1.27382600	-0.27647300
H	-6.96125200	-1.74707400	-1.27125900
H	-6.94938700	-2.07140900	0.49166000
H	-7.81525200	-0.64556200	-0.14933400
H	-5.36092900	-0.02422800	-1.03269000
H	-4.11491600	1.55256600	0.19904000
C	1.41562000	0.92604700	-2.42932500
C	1.37072100	-0.00986100	-3.60932300
C	2.80678100	-0.39157300	-3.97980800
C	3.49901200	-1.13304300	-2.83062500
C	3.15910000	-0.62950900	-1.45678000
C	2.09680800	0.33913800	-1.24770300
H	2.80758500	-1.02371700	-4.88880500
H	0.77039100	-0.91563900	-3.36918800
H	0.84811500	0.44227000	-4.48007800
H	0.01024200	2.07149900	0.75633800
H	-0.78305700	0.82782000	1.28397300
H	3.23011800	-2.21364300	-2.87544600
H	4.60018800	-1.10123500	-2.98135400
H	-1.84858600	-1.87973900	-2.68421000
H	3.37789800	0.52078400	-4.24351100
C	0.96583200	5.28518200	0.37742100
C	-0.26082900	4.88254200	-0.19373800
C	-0.25672900	3.85970100	-1.13185100
C	0.95023600	3.22558000	-1.49658900
C	2.15467500	3.64210300	-0.91357300
C	2.17597800	4.67636500	0.02780200
H	-1.18065300	5.37918300	0.10724400
H	-1.19993000	3.53350400	-1.58095000
H	3.08812200	3.15451400	-1.19550800
H	3.11745000	4.98685100	0.46668100
C	0.92497700	2.17407300	-2.52157800

O	-0.79607000	1.82311400	1.25934700
H	0.44390500	2.49351900	-3.45805300
O	0.81539000	6.31093100	1.28539600
C	2.00518500	6.81867100	1.93487800
H	1.59051500	7.60526300	2.57878800
H	2.69188000	7.23994300	1.19519200
H	2.47787000	6.03296000	2.53085700

Zero-point corrected energy = **-2786.540556**