Electronic Supplementary Information

Origin of site-selectivity of hydrogen atom transfer in carbohydrate C–H alkylations via photoredox catalysis

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Thermodynamics of the Generation of Tetracoordinated Diarylborinic Ester

The complexation of the cis-1,2-diol moieties in sugar **1** with Ph_2BOH, leading to the tetracoordinated borinic ester (**1**/BPh_2 anion), is thermodynamically favored (Fig. S1). This is consistent with prior experimental observations.

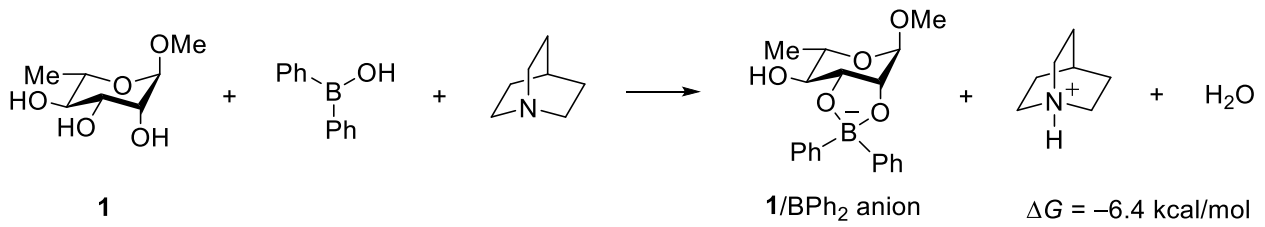
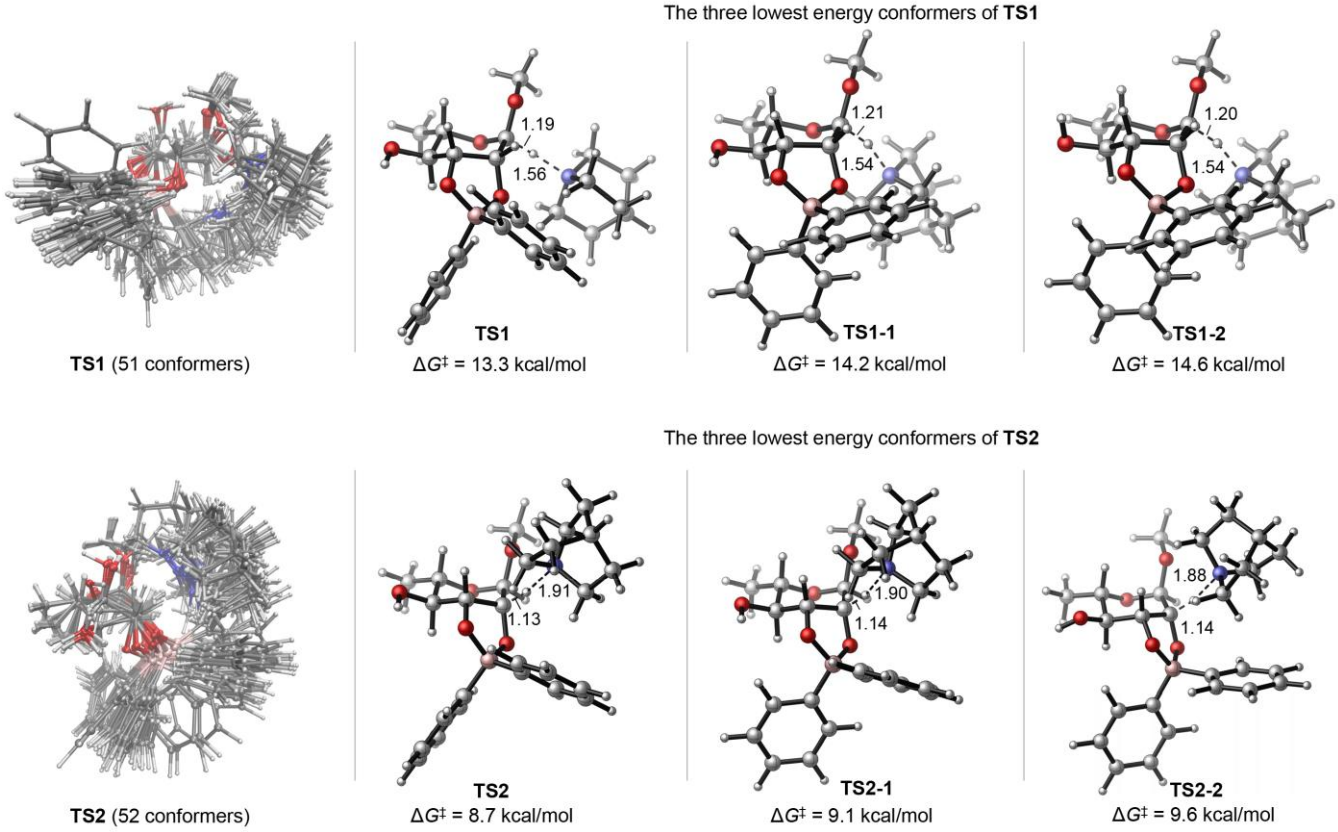


Fig. S1 Computed energetics for the formation of **1**/BPh_2 anion.

Conformational Search for the HAT Transition States

The competing HAT transition states are key to the site-selectivity. To obtain the lowest energy structures for these transition states (**TS1**~**TS5**), we carried out conformational search using CREST with the default setting. As shown in Fig. S2, the suggested 51 conformers for **TS1**, 52 conformers for **TS2**, 45 conformers for **TS3**, 51 conformers for **TS4** and 38 conformers for **TS5** were further calculated at the M06-2X/def2-TZVP-SMD(MeCN)//M06-2X/def2-SVP(MeCN) level. The three lowest energy conformers of these transition states are shown in Fig. S2.



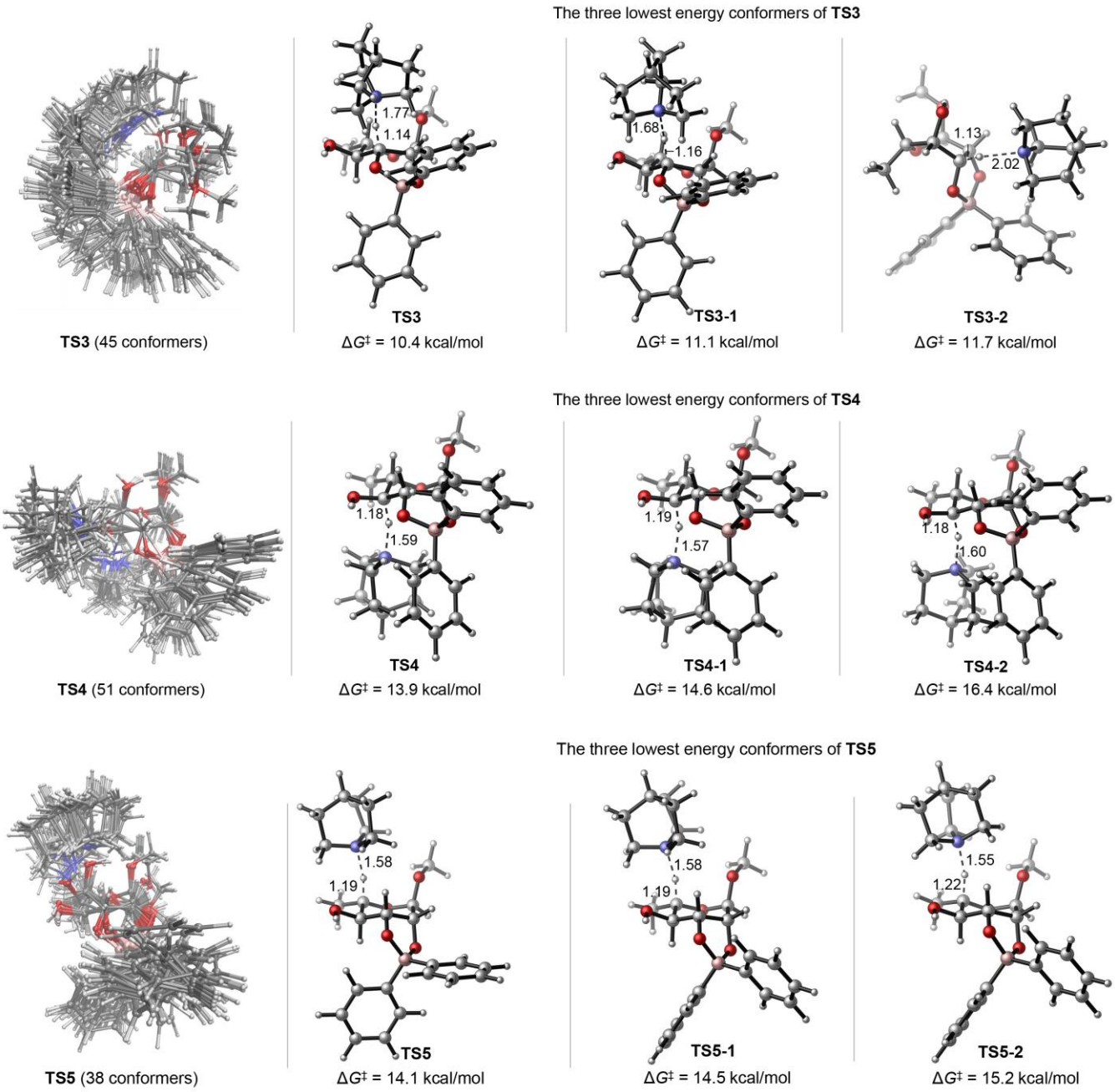


Fig. S2 Results of conformational search for **TS1**~**TS5**.

HAT of Sugar 1 without Ph_2BOH

In the absence of Ph_2BOH, the HAT transition states with sugar **1** have relatively small barrier differences (Fig. S3). Detailed conformational searches were also performed for these five HAT transition states (Fig. S4).

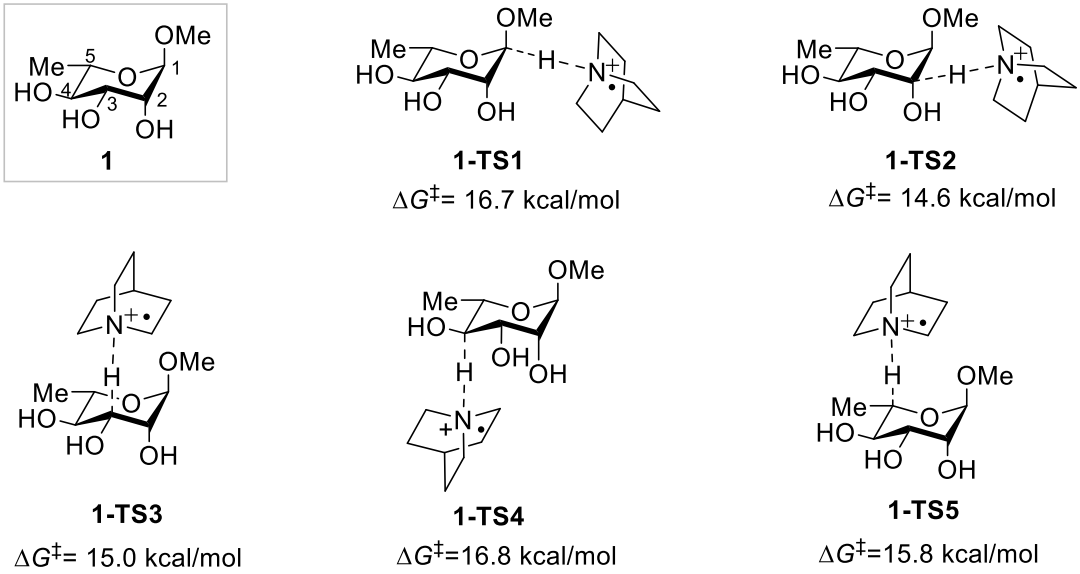
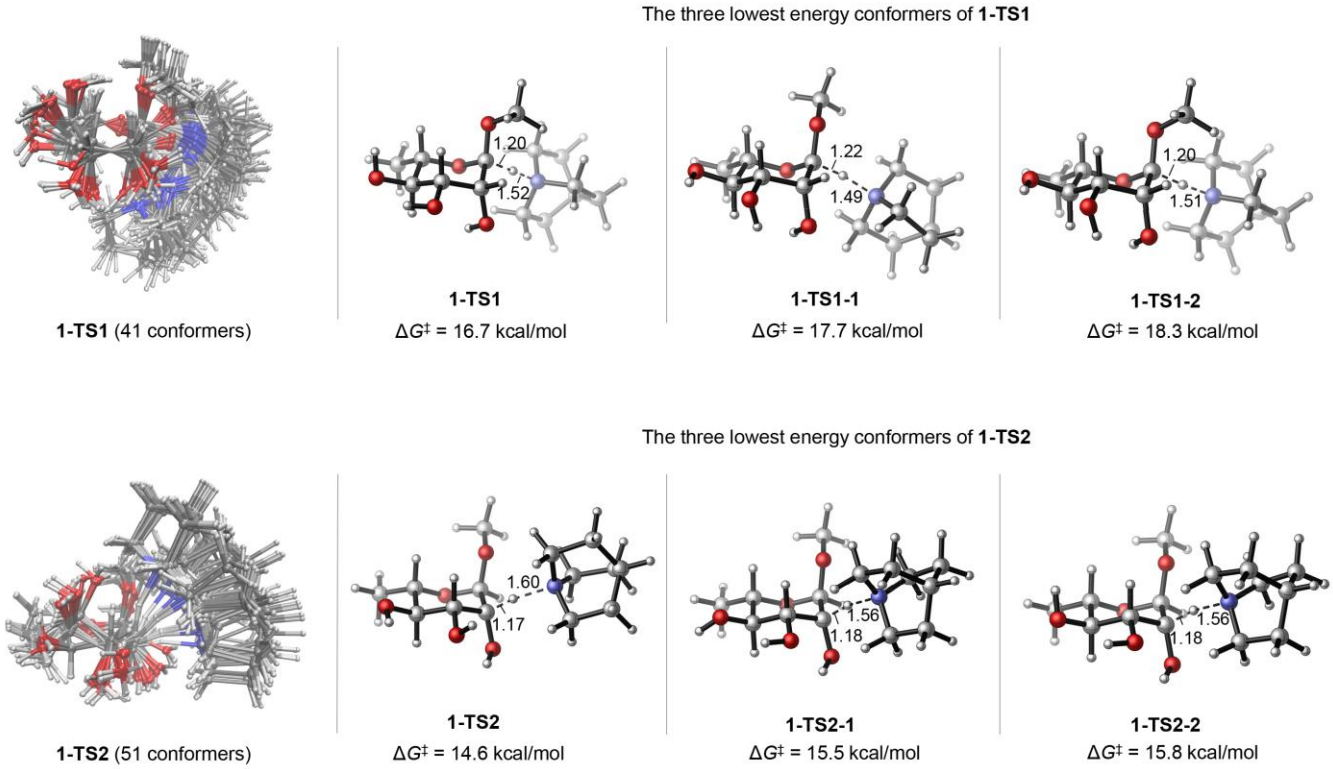


Fig. S3 Computed HAT barriers with sugar **1**.



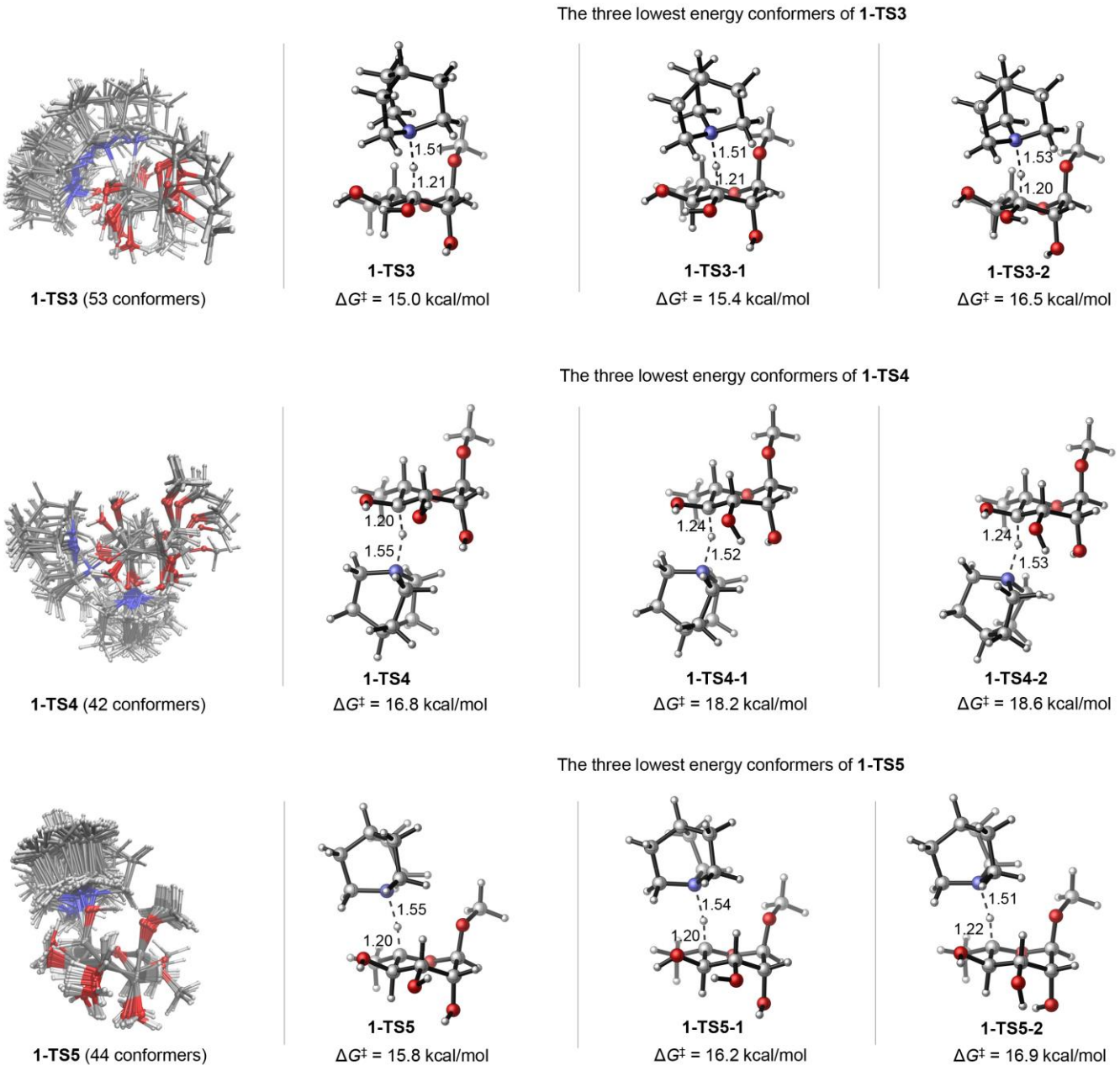


Fig. S4 Results of conformational search for **1-TS1~1-TS5**.

Role of Ph_2BOH in Lactonization Process

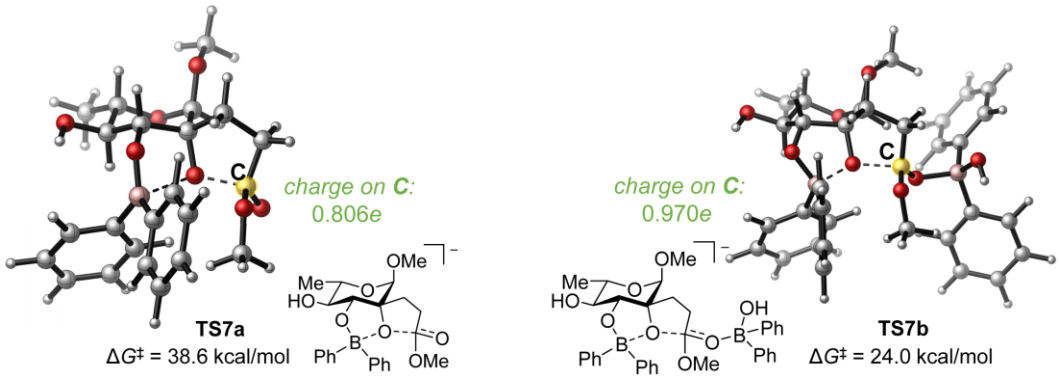


Fig. S5 NPA charges in **TS7a** and **TS7b**.

EDA Results of HAT Transition States

The comparisons of EDA results for **TS2** against **TS3**~**TS5** were given in Fig. S6-S8. The effect of charge transfer is the dominant factor accounting for the lower barrier of **TS2** than **TS3**~**TS5**. The stronger charge transfer in **TS2** ($\Delta\Delta E_{ct}$ = –2.1 ~ –9.4 kcal/mol) is mostly due to the greater orbital interactions from the C2–H σ orbital to the N SOMO (ΔE_{ct} = –7.0 ~ –17.4 kcal/mol).

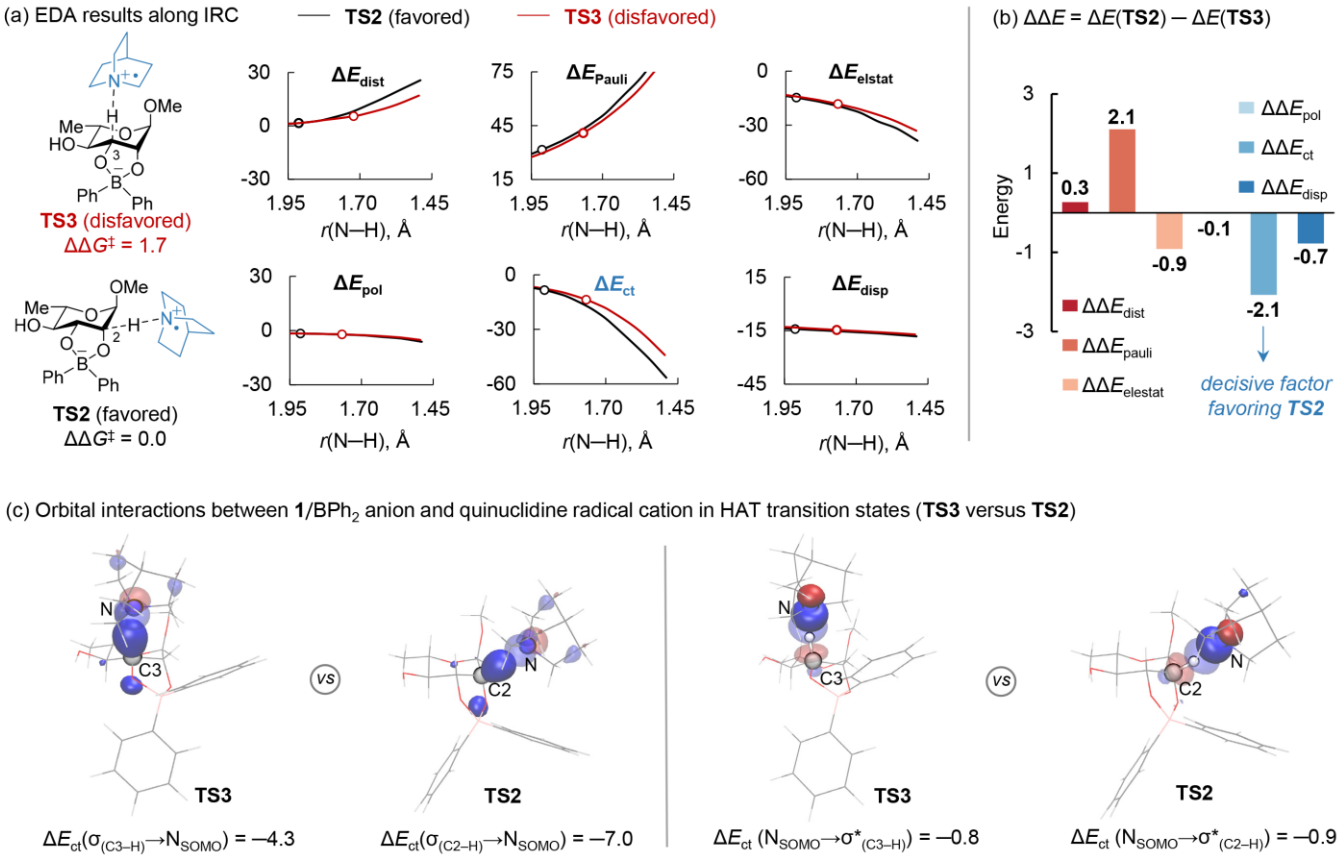


Fig. S6 EDA results for HAT transition states (**TS3** versus **TS2**). (a) EDA energy terms along IRC. (b) The bar chart of difference in six energy terms. (c) Comparison of orbital interactions. All energies are given in kcal/mol.

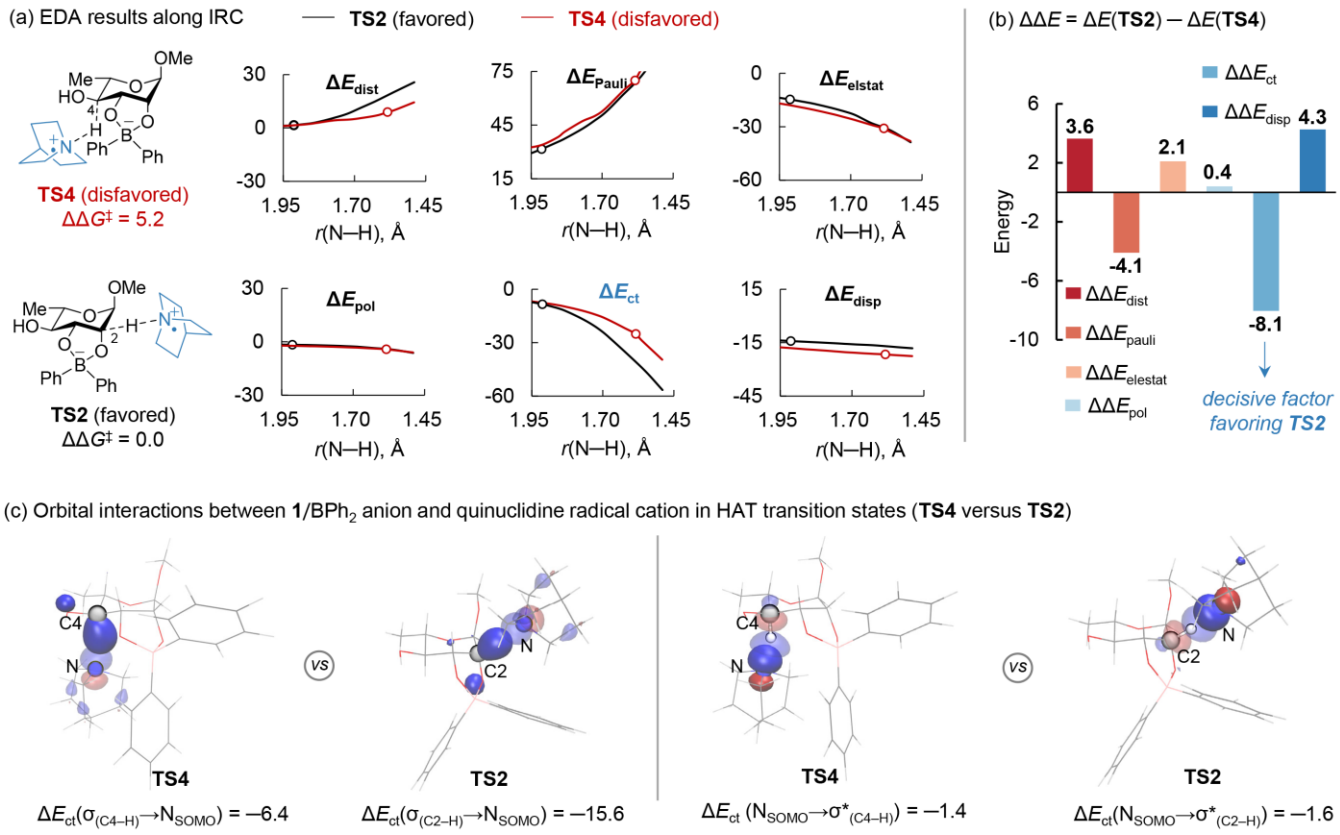


Fig. S7 EDA results for HAT transition states (**TS4** versus **TS2**). (a) EDA energy terms along IRC. (b) The bar chart of difference in six energy terms. (c) Comparison of orbital interactions. All energies are given in kcal/mol.

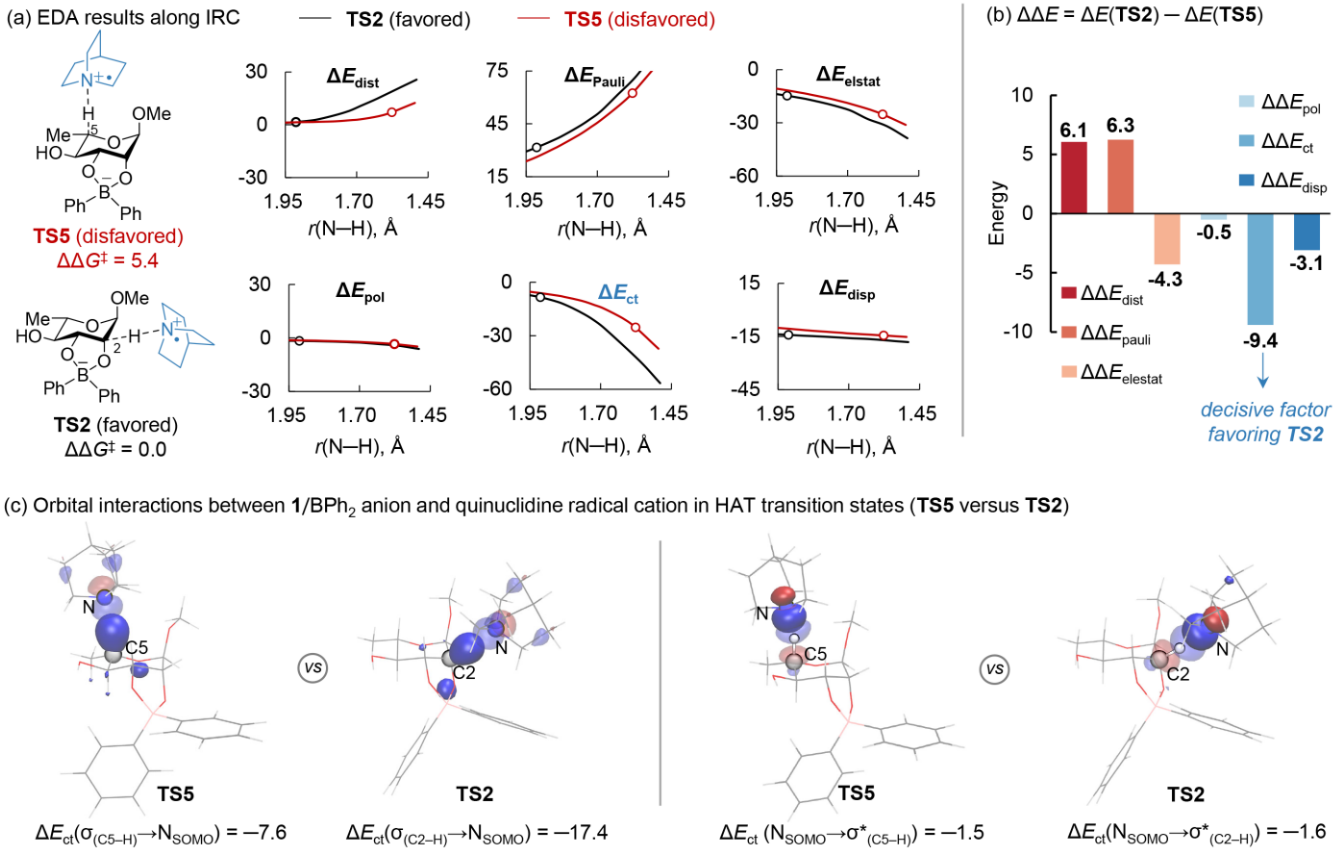


Fig. S8 EDA results for HAT transition states (**TS5** versus **TS2**). (a) EDA energy terms along IRC. (b) The bar chart of difference in six energy terms. (c) Comparison of orbital interactions. All energies are given in kcal/mol.

Relationships among HAT Barriers, Charge Transfer and C–H σ Orbital Energy

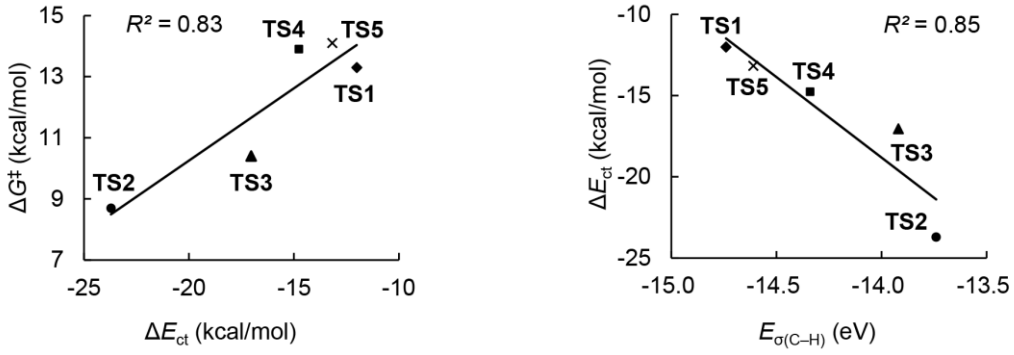


Fig. S9 Plots for $\Delta G^{\ddagger}$ against ΔE_{ct} and ΔE_{ct} against $E_{\sigma(C-H)}$.

Computed Bond Dissociation Energy and σ Orbital Energies of C–H Bonds

Table S1. Computed BDEs and $E_{\sigma(C-H)}$

1 (w/ Ph_2BOH)			**1**/BPh_2 anion		
position	*BDE* (kcal/mol)	$E\sigma_{(C-H)}$ (eV)	position	*BDE* (kcal/mol)	$E\sigma_{(C-H)}$ (eV)
C_1–H	98.0	–18.18	C_1–H	97.1	–14.74
C_2–H	95.0	–17.60	C_2–H	90.6	–13.74
C_3–H	94.9	–17.68	C_3–H	91.6	–13.92
C_4–H	96.1	–17.87	C_4–H	92.4	–14.34
C_5–H	95.1	–17.73	C_5–H	94.8	–14.61

Conformational Search for Other Transition States

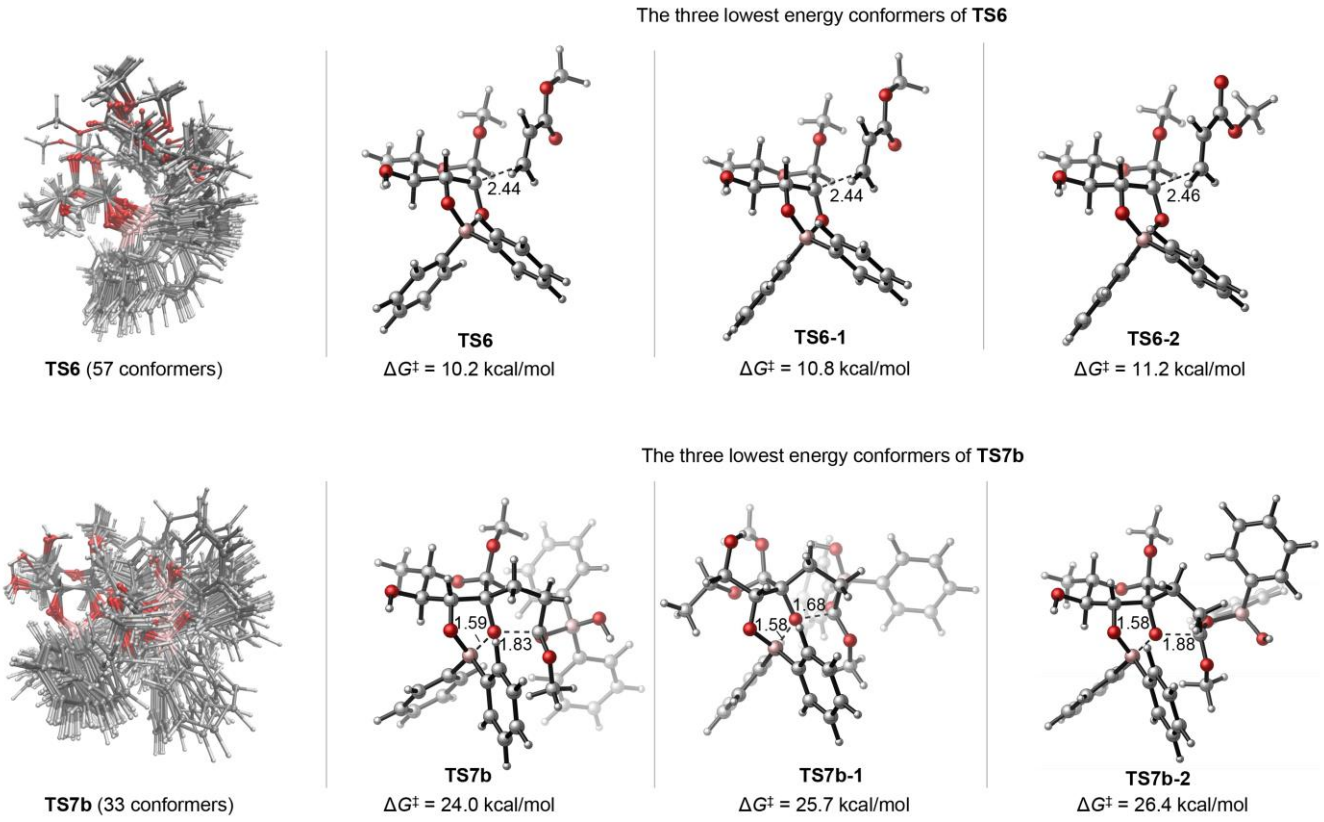


Fig. S10 Results of conformational search for **TS6 and TS7b**.

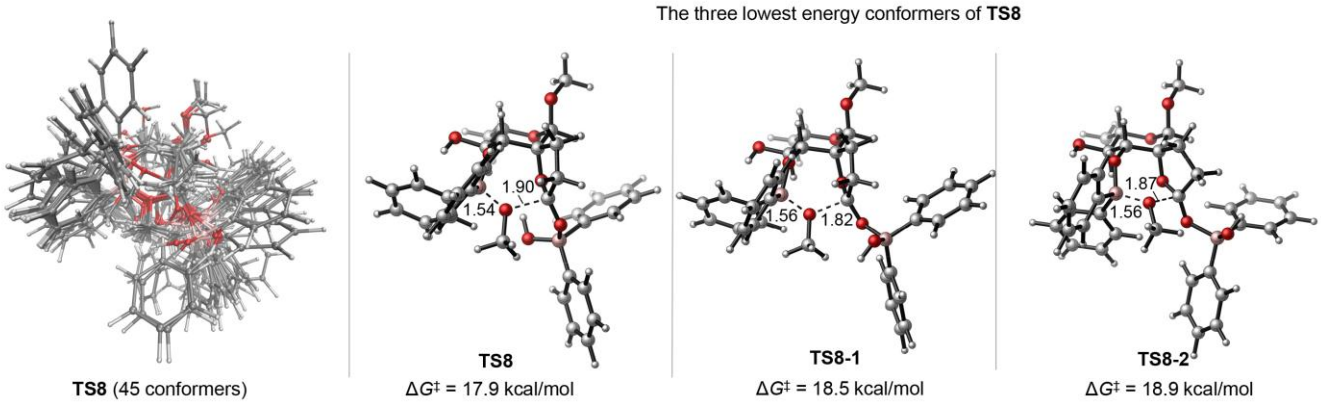


Fig. S11 Results of conformational search for **TS8**.

Energy Terms of EDA along IRC

Table S2. EDA energy terms of HAT transition state TS1

Energy terms (in kcal/mol) / *r*(N-H) In **TS1** (in Å)	ΔE_{dist}	ΔE_{Pauli}	ΔE_{ct}	ΔE_{elstat}	ΔE_{pol}	ΔE_{disp}
1.49	11.76	74.65	-35.51	-30.37	-4.81	-14.20
1.56 (TS)	7.38	63.02	-25.94	-25.91	-3.67	-13.56
1.62	4.15	53.42	-18.61	-22.26	-2.92	-12.97
1.69	2.28	45.28	-13.31	-19.38	-2.38	-12.40
1.72	1.62	41.43	-11.19	-17.97	-2.17	-12.07
1.77	1.21	36.93	-9.16	-16.40	-1.93	-11.61
1.83	0.85	31.98	-7.22	-14.66	-1.70	-11.03
1.86	0.74	29.77	-6.50	-13.88	-1.60	-10.73
1.91	0.56	26.10	-5.40	-12.57	-1.44	-10.19
1.96	0.41	23.01	-4.56	-11.46	-1.31	-9.69

Table S3. EDA energy terms of HAT transition state TS2

Energy terms (in kcal/mol) / *r*(N-H) In **TS2** (in Å)	ΔE_{dist}	ΔE_{Pauli}	ΔE_{ct}	ΔE_{elstat}	ΔE_{pol}	ΔE_{disp}
1.49	25.67	88.01	-56.52	-38.64	-6.20	-18.15
1.56	20.09	72.39	-44.14	-31.89	-4.36	-17.26
1.58	18.63	68.84	-41.08	-30.36	-4.01	-17.05
1.63	14.90	61.69	-39.03	-27.91	-3.50	-16.42
1.69	10.75	52.48	-25.92	-23.31	-2.72	-15.97
1.72	8.01	47.71	-21.17	-21.26	-2.42	-15.63
1.77	5.83	43.15	-17.02	-19.37	-2.16	-15.25
1.83	3.36	37.76	-12.42	-17.14	-1.90	-14.77
1.86	2.40	35.17	-10.50	-16.08	-1.78	-14.50
1.91 (TS)	1.60	31.61	-8.39	-14.66	-1.64	-14.07
1.96	1.06	28.63	-6.96	-13.48	-1.53	-13.64

Table S4. EDA energy terms of HAT transition state TS3

Energy terms (in kcal/mol) / *r*(N-H) In **TS3** (in Å)	ΔE_{dist}	ΔE_{Pauli}	ΔE_{ct}	ΔE_{elstat}	ΔE_{pol}	ΔE_{disp}
1.49	17.02	79.66	-44.13	-33.04	-5.14	-17.11
1.56	12.41	66.45	-33.34	-27.89	-3.83	-16.39
1.62	9.51	58.14	-26.47	-24.69	-3.16	-15.89
1.69	6.30	48.55	-18.91	-21.03	-2.52	-15.23
1.72	5.49	45.54	-16.73	-19.90	-2.35	-14.98
1.77 (TS)	4.35	40.92	-13.65	-18.18	-2.12	-14.56
1.83	3.30	35.71	-10.54	-16.25	-1.88	-14.01
1.86	2.94	32.95	-9.11	-15.24	-1.77	-13.67
1.91	2.56	29.63	-7.61	-14.03	-1.64	-13.21
1.97	2.13	26.62	-6.32	-12.91	-1.54	-12.77

Table S5. EDA energy terms of HAT transition state TS4

Energy terms (in kcal/mol) / *r*(N-H) In **TS4** (in Å)	ΔE_{dist}	ΔE_{Pauli}	ΔE_{ct}	ΔE_{elstat}	ΔE_{pol}	ΔE_{disp}
1.49	14.43	91.66	-39.50	-38.08	-5.93	-22.56
1.56	9.82	77.94	-28.72	-32.74	-4.56	-21.82
1.58 (TS)	8.96	71.48	-25.08	-30.91	-4.16	-21.55
1.62	7.00	65.90	-21.88	-29.24	-3.83	-21.29
1.69	5.30	56.71	-16.65	-26.15	-3.30	-20.70
1.72	4.68	51.94	-14.32	-24.53	-3.06	-20.31
1.77	4.27	47.50	-12.04	-22.61	-2.80	-19.74
1.83	3.92	42.13	-9.84	-20.49	-2.53	-19.02
1.86	3.73	39.37	-8.94	-19.62	-2.44	-18.74
1.91	3.56	36.42	-7.63	-17.96	-2.24	-18.05
1.96	3.34	32.96	-6.54	-16.54	-2.09	-17.45

Table S6. EDA energy terms of HAT transition state TS5

Energy terms (in kcal/mol) / *r*(N-H) In **TS5** (in Å)	ΔE_{dist}	ΔE_{Pauli}	ΔE_{ct}	ΔE_{elstat}	ΔE_{pol}	ΔE_{disp}
1.50	12.43	77.50	-37.27	-31.09	-4.80	-15.21
1.58 (TS)	7.15	62.48	-25.30	-25.18	-3.39	-14.40
1.62	5.00	55.81	-20.29	-22.58	-2.89	-14.00
1.69	3.08	47.12	-14.75	-19.34	-2.33	-13.36
1.72	2.65	43.24	-12.76	-17.93	-2.12	-12.98
1.77	2.03	38.62	-10.46	-16.19	-1.88	-12.49
1.83	1.68	32.88	-8.16	-14.10	-1.61	-11.74
1.85	1.60	30.76	-7.41	-13.32	-1.52	-11.42
1.91	1.42	26.21	-6.04	-11.63	-1.33	-10.60
1.96	1.16	22.77	-5.05	-10.31	-1.19	-9.91

Cartesian Coordinates (Å) and Energies of the Optimized Structures

1
M06-2X SCF energy: -650.53483641 a.u.
M06-2X enthalpy: -650.298768 a.u.
M06-2X free energy: -650.349501 a.u.
M06-2X SCF energy in solution: -651.29694262 a.u.
M06-2X enthalpy in solution: -651.060874 a.u.
M06-2X free energy in solution: -651.111607 a.u.
Three lowest frequencies (cm-1): 74.6344 93.9196 129.9765

Cartesian coordinates

ATOM	X	Y	Z
C	-0.096791	1.358565	0.071522
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H	-0.514706	1.446857	-0.948246
H	0.637397	-0.644255	-1.638241
H	1.647720	0.510601	0.993845
O	-0.977216	0.591957	0.886139
C	-1.246088	-0.696848	0.408048
H	-1.886072	-1.160677	1.180275
O	-1.893468	-0.674044	-0.824006
C	-3.143640	-0.025269	-0.794606
H	-3.039490	1.050183	-0.578504
H	-3.604972	-0.148744	-1.782250
H	-3.804467	-0.473011	-0.031539
C	0.028282	2.731231	0.693413
H	0.670601	3.373451	0.074833
H	-0.959581	3.206375	0.770670
H	0.462548	2.655126	1.701763
O	2.163827	1.285171	-0.869797
H	2.570160	2.012169	-0.380843
O	2.236167	-1.489790	-0.605335
H	2.930754	-0.885000	-0.906396
C	0.021286	-1.527205	0.228216
H	-0.257153	-2.457878	-0.298133
O	0.551085	-1.797161	1.499506
H	1.467685	-2.075284	1.352456

2
M06-2X SCF energy: -306.10893708 a.u.
M06-2X enthalpy: -306.005194 a.u.
M06-2X free energy: -306.043092 a.u.
M06-2X SCF energy in solution: -306.46736807 a.u.
M06-2X enthalpy in solution: -306.363625 a.u.
M06-2X free energy in solution: -306.401523 a.u.
Three lowest frequencies (cm-1): 73.3894 175.8287 205.3457

Cartesian coordinates

ATOM	X	Y	Z
C	-1.314282	1.131332	-0.000352
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H	-1.876777	2.067842	-0.000838
H	-1.877686	0.195530	-0.000463
H	0.596869	0.200162	0.000789
C	0.848913	2.359826	0.000437
O	2.055229	2.350117	0.000694
O	0.128635	3.482102	0.000191
C	0.862143	4.701269	0.000052
H	0.120575	5.506585	-0.000380
H	1.495657	4.772559	0.894975
H	1.496165	4.772063	-0.894547

3

M06-2X SCF energy: -841.10190398 a.u.
M06-2X enthalpy: -840.817176 a.u.
M06-2X free energy: -840.874575 a.u.
M06-2X SCF energy in solution: -842.07544720 a.u.
M06-2X enthalpy in solution: -841.790719 a.u.
M06-2X free energy in solution: -841.848118 a.u.
Three lowest frequencies (cm-1): 66.7830 78.9069 86.2632

Cartesian coordinates

ATOM	X	Y	Z
C	3.283028	0.777276	0.277303
C	1.346898	-0.736102	0.726735
C	1.952725	0.626492	1.016786
H	3.972131	0.001215	0.657610
H	2.053799	-1.507225	1.087350
H	1.253427	1.397809	0.647559
O	3.064213	0.582831	-1.117392
C	2.533189	-0.662380	-1.464879
H	2.378050	-0.618476	-2.558379
O	3.373073	-1.713882	-1.121053
C	4.613307	-1.691036	-1.794376
H	5.200442	-0.797600	-1.529282
H	5.168314	-2.588263	-1.495218
H	4.465928	-1.704444	-2.888019
C	3.899951	2.145837	0.457525
H	3.219037	2.922514	0.078429
H	4.101721	2.335450	1.520941
H	4.850430	2.211667	-0.089687
O	2.105991	0.703178	2.416286
H	2.140567	1.632271	2.678132
O	0.090364	-0.870586	1.334793
C	1.192494	-0.927893	-0.778092
O	0.269610	0.056643	-1.265051
C	0.564406	-2.276332	-1.157977

C	-0.925880	-1.958259	-1.208356
H	0.930814	-2.578314	-2.149884
C	-0.963718	-0.463000	-1.436073
O	-1.897569	0.223585	-1.734585
H	0.828583	-3.059333	-0.438285
H	0.184599	-0.533745	2.238648
H	-1.478336	-2.465887	-2.008619
H	-1.431185	-2.154411	-0.252991

4

M06-2X SCF energy: -1137.15583917 a.u.
M06-2X enthalpy: -1136.744922 a.u.
M06-2X free energy: -1136.821307 a.u.
M06-2X SCF energy in solution: -1138.43804469 a.u.
M06-2X enthalpy in solution: -1138.027128 a.u.
M06-2X free energy in solution: -1138.103513 a.u.
Three lowest frequencies (cm-1): 17.0443 30.4799 36.1981

Cartesian coordinates

ATOM	X	Y	Z
C	3.310683	0.413646	0.423766
C	1.119611	-0.593978	1.117799
C	1.969649	0.673276	1.091526
H	3.830961	-0.396479	0.968262
H	1.543260	-1.269605	1.884144
H	1.442738	1.421363	0.468711
O	3.055478	-0.000651	-0.915288
C	2.377538	-1.222233	-1.024907
H	2.188236	-1.348754	-2.106878
O	3.150542	-2.280034	-0.539322
C	4.384992	-2.427258	-1.197230
H	5.066898	-1.587588	-0.984609
H	4.844530	-3.358026	-0.840499
H	4.246904	-2.492936	-2.291461
C	4.189267	1.643122	0.371678
H	4.397918	1.993803	1.390794
H	5.140693	1.420375	-0.131725
H	3.679262	2.447897	-0.179518
O	2.168974	1.161818	2.397736
H	1.292164	1.181978	2.808301
O	-0.210811	-0.276678	1.411044
C	1.053886	-1.252006	-0.265220
H	0.776923	-2.320959	-0.154474
O	0.063849	-0.524681	-0.919966
C	-2.256303	-1.073440	0.091407
C	-3.210618	-1.000019	-0.939744
C	-2.462520	-2.059615	1.069228
C	-4.305099	-1.864370	-1.001557
H	-3.094425	-0.238144	-1.718881

C	-3.555770	-2.931628	1.025477
H	-1.740013	-2.134442	1.886803
C	-4.482414	-2.837527	-0.013523
H	-5.026876	-1.780243	-1.817835
H	-3.687126	-3.687199	1.804403
H	-5.338680	-3.514431	-0.053202
C	-1.345246	1.464676	-0.178121
C	-0.673777	2.232073	-1.144170
C	-2.365779	2.110693	0.541267
C	-0.995244	3.571532	-1.382941
H	0.126705	1.751986	-1.714775
C	-2.694408	3.450725	0.321764
H	-2.925888	1.547169	1.296078
C	-2.008440	4.188228	-0.647081
H	-0.454542	4.137902	-2.145626
H	-3.490659	3.923697	0.902149
H	-2.264235	5.234606	-0.828007
B	-0.935812	-0.097109	0.105540

5a

M06-2X SCF energy: -328.91713790 a.u.
M06-2X enthalpy: -328.714158 a.u.
M06-2X free energy: -328.752715 a.u.
M06-2X SCF energy in solution: -329.28354200 a.u.
M06-2X enthalpy in solution: -329.080562 a.u.
M06-2X free energy in solution: -329.119119 a.u.
Three lowest frequencies (cm-1): 41.4785 304.3235 313.6103

Cartesian coordinates

ATOM	X	Y	Z
C	-0.766279	-0.808735	1.118020
C	1.317841	-0.001085	0.000318
C	0.786691	-0.857072	1.157313
H	-1.169543	-0.381190	2.048556
H	-1.188573	-1.819812	1.015412
H	1.168605	-0.469354	2.114217
H	1.152514	-1.890283	1.055443
C	-0.763888	1.373406	0.140697
H	-1.165109	1.963514	-0.697148
H	-1.186445	1.793026	1.066198
C	0.788850	1.429630	0.164374
H	1.172121	2.066392	-0.647581
H	1.154003	1.854467	1.112033
H	2.417560	-0.001938	0.000790
C	0.787009	-0.574070	-1.320322
H	1.151826	0.032154	-2.163709
H	1.169183	-1.596083	-1.465107
C	-0.765715	-0.563618	-1.259353
H	-1.187462	0.030044	-2.084498

H	-1.169563	-1.583064	-1.353223
N	-1.251040	0.000973	0.000149

5b

M06-2X SCF energy: -328.72185941 a.u.
M06-2X enthalpy: -328.518755 a.u.
M06-2X free energy: -328.558007 a.u.
M06-2X SCF energy in solution: -329.08785726 a.u.
M06-2X enthalpy in solution: -328.884753 a.u.
M06-2X free energy in solution: -328.924005 a.u.
Three lowest frequencies (cm-1): 44.3730 306.3753 310.2778

Cartesian coordinates

ATOM	X	Y	Z
C	0.948452	1.191538	-0.565839
C	-1.270462	0.112115	-0.034402
C	-0.625232	1.366389	-0.627108
H	1.410376	1.955301	0.069290
H	1.388813	1.196576	-1.569025
H	-0.903259	2.260247	-0.054538
H	-0.923980	1.507064	-1.673546
C	0.772063	-0.193498	1.415570
H	1.088653	-1.165449	1.809843
H	1.243236	0.626049	1.969697
C	-0.806019	-0.057409	1.413584
H	-1.238681	-0.960210	1.862978
H	-1.085719	0.811879	2.021982
H	-2.365633	0.209554	-0.064029
C	-0.838389	-1.109921	-0.846919
H	-1.269605	-2.030445	-0.433486
H	-1.144003	-1.014062	-1.896381
C	0.741301	-1.214230	-0.783798
H	1.060613	-2.146208	-0.304367
H	1.188387	-1.112568	-1.778858
N	1.145788	-0.101090	0.030558

5c

M06-2X SCF energy: -329.39125656 a.u.
M06-2X enthalpy: -329.172942 a.u.
M06-2X free energy: -329.210943 a.u.
M06-2X SCF energy in solution: -329.75789804 a.u.
M06-2X enthalpy in solution: -329.539583 a.u.
M06-2X free energy in solution: -329.577584 a.u.
Three lowest frequencies (cm-1): 97.9544 290.0189 296.4187

Cartesian coordinates

ATOM	X	Y	Z

C	-0.743068	-0.742962	1.211086
C	1.311023	-0.001660	-0.000033
C	0.777569	-0.938356	1.092010
H	-1.025342	-0.132045	2.077063
H	-1.295672	-1.688549	1.246185
H	1.250882	-0.715589	2.057367
H	1.011316	-1.981506	0.836759
C	-0.740181	1.420970	0.037996
H	-1.021992	1.868118	-0.923181
H	-1.291650	1.924605	0.839957
C	0.780278	1.413097	0.267282
H	1.253673	2.138573	-0.407194
H	1.013898	1.710321	1.299402
H	2.408105	-0.002666	0.000538
C	0.778779	-0.476183	-1.358209
H	1.011673	0.269529	-2.131378
H	1.252193	-1.422513	-1.650848
C	-0.741610	-0.677780	-1.249872
H	-1.293039	-0.235536	-2.087306
H	-1.023880	-1.733272	-1.154099
N	-1.220369	0.000706	-0.000945
H	-2.246348	0.001428	-0.001798

TS1

M06-2X SCF energy: -1465.88021939 a.u.
M06-2X enthalpy: -1465.268720 a.u.
M06-2X free energy: -1465.364044 a.u.
M06-2X SCF energy in solution: -1467.52251413 a.u.
M06-2X enthalpy in solution: -1466.911015 a.u.
M06-2X free energy in solution: -1467.006339 a.u.
Three lowest frequencies (cm-1): -663.1492 9.3111 17.2707
Imaginary frequency: -663.1492 cm-1

Cartesian coordinates

ATOM	X	Y	Z
C	-0.746796	3.501023	-0.402100
C	0.804085	1.839434	-1.472338
C	0.681045	2.980625	-0.462667
H	-1.061169	3.814539	-1.415001
H	0.741388	2.269963	-2.488321
H	0.919050	2.574570	0.538999
O	-1.586040	2.412651	0.027269
C	-1.630651	1.362084	-0.860920
O	-2.345213	1.625404	-1.999051
C	-3.557441	2.337302	-1.813370
H	-3.369781	3.396187	-1.580246
H	-4.113714	2.266113	-2.755096
H	-4.153915	1.893944	-1.000624
C	-0.932816	4.636282	0.575010

H	-0.299445	5.482181	0.278452
H	-1.981621	4.963893	0.592518
H	-0.642552	4.315953	1.586732
O	1.550011	4.034386	-0.798524
H	2.422460	3.633470	-0.925786
O	2.003023	1.149184	-1.286763
C	-0.275053	0.772677	-1.225226
H	-0.414989	0.155801	-2.135985
O	0.248685	0.040311	-0.164794
C	2.148800	-1.410671	-1.118493
C	1.887814	-2.651457	-0.507873
C	2.733632	-1.444316	-2.392929
C	2.184579	-3.862697	-1.134917
H	1.438933	-2.670105	0.492101
C	3.045352	-2.649729	-3.032066
H	2.943433	-0.494965	-2.893931
C	2.769822	-3.864953	-2.404737
H	1.965790	-4.809064	-0.633996
H	3.502861	-2.641622	-4.024588
H	3.008406	-4.808533	-2.900305
C	2.477963	0.137722	1.077140
C	1.772281	0.490626	2.239039
C	3.863089	-0.057800	1.213680
C	2.409649	0.644428	3.474261
H	0.692754	0.652341	2.162542
C	4.516708	0.101897	2.437588
H	4.450328	-0.346529	0.334858
C	3.788160	0.451955	3.577511
H	1.830069	0.915926	4.360220
H	5.596315	-0.052172	2.507103
H	4.292125	0.572529	4.538963
B	1.734221	-0.014417	-0.370136
N	-2.688830	-0.832939	0.391222
C	-4.150089	-0.746345	0.407197
C	-3.491203	-2.953830	1.403577
C	-4.681321	-2.122895	0.909514
H	-4.429370	0.076700	1.076300
H	-4.490632	-0.522763	-0.611435
H	-5.405714	-1.959360	1.718326
H	-5.195304	-2.645795	0.091284
C	-2.104425	-0.888356	1.732618
H	-1.018142	-0.960560	1.606337
H	-2.349639	0.046559	2.252584
C	-2.715846	-2.133820	2.441508
H	-1.906713	-2.729980	2.883871
H	-3.387817	-1.815895	3.250665
H	-3.846887	-3.892222	1.850239
C	-2.570186	-3.251314	0.214652
H	-1.656016	-3.754919	0.559273
H	-3.069888	-3.908257	-0.509505
C	-2.200629	-1.905326	-0.478677

H	-1.116408	-1.779115	-0.587503
H	-2.691635	-1.790941	-1.453738
H	-2.174715	0.484015	-0.260178

TS2

M06-2X SCF energy: -1465.89015806 a.u.
M06-2X enthalpy: -1465.276665 a.u.
M06-2X free energy: -1465.370331 a.u.
M06-2X SCF energy in solution: -1467.53346566 a.u.
M06-2X enthalpy in solution: -1466.919973 a.u.
M06-2X free energy in solution: -1467.013639 a.u.
Three lowest frequencies (cm-1): -123.7369 16.4672 26.0405
Imaginary frequency: -123.7369 cm-1

Cartesian coordinates

ATOM	X	Y	Z
C	-1.750958	3.282601	0.411991
C	-0.614626	1.105446	0.923158
C	-1.898089	1.922263	1.079141
H	-0.888719	3.809583	0.860915
H	0.147439	1.549978	1.588852
H	-2.707578	1.387190	0.545369
O	-1.506642	3.066999	-0.975645
C	-0.303780	2.414124	-1.263623
H	-0.311092	2.256441	-2.356986
O	0.804807	3.176050	-0.883156
C	0.888069	4.424738	-1.530272
H	0.047023	5.081888	-1.257414
H	1.827793	4.897624	-1.218097
H	0.894022	4.301310	-2.627513
C	-2.993637	4.135038	0.533717
H	-3.219475	4.315289	1.592635
H	-2.850055	5.101455	0.030052
H	-3.850036	3.620880	0.071954
O	-2.215625	2.089141	2.438648
H	-2.198698	1.204108	2.831609
O	-0.833854	-0.238173	1.237445
C	-0.171065	1.077392	-0.542173
O	-0.921586	0.072430	-1.105413
C	-0.168447	-2.228912	-0.221269
C	0.112295	-2.756113	-1.492924
C	0.482910	-2.823364	0.871944
C	1.018605	-3.803450	-1.673946
H	-0.375808	-2.317048	-2.369062
C	1.389026	-3.876386	0.708338
H	0.291169	-2.430324	1.875350
C	1.666293	-4.365395	-0.570142
H	1.227249	-4.181810	-2.677760
H	1.885166	-4.314497	1.578152

H	2.380623	-5.180247	-0.705630
C	-2.740172	-1.419581	-0.097881
C	-3.658462	-0.844666	-0.990597
C	-3.232312	-2.407775	0.772160
C	-5.001908	-1.232154	-1.017915
H	-3.302541	-0.066774	-1.672473
C	-4.572672	-2.798523	0.763929
H	-2.545061	-2.888103	1.477252
C	-5.464701	-2.211417	-0.137393
H	-5.692726	-0.768572	-1.726743
H	-4.926012	-3.565234	1.457806
H	-6.513479	-2.516094	-0.152535
B	-1.175251	-0.954746	-0.040619
C	3.035670	-0.760130	-0.864475
C	4.958521	-0.300967	0.680228
C	4.537343	-1.096945	-0.559345
H	2.370399	-1.580913	-0.571960
H	2.881612	-0.504325	-1.920371
H	4.623769	-2.178336	-0.388194
H	5.162472	-0.828664	-1.421891
C	2.575813	0.088181	1.364680
H	2.390411	1.027370	1.899195
H	1.723264	-0.592006	1.496725
C	3.937079	-0.559855	1.794815
H	4.255742	-0.110641	2.744557
H	3.801820	-1.640060	1.947976
H	5.962560	-0.607485	1.005355
C	4.949645	1.192986	0.332439
H	5.109049	1.798745	1.234955
H	5.737959	1.435523	-0.392120
C	3.556340	1.547008	-0.302614
H	3.098409	2.427437	0.163289
H	3.623987	1.692346	-1.387336
N	2.720651	0.393088	-0.044395
H	0.933574	0.829652	-0.568901

TS3

M06-2X SCF energy: -1465.88737279 a.u.
M06-2X enthalpy: -1465.274248 a.u.
M06-2X free energy: -1465.368530 a.u.
M06-2X SCF energy in solution: -1467.52981882 a.u.
M06-2X enthalpy in solution: -1466.916694 a.u.
M06-2X free energy in solution: -1467.010976 a.u.
Three lowest frequencies (cm-1): -105.3746 24.0249 28.4533
Imaginary frequency: -105.3746 cm-1

Cartesian coordinates

ATOM	X	Y	Z
C	-0.525915	3.534632	-0.267126

C	-0.105645	1.068505	-0.349065
C	0.072295	2.398580	-1.081427
H	-1.600379	3.331907	-0.101490
H	1.162232	2.585763	-1.149818
O	0.152615	3.563757	0.983437
C	-0.112700	2.465791	1.811690
H	0.542769	2.601318	2.690872
O	-1.455888	2.434299	2.196739
C	-1.879408	3.589691	2.880230
H	-2.899512	3.406686	3.240780
H	-1.225728	3.799900	3.745427
H	-1.884562	4.476714	2.226233
C	-0.353456	4.883276	-0.928614
H	-0.861143	4.888479	-1.901617
H	-0.780335	5.676984	-0.299663
H	0.715007	5.093483	-1.086427
O	-0.518130	2.358863	-2.355477
H	-0.132805	1.605361	-2.824564
O	0.718434	0.098410	-0.860461
C	0.180048	1.114839	1.162333
H	-0.478592	0.383907	1.671662
O	1.515384	0.728745	1.253917
B	1.675691	-0.345628	0.240471
C	-1.916941	-1.195732	-1.839723
C	-4.051696	-2.277693	-1.092584
C	-2.812636	-2.470471	-1.975564
H	-1.957178	-0.565765	-2.737197
H	-0.869518	-1.434573	-1.605821
H	-3.091580	-2.598035	-3.029910
H	-2.250286	-3.359742	-1.656994
C	-3.723470	0.219312	-1.043458
H	-4.057784	0.764488	-0.152394
H	-3.564629	0.922671	-1.869947
C	-4.708949	-0.934261	-1.435838
H	-5.648875	-0.805334	-0.883237
H	-4.929831	-0.882247	-2.510758
H	-4.765134	-3.097183	-1.255523
C	-3.605703	-2.250564	0.373460
H	-4.452265	-2.000291	1.027467
H	-3.204656	-3.224937	0.683246
C	-2.484235	-1.167312	0.520006
H	-2.697580	-0.462981	1.334289
H	-1.493157	-1.618471	0.667901
N	-2.462783	-0.432767	-0.733490
H	-1.202468	0.788374	-0.518350
C	1.155774	-1.790961	0.811431
C	0.903971	-2.866400	-0.058721
C	0.874561	-1.995938	2.170568
C	0.376362	-4.077190	0.395529
H	1.117839	-2.750391	-1.127266
C	0.345691	-3.202083	2.642579

H	1.057345	-1.176518	2.873038
C	0.088626	-4.246868	1.753584
H	0.188674	-4.892499	-0.307677
H	0.129787	-3.327357	3.706476
H	-0.326274	-5.190042	2.115821
C	3.198126	-0.394898	-0.322109
C	4.219441	-1.062645	0.374586
C	3.560546	0.260899	-1.509171
C	5.540902	-1.064928	-0.077917
H	3.974262	-1.600563	1.296534
C	4.876843	0.261102	-1.979045
H	2.783372	0.779831	-2.077744
C	5.874033	-0.401876	-1.261400
H	6.314079	-1.589553	0.488606
H	5.127232	0.779913	-2.907599
H	6.904590	-0.405239	-1.622931

TS4

M06-2X SCF energy: -1465.88521627 a.u.
M06-2X enthalpy: -1465.273427 a.u.
M06-2X free energy: -1465.366175 a.u.
M06-2X SCF energy in solution: -1467.52448366 a.u.
M06-2X enthalpy in solution: -1466.912694 a.u.
M06-2X free energy in solution: -1467.005442 a.u.
Three lowest frequencies (cm-1): -431.2418 14.4156 25.3717
Imaginary frequency: -431.2418 cm-1

Cartesian coordinates

ATOM	X	Y	Z
C	-1.533246	3.010106	0.578464
C	0.427182	1.517231	1.042746
C	-1.073030	1.720366	1.236672
H	0.907661	2.240471	1.733794
H	-1.633921	0.894282	0.605515
O	-1.320505	2.823265	-0.816948
C	0.035583	2.790240	-1.189627
H	0.031796	2.514112	-2.259443
O	0.630530	4.036475	-1.001141
C	0.047552	5.067979	-1.761843
H	0.056925	4.819950	-2.838189
H	-0.993689	5.262701	-1.458899
H	0.642214	5.975613	-1.600058
C	-2.985248	3.352658	0.811810
H	-3.180500	3.449761	1.887756
H	-3.229804	4.304709	0.321001
H	-3.638060	2.570970	0.400651
O	-1.466520	1.581704	2.547925
H	-0.918140	0.882450	2.942700
O	0.803722	0.204551	1.330033

C	0.877964	1.774018	-0.413941
H	1.903193	2.188866	-0.393334
O	0.877384	0.501921	-0.988018
C	3.079125	-0.172370	0.181493
C	3.894062	-0.322364	-0.954424
C	3.727168	0.118654	1.391738
C	5.281928	-0.186919	-0.891464
H	3.426305	-0.549249	-1.918715
C	5.117406	0.251653	1.473078
H	3.117747	0.249844	2.291239
C	5.901133	0.099239	0.328837
H	5.886527	-0.305248	-1.794205
H	5.592542	0.477554	2.431120
H	6.986883	0.203621	0.384582
C	1.108650	-1.930289	-0.146796
C	0.807695	-2.448065	-1.416792
C	1.189856	-2.852294	0.911984
C	0.594083	-3.815332	-1.625777
H	0.736137	-1.759181	-2.264484
C	0.974072	-4.218307	0.719976
H	1.426688	-2.489267	1.917757
C	0.677184	-4.706936	-0.555611
H	0.362376	-4.185342	-2.627679
H	1.040371	-4.908111	1.564749
H	0.511422	-5.774847	-0.712505
B	1.446942	-0.359433	0.085269
C	-2.165974	-0.595312	-1.197571
C	-3.629632	-2.484237	-0.436931
C	-2.961135	-1.851802	-1.663629
H	-2.425324	0.300732	-1.775311
H	-1.079233	-0.732828	-1.228715
H	-3.717866	-1.564990	-2.407150
H	-2.266821	-2.563026	-2.133540
C	-3.973829	-0.114171	0.343343
H	-4.162400	0.295375	1.344266
H	-4.284033	0.609703	-0.419316
C	-4.662624	-1.501217	0.133059
H	-5.053302	-1.874746	1.089843
H	-5.507431	-1.376636	-0.557049
H	-4.120395	-3.426941	-0.714330
C	-2.547582	-2.734133	0.621180
H	-2.939796	-3.318946	1.464107
H	-1.704525	-3.287056	0.178960
C	-2.054631	-1.354900	1.137289
H	-2.480125	-1.108294	2.118970
H	-0.961852	-1.283891	1.186783
N	-2.541738	-0.347858	0.193165
H	-0.893257	3.835752	0.942243

TS5
M06-2X SCF energy: -1465.88109266 a.u.
M06-2X enthalpy: -1465.269469 a.u.
M06-2X free energy: -1465.363461 a.u.
M06-2X SCF energy in solution: -1467.52269379 a.u.
M06-2X enthalpy in solution: -1466.911070 a.u.
M06-2X free energy in solution: -1467.005062 a.u.
Three lowest frequencies (cm-1): -524.7712 12.5855 28.0917
Imaginary frequency: -524.7712 cm-1

Cartesian coordinates

ATOM	X	Y	Z
C	-1.503816	1.236003	0.886900
C	0.113017	-0.169241	-0.457667
C	-0.413797	1.233742	-0.173289
H	-0.636355	-0.716016	-1.055871
H	0.421135	1.822883	0.255774
O	-1.081091	0.627233	2.057617
C	-0.578729	-0.693463	1.956896
H	-0.107620	-0.884464	2.935077
O	-1.625787	-1.584040	1.732220
C	-2.386025	-1.861889	2.890942
H	-2.860707	-0.952162	3.292152
H	-3.163354	-2.585993	2.616555
H	-1.748894	-2.305390	3.674642
C	-2.073104	2.595527	1.202644
H	-2.407839	3.092996	0.284323
H	-2.912501	2.512043	1.907601
H	-1.287848	3.211688	1.668333
O	-0.902634	1.839579	-1.344981
H	-0.254963	1.651020	-2.041360
O	1.332068	-0.084793	-1.132477
C	0.453900	-0.880984	0.852907
H	0.520355	-1.973591	0.674760
O	1.688962	-0.333384	1.191061
C	3.416059	-1.397330	-0.411694
C	3.634141	-2.416906	0.527467
C	4.087401	-1.515503	-1.641926
C	4.473129	-3.504239	0.259451
H	3.124467	-2.351037	1.493767
C	4.926049	-2.594351	-1.926404
H	3.949004	-0.738554	-2.402011
C	5.122768	-3.597162	-0.971670
H	4.620353	-4.282099	1.013042
H	5.431698	-2.658028	-2.893256
H	5.778916	-4.442951	-1.188525
C	3.267377	1.267758	-0.037563
C	4.363573	1.415654	0.830691
C	2.935326	2.378383	-0.828854
C	5.080646	2.609796	0.921828
H	4.666474	0.568311	1.455656

C	3.649030	3.579575	-0.757169
H	2.088000	2.296960	-1.516788
C	4.725085	3.700330	0.122721
H	5.922362	2.693003	1.613740
H	3.365398	4.424944	-1.389128
H	5.285688	4.635623	0.184621
B	2.425206	-0.131161	-0.097614
C	-4.194921	1.243314	-1.109714
C	-5.838265	-0.630533	-1.356159
C	-5.390738	0.709606	-1.952222
H	-4.503206	2.048257	-0.430873
H	-3.354732	1.586349	-1.726152
H	-6.205069	1.445599	-1.923971
H	-5.085027	0.577041	-2.999528
C	-4.645882	-0.193018	0.802804
H	-4.263854	-1.085050	1.310838
H	-4.664585	0.651953	1.503661
C	-6.038366	-0.450858	0.154109
H	-6.480100	-1.349815	0.604196
H	-6.710812	0.395693	0.350916
H	-6.772453	-0.965966	-1.826208
C	-4.726511	-1.663185	-1.583848
H	-4.947542	-2.587474	-1.032102
H	-4.633266	-1.914167	-2.648751
C	-3.382250	-1.052401	-1.088152
H	-2.812768	-1.741090	-0.450364
H	-2.753894	-0.712653	-1.920982
N	-3.725761	0.124290	-0.288133
H	-2.394885	0.609409	0.405524

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M06-2X SCF energy: -1136.50487309 a.u.
M06-2X enthalpy: -1136.106767 a.u.
M06-2X free energy: -1136.183614 a.u.
M06-2X SCF energy in solution: -1137.78567128 a.u.
M06-2X enthalpy in solution: -1137.387565 a.u.
M06-2X free energy in solution: -1137.464412 a.u.
Three lowest frequencies (cm-1): 19.2413 23.8264 31.9268

Cartesian coordinates

ATOM	X	Y	Z
C	-1.743956	3.290064	0.541177
C	-0.645632	1.067883	0.940799
C	-1.896799	1.918275	1.194553
H	-0.835076	3.772647	0.948646
H	0.150766	1.472994	1.597682
H	-2.747945	1.412879	0.695249
O	-1.598473	3.113852	-0.863278
C	-0.417541	2.422257	-1.240540

H	-0.522208	2.257486	-2.328272
O	0.710544	3.202692	-0.965572
C	0.696493	4.459551	-1.595967
H	-0.068199	5.129339	-1.169566
H	1.685705	4.914263	-1.454264
H	0.502800	4.361103	-2.679646
C	-2.942833	4.183154	0.772095
H	-3.092559	4.341181	1.847857
H	-2.796832	5.157690	0.284761
H	-3.847323	3.714628	0.355193
O	-2.138504	2.078337	2.570906
H	-2.115070	1.191120	2.957678
O	-0.877856	-0.282799	1.214655
C	-0.286496	1.117882	-0.521605
O	-0.732569	0.007677	-1.124140
C	-0.112283	-2.307016	-0.158270
C	-0.231090	-3.268541	-1.177504
C	0.937919	-2.480343	0.756188
C	0.654777	-4.342477	-1.287065
H	-1.043167	-3.175872	-1.907079
C	1.829159	-3.553783	0.665029
H	1.048503	-1.748607	1.561078
C	1.690759	-4.490092	-0.360597
H	0.537371	-5.071683	-2.092375
H	2.633657	-3.662711	1.396657
H	2.383566	-5.330864	-0.437555
C	-2.679700	-1.418459	-0.268895
C	-3.541266	-0.671936	-1.089543
C	-3.248949	-2.503384	0.420611
C	-4.899201	-0.981063	-1.213859
H	-3.131691	0.180719	-1.639579
C	-4.604064	-2.823357	0.310965
H	-2.611413	-3.120816	1.063090
C	-5.437194	-2.060336	-0.511088
H	-5.540860	-0.378078	-1.861334
H	-5.014523	-3.671776	0.864213
H	-6.497138	-2.306849	-0.603619
B	-1.106188	-1.014222	-0.064633

TS6
M06-2X SCF energy: -1442.62305399 a.u.
M06-2X enthalpy: -1442.121057 a.u.
M06-2X free energy: -1442.215051 a.u.
M06-2X SCF energy in solution: -1444.25757556 a.u.
M06-2X enthalpy in solution: -1443.755579 a.u.
M06-2X free energy in solution: -1443.849573 a.u.
Three lowest frequencies (cm-1): -131.4653 18.5330 23.0396
Imaginary frequency: -131.4653 cm-1

Cartesian coordinates

ATOM	X	Y	Z
C	-0.924724	-3.052807	0.536328
C	-0.082721	-0.788466	1.259333
C	0.255956	-2.282313	1.122302
H	-1.795065	-2.921424	1.205537
H	-0.797715	-0.677453	2.096917
H	1.086222	-2.364558	0.393156
O	-1.229793	-2.522235	-0.750677
C	-1.662008	-1.169564	-0.724930
H	-1.791863	-0.886339	-1.784246
O	-2.858825	-1.064115	-0.022290
C	-3.943326	-1.709966	-0.642461
H	-3.783941	-2.798594	-0.714281
H	-4.833273	-1.516363	-0.029489
H	-4.109166	-1.307951	-1.657842
C	-0.628079	-4.526740	0.368732
H	0.224106	-4.664654	-0.313981
H	-0.376189	-4.969518	1.341008
H	-1.500222	-5.050319	-0.047614
O	0.615628	-2.840333	2.361252
H	1.311116	-2.273080	2.722852
O	1.068392	-0.023244	1.465173
C	-0.628954	-0.308149	-0.057727
O	0.377577	0.162905	-0.789884
C	1.932560	2.010807	0.174778
C	1.950030	2.727275	1.381264
C	2.250568	2.722454	-0.994931
C	2.266321	4.088697	1.425958
H	1.697658	2.197355	2.304083
C	2.557116	4.084377	-0.967633
H	2.257020	2.197249	-1.956155
C	2.567942	4.773801	0.248038
H	2.273325	4.619780	2.381068
H	2.790748	4.613262	-1.894894
H	2.810479	5.838392	0.275014
C	2.834227	-0.455855	-0.388675
C	2.910336	-0.987224	-1.685787
C	3.920713	-0.706467	0.467308
C	4.014568	-1.732019	-2.112967
H	2.074036	-0.825761	-2.372269
C	5.027071	-1.452051	0.056619
H	3.895667	-0.311318	1.488427
C	5.078680	-1.968067	-1.241262
H	4.043814	-2.134172	-3.128721
H	5.853120	-1.634125	0.748505
H	5.941669	-2.552533	-1.567660
B	1.564243	0.424384	0.135924
C	-1.670060	1.859571	0.383174
C	-2.962454	1.765048	0.765915
H	-0.866362	2.022902	1.104963

H	-3.265706	1.717466	1.813110
C	-3.998111	1.547831	-0.249234
O	-3.832237	1.552877	-1.450011
O	-5.206759	1.334415	0.302310
C	-6.282844	1.143947	-0.601454
H	-7.174800	0.965062	0.009009
H	-6.431963	2.035906	-1.226988
H	-6.100315	0.281898	-1.258228
H	-1.422339	1.970093	-0.673994

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M06-2X SCF energy: -1442.66324470 a.u.
M06-2X enthalpy: -1442.158709 a.u.
M06-2X free energy: -1442.251150 a.u.
M06-2X SCF energy in solution: -1444.29294412 a.u.
M06-2X enthalpy in solution: -1443.788408 a.u.
M06-2X free energy in solution: -1443.880849 a.u.
Three lowest frequencies (cm-1): 23.4511 30.2308 34.3962

Cartesian coordinates

ATOM	X	Y	Z
C	3.273990	0.498962	0.485097
C	0.988795	-0.553775	0.654820
C	1.923779	0.540516	1.175783
H	3.740101	-0.490340	0.646652
H	1.269789	-1.499888	1.149135
H	1.480585	1.519979	0.925252
O	3.031863	0.690867	-0.905368
C	2.376923	-0.382924	-1.517732
H	2.207557	-0.062624	-2.562711
O	3.171550	-1.530602	-1.486161
C	4.396616	-1.389234	-2.162894
H	5.034830	-0.620789	-1.698000
H	4.913939	-2.356091	-2.119852
H	4.235224	-1.115580	-3.220981
C	4.209628	1.590391	0.953958
H	3.757857	2.577900	0.773287
H	4.396686	1.481962	2.030227
H	5.167920	1.537933	0.417894
O	2.092252	0.417126	2.570518
H	1.202270	0.391750	2.948827
O	-0.341817	-0.230318	0.951566
C	1.004766	-0.692914	-0.884355
O	0.084507	0.268016	-1.308929
C	-2.400724	0.236581	-0.494233
C	-3.020616	0.646176	-1.687325
C	-3.195191	-0.465530	0.425044
C	-4.360329	0.361126	-1.960296
H	-2.436564	1.203026	-2.428235

C	-4.540266	-0.750226	0.171112
H	-2.731979	-0.821926	1.349736
C	-5.129081	-0.339024	-1.026154
H	-4.810328	0.687456	-2.901449
H	-5.130722	-1.304666	0.905408
H	-6.178390	-0.562396	-1.231741
C	-0.762523	2.217229	0.131791
C	-0.195267	3.125942	-0.775784
C	-1.281512	2.752913	1.323589
C	-0.141675	4.498388	-0.512389
H	0.232483	2.734223	-1.703507
C	-1.228333	4.119492	1.605633
H	-1.733898	2.076491	2.057448
C	-0.657365	5.001512	0.683331
H	0.307561	5.180195	-1.239258
H	-1.632002	4.503104	2.546263
H	-0.614851	6.071814	0.896699
B	-0.841999	0.605164	-0.181498
C	0.567907	-2.119825	-1.329269
C	-0.774228	-2.517873	-0.849335
H	0.583090	-2.122366	-2.431271
H	-1.677164	-2.250052	-1.395464
C	-0.927143	-3.250080	0.392122
O	-0.015891	-3.606415	1.116130
O	-2.213630	-3.525999	0.672852
C	-2.456925	-4.183798	1.903583
H	-2.122190	-3.567556	2.750997
H	-3.539487	-4.341052	1.964079
H	-1.935938	-5.150964	1.945572
H	1.316771	-2.834728	-0.965754

Ir(II)

M06-2X SCF energy: -2939.60353188 a.u.
M06-2X enthalpy: -2938.866849 a.u.
M06-2X free energy: -2939.007519 a.u.
M06-2X SCF energy in solution: -2942.83258975 a.u.
M06-2X enthalpy in solution: -2942.095907 a.u.
M06-2X free energy in solution: -2942.236577 a.u.
Three lowest frequencies (cm-1): 12.2038 14.2031 18.3202

Cartesian coordinates

ATOM	X	Y	Z
Ir	2.030134	2.097225	0.435870
C	0.232309	-0.354577	0.500216
C	-0.158271	-1.727052	0.466800
C	0.769003	-2.744600	0.373253
C	2.144869	-2.378207	0.321282
C	2.476344	-1.034980	0.371083
H	-1.220019	-1.971053	0.509996

H	2.940691	-3.115438	0.244391
H	3.525663	-0.724298	0.338636
C	-0.685261	0.737921	0.571108
C	-2.103923	0.588284	0.626806
C	-2.947481	1.677933	0.698030
H	-2.524414	-0.417447	0.607413
C	-0.970948	3.067793	0.650358
C	-2.350010	2.971803	0.717718
H	-0.485366	4.049096	0.652325
H	-2.940113	3.883575	0.775544
N	-0.151017	2.015134	0.571326
N	1.581143	-0.046660	0.461213
C	1.025685	1.977728	-2.407089
C	3.349471	1.796744	-2.163049
C	1.119904	1.859164	-3.788118
H	0.063164	2.109069	-1.905797
C	3.497505	1.678361	-3.551552
C	2.376353	1.708177	-4.368767
H	4.484880	1.565514	-3.988369
H	2.482495	1.617996	-5.450628
C	4.004582	1.946148	0.192743
C	4.421723	1.788818	-1.159316
C	4.979796	1.949287	1.199030
C	5.785735	1.631728	-1.437912
C	6.316910	1.791188	0.860698
H	4.723651	2.068952	2.254069
C	6.754919	1.628309	-0.448970
H	7.808983	1.503661	-0.693479
N	2.107033	1.946102	-1.627614
C	1.982883	1.347403	3.359825
C	2.186126	3.641944	2.920528
C	2.003154	1.566221	4.728678
H	1.896275	0.344893	2.935614
C	2.212167	3.916053	4.297471
C	2.120794	2.873461	5.204263
H	2.304535	4.938566	4.650850
H	2.141113	3.075139	6.277418
C	2.233157	4.077705	0.513466
C	2.274258	4.619892	1.828859
C	2.313233	4.952513	-0.578066
C	2.383385	6.007640	1.988554
C	2.420741	6.318256	-0.355965
H	2.290548	4.593370	-1.609215
C	2.457329	6.880065	0.915516
H	2.539331	7.955258	1.069481
N	2.073680	2.357999	2.490504
C	-4.466510	1.476106	0.732616
C	0.305226	-4.205050	0.327818
C	-4.842381	0.570289	1.915430
H	-5.933737	0.427177	1.947336
H	-4.375006	-0.421600	1.830327

H	-4.526798	1.018007	2.870337
C	-4.913085	0.809870	-0.578279
H	-6.005146	0.666723	-0.578170
H	-4.649132	1.434668	-1.445601
H	-4.441372	-0.175219	-0.709534
C	-5.212091	2.804748	0.880680
H	-4.932362	3.327751	1.807620
H	-5.013786	3.477459	0.033109
H	-6.295449	2.615800	0.912568
C	-0.452276	-4.536888	1.623021
H	-1.337862	-3.895820	1.743408
H	-0.790305	-5.585009	1.605830
H	0.194433	-4.398858	2.503157
C	-0.632844	-4.405154	-0.872165
H	-0.119698	-4.164528	-1.815977
H	-0.966072	-5.453759	-0.920107
H	-1.527745	-3.769935	-0.797372
C	1.483915	-5.172153	0.188580
H	2.051685	-4.987948	-0.735878
H	2.177541	-5.096393	1.039417
H	1.108457	-6.205794	0.152396
C	1.887882	0.423842	5.695946
F	1.876836	-0.757814	5.081267
F	0.767984	0.507446	6.421096
F	2.903986	0.415446	6.563964
F	2.415207	6.545585	3.212502
F	2.492000	7.140456	-1.405898
F	7.233002	1.793665	1.832071
F	6.201972	1.472333	-2.699339
C	-0.138953	1.865814	-4.607924
F	-0.825332	0.727090	-4.468901
F	0.119599	2.014714	-5.906563
F	-0.959897	2.854083	-4.242489

Ir(III)
M06-2X SCF energy: -2939.50745014 a.u.
M06-2X enthalpy: -2938.767479 a.u.
M06-2X free energy: -2938.907974 a.u.
M06-2X SCF energy in solution: -2942.73480865 a.u.
M06-2X enthalpy in solution: -2941.994838 a.u.
M06-2X free energy in solution: -2942.135333 a.u.
Three lowest frequencies (cm-1): 7.8545 12.9172 16.3036

Cartesian coordinates

ATOM	X	Y	Z
Ir	2.033061	2.096327	0.390862
C	0.222929	-0.390026	0.457884
C	-0.196398	-1.714768	0.387654
C	0.736191	-2.753409	0.253557

C	2.084252	-2.389899	0.206646
C	2.435574	-1.045684	0.287373
H	-1.260022	-1.946460	0.424067
H	2.877164	-3.128566	0.102986
H	3.483794	-0.738042	0.250564
C	-0.728180	0.752596	0.576690
C	-2.099119	0.578347	0.741278
C	-2.953314	1.686628	0.835054
H	-2.509468	-0.428845	0.803648
C	-0.982450	3.052489	0.596879
C	-2.360890	2.949484	0.757091
H	-0.496131	4.029439	0.535021
H	-2.946609	3.865061	0.817255
N	-0.187108	1.986368	0.508963
N	1.532957	-0.072153	0.408520
C	1.149359	1.933744	-2.494535
C	3.459598	1.750891	-2.145609
C	1.304006	1.796191	-3.867803
H	0.164110	2.074293	-2.043166
C	3.668667	1.609465	-3.523760
C	2.584244	1.630620	-4.389534
H	4.673686	1.487427	-3.915827
H	2.737290	1.524337	-5.464309
C	4.007850	1.946444	0.232763
C	4.484309	1.761818	-1.094461
C	4.928878	1.965325	1.286202
C	5.859610	1.595989	-1.303651
C	6.280447	1.795856	1.014661
H	4.622933	2.105248	2.324709
C	6.779591	1.607754	-0.268892
H	7.843756	1.475749	-0.460670
N	2.194882	1.907990	-1.667335
C	1.891002	1.411085	3.335891
C	2.114954	3.692376	2.849626
C	1.866597	1.662611	4.702187
H	1.822524	0.393961	2.941946
C	2.097806	3.998310	4.216698
C	1.971037	2.977472	5.148054
H	2.186214	5.028137	4.549304
H	1.959527	3.204862	6.214733
C	2.252917	4.070921	0.436168
C	2.249457	4.641700	1.738061
C	2.374417	4.913277	-0.674646
C	2.364592	6.032079	1.866635
C	2.484152	6.284163	-0.482390
H	2.384008	4.530151	-1.696710
C	2.482824	6.876099	0.775030
H	2.569688	7.954130	0.904980
N	2.007387	2.396852	2.445394
C	-4.454484	1.476986	1.012648
C	0.252639	-4.197990	0.158238

C	-4.695860	0.683969	2.306927
H	-5.776464	0.533919	2.451477
H	-4.219775	-0.306721	2.270713
H	-4.303278	1.226454	3.180227
C	-4.985988	0.678232	-0.187505
H	-6.068205	0.514980	-0.072555
H	-4.817665	1.223330	-1.128549
H	-4.501728	-0.306140	-0.267326
C	-5.205680	2.806511	1.096127
H	-4.873748	3.408772	1.955214
H	-5.075371	3.403188	0.181094
H	-6.280210	2.608062	1.219469
C	-0.517377	-4.548158	1.441569
H	-1.390228	-3.893681	1.580387
H	-0.877541	-5.586473	1.384398
H	0.129710	-4.455815	2.326902
C	-0.683065	-4.327901	-1.054156
H	-0.158953	-4.065466	-1.985541
H	-1.035610	-5.366934	-1.137633
H	-1.566095	-3.678837	-0.959767
C	1.418085	-5.174917	-0.006664
H	1.992792	-4.969026	-0.922081
H	2.105966	-5.136711	0.851306
H	1.025501	-6.199635	-0.078401
C	1.705149	0.511444	5.655220
F	2.515494	-0.502930	5.340796
F	0.459988	0.025269	5.639290
F	1.973304	0.870242	6.909151
F	2.360021	6.598103	3.076458
F	2.596338	7.077509	-1.548772
F	7.146788	1.812446	2.028993
F	6.332361	1.413661	-2.540213
C	0.083422	1.797731	-4.744649
F	-0.601992	0.655112	-4.637126
F	0.401020	1.948881	-6.029072
F	-0.757014	2.781520	-4.415023

9
M06-2X SCF energy: -1443.31500078 a.u.
M06-2X enthalpy: -1442.796938 a.u.
M06-2X free energy: -1442.886358 a.u.
M06-2X SCF energy in solution: -1444.94591025 a.u.
M06-2X enthalpy in solution: -1444.427847 a.u.
M06-2X free energy in solution: -1444.517267 a.u.
Three lowest frequencies (cm-1): 30.1719 40.0180 40.8272

Cartesian coordinates

ATOM	X	Y	Z
C	3.228084	0.475628	0.500967

C	0.990466	-0.672313	0.611791
C	1.874247	0.439219	1.182106
H	3.729627	-0.502366	0.622444
H	1.309828	-1.614320	1.086460
H	1.401272	1.411813	0.968262
O	2.980447	0.717788	-0.879905
C	2.379720	-0.359076	-1.540965
H	2.194094	0.001430	-2.570186
O	3.239529	-1.460405	-1.567051
C	4.472035	-1.202175	-2.192835
H	5.103966	-0.525254	-1.594732
H	4.991795	-2.161938	-2.310276
H	4.326629	-0.749638	-3.190275
C	4.121835	1.580015	1.018454
H	3.634016	2.556645	0.876806
H	4.312359	1.434483	2.089744
H	5.081276	1.586069	0.481837
O	2.034877	0.267264	2.573828
H	1.142694	0.184743	2.938390
O	-0.360699	-0.418607	0.904150
C	1.023432	-0.780049	-0.933258
O	0.045820	0.143304	-1.341595
C	-2.432434	0.154141	-0.514943
C	-2.984719	0.443346	-1.774113
C	-3.310163	-0.336558	0.465201
C	-4.340673	0.250803	-2.050091
H	-2.328949	0.822485	-2.565020
C	-4.670459	-0.527792	0.207219
H	-2.908111	-0.595467	1.449113
C	-5.192636	-0.234513	-1.054573
H	-4.737221	0.479455	-3.042699
H	-5.328477	-0.914073	0.990229
H	-6.254410	-0.385417	-1.261767
C	-0.771645	2.062714	0.172513
C	-0.280706	3.009461	-0.740383
C	-1.222440	2.552508	1.411012
C	-0.232174	4.373889	-0.437393
H	0.092605	2.655440	-1.706228
C	-1.174145	3.910554	1.732266
H	-1.613481	1.845316	2.150962
C	-0.677780	4.831006	0.804384
H	0.159892	5.085052	-1.169283
H	-1.523919	4.257338	2.708124
H	-0.638927	5.894935	1.048311
B	-0.861078	0.459595	-0.196857
C	0.684045	-2.196545	-1.438440
C	-0.707700	-2.701186	-1.087963
H	0.774603	-2.175668	-2.536626
H	-0.954601	-3.575356	-1.715061
C	-0.855987	-3.177221	0.333288
O	0.034916	-3.580738	1.040385

O	-2.134542	-3.190326	0.716511
C	-2.383213	-3.570712	2.059588
H	-1.815913	-2.932323	2.751524
H	-3.458622	-3.443100	2.226603
H	-2.101289	-4.619173	2.233415
H	1.437917	-2.904398	-1.069716
H	-1.476817	-1.944333	-1.285252

Ph_2BOH

M06-2X SCF energy: -563.41414210 a.u.
M06-2X enthalpy: -563.198860 a.u.
M06-2X free energy: -563.249635 a.u.
M06-2X SCF energy in solution: -564.03553568 a.u.
M06-2X enthalpy in solution: -563.820254 a.u.
M06-2X free energy in solution: -563.871029 a.u.
Three lowest frequencies (cm-1): 39.8980 56.2649 79.8223

Cartesian coordinates

ATOM	X	Y	Z
B	-2.728184	-0.366802	0.861803
C	-3.666092	-1.518403	0.337934
C	-3.169563	-2.633254	-0.357929
C	-5.048428	-1.462568	0.589686
C	-4.018180	-3.654581	-0.787684
H	-2.098110	-2.712700	-0.558285
C	-5.904732	-2.472086	0.152704
H	-5.455399	-0.608590	1.136820
C	-5.388515	-3.571561	-0.537120
H	-3.610250	-4.516839	-1.318720
H	-6.976301	-2.406513	0.351499
H	-6.055975	-4.365916	-0.877464
C	-1.301362	-0.061083	0.261313
C	-1.029631	-0.199576	-1.110648
C	-0.264605	0.399135	1.092217
C	0.224301	0.115785	-1.634608
H	-1.816741	-0.548877	-1.783771
C	0.996658	0.700158	0.578910
H	-0.437882	0.515383	2.166528
C	1.241278	0.561384	-0.788452
H	0.410751	0.011913	-2.705276
H	1.789977	1.045500	1.244642
H	2.225877	0.800977	-1.195232
O	-3.212762	0.379171	1.889433
H	-2.626938	1.104563	2.148030

TS7a

M06-2X SCF energy: -1443.25001768 a.u.

M06-2X enthalpy: -1442.733903 a.u.
M06-2X free energy: -1442.820436 a.u.
M06-2X SCF energy in solution: -1444.88535043 a.u.
M06-2X enthalpy in solution: -1444.369236 a.u.
M06-2X free energy in solution: -1444.455769 a.u.
Three lowest frequencies (cm-1): -89.6962 32.8300 37.7470
Imaginary frequency: -89.6962 cm-1

Cartesian coordinates

ATOM	X	Y	Z
C	-3.242405	1.093907	-0.685200
C	-1.140687	-0.055904	-1.360485
C	-1.775049	1.290534	-1.029331
H	-3.754992	0.593409	-1.527252
H	-1.601184	-0.417572	-2.295332
H	-1.312480	1.694992	-0.116492
O	-3.291051	0.263470	0.466643
C	-2.819926	-1.039865	0.257498
H	-2.872654	-1.517029	1.252082
O	-3.628395	-1.718798	-0.657491
C	-4.966844	-1.853286	-0.244697
H	-5.471787	-0.876999	-0.162825
H	-5.487210	-2.462550	-0.994601
H	-5.030554	-2.359661	0.735126
C	-3.942309	2.393310	-0.356765
H	-3.438958	2.892624	0.485306
H	-3.919319	3.062571	-1.226510
H	-4.989227	2.204305	-0.080202
O	-1.648265	2.186386	-2.106118
H	-0.703776	2.276837	-2.293589
O	0.246516	0.044614	-1.597427
C	-1.351282	-1.092642	-0.239845
O	-0.482234	-0.776692	0.798733
C	2.611002	-0.133983	-0.837191
C	3.730649	0.441290	-0.217232
C	2.826268	-1.240796	-1.674471
C	5.016217	-0.068223	-0.416061
H	3.597130	1.304583	0.440786
C	4.102724	-1.762497	-1.875916
H	1.966918	-1.697642	-2.171309
C	5.203317	-1.175024	-1.244375
H	5.872286	0.397165	0.076979
H	4.246596	-2.626877	-2.527812
H	6.205442	-1.580557	-1.400220
C	0.993794	1.752937	0.259616
C	0.685223	1.799027	1.628983
C	1.261438	2.969134	-0.392304
C	0.635859	3.014850	2.312669
H	0.440184	0.866781	2.141512
C	1.202464	4.189970	0.284779
H	1.524496	2.968020	-1.456227

C	0.889571	4.215222	1.643565
H	0.389143	3.028557	3.376829
H	1.404775	5.121048	-0.249151
H	0.843487	5.164880	2.180570
B	1.145365	0.441635	-0.634038
C	-0.976433	-2.522627	-0.660486
C	-0.728572	-3.184782	0.683854
H	-1.750907	-2.997686	-1.274401
H	-0.118850	-4.096211	0.622789
C	0.012233	-2.138933	1.553830
O	-0.193849	-2.059285	2.783670
O	1.380439	-2.215465	1.128589
C	2.301333	-1.650379	2.010352
H	2.219133	-2.085640	3.019977
H	3.307341	-1.846015	1.608591
H	2.181258	-0.555140	2.107177
H	-0.036299	-2.474826	-1.229858
H	-1.673599	-3.430805	1.190735

TS7b

M06-2X SCF energy: -2006.72480389 a.u.
M06-2X enthalpy: -2005.991838 a.u.
M06-2X free energy: -2006.107204 a.u.
M06-2X SCF energy in solution: -2008.96746012 a.u.
M06-2X enthalpy in solution: -2008.234494 a.u.
M06-2X free energy in solution: -2008.349860 a.u.
Three lowest frequencies (cm-1): -136.6936 16.0259 26.4119
Imaginary frequency: -136.6936 cm-1

Cartesian coordinates

ATOM	X	Y	Z
C	1.427655	3.743129	0.618592
C	2.442863	1.964000	-0.834730
C	2.582406	2.773108	0.456523
H	1.374819	4.407455	-0.262547
H	2.770720	2.620489	-1.661098
H	2.526047	2.079433	1.313116
O	0.248201	2.947289	0.686817
C	-0.098691	2.338729	-0.522220
H	-0.966940	1.706421	-0.278296
O	-0.440103	3.289140	-1.485127
C	-1.649518	3.956302	-1.201646
H	-1.799071	4.718834	-1.976619
H	-2.498394	3.250579	-1.221947
H	-1.616242	4.448462	-0.216096
C	1.517111	4.567779	1.882147
H	1.536311	3.908484	2.763207
H	2.436947	5.166887	1.871749
H	0.653013	5.242042	1.964883

O	3.807719	3.466496	0.458173
H	4.499021	2.808093	0.301498
O	3.239201	0.817883	-0.786308
C	1.020475	1.450217	-1.113724
O	0.993972	0.163125	-0.494829
C	2.986446	-1.672293	-0.894851
C	3.154295	-2.880760	-0.202258
C	3.371389	-1.664648	-2.247113
C	3.649952	-4.031625	-0.824267
H	2.890708	-2.931725	0.858601
C	3.858984	-2.804449	-2.886120
H	3.299977	-0.729130	-2.808163
C	3.997623	-3.999372	-2.174270
H	3.766649	-4.955370	-0.252549
H	4.142709	-2.762912	-3.940627
H	4.385823	-4.893781	-2.666532
C	2.555128	-0.396545	1.440216
C	1.406125	-0.540808	2.233013
C	3.793715	-0.386073	2.103764
C	1.483674	-0.669926	3.623619
H	0.428005	-0.536644	1.739960
C	3.885360	-0.505207	3.491527
H	4.713427	-0.276330	1.518801
C	2.726017	-0.650235	4.258963
H	0.570447	-0.780508	4.213934
H	4.862376	-0.485625	3.980557
H	2.792380	-0.745068	5.344956
B	2.480411	-0.290999	-0.183370
C	0.739368	1.125817	-2.577974
C	-0.495930	0.233933	-2.512309
H	0.573979	2.021687	-3.185357
H	-0.634897	-0.376240	-3.412230
C	-0.377235	-0.718941	-1.324201
O	-1.250009	-0.727391	-0.373441
O	0.157764	-1.885454	-1.670089
C	0.018042	-2.964151	-0.752592
H	0.627369	-3.782320	-1.150709
H	0.377484	-2.685445	0.247905
H	-1.033974	-3.277328	-0.687792
H	1.599291	0.567475	-2.975187
H	-1.402904	0.835969	-2.367154
B	-2.797638	-0.900480	-0.656560
C	-3.517486	0.531851	-0.365642
C	-4.449967	1.078498	-1.259740
C	-3.291187	1.236846	0.830593
C	-5.131702	2.267892	-0.977527
H	-4.643676	0.552426	-2.198628
C	-3.964126	2.422433	1.126658
H	-2.564178	0.844690	1.550459
C	-4.893323	2.942650	0.220010
H	-5.853447	2.668753	-1.693707

H	-3.765966	2.946549	2.064802
H	-5.426096	3.868673	0.446906
C	-3.300901	-2.017130	0.420484
C	-4.479246	-2.740037	0.169446
C	-2.633899	-2.285567	1.627702
C	-4.973627	-3.684259	1.073041
H	-5.022237	-2.561758	-0.764582
C	-3.117226	-3.226114	2.540871
H	-1.704142	-1.752109	1.847315
C	-4.292166	-3.930061	2.266338
H	-5.891217	-4.232460	0.846102
H	-2.574209	-3.416025	3.469932
H	-4.672642	-4.667146	2.976794
O	-3.006575	-1.296378	-2.028348
H	-2.874890	-2.245639	-2.130725

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M06-2X SCF energy: -2006.72825251 a.u.
M06-2X enthalpy: -2005.992916 a.u.
M06-2X free energy: -2006.114919 a.u.
M06-2X SCF energy in solution: -2008.97450414 a.u.
M06-2X enthalpy in solution: -2008.239168 a.u.
M06-2X free energy in solution: -2008.361171 a.u.
Three lowest frequencies (cm-1): 5.7352 16.0008 19.5410

Cartesian coordinates

ATOM	X	Y	Z
C	1.492867	2.913662	0.901026
C	1.891035	0.569303	0.162546
C	2.053090	1.553858	1.314251
H	2.100975	3.280933	0.053345
H	2.466034	0.952085	-0.694311
H	1.470214	1.180662	2.175041
O	0.140246	2.767877	0.489977
C	-0.065866	1.891341	-0.581754
H	-1.161072	1.873273	-0.727978
O	0.582129	2.319725	-1.737826
C	0.094841	3.547779	-2.229840
H	0.629136	3.770029	-3.161726
H	-0.987502	3.485557	-2.439692
H	0.264563	4.366826	-1.512611
C	1.525601	3.920295	2.028927
H	0.897269	3.572295	2.862238
H	2.555122	4.044684	2.388241
H	1.147481	4.893038	1.684785
O	3.412851	1.715740	1.639974
H	3.706714	0.927387	2.114886
O	2.384101	-0.686438	0.577258
C	0.426919	0.468851	-0.249667

O	-0.323373	-0.011787	0.847538
C	4.397882	-0.760705	-1.047149
C	5.784201	-0.578667	-0.909499
C	3.823768	-0.500092	-2.303507
C	6.565900	-0.136035	-1.977691
H	6.262570	-0.783220	0.052474
C	4.601959	-0.076720	-3.380958
H	2.748580	-0.636679	-2.447563
C	5.975353	0.111841	-3.217732
H	7.639708	0.009606	-1.844393
H	4.134492	0.108369	-4.350074
H	6.586050	0.448195	-4.057954
C	3.938507	-2.567800	0.986357
C	3.319199	-2.836878	2.220476
C	4.890684	-3.487022	0.514629
C	3.639193	-3.975761	2.957690
H	2.575990	-2.134024	2.605265
C	5.212061	-4.633347	1.243447
H	5.384292	-3.310221	-0.444618
C	4.587318	-4.877410	2.467295
H	3.149878	-4.163912	3.915495
H	5.949751	-5.338833	0.856003
H	4.838439	-5.772177	3.040745
B	3.533848	-1.282408	0.166608
C	0.144956	-0.521576	-1.379734
C	-1.307371	-0.900618	-1.110838
H	0.314775	-0.071161	-2.365723
H	-1.574111	-1.922197	-1.404950
C	-1.494481	-0.694149	0.417749
O	-2.574014	0.031012	0.771575
O	-1.547355	-1.909287	1.141330
C	-0.458520	-2.783062	0.967926
H	-0.555042	-3.580443	1.717438
H	-0.455980	-3.253962	-0.031736
H	0.501345	-2.264713	1.119543
H	0.810334	-1.390463	-1.264822
H	-1.996359	-0.218628	-1.625099
B	-3.959196	-0.316508	0.281194
C	-4.356786	0.653371	-0.984512
C	-4.962133	0.151556	-2.147587
C	-4.110505	2.037574	-0.948308
C	-5.307894	0.980402	-3.220572
H	-5.153214	-0.923708	-2.210560
C	-4.444928	2.878842	-2.012359
H	-3.637224	2.467447	-0.058483
C	-5.049001	2.350462	-3.157249
H	-5.776834	0.556290	-4.112279
H	-4.235676	3.950126	-1.952697
H	-5.314772	3.002225	-3.992448
C	-4.976213	0.008079	1.539658
C	-6.364552	-0.168211	1.393102

C	-4.529501	0.439843	2.798326
C	-7.259391	0.065400	2.438357
H	-6.757148	-0.501320	0.425568
C	-5.412587	0.683981	3.856402
H	-3.455338	0.582602	2.943923
C	-6.784012	0.496553	3.680944
H	-8.331587	-0.085343	2.288448
H	-5.030082	1.021525	4.823381
H	-7.478751	0.684444	4.502578
O	-4.052965	-1.706407	-0.159226
H	-3.551490	-2.243555	0.465965

TS8

M06-2X SCF energy: -2006.73935640 a.u.
M06-2X enthalpy: -2006.005572 a.u.
M06-2X free energy: -2006.119735 a.u.
M06-2X SCF energy in solution: -2008.97942363 a.u.
M06-2X enthalpy in solution: -2008.245639 a.u.
M06-2X free energy in solution: -2008.359802 a.u.
Three lowest frequencies (cm-1): -175.0699 14.0346 26.3619
Imaginary frequency: -175.0699 cm-1

Cartesian coordinates

ATOM	X	Y	Z
C	0.516276	3.580176	1.067877
C	1.542409	1.924378	-0.500265
C	1.343154	2.294266	0.971970
H	1.103987	4.385967	0.590487
H	2.041812	2.791434	-0.969531
H	0.781023	1.487201	1.478035
O	-0.721606	3.431476	0.380494
C	-0.609556	3.118572	-0.974918
H	-1.648139	2.979982	-1.329427
O	0.038828	4.106070	-1.705742
C	-0.647855	5.337997	-1.729804
H	-1.655561	5.219227	-2.164481
H	-0.748875	5.764123	-0.719151
H	-0.065967	6.026607	-2.354320
C	0.198624	3.955818	2.497732
H	-0.368993	4.896424	2.530224
H	-0.403636	3.165153	2.970452
H	1.129518	4.079245	3.065332
O	2.566709	2.543461	1.611832
H	3.056511	1.709468	1.629990
O	2.337557	0.813420	-0.758628
C	0.174506	1.822965	-1.180407
O	-0.613723	0.811687	-0.527162
C	3.354160	-1.423229	-1.092097
C	3.956707	-2.609519	-0.638313

C	3.641098	-1.043537	-2.414518
C	4.780864	-3.386315	-1.456792
H	3.785155	-2.938396	0.391833
C	4.464142	-1.807703	-3.246908
H	3.210354	-0.112168	-2.792600
C	5.036092	-2.988298	-2.770288
H	5.228463	-4.303807	-1.067227
H	4.664005	-1.480006	-4.270117
H	5.680255	-3.590795	-3.414527
C	2.777792	-0.539500	1.417407
C	4.114879	-0.300568	1.783603
C	1.854891	-0.710111	2.463696
C	4.511962	-0.205812	3.120899
H	4.867581	-0.171914	0.998277
C	2.239006	-0.625091	3.804219
H	0.804928	-0.901781	2.215123
C	3.570403	-0.368391	4.138786
H	5.557471	-0.008495	3.369273
H	1.495897	-0.757530	4.594323
H	3.872542	-0.297747	5.185836
B	2.334135	-0.524286	-0.164338
C	0.252038	1.359988	-2.640603
C	0.034690	-0.156963	-2.562884
H	-0.551278	1.839335	-3.217514
H	0.962775	-0.728754	-2.665256
C	-0.554575	-0.349273	-1.177931
O	-1.465010	-1.200821	-0.958677
O	0.914541	-1.110026	-0.242418
C	0.766508	-2.488623	-0.023088
H	0.942307	-3.071134	-0.946016
H	1.483009	-2.830246	0.739946
H	-0.246907	-2.692287	0.348150
H	1.214322	1.632797	-3.088349
H	-0.693705	-0.526235	-3.295529
B	-2.392652	-1.099138	0.327418
C	-3.130579	-2.541462	0.424250
C	-3.800276	-2.895988	1.608362
C	-3.175583	-3.463233	-0.633474
C	-4.481029	-4.107956	1.735532
H	-3.781453	-2.203738	2.455754
C	-3.852886	-4.681426	-0.519151
H	-2.656077	-3.227476	-1.566136
C	-4.510942	-5.007907	0.667102
H	-4.990850	-4.354791	2.669943
H	-3.865041	-5.380238	-1.359086
H	-5.040823	-5.958261	0.761255
C	-3.453569	0.103642	0.008960
C	-3.829700	1.006317	1.015213
C	-4.041831	0.279174	-1.255651
C	-4.740301	2.040438	0.778545
H	-3.387057	0.902816	2.010806

C	-4.951349	1.308438	-1.507818
H	-3.776004	-0.403780	-2.069293
C	-5.305271	2.196124	-0.487878
H	-5.007925	2.728776	1.583928
H	-5.388756	1.421514	-2.502897
H	-6.016716	3.002139	-0.679690
O	-1.599032	-0.866001	1.505846
H	-1.231078	0.026018	1.474232

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M06-2X SCF energy: -1443.31167023 a.u.
M06-2X enthalpy: -1442.794414 a.u.
M06-2X free energy: -1442.882399 a.u.
M06-2X SCF energy in solution: -1444.94241078 a.u.
M06-2X enthalpy in solution: -1444.425155 a.u.
M06-2X free energy in solution: -1444.513140 a.u.
Three lowest frequencies (cm-1): 26.3051 41.5188 45.5629

Cartesian coordinates

ATOM	X	Y	Z
C	2.429927	3.236452	1.267616
C	2.071401	1.491656	-0.500558
C	2.557141	1.746699	0.927907
H	3.150371	3.766492	0.617016
H	2.686938	2.154659	-1.138486
H	1.937071	1.155842	1.629543
O	1.121189	3.728093	1.014279
C	0.664391	3.544365	-0.292742
H	-0.373272	3.926741	-0.292885
O	1.435543	4.220344	-1.231786
C	1.389802	5.622197	-1.095379
H	2.003903	6.054068	-1.895142
H	0.355417	5.995995	-1.193850
H	1.787484	5.946814	-0.120494
C	2.748571	3.523367	2.718533
H	2.011461	3.030401	3.369886
H	3.747970	3.139891	2.960175
H	2.722667	4.604642	2.914254
O	3.924969	1.447673	1.063932
H	4.037679	0.511758	0.849830
O	2.250838	0.205122	-0.989329
C	0.649213	2.060436	-0.668486
O	-0.291956	1.476719	0.245909
C	2.089013	-2.214013	-1.574923
C	2.258414	-3.591135	-1.341501
C	1.949079	-1.825071	-2.917729
C	2.273766	-4.528385	-2.377049
H	2.391058	-3.945576	-0.313330
C	1.966595	-2.748041	-3.968601

H	1.834513	-0.759386	-3.135042
C	2.126584	-4.108415	-3.701384
H	2.405984	-5.590014	-2.153715
H	1.859294	-2.405164	-5.000920
H	2.142614	-4.835123	-4.516652
C	3.199958	-1.470222	0.770522
C	2.943118	-1.463931	2.151687
C	4.529157	-1.721726	0.381941
C	3.948664	-1.683541	3.097390
H	1.921627	-1.263446	2.490275
C	5.550073	-1.931665	1.313492
H	4.775444	-1.740907	-0.685523
C	5.260737	-1.913870	2.680110
H	3.712387	-1.667747	4.164329
H	6.573690	-2.111540	0.975776
H	6.052775	-2.077305	3.414103
B	2.023787	-1.112078	-0.343103
C	0.065280	1.786061	-2.062140
C	-0.775533	0.535314	-1.833523
H	-0.569252	2.631168	-2.368979
H	-0.184493	-0.383246	-1.962232
C	-1.122004	0.613725	-0.363316
O	-2.022253	0.075109	0.219135
O	0.708328	-1.093953	0.318649
C	0.082520	-2.275291	0.675784
H	-0.264308	-2.861666	-0.199972
H	0.731212	-2.950182	1.272095
H	-0.806175	-2.045165	1.286932
H	0.857627	1.654972	-2.808500
H	-1.689273	0.470251	-2.436281

MeOH

M06-2X SCF energy: -115.57616231 a.u.
M06-2X enthalpy: -115.520287 a.u.
M06-2X free energy: -115.547192 a.u.
M06-2X SCF energy in solution: -115.72041131 a.u.
M06-2X enthalpy in solution: -115.664536 a.u.
M06-2X free energy in solution: -115.691441 a.u.
Three lowest frequencies (cm-1): 365.2264 1077.0690 1107.3165

Cartesian coordinates

ATOM	X	Y	Z
C	-0.957372	0.588603	-0.027019
H	-0.591762	1.105214	0.872076
H	-0.602055	1.154750	-0.906813
H	-2.061161	0.635781	-0.014580
O	-0.471483	-0.729214	0.002231
H	-0.801965	-1.179429	-0.784940