Origins of Stereoselectivity of Chiral Vicinal Diamine-Catalyzed Aldol Reactions

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Supporting Information

A. Complete set of TS-1a–1p (M06-2X/def2-TZVPP–IEF-PCM (cyclohexanone)//B3LYP/6-31G(d))–IEF-PCM (cyclohexanone))

The four transition structures **TS-1a–1d** are shown in Figure S1. Twelve additional transition structures (**TS-1e–1p)** are shown below in Figure S2, S3, and S4, where the aldol acceptor is benzaldehyde and the cinchona primary amine's vinyl group is truncated to a methyl group. They vary based on the conformation of the cyclic transition state. The conformations and free energies of activation of **TS-1e–1p** are listed in Table S1. **TS-1i–1l** are the twisted conformations, with the exception of the boat–boat (**TS-1k**). **TS-1m–1p** have conformations where the quinoline ring is rotated, except **TS-1p**.

Table S1. Intermolecular Aldol Addition Transition Structures

Entry	TS	Ring Conformation	$\Delta\Delta G^{\ddagger}$
1	**TS-1e**	crown	0
2	**TS-1f**	crown (axial)	2.0
3	**TS-1g**	chair-boat	2.9
4	**TS-1h**	boat-chair	3.4
5	**TS-1i**	twist-crown	1.7
6	**TS-1j**	twist-chair-boat	6.0
7	**TS-1k**	boat-boat	7.0
8	**TS-1l**	twist-boat-chair	13.1
9	**TS-1m**	crown	1.9
10	**TS-1n**	crown (axial)	3.1
11	**TS-1o**	boat-chair	4.3
12	**TS-1p**	t-crown	5.0

M06-2X/def2-TZVPP IEF PCM (cyclohexanone)//B3LYP/6-31G(d) IEF PCM (cyclohexanone). The relative free energies of activation ($\Delta\Delta G^{\ddagger}$) are reported in kcal/mol relative to the lowest-energy transition structure, **TS-1e**.

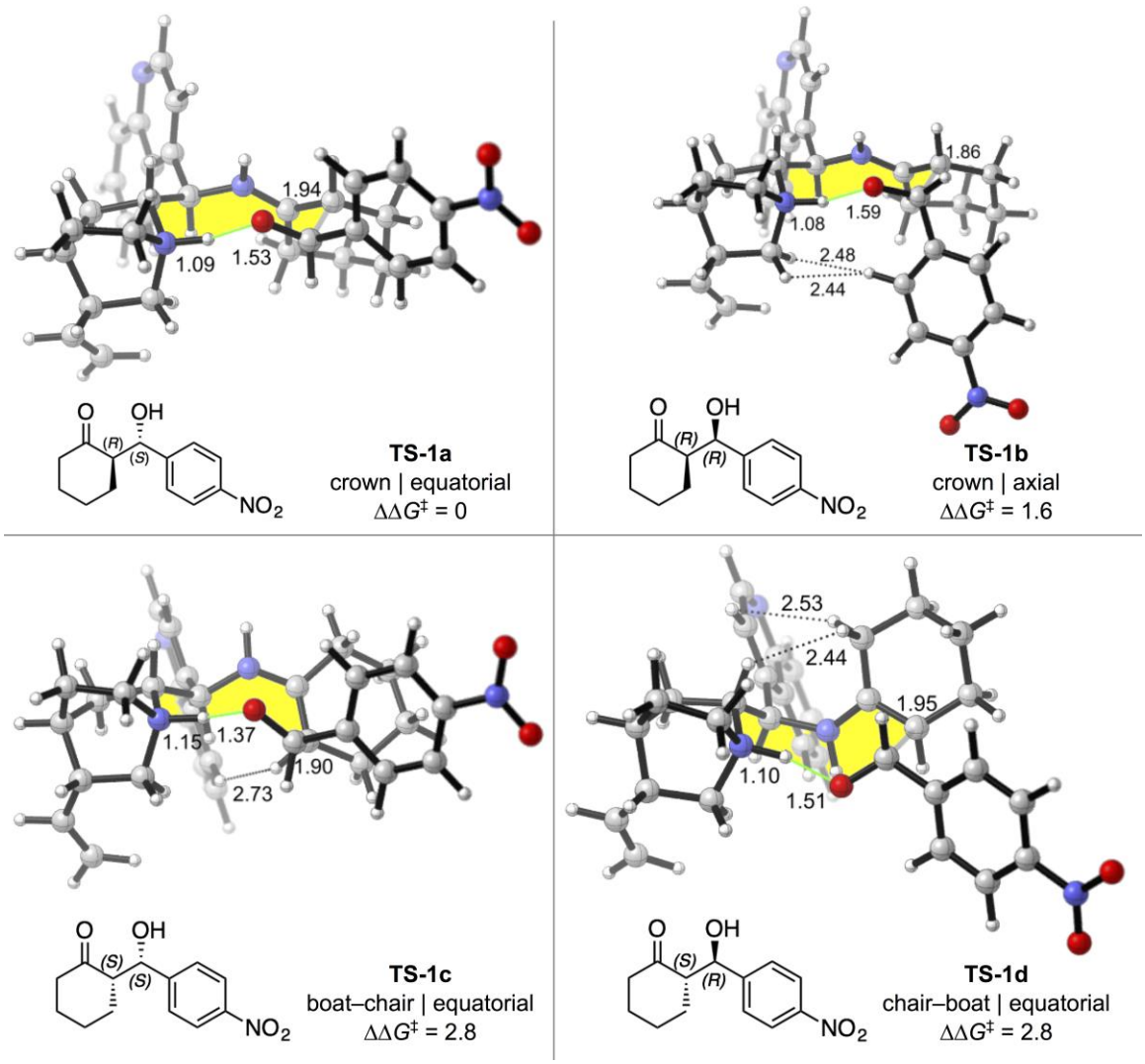


Figure S1. Lowest-energy transition structures **TS-1a–d** for the aldol addition of *p*-nitrobenzaldehyde and the enamine formed by **1** and cyclohexanone (M06-2X/def2-TZVPP–IEF-PCM//B3LYP/6-31G(d)–IEF-PCM (cyclohexanone)). The free energies of activation ($\Delta\Delta G^{\ddagger}$), relative to **TS-1a**, are reported in kcal/mol.

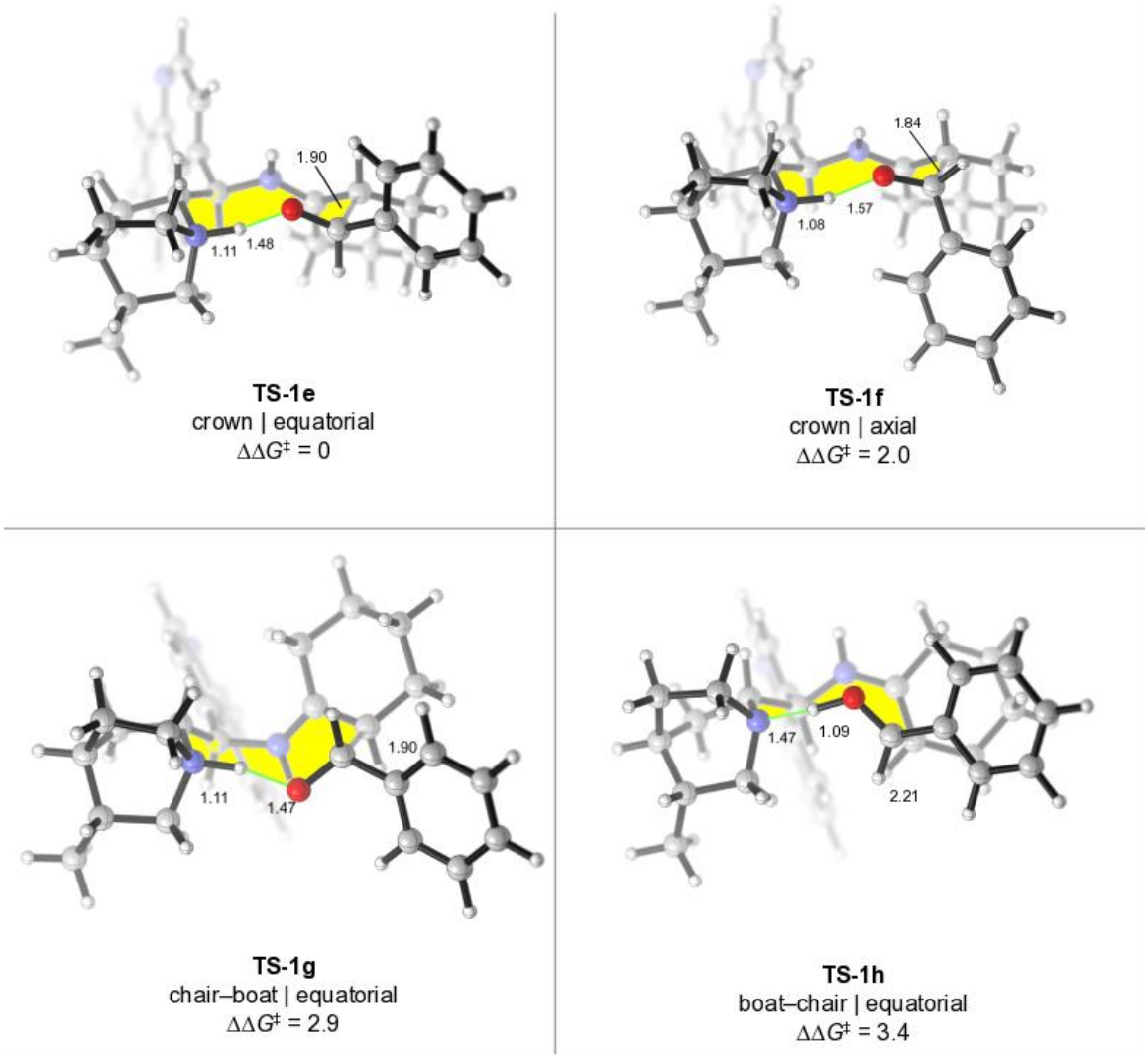


Figure S2. Lowest-energy transition structures **TS-1e–h** for the aldol addition of benzaldehyde and the enamine formed by truncated **1** and cyclohexanone (M06-2X/def2-TZVPP–IEF-PCM//B3LYP/6-31G(d)–IEF-PCM (cyclohexanone)). The free energies of activation ($\Delta\Delta G^{\ddagger}$), relative to **TS-1e**, are reported in kcal/mol.

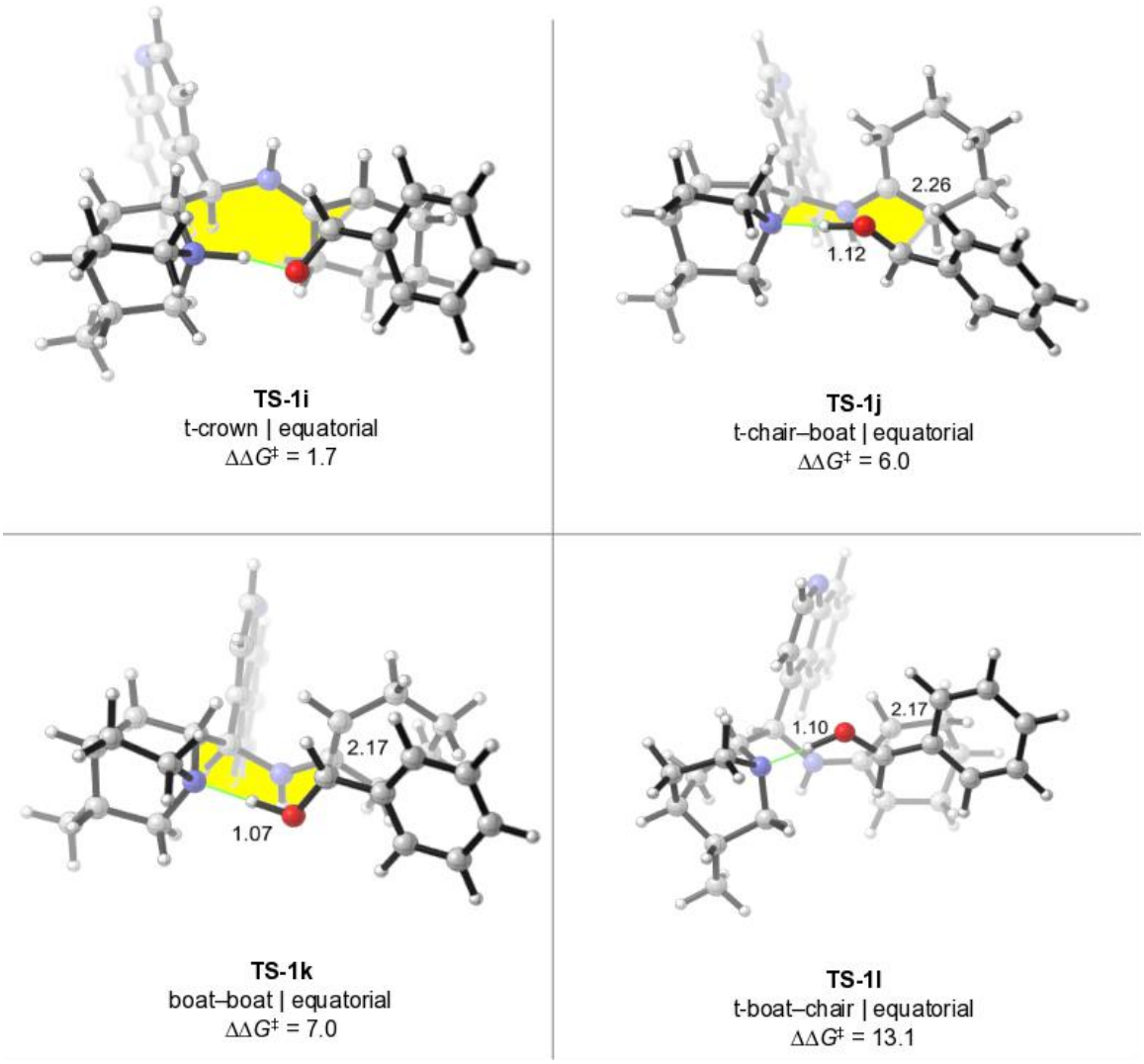


Figure S3. Transition structures **TS-1i–l** for the aldol addition of benzaldehyde and the enamine formed by truncate **1** and cyclohexanone (M06-2X/def2-TZVPP–IEF-PCM//B3LYP/6-31G(d)–IEF-PCM (cyclohexanone)). The free energies of activation ($\Delta\Delta G^{\ddagger}$), relative to **TS-1e**, are reported in kcal/mol.

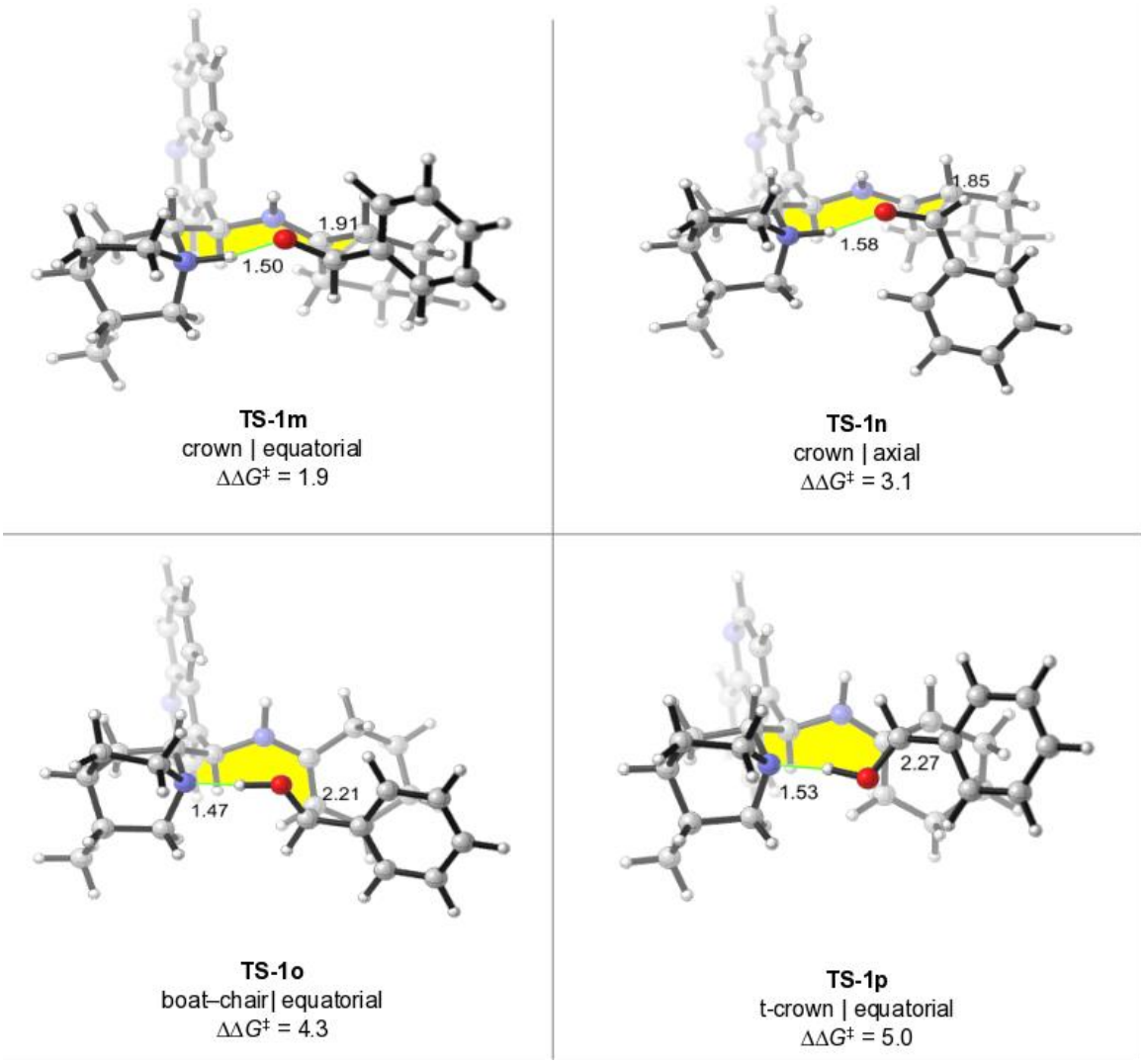


Figure S4. Transition structures **TS-1m–p** for the aldol addition of benzaldehyde and the enamine formed by truncated **1** and cyclohexanone (M06-2X/def2-TZVPP–IEF-PCM//B3LYP/6-31G(d)–IEF-PCM (cyclohexanone)). The free energies of activation ($\Delta\Delta G^{\ddagger}$), relative to **TS-1e**, are reported in kcal/mol.

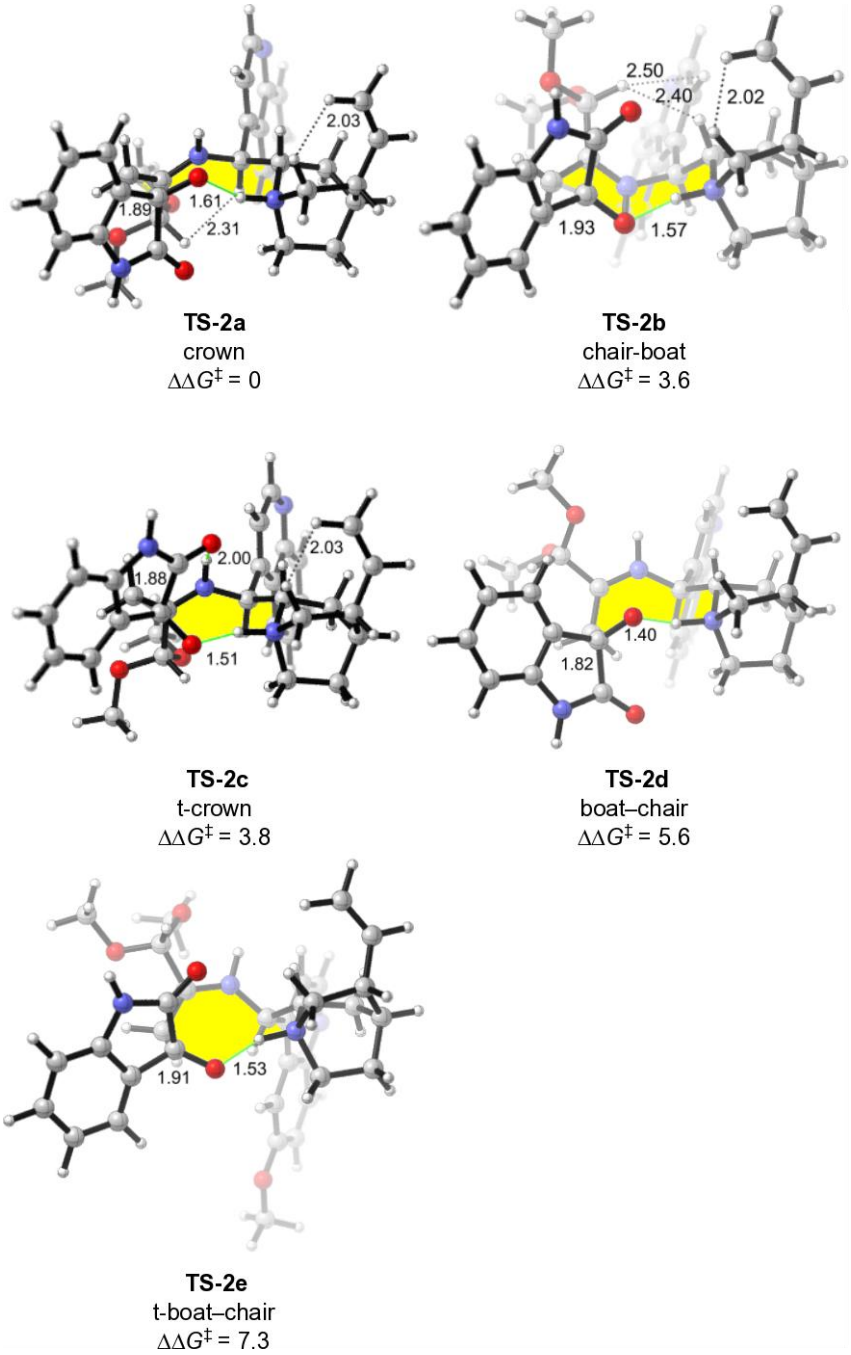
B. Complete set of TS-2a–2e (M06-2X/def2-TZVPP–IEF-PCM (1,4-dioxane)//B3LYP/6-31G(d))–IEF-PCM (1,4-dioxane))

The five transition structures **TS-2a–2e** are shown in Figure S5. The conformations and free energies of activation of **TS-2a–2e** are listed in Table S2.

Table S2. Intermolecular Aldol Addition Transition Structures

Entry	TS	Ring Conformation	$\Delta\Delta G^{\ddagger}$
1	**TS-2a**	crown	0
2	**TS-2b**	chair-boat	3.6
3	**TS-2c**	t-crown	3.8
4	**TS-2d**	boat-chair	5.6
5	**TS-2e**	twist-boat-chair	7.3

M06-2X/def2-TZVPP–IEF-PCM (1,4-dioxane)//B3LYP/6-31G(d)–IEF-PCM (1,4-dioxane). The relative free energies of activation ($\Delta\Delta G^{\ddagger}$) are reported in kcal/mol relative to the lowest-energy transition structure, **TS-2a**.



TS-2a
crown
$\Delta\Delta G^{\ddagger} = 0$

TS-2b
chair-boat
$\Delta\Delta G^{\ddagger} = 3.6$

TS-2c
t-crown
$\Delta\Delta G^{\ddagger} = 3.8$

TS-2d
boat–chair
$\Delta\Delta G^{\ddagger} = 5.6$

TS-2e
t-boat–chair
$\Delta\Delta G^{\ddagger} = 7.3$

Figure S5. Transition structures **TS-2a–2e** for the aldol addition of isatin and the enamine formed by **2a** and pyruvic aldehyde dimethyl acetal (M06-2X/def2-TZVPP–IEF-PCM//B3LYP/6-31G(d)–IEF-PCM (1,4-dioxane)). The free energies of activation ($\Delta\Delta G^{\ddagger}$), relative to **TS-2a**, are reported in kcal/mol.

C. Complete set of TS-3a–3g (M06-2X/def2-TZVPP–IEF-PCM (THF)//B3LYP/6-31G(d))–IEF-PCM (THF))

The two stereodetermining transition structures **TS-3a–3b** are shown in Figure S6. Higher energy conformations **TS-3c–3g** are shown in Figure S7. The conformations and free energies of activation of **TS-3a–3g** are listed in Table S3. The model crown and chair-boat transition structures **TS-4a–4b** are shown in Figure S8.

Table S3. Intermolecular Aldol Addition Transition Structures

Entry	TS	Ring Conformation	$\Delta\Delta G^{\ddagger}$
1	**TS-3a**	chair-boat	0
2	**TS-3b**	crown	1.5
3	**TS-3c**	boat-chair	5.8
4	**TS-3d**	t-crown	6.2
5	**TS-3e**	t-chair-boat	8.0
6	**TS-3f**	t-boat-chair	9.4
7	**TS-3g**	boat-chair	9.7

M06-2X/def2-TZVPP–IEF-PCM (THF)//B3LYP/6-31G(d)–IEF-PCM (THF). The relative free energies of activation ($\Delta\Delta G^{\ddagger}$) are reported in kcal/mol relative to the lowest-energy transition structure, **TS-3a**.

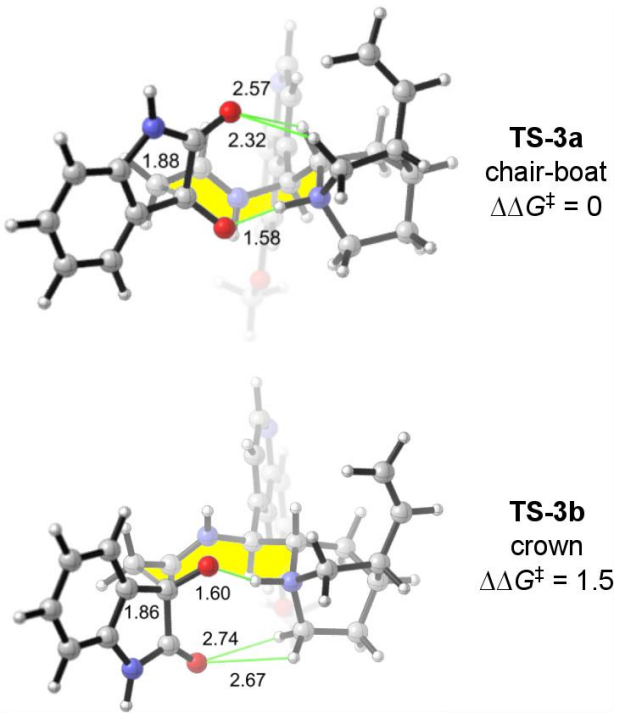
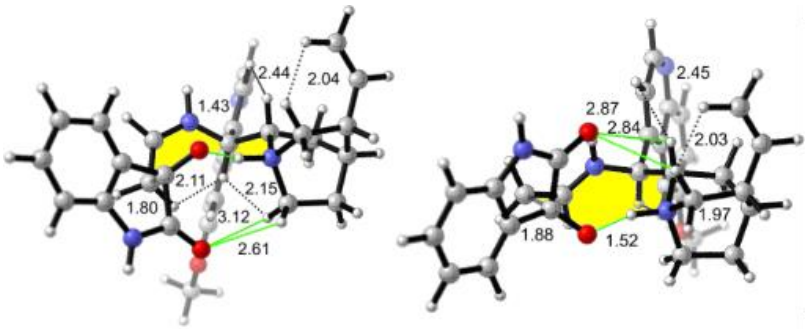
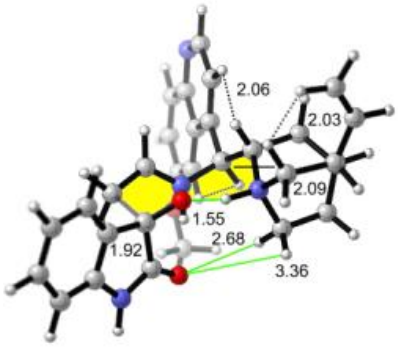


Figure S6. Transition structures **TS-3a–3b** for the aldol addition of isatin and the enamine formed by **2b** and acetaldehyde (M06-2X/def2-TZVPP–IEF-PCM//B3LYP/6-31G(d)–IEF-PCM (THF)). The free energies of activation ($\Delta\Delta G^{‡}$), relative to **TS-3a**, are reported in kcal/mol.

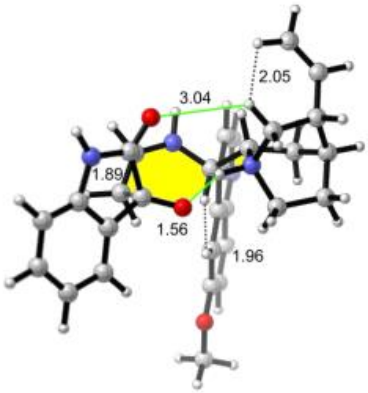


TS-3c
boat–chair
$\Delta\Delta G^{\ddagger}$ = 5.8

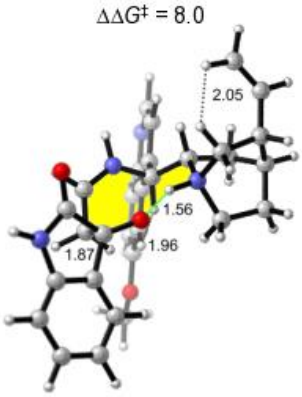
TS-3d
t–crown
$\Delta\Delta G^{\ddagger}$ = 6.2



TS-3e
t–chair–boat
$\Delta\Delta G^{\ddagger}$ = 8.0



TS-3f
t–boat–chair
$\Delta\Delta G^{\ddagger}$ = 9.4



TS-3g
boat–chair
$\Delta\Delta G^{\ddagger}$ = 9.7

Figure S7. Transition structures **TS-3c–3g** for the aldol addition of isatin and the enamine formed by **2b** and acetaldehyde (M06-2X/def2-TZVPP–IEF-PCM//B3LYP/6-31G(d)–IEF-PCM (THF)). The free energies of activation ($\Delta\Delta G^{\ddagger}$), relative to **TS-3a**, are reported in kcal/mol.

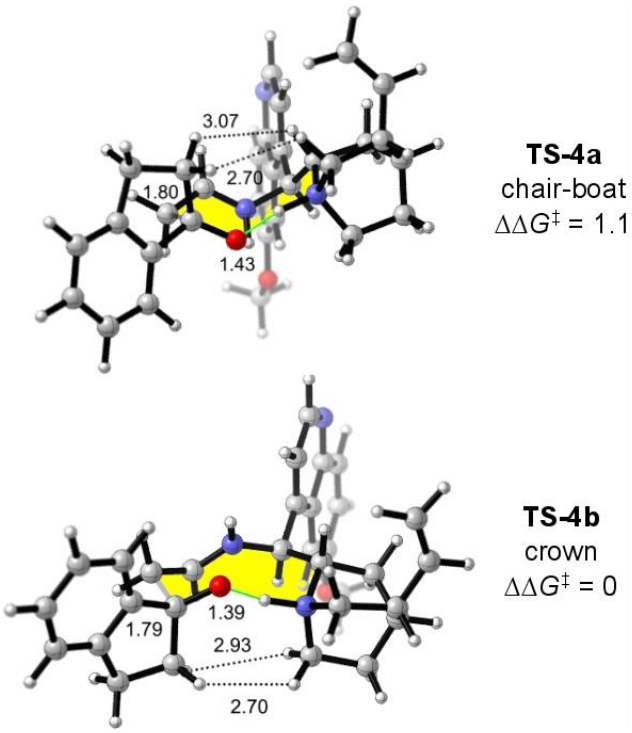


Figure S8. Transition structures **TS-4a–4b** for the aldol addition of the model substrate and the enamine formed by **2b** and acetaldehyde (M06-2X/def2-TZVPP–IEF-PCM//B3LYP/6-31G(d)–IEF-PCM (THF)). The free energies of activation ($\Delta\Delta G^{\ddagger}$), relative to **TS-4b**, are reported in kcal/mol.

D. Complete set of TS-5a–5e (M06-2X/def2-TZVPP–IEF-PCM (cyclohexanone) //B3LYP/6-31G(d))–IEF-PCM (cyclohexanone))

The four stereodetermining transition structures **TS-5a–5d** are shown in Figure S9. **TS-5e** is the higher-energy stereoisomer leading to the (*R*,*R*)-diastereomer, and shown in Figure S10. Their conformations and energies are listed in Table S4.

Table S4. Intermolecular Aldol Addition Transition Structures

Entry	TS	Ring Conformation	$\Delta\Delta G^{\ddagger}$
1	**TS-5a**	crown	0
2	**TS-5b**	crown (axial)	1.5
3	**TS-5c**	boat-chair	3.6
4	**TS-5d**	chair-boat	4.2
5	**TS-5e**	t-crown	3.8

M06-2X/def2-TZVPP–IEF-PCM (cyclohexanone)//B3LYP/6-31G(d)–IEF-PCM (cyclohexanone). The relative free energies of activation ($\Delta\Delta G^{\ddagger}$) are reported in kcal/mol relative to the lowest-energy transition structure, **TS-5a**.

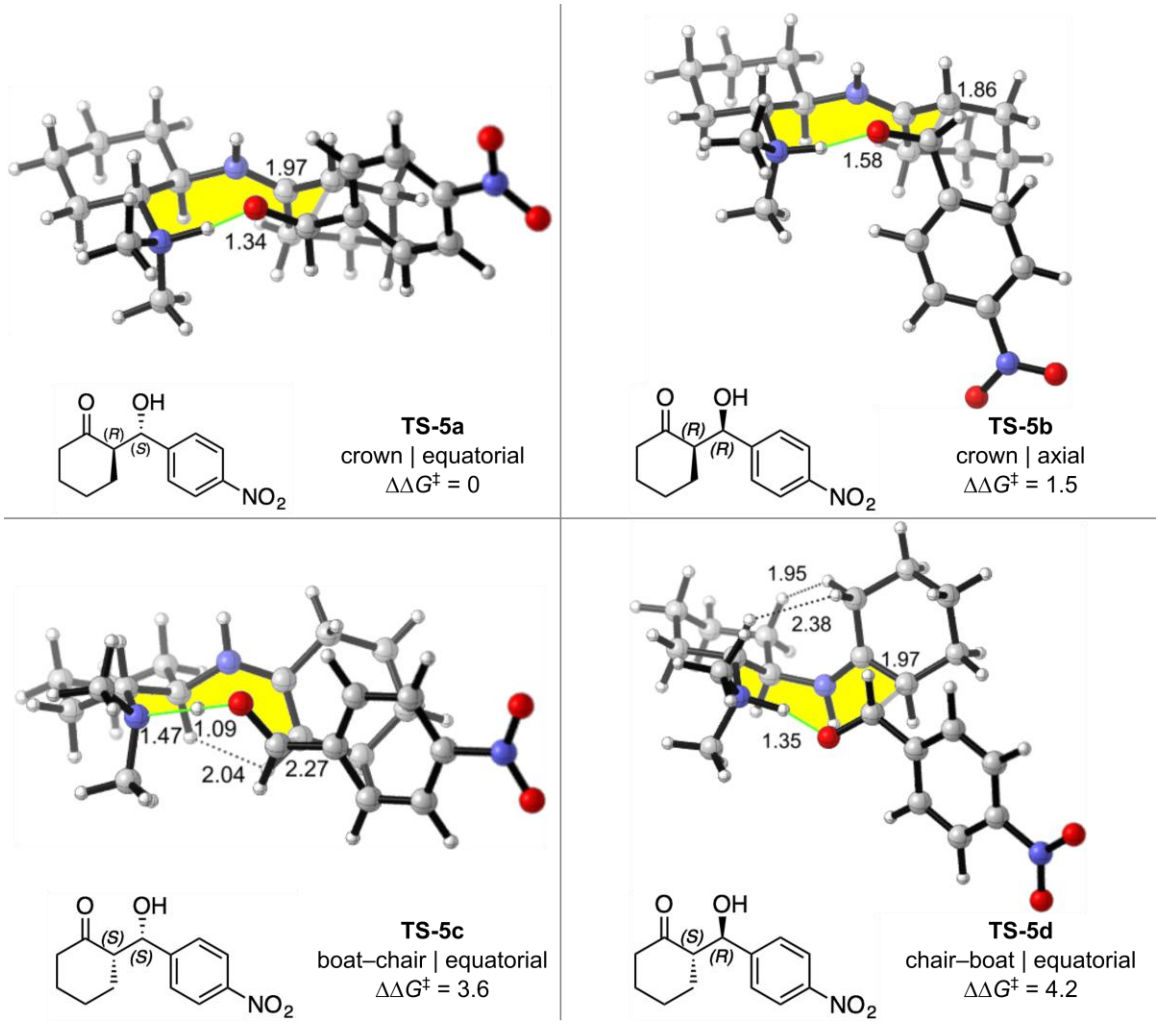
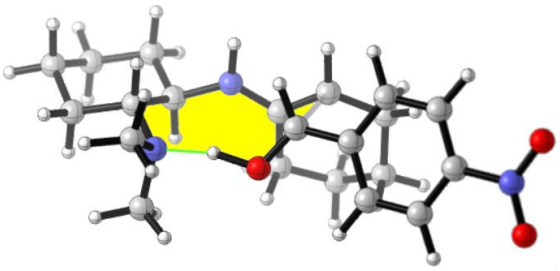


Figure S9. Transition structures **TS-5a–5d** for the aldol addition of the *p*-nitrobenzaldehyde and the enamine formed by **3** and cyclohexanone (M06-2X/def2-TZVPP–IEF-PCM//B3LYP/6-31G(d)–IEF-PCM (cyclohexanone)). The free energies of activation ($\Delta\Delta G^{\ddagger}$), relative to **TS-5a**, are reported in kcal/mol.



TS-5e
t-crown
$\Delta\Delta G^{\ddagger}$ = 3.8

Figure S10. Transition structure **TS-5e** for the aldol addition of the *p*-nitrobenzaldehyde and the enamine formed by **3** and cyclohexanone (M06-2X/def2-TZVPP–IEF-PCM//B3LYP/6-31G(d)–IEF-PCM (cyclohexanone)). The free energies of activation ($\Delta\Delta G^{\ddagger}$), relative to **TS-5a**, are reported in kcal/mol.

E. Cartesian coordinates and energies

TS-1a

N	-0.68500	2.18382	-0.18836
C	-1.73739	-0.13341	-0.32429
C	-1.70629	1.30768	-0.89383
C	-3.07152	2.03950	-0.85302
C	-2.82985	3.52124	-0.50713
C	-2.36201	3.62745	0.97257
C	-1.17359	2.65201	1.15697
C	-0.39293	3.37849	-1.06648
C	-1.72153	4.08538	-1.41606
H	0.26175	1.64829	-0.09211
N	-0.39056	-0.72000	-0.41130
H	-1.34822	1.24829	-1.92624
H	-3.73417	1.59206	-0.10595
H	-3.56465	1.93921	-1.82328
H	-3.75521	4.08768	-0.64417
H	-1.99455	4.65349	1.11455
H	-1.44887	1.76387	1.72481
H	-0.32298	3.11535	1.65942
H	0.28903	4.01422	-0.49869
H	0.14268	3.00519	-1.94093
C	0.29941	-1.35102	0.53723
H	0.14396	-0.48374	-1.24247
H	-2.00333	-0.09273	0.72882
H	-1.61663	5.16424	-1.26928
H	-1.97948	3.92295	-2.46743
C	-0.34437	-1.67001	1.86378
C	1.69578	-1.54519	0.31416
H	-1.40299	-1.90793	1.72366
H	-0.30592	-0.76283	2.48697
C	0.36091	-2.81954	2.60348
H	0.12175	-3.76902	2.10757
H	-0.04328	-2.88026	3.61923
C	1.87760	-2.61856	2.62230
C	2.42416	-2.55951	1.19109
H	2.36132	-3.43619	3.16810
H	2.11973	-1.69171	3.16084
H	3.49630	-2.34016	1.19714
H	2.32355	-3.55176	0.72845
H	1.95874	-1.62257	-0.74152
C	5.57431	0.10706	-1.45503
C	6.48569	-0.06341	-0.40938
C	2.30703	0.28280	0.48518
C	4.22340	0.21046	-1.15110

C	3.77824	0.13292	0.17799
C	6.07679	-0.12860	0.92213
C	4.71744	-0.02859	1.20686
O	1.62789	1.01596	-0.34816
H	5.93014	0.16251	-2.47620
H	3.49576	0.36898	-1.93963
H	6.81081	-0.24957	1.70876
H	4.38698	-0.06286	2.24138
H	2.13833	0.43776	1.56445
C	-2.76087	-0.98398	-1.08173
C	-3.99547	-1.40058	-0.48973
C	-2.49303	-1.37143	-2.37801
C	-4.41694	-1.07611	0.83102
C	-4.86875	-2.20776	-1.29866
C	-3.42747	-2.16216	-3.08492
H	-1.56923	-1.09150	-2.87462
C	-5.62352	-1.52614	1.32127
H	-3.79840	-0.45707	1.47223
C	-6.10412	-2.65593	-0.76046
N	-4.57239	-2.57402	-2.58084
H	-3.20575	-2.46093	-4.10806
C	-6.47586	-2.32402	0.52179
H	-5.92344	-1.26455	2.33155
H	-6.73707	-3.26416	-1.39889
H	-7.42282	-2.67081	0.92458
N	7.91160	-0.16766	-0.71987
O	8.70296	-0.31340	0.21549
O	8.25578	-0.10641	-1.90320
C	-3.50339	3.44029	1.94574
H	-4.33685	4.11925	1.76174
C	-3.59675	2.59326	2.97295
H	-2.81244	1.89551	3.25487
H	-4.48389	2.58180	3.59976

Electronic energy = -1686.08277
Zero-point electronic energy = -1685.434139
Enthalpy = -1685.400529
Free energy = -1685.500022
Free energy with quasiharmonic approximation = -1685.491371
Frequencies = -277.1955 17.7545 26.0197
SCF (M06-2X/def2-TZVPP–IEF-PCM) = -1686.018504

TS-1b

N	-0.44167	1.93727	-1.31237
C	-1.59833	-0.19623	-0.52452
C	-1.75595	1.17019	-1.23751
C	-2.81837	2.11448	-0.62663

C	-2.32118	3.56715	-0.76094
C	-1.13519	3.78515	0.22091
C	-0.12546	2.63690	-0.01448
C	-0.54920	2.95714	-2.42541
C	-1.81798	3.80976	-2.19754
H	0.36266	1.27291	-1.58031
N	-0.60116	-0.98210	-1.26983
H	-2.00852	0.96206	-2.28166
H	-2.99520	1.88287	0.42821
H	-3.76609	1.97309	-1.15200
H	-3.13326	4.25956	-0.52332
H	-0.65607	4.73228	-0.06386
H	-0.16300	1.88280	0.77201
H	0.90304	2.99334	-0.09000
H	0.36937	3.54572	-2.38909
H	-0.56050	2.40173	-3.36469
C	0.32808	-1.79820	-0.79247
H	-0.45371	-0.71395	-2.24271
H	-1.21322	-0.04147	0.48243
H	-1.58262	4.86715	-2.34829
H	-2.59688	3.54383	-2.91924
C	0.37628	-2.14347	0.67011
C	1.35644	-2.19125	-1.71758
H	-0.63671	-2.17973	1.08328
H	0.89906	-1.32784	1.19391
C	1.11501	-3.46873	0.92482
H	0.48851	-4.30274	0.58337
H	1.25058	-3.59248	2.00411
C	2.46166	-3.49673	0.19588
C	2.26480	-3.35519	-1.32021
H	2.98530	-4.43571	0.40746
H	3.09821	-2.68741	0.57360
H	3.23328	-3.25286	-1.82374
H	1.82198	-4.28232	-1.70880
H	0.95364	-2.31801	-2.72407
C	3.99080	0.71084	1.00930
C	5.27401	0.20091	0.80379
C	2.22988	-0.60554	-2.13142
C	3.00826	0.44358	0.06354
C	3.28357	-0.33180	-1.07340
C	5.59027	-0.55889	-0.32191
C	4.58962	-0.81475	-1.25456
O	1.34900	0.32893	-2.39076
H	3.78103	1.30551	1.88948
H	2.01426	0.84756	0.21209
H	6.59877	-0.92771	-0.46069

H	4.83239	-1.38572	-2.14609
H	2.72605	-1.03148	-3.02104
C	-2.94273	-0.92527	-0.45713
C	-3.69017	-1.03289	0.75868
C	-3.46022	-1.50018	-1.59900
C	-3.28423	-0.50160	2.01568
C	-4.94096	-1.74001	0.69560
C	-4.70582	-2.16691	-1.54814
H	-2.92484	-1.46498	-2.54260
C	-4.06550	-0.66248	3.13926
H	-2.35335	0.04760	2.10898
C	-5.72126	-1.88588	1.87312
N	-5.42977	-2.29092	-0.45473
H	-5.10761	-2.61360	-2.45603
C	-5.29489	-1.35984	3.07066
H	-3.73396	-0.24875	4.08688
H	-6.65910	-2.42572	1.78835
H	-5.89796	-1.47737	3.96600
N	6.31705	0.48139	1.79087
O	7.44518	0.02431	1.59176
O	6.01751	1.16060	2.77640
C	-1.59401	3.94716	1.65159
H	-2.33395	4.73846	1.77604
C	-1.19580	3.27874	2.73571
H	-0.44774	2.49057	2.71779
H	-1.60696	3.51570	3.71280

Electronic energy = -1686.078159
Zero-point electronic energy = -1685.428035
Enthalpy = -1685.394717
Free energy = -1685.4925
Free energy with quasiharmonic approximation = -1685.484753
Frequencies = -189.3077 23.1599 28.8739
SCF (M06-2X/def2-TZVPP–IEF-PCM) = -1686.017906

TS-1c

N	-0.99087	2.41039	-0.34003
C	-1.67430	-0.02692	-0.54004
C	-1.91590	1.42764	-1.02236
C	-3.36528	1.94672	-0.82977
C	-3.30849	3.45600	-0.51816
C	-2.76209	3.64741	0.92328
C	-1.48195	2.78515	1.03283
C	-0.90707	3.64783	-1.19396
C	-2.33936	4.14739	-1.49719
H	0.06963	1.98145	-0.25917
N	-0.43651	-0.61288	-1.11358

H	-1.64435	1.47948	-2.08028
H	-3.86643	1.41805	-0.01121
H	-3.94438	1.75656	-1.73641
H	-4.30853	3.89098	-0.60231
H	-2.48162	4.70615	1.02077
H	-1.66082	1.85741	1.57822
H	-0.66257	3.30761	1.53074
H	-0.31922	4.37498	-0.62972
H	-0.34616	3.38474	-2.09316
C	0.60683	-1.15719	-0.49909
H	-0.52833	-0.84741	-2.09867
H	-1.55264	-0.02186	0.53877
H	-2.38591	5.23432	-1.38139
H	-2.61991	3.91830	-2.53064
C	1.49304	-2.04634	-1.33001
C	0.99422	-0.82183	0.83612
H	2.36765	-1.46094	-1.64551
H	0.97179	-2.36323	-2.23919
C	1.96936	-3.25965	-0.50793
H	2.64794	-3.85872	-1.12407
H	1.10848	-3.89620	-0.26635
C	2.66657	-2.79464	0.77418
C	1.75108	-1.89992	1.62381
H	3.58240	-2.25572	0.50856
H	2.97375	-3.66070	1.37139
H	0.99877	-2.52968	2.11839
H	2.32178	-1.43014	2.43218
H	0.18117	-0.41448	1.43522
C	5.30134	0.35104	-1.07704
C	6.11137	0.11685	0.03603
C	1.91901	0.82509	0.60862
C	3.94381	0.57267	-0.87820
C	3.38987	0.54288	0.41215
C	5.59965	0.11786	1.33389
C	4.23744	0.33844	1.51220
O	1.36903	1.54295	-0.33750
H	5.73709	0.36608	-2.06815
H	3.29673	0.79656	-1.71898
H	6.26066	-0.04180	2.17637
H	3.83412	0.36694	2.52001
H	1.72832	1.13264	1.65166
C	-2.82702	-0.95934	-0.92246
C	-3.47549	-1.80106	0.03713
C	-3.23169	-1.03789	-2.24020
C	-3.17278	-1.83888	1.42717
C	-4.51307	-2.66998	-0.45104

C	-4.26295	-1.93156	-2.61054
H	-2.78172	-0.42212	-3.01425
C	-3.85141	-2.68256	2.27893
H	-2.40008	-1.20067	1.84156
C	-5.19329	-3.52606	0.45489
N	-4.88837	-2.72203	-1.76368
H	-4.57397	-1.98236	-3.65253
C	-4.87104	-3.53454	1.79214
H	-3.60157	-2.69277	3.33562
H	-5.97067	-4.16640	0.05032
H	-5.39640	-4.19230	2.47809
N	7.54246	-0.11831	-0.16317
O	8.24409	-0.31680	0.83180
O	7.97802	-0.10973	-1.31726
C	-3.80797	3.38068	1.97995
H	-4.72623	3.94993	1.82976
C	-3.72623	2.58280	3.04627
H	-4.55768	2.49826	3.74031
H	-2.84447	1.99681	3.29136

Electronic energy = -1686.074031
Zero-point electronic energy = -1685.426894
Enthalpy = -1685.393399
Free energy = -1685.492504
Free energy with quasiharmonic approximation = -1685.483841
Frequencies = -277.9563 15.0895 17.8692
SCF (M06-2X/def2-TZVPP–IEF-PCM) = -1686.01282

TS-1d

N	-0.80989	2.29740	-0.52953
C	-1.98260	0.13723	0.09344
C	-1.97946	1.37703	-0.83463
C	-3.27258	2.23149	-0.74823
C	-2.89689	3.72487	-0.80878
C	-2.17104	4.12770	0.50356
C	-1.02692	3.11088	0.72357
C	-0.61271	3.22148	-1.70608
C	-1.94033	3.96089	-1.99295
H	0.12188	1.74285	-0.36845
N	-0.65114	-0.51431	0.17898
H	-1.80184	1.05498	-1.86298
H	-3.81316	2.01959	0.18107
H	-3.94096	1.97641	-1.57314
H	-3.80217	4.32620	-0.93124
H	-1.72914	5.11915	0.32964
H	-1.24314	2.40752	1.52749
H	-0.07098	3.58476	0.95215

H	0.19803	3.89935	-1.43254
H	-0.27541	2.60649	-2.54287
C	0.07830	-1.18515	-0.71829
H	-0.12768	-0.26356	1.01250
H	-2.15133	0.50546	1.10892
H	-1.74838	5.02970	-2.12407
H	-2.39265	3.59546	-2.92032
C	-0.44132	-1.48937	-2.09904
C	1.44163	-1.43284	-0.38098
H	-0.24565	-0.60744	-2.72944
H	-1.52302	-1.62377	-2.08029
C	0.24313	-2.71277	-2.73199
H	-0.07692	-2.78937	-3.77636
H	-0.10071	-3.62302	-2.22425
C	1.76541	-2.60691	-2.62668
C	2.19213	-2.51105	-1.15714
H	2.11055	-1.72327	-3.18106
H	2.24131	-3.47710	-3.09221
H	2.00665	-3.47728	-0.66654
H	3.27024	-2.33947	-1.07950
H	1.62464	-1.47310	0.69361
C	5.24128	0.15603	1.60338
C	6.21899	-0.11476	0.64224
C	2.14619	0.37151	-0.59577
C	3.92409	0.30628	1.19029
C	3.57812	0.17706	-0.16407
C	5.90963	-0.23301	-0.71227
C	4.58290	-0.08439	-1.10700
O	1.43136	1.17463	0.13562
H	5.52104	0.24939	2.64521
H	3.14763	0.53859	1.91108
H	6.69391	-0.43179	-1.43163
H	4.33047	-0.16032	-2.16099
H	2.06438	0.46171	-1.69248
C	-3.11491	-0.85902	-0.18174
C	-3.47877	-1.80820	0.83075
C	-3.82688	-0.87401	-1.36220
C	-2.84480	-1.91435	2.09883
C	-4.56046	-2.70618	0.53924
C	-4.87774	-1.80632	-1.54588
H	-3.60913	-0.19154	-2.17526
C	-3.25810	-2.84985	3.02274
H	-2.01858	-1.26047	2.35361
C	-4.96078	-3.66006	1.51151
N	-5.24323	-2.69194	-0.64540
H	-5.42755	-1.80343	-2.48548

C	-4.32420	-3.73242	2.72923
H	-2.75921	-2.91104	3.98531
H	-5.78246	-4.32167	1.25609
H	-4.63654	-4.46446	3.46799
N	7.61005	-0.27205	1.06844
O	8.45989	-0.51258	0.20705
O	7.86710	-0.15820	2.26971
C	-3.12439	4.27916	1.66688
H	-3.96498	4.93959	1.45048
C	-3.03934	3.74388	2.88611
H	-2.22706	3.09549	3.20392
H	-3.79485	3.95586	3.63734

Electronic energy = -1686.076946
Zero-point electronic energy = -1685.428827
Enthalpy = -1685.394997
Free energy = -1685.495985
Free energy with quasiharmonic approximation = -1685.486174
Frequencies = -289.4083 19.7425 27.4298
SCF (M06-2X/def2-TZVPP–IEF-PCM) = -1686.013487

TS-1e

N	-0.07050	2.21529	0.03812
C	1.14615	-0.01653	0.24273
C	1.08635	1.46986	0.67578
C	2.38637	2.26385	0.38871
C	2.01199	3.69205	-0.05903
C	1.33634	3.65675	-1.45183
C	0.21441	2.58657	-1.39292
C	-0.31631	3.47431	0.83687
C	1.00138	4.27581	0.94822
H	-1.00376	1.62011	0.11365
N	-0.14536	-0.66149	0.53212
H	0.86779	1.49147	1.74778
H	2.98466	1.76733	-0.38106
H	2.99980	2.29137	1.29313
H	2.91178	4.31327	-0.09592
H	0.86875	4.63622	-1.61067
C	2.29491	3.40778	-2.62081
H	0.49663	1.67527	-1.92485
H	-0.72684	2.93823	-1.82069
H	-1.09962	4.02114	0.30855
H	-0.71403	3.16461	1.80504
C	-0.88800	-1.41154	-0.27911
H	-0.63257	-0.33410	1.36294
H	1.29997	-0.06363	-0.83267
H	0.81076	5.33116	0.73220

H	1.40228	4.21886	1.96541
H	3.04829	4.20069	-2.67554
H	1.75097	3.39656	-3.57215
H	2.81819	2.44916	-2.52783
C	-0.34898	-1.84729	-1.61793
C	-2.25407	-1.62033	0.08710
H	0.72696	-2.03287	-1.54984
H	-0.48029	-1.01204	-2.32319
C	-1.06640	-3.09059	-2.17051
H	-0.74968	-3.97377	-1.60087
H	-0.74621	-3.24709	-3.20589
C	-2.58594	-2.93887	-2.07589
C	-3.01102	-2.74525	-0.61547
H	-3.08129	-3.82423	-2.49012
H	-2.90956	-2.08220	-2.68328
H	-4.08673	-2.55624	-0.54970
H	-2.83225	-3.68010	-0.06529
H	-2.41552	-1.61022	1.16583
C	-6.13559	-0.02736	1.89334
C	-7.10719	-0.26660	0.91511
C	-2.95012	0.12546	-0.19132
C	-4.79399	0.09118	1.53487
C	-4.40188	-0.03633	0.19471
C	-6.72721	-0.38317	-0.42306
C	-5.38074	-0.26872	-0.77987
O	-2.25230	0.95471	0.54638
H	-6.42775	0.07324	2.93542
H	-8.15332	-0.35468	1.19535
H	-4.03753	0.30045	2.28527
H	-7.47640	-0.55833	-1.19048
H	-5.09032	-0.34862	-1.82526
H	-2.84198	0.21439	-1.28658
C	2.29407	-0.73110	0.96110
C	3.46849	-1.17529	0.27395
C	2.20454	-0.96158	2.31831
C	3.70692	-1.01646	-1.12089
C	4.47737	-1.83327	1.06004
C	3.25876	-1.61801	2.99334
H	1.33326	-0.65677	2.88994
C	4.86882	-1.47797	-1.70028
H	2.97492	-0.52610	-1.75371
C	5.66310	-2.29634	0.43029
N	4.35795	-2.04235	2.40454
H	3.17705	-1.79284	4.06480
C	5.85771	-2.12318	-0.92048
H	5.02617	-1.34563	-2.76649

H	6.40219	-2.78807	1.05489
H	6.76762	-2.48085	-1.39305

Electronic energy = -1443.502063
Zero-point electronic energy = -1442.861333
Enthalpy = -1442.831123
Free energy = -1442.92167
Free energy with quasiharmonic approximation = -1442.915128
Frequencies = -270.0518 19.6269 27.3274
SCF (M06-2X/def2-TZVPP–IEF-PCM) = -1443.42344

TS-1f

N	0.20779	2.21084	-0.69561
C	-0.97182	-0.03848	-0.46564
C	-1.06766	1.42403	-0.96919
C	-2.25398	2.24245	-0.40550
C	-1.80473	3.70774	-0.22091
C	-0.79946	3.80385	0.95282
C	0.26574	2.70158	0.73014
C	0.23972	3.39477	-1.63726
C	-1.08807	4.17633	-1.50418
H	1.07700	1.61051	-0.93023
N	0.14510	-0.68488	-1.17781
H	-1.13727	1.38402	-2.06072
H	-2.59934	1.82824	0.54600
H	-3.09468	2.17706	-1.10115
H	-2.67617	4.33823	-0.02215
H	-0.30519	4.78037	0.88263
C	-1.42924	3.70301	2.34593
H	0.09750	1.84024	1.38139
H	1.28357	3.05646	0.90323
H	1.11128	3.98742	-1.35292
H	0.41171	2.99714	-2.63878
C	1.00579	-1.57584	-0.70211
H	0.50840	-0.18484	-1.99554
H	-0.73759	-0.03807	0.59864
H	-0.87880	5.24891	-1.45722
H	-1.72345	4.00652	-2.37921
H	-2.13638	4.52333	2.50701
H	-0.66022	3.76617	3.12409
H	-1.96685	2.75835	2.48799
C	0.80621	-2.20276	0.64910
C	2.20056	-1.76687	-1.48205
H	-0.26177	-2.34081	0.84656
H	1.17699	-1.49479	1.40688
C	1.56634	-3.53323	0.78865
H	1.06659	-4.30164	0.18471

H	1.51077	-3.86114	1.83186
C	3.02182	-3.38129	0.33698
C	3.09314	-2.96021	-1.13770
H	3.55845	-4.32744	0.47086
H	3.52516	-2.63793	0.96695
H	4.12825	-2.73208	-1.41793
H	2.78997	-3.80975	-1.76474
H	1.97925	-1.72406	-2.55006
C	4.15095	0.62060	2.15295
C	5.49509	0.23854	2.11395
C	3.04696	-0.13546	-1.44698
C	3.35415	0.49969	1.01420
C	3.87703	-0.01086	-0.18254
C	6.03374	-0.25845	0.92583
C	5.23037	-0.37740	-0.21070
O	2.17382	0.81228	-1.72705
H	3.72410	1.01708	3.07044
H	6.11708	0.33570	2.99940
H	2.31588	0.80929	1.06176
H	7.08069	-0.54590	0.87906
H	5.66406	-0.74617	-1.13743
H	3.72142	-0.38698	-2.28455
C	-2.28863	-0.77987	-0.70604
C	-3.18459	-1.11198	0.36004
C	-2.63590	-1.14181	-1.99080
C	-2.96016	-0.82129	1.73590
C	-4.39608	-1.80087	0.00458
C	-3.85741	-1.81273	-2.22717
H	-1.98255	-0.93139	-2.83149
C	-3.87627	-1.18771	2.69776
H	-2.05924	-0.30630	2.05160
C	-5.31921	-2.16189	1.02176
N	-4.71490	-2.13569	-1.28070
H	-4.12415	-2.08934	-3.24583
C	-5.06756	-1.86273	2.34073
H	-3.68067	-0.95704	3.74068
H	-6.22252	-2.68061	0.71659
H	-5.77881	-2.14413	3.11152

Electronic energy = -1443.497738
Zero-point electronic energy = -1442.855647
Enthalpy = -1442.825738
Free energy = -1442.914734
Free energy with quasiharmonic approximation = -1442.90889
Frequencies = -203.9554 21.7766 24.5932
SCF (M06-2X/def2-TZVPP–IEF-PCM) = -1443.422125

TS-1g

N	0.09865	2.34370	-0.19516
C	-1.34268	0.29730	0.15917
C	-1.12563	1.58520	-0.67375
C	-2.32602	2.57031	-0.64143
C	-1.79502	4.01708	-0.55684
C	-1.14899	4.26906	0.82622
C	-0.16692	3.09967	1.08451
C	0.50431	3.32151	-1.26960
C	-0.70981	4.20746	-1.63584
H	0.96149	1.67289	0.01722
N	-0.10535	-0.51221	0.28520
H	-0.88855	1.30886	-1.70338
H	-2.98026	2.34861	0.20820
H	-2.93036	2.44455	-1.54259
H	-2.61809	4.71910	-0.72037
H	-0.57033	5.19796	0.75279
C	-2.14739	4.43733	1.97646
H	-0.56606	2.38843	1.81094
H	0.80593	3.43013	1.45372
H	1.33801	3.89663	-0.86207
H	0.87726	2.73940	-2.11478
C	0.63201	-1.15973	-0.61952
H	0.37985	-0.38005	1.16832
H	-1.53771	0.61834	1.18551
H	-0.40003	5.25542	-1.68780
H	-1.10212	3.93531	-2.62112
H	-2.79436	5.30291	1.79895
H	-1.62175	4.60077	2.92407
H	-2.78700	3.55578	2.10075
C	0.20692	-1.27189	-2.05917
C	1.93952	-1.56242	-0.20425
H	0.52614	-0.34962	-2.57080
H	-0.88051	-1.30933	-2.13411
C	0.83805	-2.48134	-2.77022
H	0.60618	-2.41783	-3.83862
H	0.37258	-3.40262	-2.39680
C	2.34908	-2.53368	-2.53466
C	2.65554	-2.62535	-1.03483
H	2.81876	-1.63876	-2.96567
H	2.78395	-3.39640	-3.05186
H	2.34722	-3.61443	-0.66731
H	3.73359	-2.56010	-0.85806
H	2.00807	-1.75017	0.86844
C	5.62793	-0.61421	2.32164
C	6.70994	-0.84838	1.46563

C	2.82170	0.12031	-0.14767
C	4.37311	-0.30910	1.79770
C	4.17805	-0.24150	0.41073
C	6.52787	-0.77091	0.08386
C	5.26753	-0.46911	-0.43977
O	2.10411	0.93761	0.58434
H	5.76667	-0.66404	3.39849
H	7.68867	-1.08302	1.87514
H	3.53429	-0.10403	2.45625
H	7.36519	-0.94019	-0.58778
H	5.13404	-0.39683	-1.51691
H	2.88249	0.33743	-1.22831
C	-2.55461	-0.54304	-0.25459
C	-3.10574	-1.48698	0.67519
C	-3.16320	-0.42217	-1.48538
C	-2.59821	-1.71973	1.98295
C	-4.25287	-2.23997	0.25269
C	-4.29237	-1.21798	-1.80021
H	-2.80354	0.26848	-2.23916
C	-3.19093	-2.63931	2.82116
H	-1.73012	-1.17701	2.33997
C	-4.83868	-3.18156	1.13920
N	-4.82785	-2.09491	-0.97961
H	-4.75842	-1.11011	-2.77819
C	-4.32021	-3.37917	2.39837
H	-2.78603	-2.79775	3.81623
H	-5.70499	-3.73152	0.78543
H	-4.77477	-4.10033	3.07108

Electronic energy = -1443.496514
Zero-point electronic energy = -1442.855696
Enthalpy = -1442.825588
Free energy = -1442.91549
Free energy with quasiharmonic approximation = -1442.909528
Frequencies = -279.4982 21.0332 25.6504
SCF (M06-2X/def2-TZVPP–IEF-PCM) = -1443.418856

TS-1h

N	-0.19088	2.43409	-0.29486
C	-1.14058	0.09945	-0.43933
C	-1.30850	1.59001	-0.83000
C	-2.66294	2.22447	-0.41268
C	-2.41509	3.71047	-0.07263
C	-1.62590	3.81242	1.25362
C	-0.43677	2.82088	1.13018
C	-0.13925	3.68171	-1.11946
C	-1.54592	4.33672	-1.18349

H	1.12191	1.79656	-0.43099
N	0.00451	-0.50589	-1.15241
H	-1.21109	1.64974	-1.91901
H	-3.09328	1.70289	0.44964
H	-3.38456	2.12780	-1.22886
H	-3.37040	4.23927	0.00964
H	-1.22404	4.83203	1.32007
C	-2.45783	3.56326	2.51537
H	-0.63231	1.90896	1.70245
H	0.49050	3.25229	1.51846
H	0.59747	4.34203	-0.65368
H	0.23625	3.41416	-2.11133
C	1.02740	-1.22314	-0.65864
H	-0.14529	-0.60373	-2.15119
H	-0.92510	0.04072	0.62365
H	-1.46433	5.41948	-1.04175
H	-2.00707	4.17346	-2.16425
H	-3.25735	4.30701	2.60635
H	-1.83272	3.63340	3.41347
H	-2.92128	2.56956	2.51315
C	1.81472	-2.02006	-1.67240
C	1.47739	-1.14931	0.66476
H	2.65326	-1.39732	-2.01694
H	1.19355	-2.22839	-2.55043
C	2.35864	-3.32357	-1.06505
H	2.97903	-3.83344	-1.81003
H	1.52021	-3.99364	-0.83399
C	3.16685	-3.02869	0.20168
C	2.32824	-2.27042	1.24125
H	4.04954	-2.43778	-0.06713
H	3.53365	-3.96189	0.64426
H	1.64717	-2.97421	1.74317
H	2.97780	-1.87700	2.03189
H	0.80449	-0.70192	1.39167
C	6.05052	-0.01768	-0.96864
C	6.74700	-0.33357	0.20344
C	2.61427	0.72943	0.40770
C	4.70158	0.32161	-0.91104
C	4.02935	0.33959	0.32494
C	6.09247	-0.29495	1.43736
C	4.74152	0.04350	1.49980
O	2.11508	1.38526	-0.60867
H	6.56364	-0.02948	-1.92583
H	7.79985	-0.59630	0.15532
H	4.16257	0.59188	-1.81296
H	6.63556	-0.51973	2.35051

H	4.24049	0.09741	2.46246
H	2.25048	0.98400	1.40419
C	-2.38956	-0.72802	-0.75659
C	-3.04359	-1.54002	0.22545
C	-2.89489	-0.73268	-2.04182
C	-2.64909	-1.64416	1.58916
C	-4.18493	-2.30236	-0.20526
C	-4.02357	-1.52280	-2.35731
H	-2.44776	-0.13599	-2.83215
C	-3.33741	-2.44991	2.46949
H	-1.79561	-1.08678	1.95875
C	-4.87192	-3.12279	0.72854
N	-4.65618	-2.28310	-1.48764
H	-4.41062	-1.51512	-3.37504
C	-4.45919	-3.19717	2.03865
H	-3.01570	-2.51157	3.50488
H	-5.72890	-3.68259	0.36730
H	-4.99096	-3.82704	2.74568

Electronic energy = -1443.495001
Zero-point electronic energy = -1442.856114
Enthalpy = -1442.825831
Free energy = -1442.916657
Free energy with quasiharmonic approximation = -1442.909985
Frequencies = -299.3956 14.9743 15.9683
SCF (M06-2X/def2-TZVPP–IEF-PCM) = -1443.416109

TS-1i

N	0.16779	2.01128	-0.06581
C	-1.25485	-0.11036	-0.23472
C	-0.99791	1.33319	-0.74944
C	-2.23943	2.25752	-0.62076
C	-1.76832	3.68421	-0.26992
C	-1.20781	3.71504	1.17210
C	-0.21757	2.52910	1.29449
C	0.59284	3.17500	-0.92552
C	-0.62803	4.07554	-1.23056
H	1.16348	1.36386	0.08743
N	-0.08565	-0.96869	-0.49445
H	-0.70078	1.26149	-1.79976
H	-2.79221	2.25365	-1.56394
H	-2.92484	1.88197	0.14652
H	-2.60436	4.38392	-0.36541
H	-0.64370	4.64943	1.28395
C	-2.27177	3.68509	2.27400
H	-0.65682	1.69910	1.85340
H	0.70986	2.80612	1.80101

H	1.37105	3.69984	-0.36752
H	1.04865	2.76297	-1.82855
C	0.85288	-1.39487	0.34964
H	0.08480	-1.16449	-1.47739
H	-1.39746	-0.07820	0.84104
H	-0.35614	5.12695	-1.09561
H	-0.94843	3.95393	-2.27084
H	-1.80383	3.69704	3.26513
H	-2.90097	2.78912	2.21677
H	-2.92516	4.56126	2.20245
C	0.71173	-1.19967	1.82671
C	2.11701	-1.80269	-0.17829
H	-0.33618	-1.17540	2.13541
H	1.14956	-0.20397	2.01594
C	1.48580	-2.24889	2.64564
H	0.99209	-3.22429	2.54703
H	1.43164	-1.96920	3.70301
C	2.93836	-2.34775	2.17594
C	2.99668	-2.70129	0.68633
H	3.47439	-3.10618	2.75766
H	3.44672	-1.39127	2.35145
H	4.02646	-2.65501	0.31899
H	2.66756	-3.74142	0.54680
H	2.07332	-2.13491	-1.21766
C	6.50503	0.11658	0.35908
C	7.07189	-0.50712	-0.75565
C	2.79957	-0.02328	-0.48450
C	5.12078	0.26662	0.45075
C	4.28684	-0.20936	-0.56991
C	6.24719	-0.97747	-1.78216
C	4.86350	-0.82969	-1.68842
O	2.37084	0.88117	0.37583
H	7.14272	0.49232	1.15478
H	8.15003	-0.62068	-0.82809
H	4.67063	0.77043	1.29976
H	6.68231	-1.45415	-2.65625
H	4.22644	-1.19254	-2.49242
H	2.34121	0.03147	-1.48692
C	-2.48829	-0.72002	-0.90271
C	-3.61225	-1.18877	-0.14980
C	-2.52427	-0.85037	-2.27629
C	-3.73216	-1.11594	1.26634
C	-4.69950	-1.77181	-0.88915
C	-3.64611	-1.44214	-2.90163
H	-1.70868	-0.50614	-2.90611
C	-4.85310	-1.59234	1.91029

H	-2.94088	-0.67790	1.86460
C	-5.83978	-2.25426	-0.19390
N	-4.69845	-1.89076	-2.25024
H	-3.66026	-1.54020	-3.98576
C	-5.91749	-2.16792	1.17683
H	-4.91999	-1.52510	2.99199
H	-6.63992	-2.68833	-0.78508
H	-6.79362	-2.53894	1.70023

Electronic energy = -1443.494055
Zero-point electronic energy = -1442.856018
Enthalpy = -1442.825627
Free energy = -1442.916325
Free energy with quasiharmonic approximation = -1442.909931
Frequencies = -764.0351 21.1573 24.7225
SCF (M06-2X/def2-TZVPP–IEF-PCM) = -1443.417871

TS-1j

N	0.19484	2.28328	-0.18658
C	-1.42087	0.34851	0.18651
C	-1.06062	1.60494	-0.65111
C	-2.23648	2.63203	-0.63774
C	-1.67525	4.04477	-0.38508
C	-1.02323	4.13566	1.01556
C	-0.00328	2.96477	1.12862
C	0.56882	3.31836	-1.20859
C	-0.58876	4.32311	-1.43837
H	1.37891	1.47221	-0.21288
N	-0.27492	-0.51074	0.55137
H	-0.83895	1.30276	-1.67696
H	-2.96951	2.36686	0.13222
H	-2.76943	2.60942	-1.59297
H	-2.48296	4.77975	-0.46844
H	-0.46614	5.08072	1.04891
C	-2.01948	4.15271	2.18002
H	-0.33661	2.21710	1.85388
H	0.97837	3.31351	1.46184
H	1.46918	3.81131	-0.83247
H	0.84294	2.79022	-2.12608
C	0.60108	-1.21577	-0.20077
H	-0.13170	-0.59926	1.55069
H	-1.76446	0.72154	1.15433
H	-1.00269	4.21217	-2.44665
H	-0.22188	5.35098	-1.34959
H	-2.69355	5.01315	2.10287
H	-1.49290	4.22597	3.13877
H	-2.63563	3.24642	2.21196

C	0.49609	-1.20547	-1.70055
C	1.70647	-1.80606	0.41563
H	1.02466	-0.30190	-2.04547
H	-0.54491	-1.11023	-2.01278
C	1.13627	-2.44527	-2.34733
H	1.14041	-2.31151	-3.43448
H	0.51498	-3.32534	-2.13623
C	2.55463	-2.67088	-1.81931
C	2.54419	-2.84671	-0.29558
H	3.18364	-1.81269	-2.08883
H	3.00285	-3.55283	-2.29065
H	2.14534	-3.84179	-0.04408
H	3.56644	-2.82731	0.10027
H	1.66352	-1.90847	1.50002
C	6.34175	-0.40837	-0.44691
C	6.84904	-0.99250	0.71829
C	2.75463	0.19022	0.55381
C	5.00345	-0.02899	-0.51418
C	4.15699	-0.23475	0.58950
C	6.01370	-1.19702	1.82131
C	4.67410	-0.82263	1.75769
O	2.37368	0.99931	-0.39506
H	6.99259	-0.24441	-1.30071
H	7.89390	-1.28502	0.76808
H	4.60638	0.44054	-1.40794
H	6.40788	-1.64455	2.72878
H	4.02487	-0.97811	2.61570
H	2.24170	0.27513	1.51367
C	-2.59443	-0.46054	-0.39245
C	-3.32885	-1.35623	0.45658
C	-2.99238	-0.36358	-1.70906
C	-3.06911	-1.54698	1.84161
C	-4.40610	-2.10080	-0.13233
C	-4.07299	-1.14463	-2.18793
H	-2.50205	0.30082	-2.41089
C	-3.82122	-2.42257	2.59488
H	-2.27313	-0.99674	2.33034
C	-5.15921	-2.99926	0.66854
N	-4.76003	-1.98745	-1.44872
H	-4.36564	-1.05595	-3.23304
C	-4.87410	-3.16025	2.00502
H	-3.60360	-2.54608	3.65162
H	-5.96414	-3.54540	0.18671
H	-5.45643	-3.84816	2.61082

Electronic energy = -1443.48797

Zero-point electronic energy = -1442.850208

Enthalpy = -1442.819738
Free energy = -1442.910307
Free energy with quasiharmonic approximation = -1442.904395
Frequencies = -415.749 21.2048 25.1652
SCF (M06-2X/def2-TZVPP–IEF-PCM) = -1443.410518

TS-1k

N	0.11329	2.55874	-0.09966
C	1.35755	0.34663	-0.23428
C	1.05346	1.62512	0.58698
C	2.37914	2.37456	0.93156
C	2.17622	3.88358	0.68575
C	1.91939	4.16441	-0.81547
C	0.75847	3.22799	-1.26564
C	-0.30142	3.60854	0.88194
C	0.93417	4.33745	1.47483
H	-1.16848	1.87496	-0.50765
N	0.21893	-0.29886	-0.94839
H	0.54112	1.35354	1.51186
H	3.20920	1.99533	0.32461
H	2.65267	2.19571	1.97589
H	3.06209	4.43272	1.02229
H	1.57348	5.20344	-0.89210
C	3.15738	4.02973	-1.70844
H	1.11629	2.45254	-1.94938
H	-0.02339	3.77908	-1.79617
H	-0.96205	4.29552	0.34574
H	-0.89529	3.12398	1.66273
C	-0.79345	-1.04858	-0.48305
H	0.40043	-0.41867	-1.93809
H	1.99782	0.67170	-1.05540
H	0.80814	5.42271	1.40110
H	1.05277	4.09564	2.53697
H	3.94014	4.73058	-1.39705
H	2.90703	4.25076	-2.75266
H	3.58148	3.01914	-1.67938
C	-1.43506	-1.99128	-1.47166
C	-1.36254	-0.89572	0.78852
H	-0.74743	-2.19679	-2.29863
H	-2.31831	-1.49767	-1.90125
C	-1.86852	-3.29634	-0.77931
H	-0.97783	-3.83667	-0.43352
H	-2.36935	-3.93934	-1.51099
C	-2.79912	-2.99192	0.39876
C	-2.14172	-2.04281	1.41337
H	-3.08364	-3.92036	0.90678

H	-3.72341	-2.54612	0.01532
H	-1.43507	-2.60933	2.03768
H	-2.89624	-1.65126	2.10517
H	-0.79171	-0.31539	1.50743
C	-6.11142	-0.50999	0.96201
C	-6.60924	-0.70249	-0.32955
C	-2.64123	0.77619	0.24310
C	-4.81358	-0.03566	1.14553
C	-3.99677	0.24411	0.03640
C	-5.81079	-0.40402	-1.43905
C	-4.51416	0.07096	-1.26066
O	-2.09718	1.41464	-0.77003
H	-6.73608	-0.72099	1.82483
H	-7.62096	-1.07105	-0.47218
H	-4.43761	0.13613	2.15028
H	-6.20404	-0.53448	-2.44301
H	-3.90092	0.33081	-2.11696
H	-2.43683	1.15850	1.24457
C	2.14780	-0.70433	0.55751
C	3.02211	-1.61228	-0.13102
C	2.03549	-0.84012	1.92484
C	3.25752	-1.59800	-1.53358
C	3.70894	-2.59927	0.65414
C	2.75859	-1.85270	2.60194
H	1.40818	-0.18644	2.51912
C	4.11614	-2.50138	-2.12224
H	2.76503	-0.86776	-2.16644
C	4.58601	-3.51693	0.01822
N	3.56379	-2.70735	2.00984
H	2.65284	-1.94480	3.68181
C	4.78698	-3.47207	-1.34233
H	4.27964	-2.46616	-3.19522
H	5.08702	-4.24754	0.64552
H	5.46036	-4.17711	-1.82065

Electronic energy = -1443.487561
Zero-point electronic energy = -1442.84784
Enthalpy = -1442.817628
Free energy = -1442.908181
Free energy with quasiharmonic approximation = -1442.901652
Frequencies = -271.7071 11.8351 21.8945
SCF (M06-2X/def2-TZVPP–IEF-PCM) = -1443.411216

TS-1l

N	2.22856	-1.22823	-0.71295
C	1.56102	1.10088	0.23262
C	2.62910	0.19686	-0.46300

C	4.01670	0.20334	0.22805
C	4.74233	-1.10774	-0.15220
C	4.10042	-2.28270	0.62116
C	2.56672	-2.12867	0.44126
C	3.02919	-1.69347	-1.89177
C	4.53443	-1.38333	-1.65797
H	0.82486	-1.40088	-0.98457
N	0.84646	0.41037	1.33256
H	2.76915	0.63395	-1.45322
H	3.92624	0.28473	1.31806
H	4.58014	1.08160	-0.10461
H	5.80962	-1.03236	0.07996
H	4.41928	-3.21262	0.13284
C	4.50196	-2.38049	2.09617
H	2.10859	-1.71265	1.33945
H	2.08467	-3.09157	0.24724
H	2.84472	-2.76537	-2.00297
H	2.64262	-1.19818	-2.78701
C	-0.44363	0.08155	1.56319
H	1.43183	0.32240	2.15630
H	2.16160	1.86117	0.74719
H	5.14612	-2.23372	-1.97665
H	4.85043	-0.51885	-2.25269
H	5.58128	-2.54168	2.19391
H	3.99347	-3.22137	2.58249
H	4.24572	-1.47294	2.65557
C	-0.68419	-0.34060	3.00334
C	-1.48694	0.02838	0.62463
H	-0.41675	0.51294	3.64153
H	0.01969	-1.14460	3.25991
C	-2.12685	-0.76626	3.29503
H	-2.27421	-0.79853	4.37962
H	-2.30727	-1.78180	2.92142
C	-3.09370	0.21238	2.62699
C	-2.93295	0.15562	1.10045
H	-2.88324	1.22742	2.99087
H	-4.13017	-0.01431	2.89952
H	-3.52887	-0.67384	0.70273
H	-3.35182	1.06339	0.64848
H	-1.29918	0.46542	-0.34617
C	-4.18528	-2.64472	-2.15919
C	-4.83353	-3.50738	-1.26775
C	-1.00910	-1.89165	-0.26214
C	-2.94483	-2.10409	-1.83293
C	-2.33919	-2.42033	-0.60451
C	-4.23678	-3.82763	-0.04595

C	-2.99636	-3.28403	0.28652
O	-0.22953	-1.54955	-1.25861
H	-4.64801	-2.39843	-3.11043
H	-5.80007	-3.92970	-1.52714
H	-2.43179	-1.44271	-2.52339
H	-4.73368	-4.50221	0.64490
H	-2.52714	-3.54340	1.23205
H	-0.53798	-2.33555	0.61646
C	0.65278	1.89531	-0.70515
C	0.01726	3.09125	-0.22958
C	0.45630	1.54781	-2.02440
C	0.13545	3.58813	1.09781
C	-0.78513	3.83370	-1.15990
C	-0.35858	2.35251	-2.85753
H	0.89423	0.65438	-2.45092
C	-0.50133	4.74970	1.47985
H	0.72948	3.05222	1.82988
C	-1.42955	5.02503	-0.73440
N	-0.96353	3.45160	-2.46106
H	-0.50631	2.05799	-3.89536
C	-1.29264	5.47559	0.55878
H	-0.39443	5.11115	2.49837
H	-2.02708	5.56062	-1.46545
H	-1.78835	6.38832	0.87597

Electronic energy = -1443.476763
Zero-point electronic energy = -1442.838324
Enthalpy = -1442.807863
Free energy = -1442.898846
Free energy with quasiharmonic approximation = -1442.892301
Frequencies = -354.0132 15.5782 24.8679
SCF (M06-2X/def2-TZVPP–IEF-PCM) = -1443.400134

TS-1m

N	-0.19439	2.17670	-0.51327
C	-1.29887	0.12296	0.49871
C	-1.41177	1.27016	-0.53962
C	-2.66954	2.15658	-0.35809
C	-2.29310	3.62523	-0.64346
C	-1.36128	4.16064	0.47207
C	-0.22231	3.12437	0.65736
C	-0.16932	2.97392	-1.79744
C	-1.52784	3.68807	-1.98060
H	0.72955	1.57399	-0.51655
N	-0.05715	-0.63740	0.27456
H	-1.40797	0.83550	-1.54184
H	-3.07139	2.05630	0.65470

H	-3.45210	1.81602	-1.04150
H	-3.20036	4.23425	-0.69721
H	-0.91930	5.09555	0.10681
C	-2.06593	4.47025	1.79712
H	-0.35810	2.52930	1.56348
H	0.76534	3.58689	0.71296
H	0.66438	3.67245	-1.70483
H	0.06373	2.27452	-2.60234
C	0.85988	-0.97320	1.18283
H	0.28736	-0.67060	-0.68290
H	-1.22315	0.58064	1.48550
H	-1.36056	4.72684	-2.28019
H	-2.11100	3.21007	-2.77428
H	-2.82252	5.24927	1.65633
H	-1.34841	4.83113	2.54281
H	-2.56266	3.58740	2.21591
C	0.58800	-0.75148	2.64940
C	2.14397	-1.37091	0.69972
H	-0.46530	-0.95180	2.86822
H	0.75398	0.31605	2.86461
C	1.48860	-1.60077	3.56149
H	1.14616	-2.64323	3.53633
H	1.37047	-1.25160	4.59263
C	2.95097	-1.53378	3.11616
C	3.09254	-2.05424	1.68104
H	3.57882	-2.12923	3.78851
H	3.31033	-0.49748	3.18312
H	4.12270	-1.93983	1.33032
H	2.88611	-3.13413	1.67145
H	2.10398	-1.86709	-0.27064
C	5.44377	-0.99347	-2.42862
C	6.61760	-0.78751	-1.69508
C	2.78374	0.28257	-0.01876
C	4.20736	-0.65499	-1.88202
C	4.12384	-0.11395	-0.59103
C	6.54487	-0.23789	-0.41403
C	5.30341	0.09640	0.13442
O	1.89630	0.71170	-0.88176
H	5.49565	-1.41259	-3.43012
H	7.58150	-1.04839	-2.12343
H	3.29469	-0.79126	-2.45457
H	7.45220	-0.06449	0.15829
H	5.25303	0.53580	1.12830
H	2.90474	0.86740	0.90916
C	-2.54720	-0.76265	0.53228
C	-2.94385	-1.64656	-0.52469

C	-3.34695	-0.69386	1.65420
C	-2.23450	-1.84188	-1.74227
C	-4.15845	-2.39216	-0.33143
C	-4.52419	-1.47443	1.74013
H	-3.08942	-0.04261	2.48437
C	-2.69615	-2.71015	-2.70783
H	-1.31066	-1.31014	-1.93254
C	-4.60584	-3.28011	-1.34487
N	-4.92814	-2.29480	0.79475
H	-5.14424	-1.40737	2.63256
C	-3.89269	-3.43751	-2.51082
H	-2.13315	-2.83748	-3.62752
H	-5.52683	-3.82436	-1.16133
H	-4.24302	-4.11879	-3.28041

Electronic energy = -1443.500636
Zero-point electronic energy = -1442.859625
Enthalpy = -1442.829494
Free energy = -1442.919869
Free energy with quasiharmonic approximation = -1442.913275
Frequencies = -284.0145 14.0686 30.6486
SCF (M06-2X/def2-TZVPP–IEF-PCM) = -1443.420802

TS-1n

N	0.17673	2.09847	-0.75213
C	-0.97840	0.11309	0.35242
C	-1.15815	1.42192	-0.46070
C	-2.07858	2.47706	0.19684
C	-1.54078	3.88538	-0.13928
C	-0.22745	4.13975	0.64022
C	0.66785	2.89312	0.43447
C	-0.01793	3.02554	-1.93277
C	-1.22191	3.95197	-1.64718
H	0.91186	1.36734	-1.05325
N	-0.14579	-0.81477	-0.43420
H	-1.55108	1.16016	-1.44622
H	-2.12201	2.33458	1.28106
H	-3.09660	2.34573	-0.17918
H	-2.28811	4.63918	0.12438
H	0.26898	5.00171	0.17821
C	-0.41741	4.45786	2.12661
H	0.64376	2.23235	1.30457
H	1.71025	3.14936	0.23688
H	0.91966	3.57205	-2.04974
H	-0.15517	2.39327	-2.81128
C	0.78286	-1.65158	0.01682
H	0.00543	-0.56570	-1.41753

H	-0.43429	0.35401	1.26879
H	-0.97454	4.97554	-1.94303
H	-2.09279	3.64498	-2.23526
H	-0.99661	5.37909	2.24802
H	0.55056	4.60261	2.61956
H	-0.94294	3.65482	2.65608
C	0.96323	-1.89491	1.48876
C	1.68890	-2.16649	-0.97318
H	-0.00388	-1.85158	1.99909
H	1.56949	-1.06918	1.89376
C	1.67220	-3.23013	1.77132
H	0.98436	-4.05778	1.55514
H	1.90924	-3.28294	2.83903
C	2.93828	-3.36998	0.92051
C	2.59712	-3.33052	-0.57641
H	3.44514	-4.31380	1.15187
H	3.63886	-2.56410	1.17088
H	3.51561	-3.29546	-1.17415
H	2.09401	-4.26783	-0.85072
H	1.17119	-2.35950	-1.91430
C	4.71642	0.80959	1.20017
C	5.96904	0.25964	0.91258
C	2.57519	-0.67288	-1.61795
C	3.61864	0.51211	0.39255
C	3.74424	-0.34382	-0.71045
C	6.11302	-0.58257	-0.19150
C	5.00960	-0.87697	-0.99587
O	1.69332	0.26803	-1.88486
H	4.59609	1.47415	2.05164
H	6.82551	0.49320	1.53890
H	2.65630	0.95542	0.62172
H	7.08491	-1.00434	-0.43323
H	5.13528	-1.51731	-1.86591
H	2.95614	-1.20252	-2.50861
C	-2.31593	-0.49096	0.78659
C	-3.25686	-1.09974	-0.10718
C	-2.64152	-0.42335	2.12552
C	-3.06946	-1.26293	-1.50780
C	-4.48391	-1.58253	0.46672
C	-3.87983	-0.93271	2.58379
H	-1.95842	0.01941	2.84443
C	-4.03525	-1.85558	-2.29230
H	-2.15176	-0.93438	-1.97871
C	-5.45790	-2.18905	-0.36946
N	-4.77660	-1.49021	1.79938
H	-4.12247	-0.86989	3.64329

C	-5.24204	-2.32272	-1.72172
H	-3.86468	-1.96809	-3.35879
H	-6.37117	-2.54026	0.10035
H	-5.99258	-2.78868	-2.35318

Electronic energy = -1443.497032
Zero-point electronic energy = -1442.854651
Enthalpy = -1442.824781
Free energy = -1442.913435
Free energy with quasiharmonic approximation = -1442.907969
Frequencies = -210.9774 23.3714 31.0649
SCF (M06-2X/def2-TZVPP–IEF-PCM) = -1443.420586

TS-1o

N	-0.24162	2.27577	-0.49079
C	-1.07981	0.03544	0.30031
C	-1.39466	1.31624	-0.51986
C	-2.68473	2.06251	-0.08482
C	-2.44966	3.57863	-0.25762
C	-1.44150	4.07029	0.80857
C	-0.24068	3.08497	0.76685
C	-0.40384	3.20645	-1.65209
C	-1.82623	3.82966	-1.64580
H	1.04261	1.59353	-0.70717
N	-0.09773	-0.82473	-0.39183
H	-1.48533	1.02935	-1.57044
H	-2.93988	1.83394	0.95517
H	-3.52894	1.72560	-0.69446
H	-3.39815	4.11710	-0.16070
H	-1.08937	5.06171	0.49480
C	-2.02060	4.21328	2.21938
H	-0.27469	2.39541	1.61657
H	0.71674	3.61130	0.81979
H	0.37558	3.96783	-1.56110
H	-0.20689	2.63933	-2.56642
C	1.04108	-1.35112	0.09169
H	-0.45138	-1.27258	-1.22985
H	-0.61660	0.34957	1.23453
H	-1.76823	4.90343	-1.85275
H	-2.44975	3.38238	-2.42843
H	-2.83262	4.94883	2.23392
H	-1.25074	4.55163	2.92297
H	-2.41822	3.26419	2.59783
C	1.63373	-2.47811	-0.72101
C	1.75093	-0.83422	1.18202
H	2.35569	-2.04651	-1.42953
H	0.85248	-2.95863	-1.32020

C	2.34408	-3.50466	0.17650
H	2.81415	-4.26699	-0.45411
H	1.59966	-4.01837	0.79874
C	3.38672	-2.81490	1.06125
C	2.75291	-1.70923	1.91962
H	4.17221	-2.39054	0.42600
H	3.87225	-3.54694	1.71676
H	2.22316	-2.16717	2.76853
H	3.53630	-1.08544	2.36537
H	1.21856	-0.14966	1.83672
C	5.80156	-0.48039	-1.67558
C	6.74950	-0.39798	-0.64934
C	2.71908	0.81660	0.07776
C	4.48450	-0.09324	-1.44448
C	4.09778	0.37440	-0.17495
C	6.37893	0.08818	0.60707
C	5.06085	0.47599	0.84366
O	1.98168	1.10917	-0.96332
H	6.09373	-0.84051	-2.65775
H	7.77657	-0.69972	-0.83346
H	3.75090	-0.13189	-2.24281
H	7.11690	0.17232	1.39930
H	4.78018	0.87611	1.81414
H	2.56651	1.40584	0.98360
C	-2.30379	-0.79709	0.69667
C	-3.18280	-1.44035	-0.23704
C	-2.55537	-0.97120	2.04159
C	-3.07434	-1.35793	-1.65382
C	-4.25369	-2.23128	0.30546
C	-3.64750	-1.76350	2.46794
H	-1.91953	-0.50867	2.79041
C	-3.95790	-2.01845	-2.48055
H	-2.29972	-0.75455	-2.11353
C	-5.14708	-2.89927	-0.57304
N	-4.47079	-2.38025	1.64741
H	-3.83156	-1.88736	3.53403
C	-5.00410	-2.79935	-1.93800
H	-3.84999	-1.93416	-3.55771
H	-5.94238	-3.48646	-0.12478
H	-5.69297	-3.31432	-2.60087

Electronic energy = -1443.493597
Zero-point electronic energy = -1442.854692
Enthalpy = -1442.824389
Free energy = -1442.915034
Free energy with quasiharmonic approximation = -1442.9086
Frequencies = -296.9073 15.1994 25.9890

SCF (M06-2X/def2-TZVPP–IEF-PCM) = -1443.4146

TS-1p

N	0.09519	2.11422	-0.06368
C	-1.23297	-0.03724	-0.27592
C	-1.05809	1.43485	-0.73832
C	-2.33764	2.29958	-0.56321
C	-1.91038	3.73513	-0.19007
C	-1.32232	3.74811	1.24045
C	-0.28913	2.58958	1.30228
C	0.45546	3.30808	-0.89242
C	-0.79795	4.18565	-1.15821
H	1.42338	1.37564	0.12967
N	-0.04776	-0.83551	-0.61875
H	-0.78776	1.40664	-1.79901
H	-2.91684	2.29627	-1.49136
H	-2.98890	1.88261	0.21350
H	-2.77058	4.40985	-0.25416
H	-0.78699	4.69838	1.36621
C	-2.36276	3.65570	2.36108
H	-0.69869	1.73764	1.85410
H	0.62859	2.89034	1.81665
H	1.22589	3.85627	-0.34277
H	0.90582	2.94845	-1.82203
C	0.88774	-1.36816	0.19408
H	0.08375	-0.99836	-1.61189
H	-1.33045	-0.05393	0.80568
H	-0.55870	5.24278	-1.00168
H	-1.13306	4.08041	-2.19645
H	-3.04763	4.51040	2.32676
H	-1.87652	3.65634	3.34383
H	-2.96287	2.74061	2.29134
C	0.69301	-1.29208	1.68749
C	2.06694	-1.88437	-0.34707
H	-0.20891	-1.86818	1.93710
H	0.48946	-0.25551	1.98122
C	1.89449	-1.82355	2.48407
H	1.58309	-1.98936	3.52063
H	2.68333	-1.06151	2.50564
C	2.43760	-3.10688	1.85438
C	2.96628	-2.81664	0.44144
H	1.63590	-3.85646	1.80808
H	3.23649	-3.53216	2.47157
H	3.97775	-2.39290	0.50875
H	3.07479	-3.75287	-0.12050
H	2.08758	-2.01601	-1.42807

C	6.48323	0.00014	0.57620
C	7.08152	-0.55274	-0.56047
C	2.89192	0.21928	-0.54599
C	5.11284	0.24801	0.59498
C	4.32651	-0.05891	-0.53025
C	6.30549	-0.86087	-1.68297
C	4.93492	-0.61975	-1.66802
O	2.40916	1.02687	0.36597
H	7.08705	0.24188	1.44582
H	8.15092	-0.74225	-0.57256
H	4.64436	0.69104	1.46748
H	6.77043	-1.28577	-2.56743
H	4.33147	-0.85828	-2.54021
H	2.39248	0.21711	-1.51610
C	-2.46949	-0.68167	-0.90860
C	-3.52135	-1.26218	-0.12881
C	-2.57658	-0.74030	-2.28378
C	-3.56446	-1.27932	1.29390
C	-4.61317	-1.86824	-0.84253
C	-3.69440	-1.36409	-2.88346
H	-1.81702	-0.31348	-2.93259
C	-4.61745	-1.85926	1.96710
H	-2.76557	-0.82995	1.87344
C	-5.68271	-2.45750	-0.11750
N	-4.68241	-1.91167	-2.20663
H	-3.76264	-1.40317	-3.96952
C	-5.68754	-2.45467	1.25814
H	-4.62619	-1.85863	3.05302
H	-6.48883	-2.90510	-0.69035
H	-6.51011	-2.90728	1.80398

Electronic energy = -1443.491849
Zero-point electronic energy = -1442.853369
Enthalpy = -1442.822786
Free energy = -1442.914698
Free energy with quasiharmonic approximation = -1442.907472
Frequencies = -230.3321 14.9717 18.5864
SCF (M06-2X/def2-TZVPP–IEF-PCM) = -1443.412971

TS-2a

C	-1.26443	-0.01146	0.13820
H	-1.36732	-0.49230	-0.82949
N	-0.00742	-0.49743	0.73835
H	0.37691	0.08645	1.47891
C	0.83788	-1.42678	0.30496
C	2.12690	-1.45929	0.90179
H	2.15604	-1.22792	1.96471

H	2.74857	-2.30191	0.62099
C	-2.46478	-0.36784	1.02043
C	-3.63620	-1.00599	0.50174
C	-2.43769	-0.04022	2.36087
C	-3.81166	-1.42418	-0.84768
C	-4.71468	-1.23823	1.42570
C	-3.55195	-0.32867	3.18255
H	-1.57492	0.44100	2.81299
C	-4.98435	-2.01937	-1.25797
H	-3.01052	-1.30696	-1.56776
C	-5.91047	-1.85217	0.96732
H	-3.51964	-0.06792	4.23912
C	-6.04647	-2.23199	-0.34718
H	-6.70100	-2.00716	1.69432
H	-6.96361	-2.70183	-0.68968
N	-4.65483	-0.89727	2.74574
C	-1.18557	1.52879	-0.03537
C	-2.44406	2.15445	-0.68707
H	-1.03350	1.97144	0.95334
C	-0.14389	1.72305	-2.31323
C	0.25510	3.44850	-0.59657
C	-2.00454	3.27357	-1.65170
H	-3.09704	2.54229	0.09809
H	-3.01789	1.40173	-1.23765
H	0.82679	1.90308	-2.77490
H	-0.36281	0.66320	-2.44528
C	-1.27112	2.63697	-2.84722
C	-1.02980	4.24634	-0.92975
H	1.09507	3.73281	-1.23298
H	0.58188	3.54417	0.43871
H	-2.88278	3.82521	-1.99988
H	-0.85833	3.41674	-3.49553
H	-1.96879	2.05112	-3.45365
H	-0.76298	5.02359	-1.65873
N	0.02788	1.97254	-0.83666
H	0.90857	1.48880	-0.44496
C	5.17767	-0.37411	-0.01626
C	4.26647	0.05649	0.96074
C	4.70017	0.32544	2.25049
C	6.05514	0.14473	2.55779
C	6.94820	-0.29919	1.57823
C	6.52298	-0.56382	0.26888
H	3.99987	0.67703	3.00348
H	6.41498	0.35255	3.56078
H	7.99575	-0.43670	1.82966
H	7.22484	-0.89478	-0.49098

C	2.90455	0.15727	0.32216
O	2.08198	1.12222	0.58843
C	3.19327	-0.17157	-1.17133
N	4.50868	-0.53135	-1.25049
H	4.96065	-0.76770	-2.12476
O	2.38748	-0.10517	-2.09428
C	-1.69902	4.94837	0.23246
H	-2.63985	5.42732	-0.04254
C	-1.27777	5.06935	1.49215
H	-0.34392	4.65183	1.85944
H	-1.86157	5.62579	2.21941
H	-5.09235	-2.33540	-2.29142
C	0.48768	-2.24683	-0.94197
H	0.43701	-1.56396	-1.80118
O	1.50570	-3.17558	-1.12724
O	-0.79896	-2.81501	-0.85656
C	-0.95956	-3.83131	0.14560
H	-0.27670	-4.66697	-0.02995
H	-0.79235	-3.43138	1.15368
H	-1.99261	-4.16911	0.05967
C	1.55046	-3.71998	-2.45143
H	0.61387	-4.22890	-2.70183
H	1.74833	-2.92540	-3.18174
H	2.37086	-4.43882	-2.45779

Electronic energy = -1761.354957
Zero-point electronic energy = -1760.703677
Enthalpy = -1760.667669
Free energy = -1760.770820
Free energy with quasiharmonic approximation = -1760.763131
Frequencies = -240.6210 15.2836 26.0906
SCF (M06-2X/def2-TZVPP–IEF-PCM) = -1761.315275

TS-2b

C	-1.42895	0.41297	-0.74347
H	-1.73845	0.59411	-1.77736
N	-0.31800	-0.56637	-0.89638
H	0.17866	-0.46920	-1.78002
C	0.37064	-1.30599	-0.02086
C	1.60960	-1.83436	-0.45621
H	1.68399	-2.10575	-1.50658
H	2.09264	-2.52758	0.22162
C	-2.65225	-0.16018	-0.03004
C	-3.46228	-1.13278	-0.70120
C	-3.02593	0.23025	1.23633
C	-3.20926	-1.62864	-2.00890
C	-4.60620	-1.63736	0.00327

C	-4.17503	-0.33632	1.84047
H	-2.45638	0.95515	1.80737
C	-4.04186	-2.56310	-2.58676
H	-2.34676	-1.28060	-2.56785
C	-5.44358	-2.60004	-0.61872
H	-4.45613	-0.02258	2.84459
C	-5.16909	-3.05500	-1.88795
H	-6.29988	-2.95545	-0.05479
H	-5.81498	-3.79064	-2.35785
N	-4.94348	-1.23179	1.26327
C	-0.95361	1.77687	-0.17339
C	-2.04994	2.87487	-0.22701
H	-0.58736	1.63439	0.84458
C	-0.08834	2.84212	-2.28580
C	0.88661	3.42796	-0.10701
C	-1.41794	4.21161	-0.66170
H	-2.84340	2.59449	-0.92999
H	-2.51576	2.97535	0.75456
H	0.86047	3.04306	-2.78677
H	-0.58612	2.04467	-2.84048
C	-0.97664	4.09857	-2.13270
C	-0.17070	4.50949	0.21751
H	1.69733	3.82325	-0.72244
H	1.32986	2.95566	0.76672
H	-2.15048	5.01668	-0.55092
H	-0.42795	4.99599	-2.43626
H	-1.85085	4.01916	-2.78589
H	0.22515	5.48017	-0.11025
C	-0.53829	4.65567	1.67857
H	-1.25686	5.45596	1.86114
C	-0.09824	3.95371	2.72496
H	-0.44996	4.18271	3.72695
H	0.62638	3.14669	2.65132
N	0.25912	2.31433	-0.91701
C	4.75599	-0.84908	0.29461
C	4.03238	-0.87100	-0.90855
C	4.60466	-1.39210	-2.05997
C	5.90557	-1.90755	-1.99099
C	6.60808	-1.89339	-0.78250
C	6.04371	-1.35801	0.38414
H	4.05276	-1.39270	-2.99596
H	6.37236	-2.31799	-2.88105
H	7.61535	-2.29735	-0.74248
H	6.60076	-1.33563	1.31596
C	2.69115	-0.24248	-0.65586
C	2.78581	0.22163	0.82664

N	3.98394	-0.22493	1.30019
H	4.30227	-0.04606	2.24428
O	2.09453	0.51460	-1.51280
O	1.94390	0.87667	1.43624
H	1.01127	1.54873	-1.03110
C	-0.10794	-1.49682	1.42300
H	-0.46091	-0.54518	1.83406
O	-1.22823	-2.34575	1.48382
O	0.98202	-1.96928	2.15395
C	-1.02601	-3.69540	1.04511
H	-0.88007	-3.74764	-0.04102
H	-0.17193	-4.15455	1.55188
H	-1.94050	-4.22861	1.30787
C	0.81828	-1.84299	3.56941
H	-0.09377	-2.34468	3.90823
H	1.68833	-2.32097	4.02220
H	0.78996	-0.78424	3.85707
H	-3.83030	-2.92643	-3.58821

Electronic energy = -1761.346682
Zero-point electronic energy = -1760.694707
Enthalpy = -1760.659026
Free energy = -1760.760438
Free energy with quasiharmonic approximation = -1760.753958
Frequencies = -278.5172 22.4954 25.0373
SCF (M06-2X/def2-TZVPP–IEF-PCM) = -1761.310381

TS-2c

C	-1.28453	-0.08392	0.05352
H	-1.43625	-0.66193	-0.85170
N	-0.06287	-0.59691	0.71072
H	0.30539	0.03869	1.42689
C	0.78444	-1.54272	0.35407
C	2.08844	-1.55631	0.94869
H	2.11201	-1.34180	2.01659
H	2.67845	-2.42534	0.68458
C	-2.49116	-0.24472	0.98153
C	-3.71172	-0.85212	0.54583
C	-2.42181	0.23027	2.27590
C	-3.93821	-1.39543	-0.75077
C	-4.78720	-0.91143	1.49970
C	-3.54069	0.11054	3.13279
H	-1.52409	0.70358	2.66429
C	-5.15362	-1.95364	-1.08233
H	-3.14826	-1.39565	-1.49341
C	-6.02704	-1.49233	1.12261
H	-3.47565	0.48673	4.15237

C	-6.20987	-2.00114	-0.14172
H	-6.81341	-1.51588	1.86995
H	-7.16099	-2.44382	-0.42199
N	-4.68410	-0.43149	2.77292
C	-1.06255	1.41517	-0.27646
C	-2.30189	2.12199	-0.87897
H	-0.76990	1.92009	0.64655
C	-0.25177	1.33294	-2.64465
C	0.53297	3.08779	-1.10765
C	-1.82780	3.14168	-1.93493
H	-2.98086	1.39902	-1.34451
H	-2.85688	2.61186	-0.07581
H	0.68373	1.34193	-3.20696
H	-0.64145	0.31298	-2.67078
C	-1.28096	2.36861	-3.15031
C	-0.68055	4.01989	-1.35475
H	1.31744	3.23005	-1.85372
H	0.98553	3.20085	-0.12337
H	-2.66437	3.77826	-2.23752
H	-0.81437	3.05857	-3.86100
H	-2.09262	1.86060	-3.67998
H	-0.40249	4.73222	-2.14319
C	-1.14483	4.83945	-0.17019
H	-1.98029	5.49916	-0.40903
C	-0.66734	4.85703	1.07560
H	-1.10409	5.51279	1.82327
H	0.16702	4.24764	1.41375
N	0.10653	1.64350	-1.21551
H	0.99594	1.04209	-0.96308
C	4.91736	0.27203	1.28067
C	4.34591	-0.38571	0.18179
C	5.14232	-1.14576	-0.66295
C	6.51052	-1.25490	-0.38227
C	7.06074	-0.60512	0.72666
C	6.26899	0.17711	1.57883
H	4.70729	-1.64369	-1.52472
H	7.14959	-1.84582	-1.03125
H	8.12281	-0.69947	0.93262
H	6.70184	0.69316	2.43072
C	2.87619	-0.05587	0.13706
C	2.71101	0.92260	1.34445
N	3.92010	1.01886	1.95407
H	4.08193	1.59526	2.77118
O	2.30104	0.28155	-0.98317
O	1.66612	1.48591	1.69124
C	0.51615	-2.36615	-0.91100

H	0.66975	-1.66870	-1.75294
O	1.44541	-3.39752	-0.96004
O	-0.81745	-2.79853	-1.02376
C	-1.21052	-3.80676	-0.07555
H	-0.62427	-4.71947	-0.20925
H	-1.09770	-3.45073	0.95604
H	-2.26359	-4.00454	-0.27543
C	1.56186	-4.00726	-2.25115
H	0.62121	-4.47864	-2.55360
H	1.85670	-3.26408	-3.00352
H	2.34064	-4.76502	-2.15926
H	-5.30150	-2.36487	-2.07664

Electronic energy = -1761.346789
Zero-point electronic energy = -1760.696135
Enthalpy = -1760.660258
Free energy = -1760.763517
Free energy with quasiharmonic approximation = -1760.755404
Frequencies = -265.3711 14.6757 27.6435
SCF (M06-2X/def2-TZVPP–IEF-PCM) = -1761.308764

TS-2d

C	-1.27970	0.03485	0.02117
H	-1.03267	-0.00728	-1.03645
N	-0.15891	-0.60895	0.75218
H	-0.35342	-0.84230	1.72733
C	0.91750	-1.20202	0.28003
C	1.52749	-0.87886	-0.96813
H	0.85095	-0.53870	-1.75076
H	2.22303	-1.63131	-1.33561
C	-2.52059	-0.81467	0.29872
C	-3.12422	-1.63225	-0.70808
C	-3.05750	-0.83450	1.57074
C	-2.68666	-1.72523	-2.05897
C	-4.26488	-2.41512	-0.31198
C	-4.18060	-1.64728	1.85000
H	-2.64111	-0.22912	2.37248
C	-3.33693	-2.53910	-2.96010
H	-1.82773	-1.15770	-2.40251
C	-4.91198	-3.24244	-1.26737
H	-4.59875	-1.65607	2.85510
C	-4.45964	-3.30443	-2.56449
H	-5.76913	-3.81614	-0.93045
H	-4.96016	-3.93933	-3.28931
N	-4.77082	-2.41004	0.95533
C	-1.47136	1.52254	0.42821
C	-2.88172	2.10810	0.15624

H	-1.24623	1.61001	1.49400
C	-0.86536	2.73783	-1.67540
C	-0.36265	3.70366	0.52748
C	-2.73317	3.58792	-0.25540
H	-3.39140	1.55549	-0.64087
H	-3.49402	2.00516	1.05473
H	0.00443	3.19449	-2.14847
H	-1.03684	1.79242	-2.19244
C	-2.12044	3.63711	-1.66683
C	-1.77094	4.32439	0.72016
H	0.29921	4.35923	-0.04127
H	0.14438	3.45817	1.46135
H	-3.71262	4.07542	-0.24621
H	-1.86152	4.66757	-1.93272
H	-2.83940	3.28249	-2.41196
H	-1.72611	5.37037	0.38567
C	-2.31146	4.34246	2.13374
H	-3.34089	4.69906	2.19388
C	-1.69407	4.01648	3.27050
H	-2.20700	4.10305	4.22393
H	-0.66285	3.67650	3.31955
N	-0.46971	2.42309	-0.25737
C	4.72850	0.27167	-1.29115
C	3.86732	0.20178	-0.18597
C	4.36738	-0.13406	1.06432
C	5.72812	-0.44832	1.18847
C	6.56590	-0.40653	0.07036
C	6.07902	-0.03669	-1.19077
H	3.71075	-0.13934	1.93067
H	6.13660	-0.71418	2.15877
H	7.61884	-0.65001	0.17824
H	6.73930	0.02288	-2.05082
C	2.48455	0.63037	-0.62462
C	2.71628	1.04313	-2.12260
N	4.01520	0.72376	-2.42087
H	4.43740	0.94180	-3.31501
O	1.81683	1.45756	0.13093
O	1.88766	1.53643	-2.87111
H	0.56009	1.95421	-0.22666
C	1.56968	-2.21292	1.22327
H	2.65424	-2.25640	1.05161
O	1.27408	-1.81447	2.52442
O	0.97138	-3.45803	0.93333
C	1.80465	-4.42908	0.29324
H	2.75250	-4.55656	0.83050
H	1.24562	-5.36593	0.31462

H	2.01106	-4.16094	-0.75014
C	1.78631	-2.68051	3.54628
H	1.51984	-2.21725	4.49675
H	1.33681	-3.67457	3.47619
H	2.87832	-2.75783	3.47017
H	-2.98429	-2.59400	-3.98579

Electronic energy = -1761.346325
Zero-point electronic energy = -1760.696602
Enthalpy = -1760.660598
Free energy = -1760.764969
Free energy with quasiharmonic approximation = -1760.755712
Frequencies = -199.1412 16.4068 19.5357
SCF (M06-2X/def2-TZVPP–IEF-PCM) = -1761.305129

TS-2e

C	-1.01684	0.47622	0.33991
H	-0.68793	-0.32428	-0.31889
N	0.04636	0.64403	1.34803
H	-0.11208	1.36628	2.05055
C	1.18116	-0.01326	1.53081
C	1.67659	-1.09225	0.75496
H	0.93503	-1.75937	0.32483
H	2.48715	-1.61258	1.25349
C	-2.31623	0.09107	1.03900
C	-3.02496	-1.10606	0.69450
C	-2.83100	0.89102	2.03901
C	-2.62732	-2.02182	-0.30890
C	-4.22874	-1.37874	1.43565
C	-4.02490	0.52296	2.70221
H	-2.34389	1.81828	2.33124
C	-3.37291	-3.16018	-0.57767
H	-1.72874	-1.87858	-0.89945
C	-4.96608	-2.55225	1.13563
H	-4.42131	1.16185	3.48934
C	-4.55917	-3.42747	0.15657
H	-5.86822	-2.73585	1.71003
H	-5.14608	-4.31512	-0.04720
N	-4.70622	-0.56760	2.42092
O	-2.89511	-3.96504	-1.56033
C	-3.60337	-5.16177	-1.88377
H	-4.61847	-4.94316	-2.23492
H	-3.03525	-5.62924	-2.68867
H	-3.64797	-5.84369	-1.02669
C	-1.09553	1.80582	-0.49672
C	-2.48410	2.38626	-0.84990
H	-0.54441	2.56353	0.06391

C	-1.16138	1.03591	-2.88001
C	0.12945	3.03772	-2.23164
C	-2.37752	3.10318	-2.21439
H	-3.24653	1.60303	-0.90794
H	-2.79341	3.07577	-0.06056
H	-0.47627	0.77243	-3.68737
H	-1.56233	0.10574	-2.47383
C	-2.27018	2.02118	-3.30446
C	-1.09715	3.98847	-2.27623
H	0.58876	2.91761	-3.21494
H	0.91250	3.34314	-1.53798
H	-3.26258	3.72462	-2.37880
H	-2.03998	2.47428	-4.27451
H	-3.21880	1.48692	-3.41370
H	-1.10558	4.47815	-3.25968
C	-1.12784	5.09349	-1.24158
H	-2.03999	5.69087	-1.28177
C	-0.19936	5.42635	-0.34297
H	-0.35538	6.26708	0.32680
H	0.75154	4.91032	-0.23785
N	-0.32302	1.67080	-1.79558
C	4.63233	-1.00490	-0.89017
C	3.37604	-1.53917	-1.21716
C	3.27486	-2.82110	-1.73755
C	4.44535	-3.57151	-1.91055
C	5.68804	-3.03231	-1.56529
C	5.80258	-1.73317	-1.05058
H	2.30477	-3.22705	-2.01037
H	4.38849	-4.57629	-2.31790
H	6.58765	-3.62475	-1.70437
H	6.77218	-1.31341	-0.80015
C	2.33300	-0.49156	-0.93478
C	3.17764	0.74324	-0.50832
N	4.47830	0.32402	-0.43345
H	5.24595	0.95346	-0.23362
O	1.31888	-0.30614	-1.70706
O	2.74790	1.86998	-0.28291
H	0.52159	1.00085	-1.66144
C	2.05011	0.63775	2.63037
H	2.57323	1.48557	2.16245
O	1.24368	1.23891	3.62657
O	2.94332	-0.30765	3.10973
C	0.62610	0.32232	4.54887
H	0.03952	0.94111	5.22900
H	-0.03551	-0.38531	4.03435
H	1.37855	-0.23506	5.11180

C	4.06039	0.25439	3.80900
H	3.73630	0.81105	4.69431
H	4.68534	-0.58680	4.11104
H	4.63068	0.92041	3.14880

Electronic energy = -1761.347328
Zero-point electronic energy = -1760.695683
Enthalpy = -1760.659897
Free energy = -1760.762559
Free energy with quasiharmonic approximation = -1760.754777
Frequencies = -270.2044 17.3472 27.5420
SCF (M06-2X/def2-TZVPP–IEF-PCM) = -1761.304400

TS-3a

C	-1.14807	0.37616	-0.27266
H	-1.65541	0.33472	-1.23828
N	-0.25920	-0.81095	-0.25657
H	0.03179	-1.18185	-1.15792
C	0.40196	-1.26112	0.79168
H	0.16680	-0.80651	1.74865
C	1.50145	-2.13897	0.63517
H	1.43070	-2.85264	-0.18315
H	1.88628	-2.57432	1.55402
C	-2.21068	0.26898	0.81752
C	-3.36213	-0.56303	0.60178
C	-2.09889	0.92153	2.02658
C	-3.59916	-1.30789	-0.57488
C	-4.32599	-0.63126	1.66500
C	-3.11021	0.77400	3.00960
H	-1.25557	1.56268	2.25874
C	-4.74137	-2.08309	-0.71549
H	-2.89802	-1.30867	-1.40169
C	-5.48388	-1.42963	1.48939
H	-3.00834	1.29771	3.95829
C	-5.69811	-2.14204	0.33202
H	-6.20019	-1.46274	2.30398
H	-6.59329	-2.74344	0.22893
N	-4.18642	0.03546	2.84807
O	-4.86327	-2.75490	-1.88938
C	-6.00775	-3.58396	-2.09900
H	-6.05586	-4.39152	-1.35967
H	-6.93485	-3.00033	-2.06934
H	-5.88098	-4.01131	-3.09421
C	-0.33877	1.69586	-0.21307
C	-1.22233	2.94936	-0.43789
H	0.19161	1.74103	0.73919
C	0.27328	1.86153	-2.64741

C	1.71184	2.87484	-0.92779
C	-0.51370	3.90667	-1.41385
H	-2.19756	2.66358	-0.84810
H	-1.40846	3.44094	0.51926
H	1.13984	1.74755	-3.30078
H	-0.40105	1.02806	-2.85003
C	-0.42112	3.23628	-2.79781
C	0.92425	4.20713	-0.90395
H	2.47203	2.86443	-1.71090
H	2.19607	2.62671	0.01421
H	-1.08137	4.83869	-1.48962
H	0.14145	3.87218	-3.48823
H	-1.42184	3.10391	-3.21981
H	1.38196	4.88558	-1.63618
C	0.90844	4.93824	0.42081
H	0.40016	5.90232	0.36971
C	1.42189	4.55830	1.59285
H	1.33189	5.19927	2.46549
H	1.94988	3.62073	1.74726
N	0.78277	1.72055	-1.23696
C	4.84692	-1.64196	0.80803
C	3.97306	-1.94661	-0.24664
C	4.30120	-2.93566	-1.16199
C	5.50787	-3.63084	-1.00030
C	6.36150	-3.32611	0.06411
C	6.04521	-2.31951	0.98777
H	3.63464	-3.16140	-1.99009
H	5.78247	-4.40848	-1.70659
H	7.29328	-3.87237	0.17887
H	6.71808	-2.07612	1.80436
C	2.78350	-1.02066	-0.15975
C	3.14426	-0.10722	1.05284
N	4.31831	-0.57532	1.56731
H	4.78194	-0.14778	2.35971
O	2.26868	-0.48304	-1.21935
O	2.48801	0.84558	1.46601
H	1.37948	0.82408	-1.15328

Electronic energy = -1607.545437
Zero-point electronic energy = -1606.955567
Enthalpy = -1606.923489
Free energy = -1607.018414
Free energy with quasiharmonic approximation = -1607.011299
Frequencies = -225.6340 15.4370 25.0950
SCF (M06-2X/def2-TZVPP–IEF-PCM) = -1607.503363

TS-3b

C	-0.88031	-0.13831	0.37087
H	-1.05419	-0.61537	-0.59274
N	0.34711	-0.75078	0.90600
H	0.83442	-0.25006	1.64629
C	0.99298	-1.76682	0.37351
H	0.52671	-2.24581	-0.48164
C	2.33061	-2.04719	0.75355
H	2.57095	-1.87266	1.80087
H	2.73527	-2.98298	0.37539
C	-2.07427	-0.38282	1.29239
C	-3.30395	-0.93452	0.80316
C	-1.98341	-0.06762	2.63174
C	-3.54811	-1.30558	-0.54064
C	-4.35811	-1.11419	1.76641
C	-3.08561	-0.29191	3.48996
H	-1.07520	0.34858	3.05843
C	-4.77240	-1.82752	-0.93086
H	-2.79515	-1.20084	-1.31380
C	-5.59645	-1.65232	1.33368
H	-3.00042	-0.04151	4.54577
C	-5.81134	-2.00229	0.02123
H	-6.37597	-1.77893	2.07806
H	-6.76964	-2.41053	-0.27652
N	-4.23416	-0.79347	3.08635
O	-4.89159	-2.14684	-2.24567
C	-6.12978	-2.67947	-2.71954
H	-6.95103	-1.96825	-2.57515
H	-5.98439	-2.85309	-3.78622
H	-6.37159	-3.62759	-2.22612
C	-0.64507	1.37870	0.16969
C	-1.86595	2.14694	-0.39245
H	-0.36818	1.80049	1.14006
C	0.22824	1.45231	-2.18613
C	0.97439	3.10128	-0.51055
C	-1.36822	3.21424	-1.38655
H	-2.41414	2.60079	0.43623
H	-2.55711	1.46822	-0.90320
H	1.17509	1.52064	-2.72133
H	-0.12373	0.42766	-2.29952
C	-0.81223	2.50318	-2.63350
C	-0.22587	4.05366	-0.74633
H	1.78858	3.28546	-1.21305
H	1.38952	3.15174	0.49593
H	-2.19598	3.87263	-1.66519
H	-0.35465	3.23165	-3.31041
H	-1.62056	2.01363	-3.18471

H	0.07728	4.79396	-1.49882
N	0.54743	1.66721	-0.72699
H	1.39102	1.06509	-0.42396
C	5.34636	-1.43391	-0.66293
C	4.66995	-0.89383	0.44205
C	5.34129	-0.68620	1.63764
C	6.69491	-1.04163	1.72353
C	7.35122	-1.59279	0.61915
C	6.68556	-1.79547	-0.59817
H	4.82529	-0.25117	2.48952
H	7.23712	-0.88640	2.65141
H	8.39979	-1.86517	0.69791
H	7.20259	-2.21068	-1.45795
C	3.24461	-0.60191	0.02977
O	2.65537	0.49966	0.38314
C	3.23587	-0.99025	-1.48022
N	4.47106	-1.50314	-1.76715
H	4.73740	-1.81420	-2.69325
O	2.29304	-0.86345	-2.25228
C	-0.71077	4.82975	0.45903
H	-1.58708	5.44346	0.24530
C	-0.20459	4.86656	1.69278
H	0.67540	4.30829	2.00142
H	-0.65928	5.48867	2.45837

Electronic energy = -1607.544314
Zero-point electronic energy = -1606.95438
Enthalpy = -1606.922299
Free energy = -1607.016838
Free energy with quasiharmonic approximation = -1607.010161
Frequencies = -196.1872 15.5158 25.0267
SCF (M06-2X/def2-TZVPP–IEF-PCM) = -1607.50102098

TS-3c

C	0.85423	0.32184	-0.54059
H	0.73519	-0.31446	0.33209
N	-0.14417	-0.14138	-1.54169
H	0.03050	0.20143	-2.48314
C	-1.03789	-1.09952	-1.43657
H	-1.50381	-1.37873	-2.37793
C	-1.58344	-1.60725	-0.22499
H	-0.95856	-1.52829	0.66272
H	-2.02384	-2.59675	-0.33093
C	2.23305	0.09541	-1.16037
C	3.10949	-0.93969	-0.69543
C	2.64093	0.86920	-2.22825
C	2.83100	-1.81118	0.38207

C	4.36314	-1.08343	-1.38838
C	3.89691	0.63490	-2.83667
H	2.02241	1.67287	-2.61986
C	3.73784	-2.78549	0.77172
H	1.90539	-1.75399	0.94281
C	5.26776	-2.08956	-0.96440
H	4.20704	1.25292	-3.67707
C	4.97447	-2.92538	0.08756
H	6.20673	-2.17880	-1.50107
H	5.68801	-3.68379	0.38663
N	4.73434	-0.30125	-2.44199
O	3.36133	-3.56290	1.81896
C	4.24770	-4.58489	2.27894
H	3.73406	-5.06327	3.11345
H	4.44065	-5.32753	1.49648
H	5.19614	-4.16221	2.62938
C	0.62184	1.80102	-0.12425
C	1.85255	2.49776	0.51337
H	0.31204	2.35703	-1.01238
C	-0.13256	1.59241	2.25586
C	-1.00425	3.37993	0.80826
C	1.36242	3.47897	1.59878
H	2.53086	1.76498	0.96386
H	2.41411	3.01781	-0.26538
H	-1.05685	1.50721	2.82725
H	0.31717	0.59848	2.23475
C	0.84395	2.65900	2.79410
C	0.18836	4.34010	1.05186
H	-1.76612	3.47138	1.58444
H	-1.49685	3.52274	-0.15387
H	2.18563	4.12903	1.90898
H	0.34474	3.31271	3.51690
H	1.67389	2.17244	3.31555
H	-0.09559	5.03128	1.85703
C	0.61916	5.19379	-0.12115
H	1.49940	5.80154	0.09416
C	0.06162	5.30460	-1.32834
H	0.47873	5.97945	-2.07040
H	-0.82720	4.75882	-1.63469
N	-0.52940	1.94897	0.84610
C	-4.94038	-1.71602	0.29860
C	-4.14900	-1.00423	-0.61587
C	-4.56476	-0.86795	-1.93231
C	-5.76430	-1.47370	-2.33296
C	-6.53007	-2.19665	-1.41392
C	-6.13098	-2.32554	-0.07637

H	-3.97369	-0.29135	-2.63920
H	-6.10224	-1.37730	-3.36039
H	-7.45762	-2.66203	-1.73489
H	-6.73668	-2.87220	0.64017
C	-2.93652	-0.46245	0.11499
C	-3.21142	-0.90638	1.59800
N	-4.34871	-1.66894	1.57670
H	-4.77053	-2.04576	2.41669
O	-2.58378	0.78110	-0.07650
O	-2.53429	-0.62422	2.57499
H	-1.40861	1.33301	0.52464

Electronic energy = -1607.533751
Zero-point electronic energy = -1606.94486
Enthalpy = -1606.91291
Free energy = -1607.007406
Free energy with quasiharmonic approximation = -1607.000357
Frequencies = -188.9351 15.4646 25.8495
SCF (M06-2X/def2-TZVPP–IEF-PCM) = -1607.49332021

TS-3d

C	-0.93042	-0.23421	0.13845
H	-1.20178	-0.64394	-0.83377
N	0.27049	-0.96543	0.57505
H	0.78163	-0.55538	1.36664
C	0.91286	-1.86829	-0.12067
H	0.43495	-2.17829	-1.04816
C	2.25992	-2.25577	0.15994
H	2.49612	-2.42722	1.20961
H	2.61324	-3.06297	-0.47581
C	-2.07438	-0.43147	1.12985
C	-3.36067	-0.90753	0.71404
C	-1.87793	-0.15165	2.46591
C	-3.71236	-1.22717	-0.61833
C	-4.35504	-1.06135	1.74266
C	-2.93050	-0.34253	3.39216
H	-0.92449	0.21383	2.83726
C	-4.98381	-1.68022	-0.93684
H	-3.00830	-1.13105	-1.43697
C	-5.64419	-1.52924	1.38289
H	-2.76260	-0.12094	4.44447
C	-5.96311	-1.83370	0.08008
H	-6.37760	-1.63861	2.17526
H	-6.95817	-2.18832	-0.16059
N	-4.12657	-0.77992	3.05763
O	-5.20641	-1.95420	-2.24851
C	-6.49374	-2.42688	-2.64938

H	-6.73617	-3.38096	-2.16783
H	-7.27562	-1.69176	-2.42733
H	-6.42916	-2.57196	-3.72823
C	-0.56807	1.26676	0.00043
C	-1.76103	2.17544	-0.38602
H	-0.15558	1.59284	0.95830
C	0.06379	1.44356	-2.42182
C	1.13399	2.87707	-0.72583
C	-1.25982	3.27477	-1.34360
H	-2.55306	1.59871	-0.87595
H	-2.18966	2.60502	0.52216
H	0.95655	1.46357	-3.04870
H	-0.41131	0.47038	-2.56225
C	-0.89956	2.62161	-2.69071
C	0.01679	3.95055	-0.76321
H	1.88855	3.04272	-1.49630
H	1.64904	2.80470	0.23209
H	-2.04214	4.02600	-1.48590
H	-0.43223	3.35569	-3.35499
H	-1.80223	2.25859	-3.19112
H	0.31710	4.72335	-1.48346
C	-0.27261	4.65986	0.54192
H	-1.06502	5.40462	0.45462
C	0.30807	4.49786	1.73223
H	-0.00603	5.09305	2.58496
H	1.11370	3.79304	1.92154
N	0.54876	1.51210	-0.99589
H	1.39017	0.80898	-0.91394
C	5.35297	-1.01090	0.69917
C	4.61949	-1.24151	-0.47420
C	5.22934	-1.83499	-1.57043
C	6.57466	-2.21452	-1.47104
C	7.28670	-1.99289	-0.28806
C	6.68569	-1.38008	0.82057
H	4.67003	-1.99729	-2.48768
H	7.06876	-2.68096	-2.31802
H	8.32860	-2.29283	-0.22368
H	7.24700	-1.19506	1.73148
C	3.22295	-0.70362	-0.28351
C	3.29440	-0.08926	1.15431
N	4.53534	-0.35009	1.64448
H	4.83962	-0.05536	2.56488
O	2.65498	0.01088	-1.20781
O	2.38813	0.51116	1.74166

Electronic energy = -1607.534718
Zero-point electronic energy = -1606.945592

Enthalpy = -1606.913516
Free energy = -1607.008175
Free energy with quasiharmonic approximation = -1607.001351
Frequencies = -305.4571 16.0487 26.9351
SCF (M06-2X/def2-TZVPP–IEF-PCM) = -1607.492641

TS-3e

C	1.22913	0.38407	0.05624
H	1.64669	0.31121	1.06379
N	0.17062	-0.65213	0.00717
H	-0.29503	-0.88287	0.90006
C	-0.40310	-1.12529	-1.07350
H	-0.00121	-0.77732	-2.02274
C	-1.61662	-1.87334	-1.02264
H	-1.62173	-2.71406	-0.33060
H	-1.99292	-2.15428	-2.00270
C	2.34762	0.08371	-0.93733
C	3.29642	-0.95010	-0.63993
C	2.47757	0.76164	-2.13352
C	3.26845	-1.73962	0.54182
C	4.32596	-1.18641	-1.61003
C	3.53094	0.43811	-3.02016
H	1.79669	1.55362	-2.42294
C	4.22830	-2.71436	0.75556
H	2.48765	-1.58892	1.27522
C	5.29689	-2.19483	-1.35265
H	3.62294	0.98119	-3.95877
C	5.25436	-2.93909	-0.20492
H	6.06848	-2.35293	-2.09913
H	5.98888	-3.71107	0.00066
N	4.42923	-0.49457	-2.77902
O	4.29111	-3.51979	1.84403
C	3.30354	-3.37300	2.86316
H	3.33243	-2.36795	3.30044
H	2.29928	-3.57654	2.47299
H	3.55374	-4.10982	3.62680
C	0.61898	1.80065	-0.10577
C	1.62618	2.93720	0.22375
H	0.23220	1.89528	-1.12272
C	-0.32455	1.91337	2.23193
C	-1.21872	3.34085	0.43454
C	1.06043	3.81472	1.35503
H	2.58822	2.51443	0.53050
H	1.81139	3.53988	-0.66914
H	-1.26929	2.12746	2.73473
H	-0.06183	0.88401	2.47433

C	0.78402	2.93195	2.58538
C	-0.27209	4.47319	0.89929
H	-2.18999	3.37033	0.93065
H	-1.39461	3.33928	-0.64134
H	1.78733	4.59126	1.61070
H	0.46745	3.54541	3.43423
H	1.70108	2.41435	2.88554
H	-0.70823	4.94275	1.79211
C	-0.04347	5.58143	-0.10346
H	0.63918	6.35069	0.25975
C	-0.57191	5.73134	-1.31920
H	-0.32038	6.59532	-1.92769
H	-1.27562	5.03188	-1.76231
N	-0.61484	1.99323	0.75648
H	-1.37537	1.27181	0.45401
C	-4.71346	-2.00721	0.35237
C	-4.17129	-1.19483	-0.65501
C	-4.88511	-0.96453	-1.82254
C	-6.13663	-1.57527	-1.97961
C	-6.65503	-2.39603	-0.97314
C	-5.95016	-2.62277	0.21745
H	-4.47664	-0.32165	-2.59732
H	-6.70903	-1.40908	-2.88720
H	-7.62575	-2.86414	-1.10813
H	-6.36227	-3.24788	1.00363
C	-2.84260	-0.66906	-0.17714
C	-2.72508	-1.28323	1.25345
N	-3.83004	-2.04653	1.45702
H	-3.99551	-2.56930	2.30900
O	-2.52253	0.57624	-0.31438
O	-1.78695	-1.12043	2.04103

Electronic energy = -1607.533213
Zero-point electronic energy = -1606.94354
Enthalpy = -1606.911609
Free energy = -1607.005983
Free energy with quasiharmonic approximation = -1606.999031
Frequencies = -331.4134 16.7884 27.7170
SCF (M06-2X/def2-TZVPP–IEF-PCM) = -1607.490642

TS-3f

C	-0.89651	0.45267	0.65674
H	-0.44162	-0.26843	-0.01813
N	-0.00872	0.54024	1.83699
H	-0.29863	1.22722	2.52611
C	1.06016	-0.16534	2.16044
H	1.49141	0.13839	3.11025

C	1.74687	-1.14234	1.39948
H	1.17333	-1.73775	0.69461
H	2.41805	-1.73958	2.01123
C	-2.27379	-0.02673	1.10926
C	-2.83729	-1.25629	0.63381
C	-2.99727	0.71274	2.02232
C	-2.21744	-2.12388	-0.29602
C	-4.12995	-1.61936	1.15333
C	-4.26070	0.25763	2.46636
H	-2.62375	1.65408	2.41716
C	-2.83137	-3.29829	-0.70392
H	-1.24356	-1.90941	-0.72079
C	-4.73020	-2.82635	0.71368
H	-4.82024	0.85252	3.18587
C	-4.10759	-3.65315	-0.19185
H	-5.70492	-3.07829	1.11890
H	-4.59369	-4.56858	-0.50719
N	-4.81785	-0.86265	2.05575
O	-2.13968	-4.05179	-1.59765
C	-2.70640	-5.28116	-2.05396
H	-3.65117	-5.11337	-2.58345
H	-1.97473	-5.70190	-2.74446
H	-2.86703	-5.97904	-1.22437
C	-0.91315	1.85399	-0.03427
C	-2.20969	2.30669	-0.74228
H	-0.67341	2.59385	0.73296
C	-0.17759	1.42273	-2.39417
C	0.56935	3.43721	-1.17778
C	-1.81868	3.22723	-1.92099
H	-2.78263	1.45204	-1.11773
H	-2.84363	2.82844	-0.02196
H	0.74376	1.34380	-2.97195
H	-0.54810	0.41080	-2.22818
C	-1.23597	2.34066	-3.03534
C	-0.72127	4.24558	-1.48530
H	1.29892	3.51045	-1.98618
H	1.06779	3.72685	-0.25269
H	-2.69881	3.76791	-2.28010
H	-0.79274	2.95549	-3.82543
H	-2.02074	1.73316	-3.49587
H	-0.51753	4.87643	-2.36100
C	-1.21623	5.16910	-0.39265
H	-2.16547	5.64797	-0.63724
C	-0.63979	5.47463	0.77142
H	-1.10901	6.17780	1.45357
H	0.31394	5.06707	1.09634

N	0.21437	1.98029	-1.04322
C	5.02470	-0.80389	0.58589
C	3.89158	-1.23765	-0.12098
C	3.94400	-2.39348	-0.88564
C	5.14078	-3.12273	-0.92503
C	6.25730	-2.68599	-0.20567
C	6.21843	-1.51264	0.56148
H	3.07245	-2.72037	-1.44629
H	5.20249	-4.02967	-1.51895
H	7.17909	-3.25938	-0.24456
H	7.09275	-1.16725	1.10491
C	2.78330	-0.23918	0.10740
C	3.48132	0.87050	0.95324
N	4.73976	0.41131	1.24311
H	5.42532	0.96371	1.74305
O	1.99091	0.12920	-0.83975
O	2.99253	1.94485	1.27722
H	1.06751	1.38525	-0.74954

Electronic energy = -1607.531569
Zero-point electronic energy = -1606.942005
Enthalpy = -1606.909756
Free energy = -1607.005728
Free energy with quasiharmonic approximation = -1606.997827
Frequencies = -260.2266 11.9840 21.6114
SCF (M06-2X/def2-TZVPP–IEF-PCM) = -1607.488015

TS-3g

C	1.03575	0.41487	-0.48117
H	0.62241	-0.25885	0.26565
N	0.17718	0.32026	-1.68315
H	0.56331	0.78947	-2.49757
C	-0.88156	-0.43840	-1.91861
H	-1.19888	-0.41457	-2.95603
C	-1.69768	-1.12207	-0.98576
H	-1.27932	-1.35182	-0.00893
H	-2.22319	-1.96587	-1.42796
C	2.43849	-0.04927	-0.87534
C	2.94298	-1.33413	-0.48596
C	3.23170	0.75058	-1.67286
C	2.24881	-2.26401	0.32136
C	4.25625	-1.68381	-0.96038
C	4.50921	0.30113	-2.08367
H	2.90562	1.73426	-1.99985
C	2.81132	-3.48653	0.65641
H	1.25656	-2.06093	0.70640
C	4.80183	-2.94186	-0.60034

H	5.12459	0.94309	-2.71113
C	4.10710	-3.82951	0.18748
H	5.79328	-3.18295	-0.96987
H	4.55249	-4.78291	0.44483
N	5.01394	-0.86725	-1.74741
O	2.05233	-4.29619	1.43910
C	2.57474	-5.56574	1.83545
H	3.49016	-5.45275	2.42734
H	1.79899	-6.02172	2.45135
H	2.77265	-6.20500	0.96764
C	1.02676	1.86306	0.07276
C	2.15431	2.20762	1.07558
H	1.08465	2.54766	-0.77667
C	-0.35816	1.68009	2.16356
C	-0.44328	3.70591	0.75730
C	1.60587	3.21134	2.11186
H	2.51187	1.30788	1.58834
H	3.00252	2.62409	0.52908
H	-1.39840	1.78705	2.46982
H	-0.13770	0.61239	2.12668
C	0.64049	2.45755	3.04376
C	0.81537	4.34714	1.39923
H	-1.34811	3.91929	1.32833
H	-0.62005	4.01670	-0.27282
H	2.43171	3.64202	2.68469
H	0.11610	3.15809	3.70161
H	1.19042	1.76016	3.68260
H	0.47415	5.03207	2.18680
C	1.70738	5.15423	0.48021
H	2.60188	5.52868	0.98002
C	1.52843	5.46843	-0.80408
H	2.25791	6.07713	-1.33057
H	0.66351	5.16214	-1.38647
N	-0.28721	2.20431	0.74498
C	-5.09079	-1.08326	-0.68232
C	-4.02982	-0.83658	0.20237
C	-4.04810	-1.37253	1.48109
C	-5.12973	-2.17951	1.86205
C	-6.17176	-2.42963	0.96436
C	-6.17117	-1.88008	-0.32580
H	-3.23737	-1.16540	2.17483
H	-5.16059	-2.60954	2.85871
H	-7.00528	-3.05587	1.26959
H	-6.99010	-2.06519	-1.01435
C	-3.03686	0.08046	-0.48097
C	-3.71606	0.34636	-1.87097

N	-4.86858	-0.39788	-1.89280
H	-5.51869	-0.37961	-2.66887
O	-2.52761	1.07655	0.15643
O	-3.29760	1.06911	-2.76322
H	-1.13220	1.76776	0.24730

Electronic energy = -1607.530757
Zero-point electronic energy = -1606.940787
Enthalpy = -1606.908563
Free energy = -1607.004495
Free energy with quasiharmonic approximation = -1606.996567
Frequencies = -238.2164 15.2101 18.2905
SCF (M06-2X/def2-TZVPP–IEF-PCM) = -1607.48793

TS-4a

C	-1.11748	0.51332	-0.26327
H	-1.56856	0.45837	-1.25750
N	-0.21075	-0.65713	-0.18625
H	0.24400	-0.94217	-1.05450
C	0.34837	-1.14204	0.90101
H	-0.00013	-0.74937	1.85290
C	1.49474	-1.98169	0.79024
H	1.43794	-2.70981	-0.01772
H	1.80998	-2.43593	1.72714
C	-2.23854	0.39395	0.76392
C	-3.29918	-0.54857	0.53453
C	-2.27138	1.13713	1.92400
C	-3.38470	-1.38960	-0.59677
C	-4.32663	-0.63156	1.53476
C	-3.33738	0.97053	2.84468
H	-1.50402	1.86390	2.16546
C	-4.44032	-2.27704	-0.75168
H	-2.62747	-1.38130	-1.37242
C	-5.39288	-1.54606	1.34603
H	-3.35063	1.56767	3.75457
C	-5.45896	-2.35429	0.23456
H	-6.15951	-1.59053	2.11287
H	-6.28658	-3.04424	0.12082
N	-4.33110	0.12710	2.66974
O	-4.41888	-3.03687	-1.87652
C	-5.46867	-3.98096	-2.09584
H	-5.49953	-4.73422	-1.30052
H	-6.44248	-3.48421	-2.17239
H	-5.23350	-4.46493	-3.04427
C	-0.31575	1.83717	-0.17251
C	-1.16551	3.08776	-0.52338
H	0.09555	1.92102	0.83592

C	0.56193	1.90461	-2.52354
C	1.78603	2.99372	-0.69434
C	-0.37133	3.99026	-1.48596
H	-1.42111	3.62838	0.39087
H	-2.10923	2.79003	-0.99429
H	1.50340	1.80127	-3.06643
H	-0.05303	1.03785	-2.77193
C	-0.15907	3.24257	-2.81436
C	1.01729	4.32810	-0.87459
H	2.66252	2.93378	-1.34180
H	2.12064	2.82357	0.32947
H	-0.92844	4.91498	-1.66366
H	0.43584	3.85324	-3.50045
H	-1.12174	3.05362	-3.29891
H	1.55060	4.92875	-1.62383
N	0.90990	1.82387	-1.06091
H	1.53244	0.88807	-0.90384
C	4.78498	-1.89610	1.02370
C	3.91795	-1.90202	-0.07374
C	4.15328	-2.71752	-1.17873
C	5.27976	-3.54378	-1.17427
C	6.15084	-3.54569	-0.07662
C	5.91031	-2.72087	1.02708
H	3.47954	-2.69353	-2.03138
H	5.48827	-4.18158	-2.02909
H	7.02688	-4.18874	-0.08685
H	6.59764	-2.71894	1.86982
C	2.78504	-0.91071	0.12689
C	3.30978	-0.02995	1.30121
C	4.31318	-0.91363	2.07725
O	2.30290	-0.31892	-0.95615
H	5.13354	-0.33632	2.51714
H	3.81862	-1.43897	2.90658
H	2.51799	0.38549	1.93233
H	3.84420	0.80800	0.83622
C	0.88469	5.19316	0.35962
H	0.31942	6.10827	0.17716
C	1.36492	4.98741	1.58707
H	1.95444	4.11878	1.86808
H	1.19218	5.71344	2.37636

Electronic energy = -1517.462828
Zero-point electronic energy = -1516.843953
Enthalpy = -1516.812568
Free energy = -1516.905712
Free energy with quasiharmonic approximation = -1516.899059
Frequencies = -243.1771 17.0621 28.5562

SCF (M06-2X/def2-TZVPP–IEF-PCM) = -1517.399629

TS-4b

C	-0.84647	-0.19576	0.25632
H	-1.08559	-0.58144	-0.73397
N	0.38086	-0.89527	0.67082
H	0.90663	-0.49401	1.44582
C	1.00675	-1.82567	-0.01239
H	0.50766	-2.19299	-0.90610
C	2.36914	-2.13086	0.27659
H	2.61147	-2.14083	1.33823
H	2.75024	-3.01101	-0.23709
C	-2.00232	-0.47759	1.21412
C	-3.26903	-0.96108	0.74791
C	-1.83898	-0.26710	2.56723
C	-3.58699	-1.22404	-0.60560
C	-4.28019	-1.18863	1.74631
C	-2.90472	-0.52871	3.46026
H	-0.90028	0.09256	2.97930
C	-4.84064	-1.69011	-0.97221
H	-2.86957	-1.07410	-1.40440
C	-5.55128	-1.66519	1.33700
H	-2.76187	-0.36062	4.52611
C	-5.83710	-1.91259	0.01471
H	-6.29761	-1.82911	2.10763
H	-6.81886	-2.27601	-0.26418
N	-4.08468	-0.97083	3.07851
O	-5.02998	-1.90869	-2.29953
C	-6.29842	-2.38999	-2.74777
H	-7.09990	-1.68075	-2.51204
H	-6.20839	-2.48813	-3.83008
H	-6.53086	-3.36808	-2.31157
C	-0.56268	1.32601	0.16778
C	-1.75949	2.14081	-0.38611
H	-0.31740	1.67763	1.17429
C	0.39737	1.50883	-2.12998
C	1.08140	3.06182	-0.35580
C	-1.22111	3.24241	-1.31930
H	-2.32409	2.56605	0.44676
H	-2.44483	1.49528	-0.94559
H	1.35970	1.61431	-2.63513
H	0.04175	0.49264	-2.31264
C	-0.63055	2.57665	-2.57516
C	-0.09485	4.04200	-0.60577
H	1.93382	3.27559	-1.00311
H	1.44430	3.06653	0.67240

H	-2.03385	3.91915	-1.59902
H	-0.15197	3.32782	-3.21162
H	-1.42338	2.10961	-3.16713
H	0.24785	4.80563	-1.31725
N	0.66436	1.64515	-0.65788
H	1.56906	0.99247	-0.33102
C	5.44449	-1.52241	-0.77535
C	4.66572	-0.96657	0.24462
C	5.19539	-0.72421	1.51049
C	6.53200	-1.05081	1.75192
C	7.31736	-1.61120	0.73559
C	6.77967	-1.84781	-0.53368
H	4.58070	-0.27368	2.28553
H	6.96875	-0.86197	2.72892
H	8.35742	-1.85658	0.93337
H	7.39908	-2.27144	-1.32072
C	3.26156	-0.66486	-0.24858
C	3.41840	-0.75149	-1.79731
C	4.63861	-1.66681	-2.05075
O	2.66095	0.39532	0.27924
H	4.32759	-2.71041	-2.19941
H	5.20324	-1.37936	-2.94429
H	3.64656	0.26622	-2.13752
H	2.51318	-1.08414	-2.31447
C	-0.62212	4.78168	0.60463
H	-1.46453	5.43426	0.36984
C	-0.19158	4.74415	1.86677
H	0.64829	4.14073	2.20078
H	-0.67190	5.34644	2.63264

Electronic energy = -1517.464017
Zero-point electronic energy = -1516.845995
Enthalpy = -1516.814555
Free energy = -1516.907768
Free energy with quasiharmonic approximation = -1516.900971
Frequencies = -333.2733 18.4008 23.1919
SCF (M06-2X/def2-TZVPP–IEF-PCM) = -1517.400580

TS-5a

N	2.47037	-1.60924	1.06357
C	2.82633	-1.04826	2.40242
H	3.02342	0.02057	2.32294
H	1.97742	-1.20763	3.06854
H	3.70448	-1.55682	2.80104
C	2.25868	-3.08911	1.16020
H	3.17884	-3.58565	1.46921
H	1.47552	-3.26884	1.89733

H	1.93325	-3.46086	0.18814
N	1.87880	0.53892	-0.83021
H	1.41990	-0.14060	-1.43007
C	-0.72366	-0.07246	0.57918
O	0.05227	-1.06710	0.27476
H	1.47905	-1.23453	0.78989
C	-0.30400	1.41583	-0.63102
C	1.64859	2.56251	0.56015
C	1.09367	1.51140	-0.37089
H	1.65372	2.14800	1.58011
H	2.69000	2.78252	0.30891
N	-6.31527	-0.90853	-0.45669
O	-7.13681	-0.32581	0.25618
O	-6.62704	-1.66722	-1.37858
H	-0.54543	0.85450	-1.53454
C	0.81967	3.85788	0.54702
C	-0.67364	3.56165	0.70026
C	-1.15995	2.66401	-0.44390
H	-2.20440	2.37590	-0.28849
H	-1.14428	3.23905	-1.38113
H	-0.85414	3.07482	1.66870
H	-1.24704	4.49536	0.70542
H	0.99398	4.38913	-0.39764
H	1.17776	4.51057	1.35012
C	3.42420	-1.24391	-0.06664
C	3.27648	0.23764	-0.49556
H	3.57195	0.88351	0.33308
H	3.09342	-1.86852	-0.90390
C	4.88982	-1.57924	0.24710
H	4.97939	-2.63183	0.53364
H	5.23603	-0.98008	1.09762
C	5.78616	-1.29161	-0.96857
H	6.82508	-1.52055	-0.70845
H	5.51035	-1.96238	-1.79343
C	5.65378	0.16718	-1.42017
H	6.04941	0.83147	-0.63960
H	6.25327	0.34559	-2.31951
C	4.19027	0.52664	-1.70596
H	4.09073	1.58554	-1.96722
H	3.82440	-0.04992	-2.56631
C	-2.19240	-0.26328	0.29580
C	-2.59925	-1.13295	-0.72854
C	-3.16521	0.37682	1.07777
C	-3.94707	-1.34570	-0.98589
H	-1.84218	-1.64903	-1.30898
C	-4.52107	0.17151	0.83848

H	-2.86203	1.03123	1.89032
C	-4.89318	-0.68639	-0.19618
H	-4.27369	-2.01120	-1.77514
H	-5.28013	0.65731	1.43847
H	-0.56180	0.43533	1.54503

Electronic energy = -1209.179006
Zero-point electronic energy = -1208.659576
Enthalpy = -1208.633443
Free energy = -1208.714723
Free energy with quasiharmonic approximation = -1208.710211
Frequencies = -260.8843 22.9064 34.9894
SCF (M06-2X/def2-TZVPP–IEF-PCM) = -1209.12061045

TS-5b

N	-2.14539	-1.83673	0.56434
C	-1.59240	-2.55996	-0.62245
H	-1.41167	-1.85726	-1.43661
H	-0.65158	-3.02268	-0.32389
H	-2.28778	-3.33396	-0.94635
C	-2.43476	-2.79824	1.67730
H	-3.23406	-3.47975	1.38639
H	-1.52371	-3.35965	1.88497
H	-2.71960	-2.22940	2.56207
N	-1.95321	1.06440	0.46800
H	-2.10307	0.94666	1.46760
C	0.60768	0.38464	1.88633
O	-0.40609	-0.43918	1.96498
H	-1.36061	-1.21046	0.96740
C	0.04071	2.03081	1.23867
C	-0.43644	1.88468	-1.29081
C	-0.83506	1.69517	0.14748
H	0.07835	0.97078	-1.62497
H	-1.32371	1.98973	-1.92189
H	-0.52886	2.28026	2.13627
C	0.49629	3.09602	-1.46956
C	1.65996	3.04943	-0.47518
C	1.14684	3.05295	0.97237
H	1.97546	2.88758	1.67066
H	0.75289	4.05132	1.20694
H	2.26230	2.15297	-0.66345
H	2.31978	3.91095	-0.62776
H	-0.08026	4.01897	-1.32594
H	0.86342	3.10667	-2.50106
C	-3.35018	-0.94648	0.25962
C	-2.92553	0.38630	-0.39922
H	-2.44574	0.18592	-1.36018

H	-3.76564	-0.70949	1.24586
C	-4.42795	-1.66005	-0.57029
H	-4.72830	-2.58775	-0.07249
H	-4.02486	-1.93350	-1.55222
C	-5.65248	-0.75258	-0.77195
H	-6.39020	-1.28194	-1.38404
H	-6.12743	-0.55439	0.19820
C	-5.25176	0.57054	-1.43391
H	-4.88834	0.37869	-2.45276
H	-6.12111	1.23019	-1.52821
C	-4.16314	1.28232	-0.62186
H	-3.83853	2.20174	-1.12022
H	-4.55992	1.57456	0.35911
C	1.83566	-0.04612	1.10272
C	3.11393	0.32372	1.55184
C	1.73685	-0.85636	-0.03837
C	4.26100	-0.07012	0.86953
H	3.21544	0.91631	2.45650
C	2.86758	-1.26033	-0.73793
H	0.76230	-1.17799	-0.38196
C	4.12075	-0.85545	-0.27450
H	5.24770	0.21348	1.21364
H	2.79341	-1.87976	-1.62295
N	5.31801	-1.27499	-1.00243
O	5.17206	-1.97088	-2.01101
O	6.41681	-0.91141	-0.57549
H	0.94045	0.79901	2.85513

Electronic energy = -1209.173311
Zero-point electronic energy = -1208.652972
Enthalpy = -1208.627018
Free energy = -1208.707382
Free energy with quasiharmonic approximation = -1208.703142
Frequencies = -180.1472 26.2161 37.8529
SCF (M06-2X/def2-TZVPP–IEF-PCM) = -1209.11954079

TS-5c

N	2.70625	-1.92926	-0.07338
C	2.80079	-2.47048	1.31582
H	2.80674	-1.65160	2.03618
H	1.91421	-3.08361	1.48439
H	3.69677	-3.07997	1.43778
C	2.76672	-3.04074	-1.06785
H	2.55095	-2.63920	-2.05890
H	3.75343	-3.50885	-1.05968
H	2.00753	-3.77838	-0.80418
N	1.94698	0.94181	-0.76968

H	2.15078	1.10307	-1.75349
H	-0.23318	-0.96509	1.74182
C	-0.42527	-0.69567	0.68860
O	0.25728	-1.33522	-0.22653
H	1.63641	-1.54824	-0.13385
C	-1.91211	-0.62696	0.43535
C	-2.82014	-0.50019	1.49854
C	-2.40884	-0.78603	-0.86887
C	-4.19218	-0.48288	1.26887
H	-2.45399	-0.43334	2.51882
C	-3.77568	-0.76806	-1.11899
H	-1.70582	-0.94987	-1.67793
C	-4.65120	-0.60768	-0.04277
H	-4.89969	-0.38567	2.08266
H	-4.16861	-0.88524	-2.12118
N	-6.09245	-0.58999	-0.29544
O	-6.85150	-0.45913	0.66837
O	-6.48050	-0.70430	-1.46103
H	0.48887	2.36899	-2.24447
C	-0.10715	2.04971	-1.38299
C	0.76567	1.37798	-0.35809
C	-0.86758	3.23578	-0.75907
H	-0.83095	1.30714	-1.74716
C	0.23332	1.08992	0.93723
C	-1.66804	2.77508	0.46332
H	-1.52922	3.67003	-1.51594
H	-0.15106	4.01675	-0.47338
C	-0.76460	2.10497	1.50964
H	0.99526	0.84044	1.67371
H	-2.44949	2.08029	0.13665
H	-2.17817	3.62902	0.92351
H	-1.37160	1.62684	2.28556
H	-0.18113	2.88090	2.02497
H	3.79962	2.61391	0.17497
C	4.19685	1.67901	-0.23409
C	5.57602	1.35836	0.35162
C	3.14682	0.56800	0.01169
H	4.29708	1.82505	-1.31885
C	6.08421	0.01601	-0.17970
H	6.26884	2.16705	0.09428
H	5.52057	1.32507	1.44815
C	3.68942	-0.82004	-0.40788
H	2.87438	0.56003	1.06821
C	5.08946	-1.09816	0.16756
H	6.22306	0.07279	-1.26780
H	7.06027	-0.22771	0.25322

H	3.75917	-0.82441	-1.50094
H	5.44832	-2.06176	-0.21046
H	5.03403	-1.18065	1.25866

Electronic energy = -1209.169629
Zero-point electronic energy = -1208.650857
Enthalpy = -1208.625051
Free energy = -1208.705575
Free energy with quasiharmonic approximation = -1208.700921
Frequencies = -330.8629 15.5031 31.8006
SCF (M06-2X/def2-TZVPP–IEF-PCM) = -1209.11472984

TS-5d

C	-2.44035	-3.08662	0.14682
H	-2.47816	-2.94537	-0.93284
H	-1.51471	-3.60240	0.40401
H	-3.29726	-3.67272	0.47887
C	-2.42646	-1.95250	2.32152
H	-2.34785	-0.98108	2.81063
H	-3.34417	-2.45306	2.63184
H	-1.56449	-2.56549	2.58729
H	-1.17823	-0.22444	-1.74137
C	0.74901	-0.15281	0.53331
O	0.03846	-1.18156	0.18825
H	-1.42738	-1.35702	0.59876
H	0.52879	0.32895	1.50201
C	2.23345	-0.25724	0.28951
C	2.71383	-1.08567	-0.73728
C	3.14907	0.42244	1.10641
C	4.07727	-1.21967	-0.96273
H	2.00124	-1.63250	-1.34516
C	4.51987	0.29686	0.89845
H	2.79023	1.04386	1.92212
C	4.96498	-0.52162	-0.13925
H	4.46006	-1.85303	-1.75316
H	5.23559	0.81378	1.52509
N	6.40341	-0.65964	-0.36685
O	6.78009	-1.39409	-1.28408
O	7.17279	-0.03410	0.36754
C	-1.12541	1.29155	-0.47976
C	0.28775	1.35029	-0.64268
C	-1.78600	2.14620	0.57185
C	1.00399	2.65749	-0.32043
H	0.64401	0.88158	-1.56130
C	-1.14346	3.54130	0.66700
H	-2.85983	2.22965	0.40645
C	0.37305	3.43259	0.84425

H	2.06231	2.46040	-0.12057
H	0.98310	3.28661	-1.22199
H	-1.37433	4.10881	-0.24376
H	-1.59893	4.08055	1.50414
H	0.82078	4.43088	0.90452
H	0.59259	2.93244	1.79735
H	-5.98345	0.49566	0.64613
C	-5.94724	-0.34597	-0.05880
C	-5.62295	0.16919	-1.46567
C	-4.90038	-1.37044	0.40680
H	-6.93624	-0.81599	-0.04026
C	-4.22296	0.79560	-1.51035
H	-6.36166	0.91360	-1.78192
H	-5.68075	-0.66020	-2.18392
C	-3.48578	-0.77023	0.37982
H	-5.13719	-1.71615	1.41829
H	-4.94751	-2.24372	-0.25401
H	-3.95981	1.10018	-2.52847
C	-3.15104	-0.20298	-1.02117
H	-4.21821	1.70159	-0.89621
N	-2.41781	-1.75800	0.83814
H	-3.43562	0.04145	1.11072
N	-1.77217	0.32164	-1.12683
H	-3.16373	-1.03492	-1.73148
H	-1.65537	1.63156	1.53764

Electronic energy = -1209.172384
Zero-point electronic energy = -1208.652014
Enthalpy = -1208.626117
Free energy = -1208.706651
Free energy with quasiharmonic approximation = -1208.702248
Frequencies = -244.5580 19.5805 35.3121
SCF (M06-2X/def2-TZVPP–IEF-PCM) = -1209.11521842

TS-5e

N	2.45974	-1.71125	0.55379
C	2.69204	-1.67107	2.02169
H	2.90553	-0.64929	2.34281
H	3.51769	-2.32248	2.32420
C	2.24519	-3.11743	0.12489
H	1.39542	-3.52646	0.67695
H	2.01460	-3.14234	-0.94338
N	2.08959	0.90287	-0.82085
H	1.98243	0.69387	-1.80930
C	-0.60451	-0.55734	-0.37951
O	0.06890	-0.93362	0.66518
H	1.16746	-1.17572	0.47878

C	-2.06914	-0.54388	-0.30790
C	-2.72791	-0.66851	0.92873
C	-2.82331	-0.45353	-1.49202
C	-4.11666	-0.69651	0.98280
H	-2.14335	-0.76261	1.83715
C	-4.21227	-0.48588	-1.44916
H	-2.32051	-0.36623	-2.45174
C	-4.83505	-0.60376	-0.20800
H	-4.64977	-0.79602	1.92038
H	-4.81501	-0.42585	-2.34691
H	-0.16389	-0.76089	-1.35978
N	-6.31297	-0.63714	-0.15390
O	-6.83141	-0.74372	0.95375
O	-6.91521	-0.55409	-1.22058
H	0.54282	4.08719	0.99581
C	0.19000	3.17507	1.49413
C	1.15643	2.01935	1.17784
H	0.21832	3.37303	2.57072
C	-1.23305	2.85051	1.03515
C	1.04823	1.54671	-0.24829
H	2.18324	2.32039	1.40792
H	0.92395	1.15300	1.81882
C	-1.26704	2.56900	-0.47260
H	-1.90776	3.67982	1.27190
H	-1.60418	1.97577	1.58450
C	-0.17324	1.62403	-0.91977
H	-1.15821	3.51322	-1.02797
H	-2.24366	2.16627	-0.76568
H	-0.15800	1.39737	-1.98717
H	1.77914	-2.00447	2.52131
H	3.12275	-3.74436	0.31661
H	6.13706	1.07463	0.31364
C	5.91417	0.71671	-0.70117
C	4.50628	1.16375	-1.11082
C	6.03204	-0.80980	-0.74642
H	6.65073	1.18289	-1.36420
H	4.39872	2.25152	-1.03596
H	4.34035	0.90553	-2.16784
C	4.96500	-1.45898	0.14669
H	5.91792	-1.16149	-1.78135
H	7.02572	-1.13008	-0.41589
C	3.53699	-1.04059	-0.26035
H	5.05435	-2.55041	0.10794
H	5.15315	-1.16155	1.18591
H	3.36342	-1.38006	-1.29055
C	3.39005	0.50560	-0.26983

H 3.45133 0.87530 0.75585
Electronic energy = -1209.190034
Zero-point electronic energy = -1208.671188
Enthalpy = -1208.643581
Free energy = -1208.732621
Free energy with quasiharmonic approximation = -1208.723231
Frequencies = -209.5767 9.6455 15.8045
SCF (M06-2X/def2-TZVPP–IEF-PCM) = -1209.1126127