Electronic Supplementary Information

Computational insights into strain-increase allylborations for alkylidenecyclopropanes

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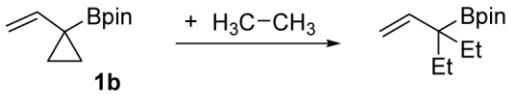
Computational Details

The M06-2X functional with dispersion corrections (D3)[1] and the def2-SVP basis set were used for geometry optimizations for all intermediates and transition states. All minima have zero imaginary frequency and all transition states have only one imaginary frequency and were confirmed by intrinsic reaction coordinate (IRC) calculations. Single-point energies were calculated by using M06-2X with dispersion corrections (D3) and the def2-TZVP basis set. Solvation energy corrections were calculated using the SMD model[2] with THF as solvent. All these calculations were carried out with Gaussian 09.[3]

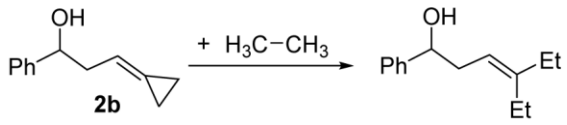
Energy decomposition analysis (EDA) calculations at the M06-2X-D3/def2-TZVP level of theory were performed by using the second-generation EDA based on absolutely localized orbitals (ALMO-EDA2) implemented in Q-Chem 5.2.[4] The complementary occupied-virtual pairs (COVPs) were computed to figure out the direction of charge transfer and the most significant orbitals. Mostly, the targeted C–C bonds in different allylboration transition states have different bond distances. To minimize the effect of early or late transition states in comparing each energy term among these transition states, we performed EDA calculations along the reaction coordinates obtained from IRC calculations. The reported energies in the bar charts are the average of $\Delta\Delta\Delta E$ values at the region of C–C bond distances that correspond to the allylboration transition states. The geometries and molecular orbitals were visualized using CYLview[5] and IQmol, respectively. The NBO donor-acceptor interactions were analyzed by using NBOPro.[6]

Ring Strain Energy

We computed the ring strain energies of allylboronate **1b** and alkylidenecyclopropane **2b** based on the homodesmotic reactions shown in Fig. S1. The much larger ring strain of **2b** than **1b** indicates the allylboration of **1b** with benzaldehyde to generate **2b** suffers from a great strain increase.



ring strain energy of **1b**: ΔH_{strain} = 19.5 kcal/mol



ring strain energy of **2b**: ΔH_{strain} = 36.9 kcal/mol

Fig. S1. Computed ring strain energies of **1b** and **2b**.

Energy Profiles with Different Allylboronates

The energy profiles of allylborations with allylboronates **1a**, **1b** and **1d** are shown in Fig. S2. The results show that **TS1**~**TS3** require barriers of 21.2, 27.3 and 15.9 kcal/mol with respect to the separated allylboronates and benzaldehyde, respectively. The barrier trend is consistent with the relative barriers of **TS1**~**TS3** with respect to the complexes of allylboronates with benzaldehyde (**IM1**~**IM2**), which are 12.3, 19.5 and 9.8 kcal/mol, respectively.

In addition, although the allylborations with **1b** and **1d** to form **IM2a** and **IM3a** intermediates are strain-increase processes, the reactions are thermodynamically favorable and exothermic by 13.8 and 16.8 kcal/mol, respectively. This indicates that the increased strain energy can be overcome by forming C−C and B−O bonds. In contrast, the unstrained allyboration with **1a** is much more thermodynamically favorable, which is exothermic by 28.7 kcal/mol.

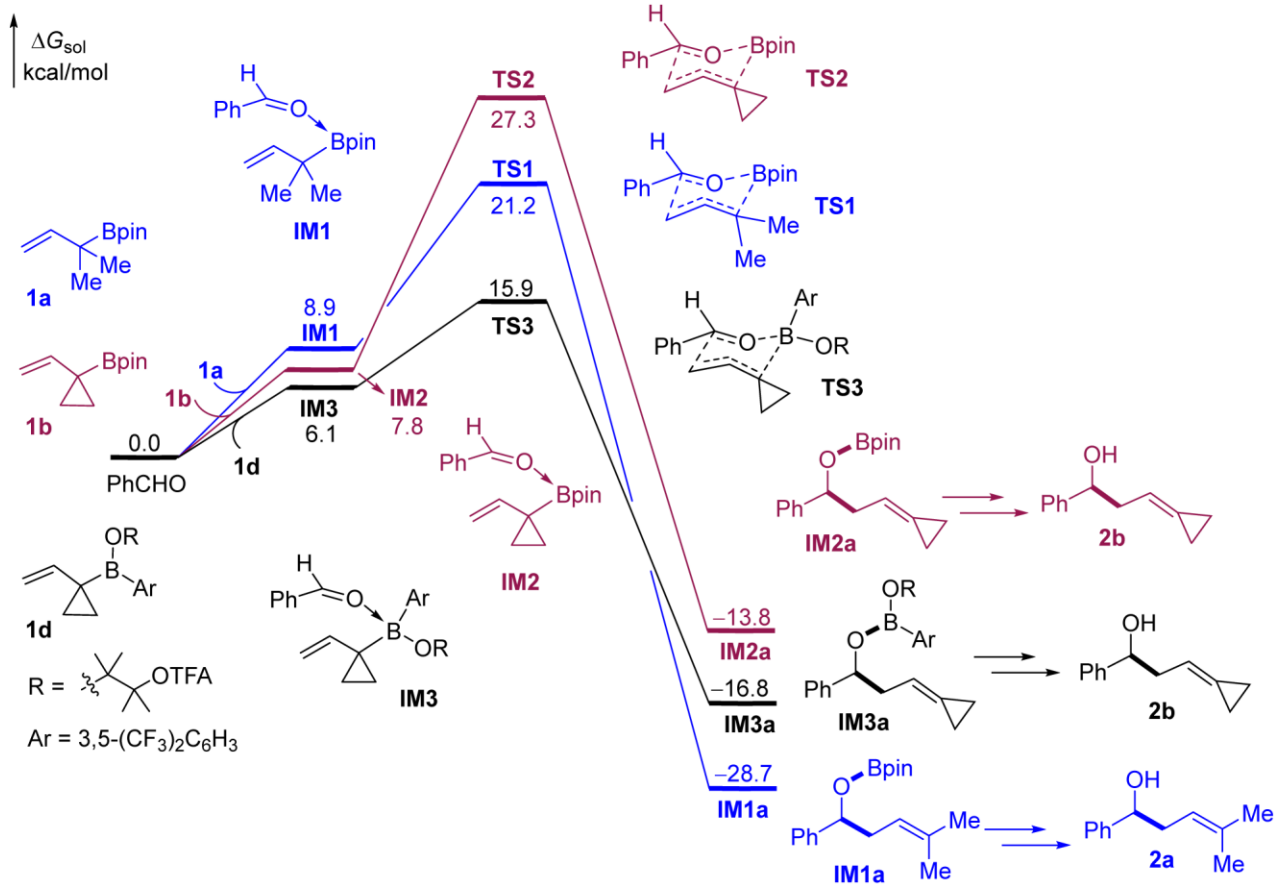


Fig. S2. Energy profiles for allylborations with substrates **1a, 1b** and **1d**.

Orbital Interactions

Fig. S3 shows the cyclopropyl "quasi π" orbital and the olefin π* orbital. These two orbitals are nearly perpendicular to each other, which leads to ineffective orbital overlaps. Thus, it is less possible for the electron donation from cyclopropyl to olefin in **TS2**.

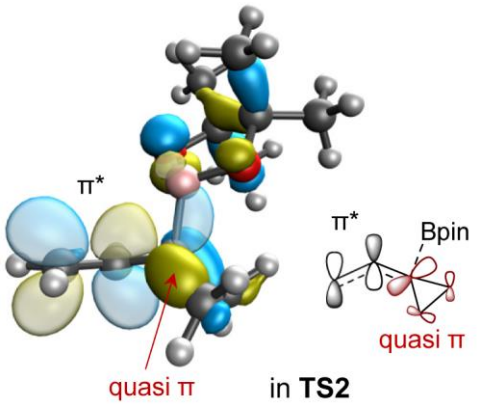


Fig. S3. The cyclopropyl "quasi π" and olefin π* orbitals.

To further understand the effects of cyclopropyl and dimethyl substituents on the reactivity of allylborations, we analyzed donor-acceptor interactions based on natural bond orbitals for **TS1** and **TS2**. As shown in Fig. S4, the donor-acceptor interaction from σ(C–B) to π*(C=C) in **TS1** (ΔE = 19.0 kcal/mol) is much stronger than that in **TS2** (ΔE = 11.6 kcal/mol). This is mostly due to the more effective orbital overlap in **TS1** with a smaller ∠BCC (100.2°) than that in **TS2** with a larger ∠BCC (104.8°). In addition, the cyclopropyl σ*(C–C) in **TS2** (ΔE = 4.1 and 1.2 kcal/mol) is a better electron acceptor than the dimethyl σ*(C–C) in **TS1** (ΔE = 0.7 and 1.9 kcal/mol). Therefore, compared with **TS1** with dimethyl substituents, the weaker σ(C–B)→π*(C=C) and stronger π(C=C)→σ*(C–C) interactions in **TS2** with cyclopropyl group result in much weaker nucleophilicity of the double bond toward aldehyde.

We further computed the allylboration transition state (**TS4**, Fig. S4) with Me and CF_3. Indeed, due to the electron-withdrawing property of CF_3, the barrier of **TS4** is 2.2 kcal/mol higher than that of **TS1** with dimethyl group. Nevertheless, **TS4** is more favorable than **TS2** with cyclopropyl group. This can be ascribed to the donor-acceptor interactions based on the results of NBO analysis. As shown Fig. S4, the barrier trend of these transition states is consistent with the strength of σ(C–B)→π*(C=C) orbital interactions.

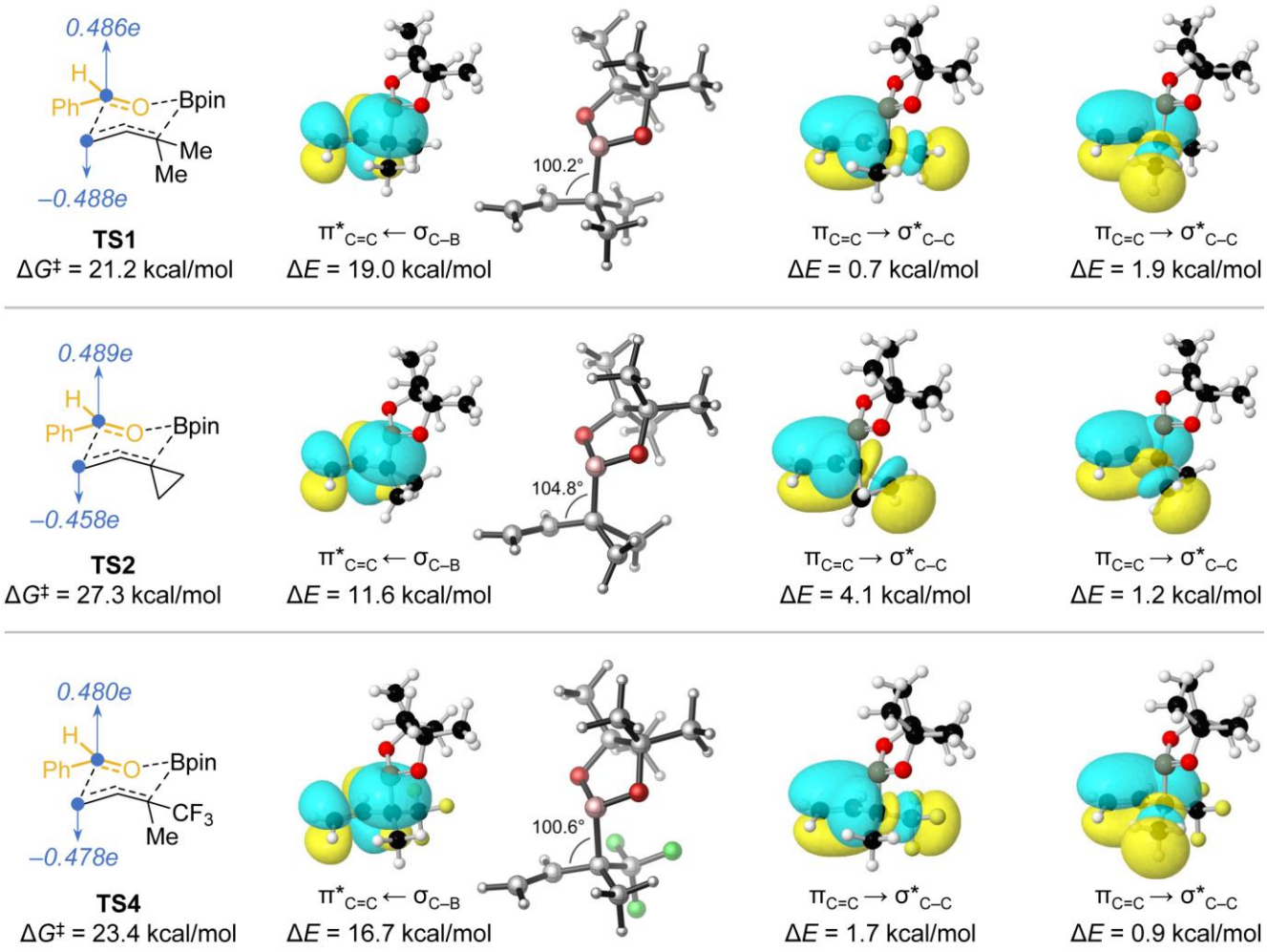


Fig. S4. NBO donor-acceptor interactions in **TS1**, **TS2** and **TS4**.

Allylboration with Ketone

The Aggarwal's experiment shows the allylboration cannot be applied for ketone even with more acidic vinylcyclopropyl boronates. The computed barrier for the allylboration with ketone (**TS5**, $\Delta G^{\ddagger}$ = 24.5 kcal/mol, Fig. S5) is much higher than that with aldehyde (**TS3**, $\Delta G^{\ddagger}$ = 15.9 kcal/mol), which is in line with the experimental result. The interaction of acetophenone with acidic boron center is weaker than that of benzaldehyde, which is evidenced by the higher energy of **IM5** and the longer B···O distance (1.73 Å) in **IM5** than that in **IM3** (1.68 Å). Thus, compared with **IM3** (ΔE_{Pauli} = 124.0 kcal/mol), **IM5** sustains smaller lp)(lp repulsion in advance (ΔE_{Pauli} = 109.2 kcal/mol). The ensuing **TS5** suffers from the rest of lp)(lp repulsion as well as π)(π repulsion (ΔE_{Pauli} = 269.7 kcal/mol), which is more repulsive than that in **TS3** (ΔE_{Pauli} = 254.7 kcal/mol). In addition, the larger deformation of acetophenone than benzaldehyde leads to greater distortion energy in **TS5** (ΔE_{dist} = 66.5 kcal/mol) than that in **TS3** (ΔE_{dist} = 54.8 kcal/mol). Taken together, the low reactivity with ketone can be ascribed to the relatively weak O(ketone)→B interaction and large geometric deformations.

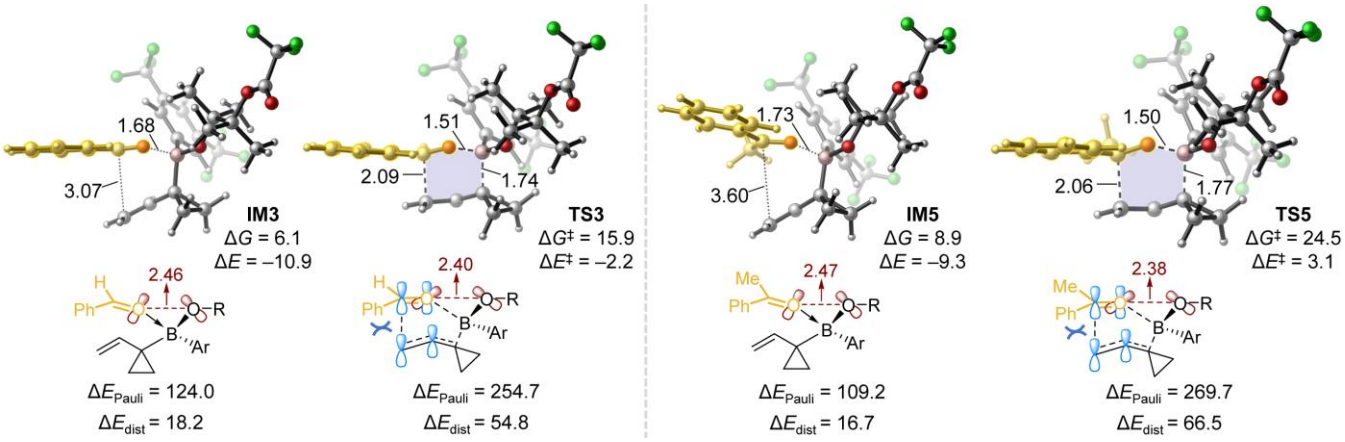


Fig. S5. Comparison of allylborations with aldehyde and ketone.

Energy Terms of EDA along IRC

Table S1. EDA energy terms of TS1 along IRC

Energy terms (in kcal/mol) / *r*(C-C) in **TS1** (in Å)	**Steric effect:** ΔE_{steric}		**Electronic effects:** ΔE_{elec}			**Dispersion effect:** ΔE_{disp}
	ΔE_{dist}	ΔE_{Pauli}	ΔE_{elstat}	ΔE_{oi}		
				ΔE_{ct}	ΔE_{pol}	
2.47	28.86	181.37	-97.570	-45.19	-43.45	-23.91
2.43	31.46	190.63	-102.21	-48.68	-46.31	-24.39
2.38	34.45	200.56	-107.22	-52.71	-49.38	-24.89
2.34	38.01	211.33	-112.68	-57.43	-52.78	-25.39
2.28 (TS)	42.23	222.97	-118.59	-62.93	-56.55	-25.92
2.23	46.84	235.57	-124.95	-69.09	-60.67	-26.46
2.19	52.15	249.12	-131.81	-76.08	-65.27	-27.02
2.14	58.24	263.64	-139.20	-83.99	-70.40	-27.60
2.04	72.62	296.06	-155.75	-102.43	-82.75	-28.83

Table S2. EDA energy terms of IM1

Energy terms (in kcal/mol) / *r*(C-C) in **IM1** (in Å)	**Steric effect:** ΔE_{steric}		**Electronic effects:** ΔE_{elec}			**Dispersion effect:** ΔE_{disp}
	ΔE_{dist}	ΔE_{Pauli}	ΔE_{elstat}	ΔE_{oi}		
				ΔE_{ct}	ΔE_{pol}	
3.13	1.0	19.8	-10.9	-2.9	-2.1	-13.4

Table S3. EDA energy terms of TS2 along IRC

Energy terms (in kcal/mol) / *r*(C-C) in **TS2** (in Å)	**Steric effect:** ΔE_{steric}		**Electronic effects:** ΔE_{elec}			**Dispersion effect:** ΔE_{disp}
	ΔE_{dist}	ΔE_{Pauli}	ΔE_{elstat}	ΔE_{oi}		
				ΔE_{ct}	ΔE_{pol}	
2.49	29.53	171.92	-92.17	-42.48	-40.46	-22.33
2.44	31.70	180.73	-96.51	-45.45	-42.92	-22.85
2.39	34.55	190.72	-101.46	-49.19	-45.82	-23.39
2.33	37.79	201.47	-106.73	-53.53	-48.97	-23.94
2.28	41.70	213.39	-112.62	-58.72	-52.51	-24.51
2.22	46.22	226.39	-119.03	-64.75	-56.46	-25.09
2.17	51.82	240.76	-126.17	-71.95	-61.07	-25.69
2.12 (TS)	58.52	256.55	-134.05	-80.40	-66.37	-26.31
2.06	65.86	273.99	-142.69	-89.88	-72.43	-26.97
2.01	74.25	293.00	-152.13	-100.52	-79.52	-27.66
1.95	83.62	313.58	-162.37	-112.12	-87.86	-28.37
1.9	93.70	336.09	-173.55	-124.21	-97.87	-29.13
1.85	104.31	360.63	-185.70	-136.14	-110.04	-29.92

Table S4. EDA energy terms of IM2

Energy terms (in kcal/mol) / *r*(C-C) in **IM2** (in Å)	**Steric effect:** ΔE_{steric}		**Electronic effects:** ΔE_{elec}			**Dispersion effect:** ΔE_{disp}
	ΔE_{dist}	ΔE_{Pauli}	ΔE_{elstat}	ΔE_{oi}		
				ΔE_{ct}	ΔE_{pol}	
3.24	0.4	17.1	-9.3	-2.4	-1.8	-12.0

Table S5. EDA energy terms of TS3 along IRC

Energy terms (in kcal/mol) / *r*(C-C) in **TS3** (in Å)	**Steric effect:** ΔE_{steric}		**Electronic effects:** ΔE_{elec}			**Dispersion effect:** ΔE_{disp}
	ΔE_{dist}	ΔE_{Pauli}	ΔE_{elstat}	ΔE_{oi}		
				ΔE_{ct}	ΔE_{pol}	
2.36	32.88	196.5487	-104.46	-52.60	-51.33	-27.13
2.3	35.58	205.7651	-108.92	-56.70	-53.80	-27.65
2.26	39.17	216.085	-113.95	-61.62	-56.66	-28.18
2.2	43.28	227.4197	-119.45	-67.27	-59.85	-28.73
2.15	48.52	240.1296	-125.70	-74.01	-63.65	-29.28
2.09 (TS)	54.83	254.6461	-132.68	-82.01	-68.17	-29.86
2.04	61.74	269.9624	-140.39	-90.92	-73.32	-30.47
1.98	69.70	287.3841	-148.97	-100.97	-79.49	-31.11
1.93	78.63	306.5061	-158.43	-111.94	-86.89	-31.78
1.88	88.26	330.2808	-170.64	-124.48	-97.47	-31.96

Table S6. EDA energy terms of IM3

Energy terms (in kcal/mol) / *r*(C-C) in **IM3** (in Å)	**Steric effect:** ΔE_{steric}		**Electronic effects:** ΔE_{elec}			**Dispersion effect:** ΔE_{disp}
	ΔE_{dist}	ΔE_{Pauli}	ΔE_{elstat}	ΔE_{oi}		
				ΔE_{ct}	ΔE_{pol}	
3.07	18.2	124.0	-69.7	-30.5	-32.7	-20.2

Table S7. EDA energy terms of IM5

Energy terms (in kcal/mol) / *r*(C-C) in **IM3** (in Å)	**Steric effect:** ΔE_{steric}		**Electronic effects:** ΔE_{elec}			**Dispersion effect:** ΔE_{disp}
	ΔE_{dist}	ΔE_{Pauli}	ΔE_{elstat}	ΔE_{oi}		
				ΔE_{ct}	ΔE_{pol}	
3.07	16.7	109.2	-60.6	-24.5	-28.0	-21.9

Table S8. EDA energy terms of TS5

Energy terms (in kcal/mol) / *r*(C-C) in **IM3** (in Å)	**Steric effect:** ΔE_{steric}		**Electronic effects:** ΔE_{elec}			**Dispersion effect:** ΔE_{disp}
	ΔE_{dist}	ΔE_{Pauli}	ΔE_{elstat}	ΔE_{oi}		
				ΔE_{ct}	ΔE_{pol}	
3.07	66.5	269.7	-138.0	-87.8	-73.0	-34.1

Cartesian Coordinates (Å) and Energies of the Optimized Structures

PhCHO
M06-2X-D3 SCF energy: -345.16763038 a.u.
M06-2X-D3 enthalpy: -345.049340 a.u.
M06-2X-D3 free energy: -345.087019 a.u.
M06-2X-D3 SCF energy in solution: -345.56590276 a.u.
M06-2X-D3 enthalpy in solution: -345.447612 a.u.
M06-2X-D3 free energy in solution: -345.485291 a.u.
Three lowest frequencies (cm-1): 125.6342 224.1846 242.8568

Cartesian coordinates

ATOM	X	Y	Z
C	1.995670	0.468525	-0.000154
O	2.828519	-0.398088	0.000306
H	2.287309	1.547785	-0.000439
C	-2.210717	-0.253999	0.000079
C	-1.318993	-1.330952	-0.000031
C	0.051217	-1.096610	-0.000189
C	0.530441	0.218497	-0.000145
C	-0.361669	1.293046	-0.000048
C	-1.735174	1.057273	0.000097
H	-3.285898	-0.440585	0.000268
H	-1.699677	-2.353279	0.000002
H	0.775769	-1.912853	-0.000184
H	0.025082	2.315442	-0.000094
H	-2.435381	1.893524	0.000343

1a
M06-2X-D3 SCF energy: -606.48643304 a.u.
M06-2X-D3 enthalpy: -606.159634 a.u.
M06-2X-D3 free energy: -606.218909 a.u.
M06-2X-D3 SCF energy in solution: -607.18564577 a.u.
M06-2X-D3 enthalpy in solution: -606.858847 a.u.
M06-2X-D3 free energy in solution: -606.918122 a.u.
Three lowest frequencies (cm-1): 21.2649 48.2182 101.5633

Cartesian coordinates

ATOM	X	Y	Z
B	0.479406	0.217066	0.173495
C	-1.677991	0.614368	-0.396998
C	-1.552689	-0.761275	0.345389
C	-1.528533	-1.946759	-0.616161
H	-1.230766	-2.844912	-0.058343
H	-2.514487	-2.121851	-1.068464
H	-0.793071	-1.783868	-1.417635
C	-2.573571	-0.986893	1.446762
H	-2.488973	-0.225345	2.231214
H	-3.594448	-0.966475	1.037228
H	-2.404845	-1.970710	1.905576
C	-2.184792	1.730480	0.512775
H	-3.251990	1.609821	0.745064
H	-1.619174	1.754375	1.455454
H	-2.041545	2.692300	0.001893

C	-2.482844	0.571070	-1.684616
H	-3.514966	0.246641	-1.485112
H	-2.515936	1.575146	-2.129321
H	-2.029471	-0.110745	-2.414013
O	-0.239058	-0.670827	0.926763
O	-0.305504	0.914005	-0.706770
C	2.535918	-0.275365	-1.016491
C	3.219115	-1.418106	-1.108540
H	3.511995	-1.818237	-2.080893
H	3.512680	-1.990301	-0.225975
H	2.267746	0.252066	-1.940405
C	2.049029	0.390687	0.252256
C	2.603257	-0.271100	1.512767
C	2.413140	1.884353	0.204673
H	3.704633	-0.239660	1.518798
H	2.283335	-1.319755	1.590496
H	2.017591	2.413584	1.085109
H	1.994440	2.364594	-0.691451
H	2.240004	0.248547	2.411480
H	3.506480	2.015273	0.190976

1b

M06-2X-D3 SCF energy: -605.26561778 a.u.
M06-2X-D3 enthalpy: -604.961537 a.u.
M06-2X-D3 free energy: -605.018523 a.u.
M06-2X-D3 SCF energy in solution: -605.96163447 a.u.
M06-2X-D3 enthalpy in solution: -605.657554 a.u.
M06-2X-D3 free energy in solution: -605.714540 a.u.
Three lowest frequencies (cm-1): 25.1823 67.8254 103.9551

Cartesian coordinates

ATOM	X	Y	Z
B	0.561748	-0.085600	0.020708
C	-1.520859	0.811196	0.112509
C	-1.607959	-0.736688	-0.116085
C	-1.853971	-1.101227	-1.578257
H	-1.690627	-2.180352	-1.703385
H	-2.880720	-0.862443	-1.888274
H	-1.153320	-0.568334	-2.237267
C	-2.595511	-1.458221	0.784856
H	-2.331899	-1.337188	1.842329
H	-3.615023	-1.077145	0.624653
H	-2.587273	-2.531642	0.550915
C	-1.764690	1.205180	1.566971
H	-2.822116	1.092863	1.843750
H	-1.154324	0.592071	2.245389
H	-1.474854	2.256203	1.700265
C	-2.388274	1.642407	-0.816933
H	-3.449507	1.381412	-0.690528
H	-2.264227	2.707747	-0.578875
H	-2.106387	1.491892	-1.865861
O	-0.273869	-1.161361	0.206670
O	-0.135299	1.078484	-0.170117
C	3.039601	0.891912	-0.099083

C	2.718754	2.177957	-0.250400
H	3.501611	2.933601	-0.335386
H	1.679547	2.506100	-0.293900
H	4.103073	0.618644	-0.063795
C	2.108064	-0.259472	0.030182
C	2.590378	-1.576161	-0.576719
C	2.596705	-1.419418	0.895086
H	3.543870	-1.540445	-1.107555
H	1.833921	-2.224642	-1.021708
H	1.844184	-1.958102	1.473125
H	3.555243	-1.274019	1.397381

1d

M06-2X-D3 SCF energy: -1960.46808769 a.u.
M06-2X-D3 enthalpy: -1960.016247 a.u.
M06-2X-D3 free energy: -1960.122426 a.u.
M06-2X-D3 SCF energy in solution: -1962.75715005 a.u.
M06-2X-D3 enthalpy in solution: -1962.305309 a.u.
M06-2X-D3 free energy in solution: -1962.411488 a.u.
Three lowest frequencies (cm-1): 13.9014 19.0412 21.2414

Cartesian coordinates

ATOM	X	Y	Z
B	0.648890	1.666841	-0.550970
C	-2.923447	0.928957	-0.053823
C	-1.494278	0.320369	-0.265622
C	-1.484112	-0.636435	-1.458377
H	-0.548311	-1.209441	-1.479396
H	-2.314481	-1.349792	-1.376337
H	-1.579982	-0.083838	-2.402495
C	-1.026279	-0.397105	1.001224
H	-0.797265	0.320448	1.801073
H	-1.817218	-1.075200	1.348529
H	-0.126395	-0.992575	0.804399
C	-3.419289	1.656317	-1.298785
H	-2.695462	2.436763	-1.566862
H	-3.525082	0.964407	-2.144647
H	-4.392310	2.121741	-1.102695
C	-2.972320	1.833446	1.173712
H	-2.165613	2.574748	1.103183
H	-3.934896	2.354756	1.227707
H	-2.837191	1.253014	2.095865
O	-0.690538	1.465859	-0.553842
C	2.575421	3.439195	-0.700856
C	3.080648	4.438784	0.022812
H	4.158082	4.598594	0.089199
H	2.437263	5.126121	0.577969
H	3.266713	2.764813	-1.220277
C	1.126291	3.124820	-0.869517
C	0.105161	4.231356	-0.735991
C	0.423572	3.721496	-2.094364
H	0.475926	5.222450	-0.471756
H	-0.860762	3.964763	-0.303693
H	-0.315073	3.100451	-2.605916

H	1.041513	4.347448	-2.741042
O	-3.738742	-0.252960	0.176856
C	-5.030006	-0.177542	0.427771
C	-5.564836	-1.611177	0.622588
O	-5.720414	0.791848	0.504489
F	-4.937048	-2.199182	1.637122
F	-5.347745	-2.332519	-0.473565
F	-6.858378	-1.593760	0.873280
C	1.712648	0.523028	-0.281892
C	2.454435	0.506987	0.908480
C	1.965454	-0.479483	-1.222551
C	3.366992	-0.512651	1.167655
H	2.322783	1.300299	1.648881
C	2.888003	-1.494300	-0.962534
H	1.438358	-0.483804	-2.179938
C	3.589579	-1.527087	0.236778
H	4.307267	-2.321860	0.439958
C	4.085874	-0.539037	2.491911
C	3.091557	-2.554705	-2.011947
F	4.389337	0.690976	2.906493
F	5.217715	-1.239585	2.424640
F	3.330402	-1.096790	3.441294
F	3.928473	-3.507195	-1.607445
F	1.931141	-3.139443	-2.327498
F	3.580418	-2.035599	-3.139533

IM1

M06-2X-D3 SCF energy: -951.67105239 a.u.

M06-2X-D3 enthalpy: -951.223909 a.u.

M06-2X-D3 free energy: -951.302370 a.u.

M06-2X-D3 SCF energy in solution: -952.75897322 a.u.

M06-2X-D3 enthalpy in solution: -952.311830 a.u.

M06-2X-D3 free energy in solution: -952.390291 a.u.

Three lowest frequencies (cm-1): 24.9212 27.8305 33.8716

Cartesian coordinates

ATOM	X	Y	Z
B	-1.503676	0.739906	0.039802
C	-2.574219	-1.073674	-0.817454
C	-2.974728	-0.867261	0.691710
C	-2.277220	-1.837651	1.640703
H	-2.480948	-1.518376	2.672098
H	-2.650269	-2.863358	1.511148
H	-1.190846	-1.816019	1.489395
C	-4.473907	-0.873905	0.949677
H	-4.983090	-0.078143	0.392970
H	-4.911180	-1.843257	0.667639
H	-4.656397	-0.711978	2.020749
C	-3.652170	-0.600947	-1.789681
H	-4.534667	-1.255141	-1.770156
H	-3.967674	0.425058	-1.550934
H	-3.233930	-0.601981	-2.805626
C	-2.129188	-2.485133	-1.162649
H	-2.940734	-3.204776	-0.979504

H	-1.857753	-2.533943	-2.226523
H	-1.255542	-2.778602	-0.567469
O	-2.462869	0.446342	0.969164
O	-1.458405	-0.181256	-0.977849
C	0.382478	2.097517	-0.986896
C	1.678942	2.333125	-0.771097
H	2.401650	2.304176	-1.589398
H	2.069833	2.552813	0.225464
H	0.055526	1.872882	-2.010120
C	1.385337	-0.682905	0.024956
O	0.723206	-0.569187	1.029711
H	0.890539	-0.786719	-0.966338
C	5.650326	-0.710055	-0.002039
C	4.964633	-0.594499	1.210713
C	3.574154	-0.589104	1.223376
C	2.869195	-0.699870	0.019930
C	3.555665	-0.816345	-1.191082
C	4.948848	-0.821112	-1.202981
H	6.741583	-0.712808	-0.009650
H	5.521359	-0.507974	2.144852
H	3.007524	-0.499547	2.151951
H	2.990270	-0.895287	-2.123127
H	5.489503	-0.909617	-2.146144
C	-0.722346	2.118303	0.035952
C	-0.239359	2.479583	1.441332
C	-1.782177	3.148651	-0.426761
H	0.212084	3.485179	1.451455
H	0.504572	1.757570	1.807089
H	-2.635903	3.161269	0.266613
H	-2.161020	2.913643	-1.434276
H	-1.084890	2.472146	2.143533
H	-1.342249	4.157762	-0.459167

TS1

M06-2X-D3 SCF energy: -951.65970704 a.u.
M06-2X-D3 enthalpy: -951.213808 a.u.
M06-2X-D3 free energy: -951.284810 a.u.
M06-2X-D3 SCF energy in solution: -952.74450227 a.u.
M06-2X-D3 enthalpy in solution: -952.298603 a.u.
M06-2X-D3 free energy in solution: -952.369605 a.u.
Three lowest frequencies (cm-1): -284.8726 41.2375 49.4155
Imaginary frequency: -284.8726 cm-1

Cartesian coordinates

ATOM	X	Y	Z
B	-0.970965	0.436144	0.172381
C	-2.586739	-0.910382	-0.808269
C	-2.527218	-1.124590	0.750177
C	-1.683106	-2.341423	1.140432
H	-1.510984	-2.308147	2.225225
H	-2.188716	-3.285247	0.891155
H	-0.703964	-2.323828	0.642832
C	-3.887650	-1.211412	1.426419
H	-4.454855	-0.282273	1.292679

H	-4.474948	-2.050716	1.024277
H	-3.747581	-1.372206	2.504584
C	-3.822746	-0.121274	-1.239170
H	-4.737222	-0.727597	-1.168367
H	-3.948452	0.777559	-0.622031
H	-3.689790	0.193040	-2.284442
C	-2.497488	-2.195389	-1.621647
H	-3.327234	-2.875576	-1.376608
H	-2.555921	-1.953773	-2.692603
H	-1.548447	-2.715012	-1.440224
O	-1.862779	0.050702	1.200165
O	-1.432533	-0.113145	-1.067225
C	0.189506	2.258074	-0.978222
C	1.549333	2.130426	-0.940964
H	2.132011	2.128439	-1.864491
H	2.105899	2.272096	-0.013345
H	-0.295575	2.229591	-1.961659
C	1.290759	-0.093835	-0.494981
O	0.458961	-0.076921	0.458299
H	0.911925	-0.280265	-1.509539
C	5.381450	-0.969747	0.313111
C	4.504781	-0.710367	1.369160
C	3.169014	-0.418624	1.112532
C	2.707695	-0.383194	-0.209227
C	3.585915	-0.649430	-1.265592
C	4.921371	-0.941604	-1.004182
H	6.428180	-1.198616	0.518678
H	4.866496	-0.740248	2.397765
H	2.464426	-0.223890	1.922807
H	3.216023	-0.625023	-2.293448
H	5.605469	-1.149934	-1.827658
C	-0.701216	2.149560	0.158086
C	-0.136105	2.551195	1.517911
C	-2.076985	2.768817	-0.084460
H	0.004039	3.643217	1.579089
H	0.825460	2.066266	1.732053
H	-2.782452	2.419495	0.682674
H	-2.468739	2.482631	-1.070961
H	-0.836097	2.245116	2.308076
H	-2.026735	3.868271	-0.035022

IM1a

M06-2X-D3 SCF energy: -951.73709194 a.u.
M06-2X-D3 enthalpy: -951.287118 a.u.
M06-2X-D3 free energy: -951.361731 a.u.
M06-2X-D3 SCF energy in solution: -952.82443868 a.u.
M06-2X-D3 enthalpy in solution: -952.374465 a.u.
M06-2X-D3 free energy in solution: -952.449078 a.u.
Three lowest frequencies (cm-1): 28.2831 32.1827 37.4641

Cartesian coordinates

ATOM	X	Y	Z
B	-0.671436	-0.449488	0.302861
C	-2.492259	-1.141815	-0.847562

C	-2.770457	-1.175209	0.700159
C	-2.644497	-2.578949	1.287388
H	-2.640093	-2.500987	2.382958
H	-3.479864	-3.223790	0.981403
H	-1.701698	-3.049839	0.973699
C	-4.085443	-0.540349	1.118929
H	-4.121019	0.519849	0.839373
H	-4.933982	-1.060930	0.650868
H	-4.194983	-0.611107	2.209817
C	-3.091318	0.085915	-1.525598
H	-4.187341	0.028885	-1.579303
H	-2.805174	0.997568	-0.984794
H	-2.689793	0.153913	-2.546253
C	-2.889781	-2.406868	-1.589012
H	-3.968738	-2.593727	-1.483432
H	-2.662629	-2.290261	-2.657601
H	-2.338347	-3.278041	-1.215836
O	-1.684683	-0.397064	1.226366
O	-1.065549	-0.995518	-0.895517
C	0.094566	2.369515	-0.889657
C	1.468352	1.797595	-0.675632
H	2.118350	2.036018	-1.530792
H	1.943957	2.231524	0.216395
H	-0.253500	2.431280	-1.927138
C	1.463474	0.266411	-0.492251
O	0.591595	-0.045909	0.575571
H	1.094010	-0.205934	-1.417428
C	5.476654	-1.088751	0.318037
C	4.571792	-0.924981	1.365758
C	3.266451	-0.505287	1.110085
C	2.854531	-0.247853	-0.199473
C	3.764571	-0.418334	-1.247174
C	5.069215	-0.834728	-0.991784
H	6.496712	-1.418904	0.520134
H	4.883240	-1.127879	2.391822
H	2.549106	-0.384693	1.922581
H	3.444305	-0.229642	-2.275343
H	5.768773	-0.968367	-1.818491
C	-0.739937	2.795540	0.073365
C	-0.441427	2.738185	1.546452
C	-2.080522	3.391496	-0.264319
H	-0.637576	3.714604	2.016730
H	0.587053	2.432749	1.766286
H	-2.885946	2.874665	0.282928
H	-2.295796	3.342343	-1.340109
H	-1.108702	1.999716	2.019894
H	-2.117840	4.447163	0.049695

IM2

M06-2X-D3 SCF energy: -950.44918026 a.u.

M06-2X-D3 enthalpy: -950.024638 a.u.

M06-2X-D3 free energy: -950.102077 a.u.

M06-2X-D3 SCF energy in solution: -951.53440682 a.u.

M06-2X-D3 enthalpy in solution: -951.109865 a.u.

M06-2X-D3 free energy in solution: -951.187304 a.u.
Three lowest frequencies (cm-1): 19.9919 29.6868 32.2341

Cartesian coordinates

ATOM	X	Y	Z
B	1.508587	0.777626	0.126083
C	2.675105	-1.063260	0.767768
C	3.115143	-0.610991	-0.674630
C	2.498940	-1.460097	-1.783097
H	2.717210	-0.981221	-2.747700
H	2.919766	-2.475346	-1.793302
H	1.408334	-1.512050	-1.668768
C	4.619349	-0.503698	-0.868497
H	5.064465	0.222728	-0.178102
H	5.099453	-1.481811	-0.716266
H	4.828959	-0.172992	-1.894900
C	3.680052	-0.670415	1.847424
H	4.603195	-1.262242	1.777868
H	3.936940	0.395721	1.771397
H	3.223512	-0.842841	2.831690
C	2.319050	-2.536198	0.882793
H	3.183423	-3.166844	0.627366
H	2.020609	-2.761405	1.916245
H	1.484585	-2.790713	0.217651
O	2.537485	0.701630	-0.774435
O	1.491205	-0.280792	0.998415
C	-0.454152	1.989759	1.314882
C	-1.771395	2.180823	1.209319
H	-2.416787	2.174015	2.090103
H	-2.254444	2.338206	0.241267
H	-0.028905	1.804443	2.308287
C	-1.336466	-0.748114	-0.111531
O	-0.673384	-0.578018	-1.106352
H	-0.845776	-0.910752	0.874237
C	-5.603058	-0.752592	-0.098844
C	-4.912206	-0.560526	-1.298815
C	-3.521501	-0.562398	-1.306176
C	-2.821699	-0.756944	-0.110605
C	-3.513239	-0.948321	1.087807
C	-4.906481	-0.946620	1.094460
H	-6.694349	-0.749838	-0.095083
H	-5.464995	-0.409143	-2.227061
H	-2.949426	-0.413557	-2.223702
H	-2.951242	-1.088936	2.014578
H	-5.451191	-1.093864	2.027923
C	0.529068	1.986201	0.196204
C	0.176630	2.619178	-1.128203
C	1.137458	3.318475	-0.231521
H	-0.821683	3.047262	-1.231944
H	0.563987	2.129879	-2.023221
H	2.194764	3.322566	-0.502915
H	0.780617	4.202476	0.300493

TS2

M06-2X-D3 SCF energy: -950.42765182 a.u.
M06-2X-D3 enthalpy: -950.004680 a.u.
M06-2X-D3 free energy: -950.074164 a.u.
M06-2X-D3 SCF energy in solution: -951.50963623 a.u.
M06-2X-D3 enthalpy in solution: -951.086664 a.u.
M06-2X-D3 free energy in solution: -951.156148 a.u.
Three lowest frequencies (cm-1): -374.9500 36.1097 46.4773
Imaginary frequency: -374.9500 cm-1

Cartesian coordinates

ATOM	X	Y	Z
B	0.916986	0.346082	-0.129414
C	2.621596	-0.905363	0.799388
C	2.609171	-1.046762	-0.764958
C	1.881438	-2.312700	-1.222116
H	1.716517	-2.245365	-2.306343
H	2.461790	-3.221438	-1.007502
H	0.899909	-2.393724	-0.733392
C	3.980518	-0.965049	-1.416760
H	4.450039	0.007741	-1.223485
H	4.641905	-1.761542	-1.043376
H	3.876291	-1.083089	-2.504501
C	3.709149	0.051248	1.289167
H	4.715553	-0.377718	1.180043
H	3.664800	1.000827	0.738602
H	3.531216	0.264640	2.352708
C	2.722831	-2.227314	1.547511
H	3.648547	-2.759719	1.281210
H	2.735725	-2.035358	2.629894
H	1.864471	-2.873300	1.325777
O	1.834952	0.078039	-1.170426
O	1.355849	-0.311831	1.065740
C	-0.181528	2.137040	1.168728
C	-1.542176	1.952477	1.048423
H	-2.180809	1.918898	1.933630
H	-2.027378	2.198665	0.101257
H	0.277323	2.053537	2.161325
C	-1.349608	-0.082392	0.502717
O	-0.502209	-0.063406	-0.457575
H	-0.990152	-0.415259	1.486369
C	-5.433603	-0.900097	-0.436834
C	-4.540476	-0.556186	-1.453757
C	-3.209061	-0.284383	-1.153550
C	-2.767232	-0.355602	0.172369
C	-3.661519	-0.705634	1.189169
C	-4.992905	-0.976633	0.884799
H	-6.476413	-1.113369	-0.676230
H	-4.885206	-0.504072	-2.487412
H	-2.492527	-0.023796	-1.933968
H	-3.307999	-0.767721	2.221356
H	-5.688206	-1.251990	1.678801
C	0.683527	2.057367	0.041645
C	0.624829	2.839150	-1.223159
C	1.846037	2.912073	-0.329671
H	-0.030473	3.713290	-1.264541
H	0.739029	2.289112	-2.159747

H	2.741876	2.407184	-0.696091
H	2.014565	3.833302	0.232113

IM2a

M06-2X-D3 SCF energy: -950.49054656 a.u.
M06-2X-D3 enthalpy: -950.064417 a.u.
M06-2X-D3 free energy: -950.137210 a.u.
M06-2X-D3 SCF energy in solution: -951.57505161 a.u.
M06-2X-D3 enthalpy in solution: -951.148922 a.u.
M06-2X-D3 free energy in solution: -951.221715 a.u.
Three lowest frequencies (cm-1): 28.1764 36.0659 43.6308

Cartesian coordinates

ATOM	X	Y	Z
B	-0.681470	-0.378548	0.291450
C	-2.515385	-1.133124	-0.801491
C	-2.805840	-0.987745	0.737024
C	-2.710600	-2.319440	1.478336
H	-2.712413	-2.119718	2.558372
H	-3.555435	-2.979664	1.238646
H	-1.774547	-2.839151	1.227669
C	-4.113290	-0.290912	1.070081
H	-4.145007	0.723355	0.653889
H	-4.965973	-0.861375	0.673088
H	-4.222628	-0.218686	2.160866
C	-3.077707	0.023729	-1.622589
H	-4.174452	-0.015088	-1.680033
H	-2.772940	0.988920	-1.194918
H	-2.669973	-0.040634	-2.641054
C	-2.941731	-2.463072	-1.400395
H	-4.026012	-2.609117	-1.285311
H	-2.704160	-2.473289	-2.473009
H	-2.416299	-3.300727	-0.926557
O	-1.706299	-0.177255	1.183128
O	-1.084554	-1.033829	-0.848147
C	0.051371	2.154512	-1.197587
C	1.449272	1.671115	-0.925030
H	2.106617	1.825726	-1.793562
H	1.873808	2.227881	-0.075871
H	-0.364350	2.026734	-2.202641
C	1.479576	0.174788	-0.545109
O	0.599408	-0.018029	0.543537
H	1.137241	-0.424530	-1.405116
C	5.511301	-0.954713	0.485089
C	4.585402	-0.682757	1.491132
C	3.274409	-0.334189	1.166797
C	2.878214	-0.257808	-0.170258
C	3.809183	-0.536118	-1.175530
C	5.119519	-0.881070	-0.851767
H	6.535861	-1.228615	0.741302
H	4.884945	-0.744151	2.538751
H	2.541011	-0.128077	1.946929
H	3.501487	-0.489077	-2.223617
H	5.835760	-1.100098	-1.645301

C	-0.704701	2.663067	-0.232692
C	-0.783399	3.031943	1.181321
C	-1.973225	3.218900	0.240755
H	-0.255290	3.927042	1.521605
H	-0.849178	2.216292	1.907097
H	-2.821299	2.542255	0.379007
H	-2.242066	4.236799	-0.054136

IM3

M06-2X-D3 SCF energy: -2305.65848300 a.u.
M06-2X-D3 enthalpy: -2305.086322 a.u.
M06-2X-D3 free energy: -2305.208542 a.u.
M06-2X-D3 SCF energy in solution: -2308.33693884 a.u.
M06-2X-D3 enthalpy in solution: -2307.764778 a.u.
M06-2X-D3 free energy in solution: -2307.886998 a.u.
Three lowest frequencies (cm-1): 13.2450 15.0795 16.7056

Cartesian coordinates

ATOM	X	Y	Z
B	0.570674	0.446633	-1.097648
C	-3.145800	0.478931	-0.834800
C	-1.789874	-0.050620	-0.251704
C	-1.797735	-1.581705	-0.178037
H	-0.928441	-1.940435	0.388745
H	-2.707313	-1.939451	0.322885
H	-1.745720	-2.015715	-1.185993
C	-1.559009	0.538257	1.144001
H	-1.335347	1.611440	1.085256
H	-2.448838	0.389060	1.770625
H	-0.717382	0.032758	1.633900
C	-3.419960	-0.083813	-2.223978
H	-2.576465	0.175104	-2.876867
H	-3.521473	-1.176576	-2.193612
H	-4.341860	0.345201	-2.634539
C	-3.191290	2.004240	-0.837236
H	-2.267703	2.376428	-1.300152
H	-4.057371	2.366323	-1.403232
H	-3.255191	2.395217	0.187279
O	-0.834065	0.404633	-1.182950
C	2.668585	0.983837	-2.597635
C	3.278202	2.163324	-2.773594
H	4.366837	2.253119	-2.759390
H	2.698754	3.071687	-2.964961
H	3.287684	0.096740	-2.406638
C	2.056370	2.219012	0.041102
O	0.920148	1.870400	-0.284434
H	2.869825	1.474991	0.070336
C	2.981936	6.181366	1.206267
C	1.683456	5.874548	0.785928
C	1.369105	4.578504	0.399721
C	2.362977	3.588475	0.436829
C	3.663566	3.897779	0.855814
C	3.971867	5.198031	1.242229
H	3.223891	7.201522	1.508568

H	0.920239	6.652842	0.761012
H	0.366060	4.309675	0.064759
H	4.426413	3.116169	0.874644
H	4.980979	5.447735	1.570565
C	1.199304	0.779010	-2.559129
C	0.329841	1.551698	-3.510744
C	0.537763	0.081858	-3.726233
H	0.815127	2.230427	-4.215096
H	-0.647283	1.872764	-3.145694
H	-0.295087	-0.588893	-3.501463
H	1.169323	-0.218582	-4.565539
O	-4.135324	-0.037686	0.102935
C	-5.417187	0.226637	-0.012574
C	-6.155707	-0.457913	1.156156
O	-5.979393	0.876391	-0.841301
F	-5.710741	0.016557	2.317572
F	-5.939929	-1.769842	1.135439
F	-7.454292	-0.239100	1.078483
C	1.342398	-0.740919	-0.303054
C	1.688435	-0.724673	1.052257
C	1.651850	-1.908494	-1.017527
C	2.289333	-1.822303	1.671749
H	1.475659	0.154702	1.667699
C	2.252405	-3.005077	-0.402552
H	1.406353	-1.965239	-2.082010
C	2.574558	-2.977599	0.953037
H	3.039163	-3.836756	1.435753
C	2.607699	-1.721307	3.138388
C	2.574251	-4.213442	-1.241457
F	3.420924	-0.686935	3.384805
F	3.200364	-2.818311	3.604549
F	1.503398	-1.518164	3.862003
F	2.979292	-5.244677	-0.499902
F	1.514514	-4.612610	-1.947069
F	3.545448	-3.947050	-2.119429

TS3

M06-2X-D3 SCF energy: -2305.64885659 a.u.
M06-2X-D3 enthalpy: -2305.077570 a.u.
M06-2X-D3 free energy: -2305.195614 a.u.
M06-2X-D3 SCF energy in solution: -2308.32468391 a.u.
M06-2X-D3 enthalpy in solution: -2307.753397 a.u.
M06-2X-D3 free energy in solution: -2307.871441 a.u.
Three lowest frequencies (cm-1): -345.2893 13.0751 14.7029
Imaginary frequency: -345.2893 cm-1

Cartesian coordinates

ATOM	X	Y	Z
B	0.578063	0.505768	-1.036363
C	-3.134933	0.407303	-0.805594
C	-1.762095	-0.077822	-0.225104
C	-1.736786	-1.606439	-0.111094
H	-0.854860	-1.931706	0.456387
H	-2.633836	-1.969746	0.408179

H	-1.685065	-2.066834	-1.107458
C	-1.522880	0.553674	1.149535
H	-1.324097	1.629262	1.058745
H	-2.396679	0.397422	1.796505
H	-0.657594	0.084095	1.634743
C	-3.415803	-0.205142	-2.172674
H	-2.580216	0.036267	-2.842232
H	-3.507519	-1.296995	-2.102962
H	-4.344723	0.200941	-2.590597
C	-3.211976	1.930507	-0.852124
H	-2.302390	2.308978	-1.337040
H	-4.093702	2.258288	-1.414922
H	-3.268235	2.349374	0.161655
O	-0.822609	0.372427	-1.178844
C	2.529552	1.142058	-2.516035
C	2.896564	2.423522	-2.168038
H	3.943206	2.673923	-1.982983
H	2.229151	3.251046	-2.419048
H	3.268231	0.336152	-2.411314
C	2.126453	2.232701	-0.232365
O	0.917286	1.828660	-0.392248
H	2.883419	1.503859	0.089560
C	2.714391	6.222220	1.162691
C	1.483693	5.850872	0.616607
C	1.286984	4.553390	0.154626
C	2.327651	3.621323	0.240658
C	3.558434	3.992936	0.791394
C	3.751033	5.292820	1.251641
H	2.864314	7.240373	1.524531
H	0.673025	6.577919	0.554563
H	0.330458	4.241780	-0.268090
H	4.363901	3.257899	0.864818
H	4.709296	5.580478	1.685546
C	1.157188	0.783124	-2.658968
C	0.188218	1.410714	-3.601281
C	0.524411	-0.060152	-3.717775
H	0.583165	2.078778	-4.370472
H	-0.801733	1.660334	-3.216278
H	-0.248659	-0.763851	-3.400188
H	1.133836	-0.381140	-4.565471
O	-4.102154	-0.100679	0.159521
C	-5.390711	0.131884	0.049235
C	-6.103325	-0.533868	1.244590
O	-5.974704	0.742524	-0.794093
F	-5.651191	-0.025297	2.388171
F	-5.867563	-1.842684	1.251850
F	-7.406020	-0.336842	1.178299
C	1.385265	-0.714599	-0.328358
C	1.775723	-0.674047	1.015304
C	1.668315	-1.892836	-1.032972
C	2.395841	-1.761174	1.633305
H	1.582580	0.222038	1.613650
C	2.292317	-2.977946	-0.419794
H	1.382786	-1.974658	-2.085059
C	2.658662	-2.927954	0.923612
H	3.138960	-3.779248	1.404941

C	2.760189	-1.639245	3.088027
C	2.588435	-4.199361	-1.248574
F	3.568833	-0.593997	3.296226
F	3.380548	-2.725062	3.545905
F	1.677473	-1.441979	3.844288
F	2.993126	-5.226590	-0.502147
F	1.514432	-4.594384	-1.935401
F	3.549834	-3.954065	-2.144462

IM3a

M06-2X-D3 SCF energy: -2305.69859892 a.u.
M06-2X-D3 enthalpy: -2305.124550 a.u.
M06-2X-D3 free energy: -2305.246118 a.u.
M06-2X-D3 SCF energy in solution: -2308.37601436 a.u.
M06-2X-D3 enthalpy in solution: -2307.801965 a.u.
M06-2X-D3 free energy in solution: -2307.923533 a.u.
Three lowest frequencies (cm-1): 12.6399 14.5825 18.4260

Cartesian coordinates

ATOM	X	Y	Z
B	0.479623	0.757215	-0.269711
C	-3.205941	1.077921	-0.241061
C	-1.946575	0.226738	0.137401
C	-2.073781	-1.188115	-0.431179
H	-1.325668	-1.857275	0.011019
H	-3.069331	-1.589655	-0.198840
H	-1.938461	-1.190638	-1.521297
C	-1.761665	0.169065	1.654265
H	-1.534672	1.164076	2.059301
H	-2.668399	-0.216166	2.137716
H	-0.928657	-0.504282	1.900359
C	-3.466147	1.053616	-1.743625
H	-2.545919	1.337788	-2.269834
H	-3.765135	0.050104	-2.074714
H	-4.262279	1.759294	-2.007498
C	-3.108908	2.505923	0.283472
H	-2.181155	2.958172	-0.089212
H	-3.965728	3.095104	-0.063627
H	-3.094178	2.522876	1.381133
O	-0.860674	0.945409	-0.445642
C	2.191584	0.897930	-2.826671
C	2.881317	2.002986	-2.079089
H	3.967658	1.997687	-2.250808
H	2.488665	2.978804	-2.402135
H	2.678970	-0.081196	-2.892288
C	2.633313	1.885604	-0.558872
O	1.240475	1.882282	-0.327742
H	3.078697	0.939919	-0.206035
C	4.526095	5.172407	1.489078
C	3.166758	5.232060	1.185068
C	2.542816	4.166034	0.537907
C	3.276511	3.028816	0.191988
C	4.638059	2.971280	0.503292
C	5.261868	4.037911	1.146903

H	5.011492	6.006918	1.997130
H	2.585808	6.115234	1.455649
H	1.478271	4.201383	0.304041
H	5.214314	2.078391	0.246230
H	6.324048	3.979965	1.389180
C	0.967284	1.059686	-3.311906
C	-0.144964	1.993299	-3.488447
C	-0.249940	0.531132	-3.927713
H	-0.069344	2.747567	-4.276491
H	-0.690299	2.304674	-2.592272
H	-0.886993	-0.128423	-3.327920
H	-0.258670	0.318494	-4.999831
O	-4.277647	0.375292	0.449728
C	-5.534839	0.757681	0.366010
C	-6.390599	-0.225558	1.190832
O	-5.997292	1.682981	-0.227833
F	-5.976117	-0.249361	2.454308
F	-6.276016	-1.454457	0.693828
F	-7.659980	0.128300	1.164756
C	1.140113	-0.660090	0.021169
C	1.780020	-0.928891	1.236700
C	1.133305	-1.667178	-0.950417
C	2.372913	-2.169277	1.477269
H	1.822062	-0.162178	2.016514
C	1.740468	-2.898248	-0.713347
H	0.653009	-1.487540	-1.916330
C	2.360476	-3.164917	0.504791
H	2.828251	-4.131169	0.691650
C	3.046384	-2.397678	2.805426
C	1.715268	-3.924500	-1.814543
F	4.085775	-1.575866	2.965888
F	3.495560	-3.645274	2.929256
F	2.207888	-2.164503	3.817058
F	2.281796	-5.071260	-1.445520
F	0.464112	-4.191883	-2.195427
F	2.362478	-3.481865	-2.896205

TS4

M06-2X-D3 SCF energy: -1249.09151959 a.u.
M06-2X-D3 enthalpy: -1248.665499 a.u.
M06-2X-D3 free energy: -1248.741115 a.u.
M06-2X-D3 SCF energy in solution: -3424.28010821 a.u.
M06-2X-D3 enthalpy in solution: -3423.854088 a.u.
M06-2X-D3 free energy in solution: -3423.929704 a.u.
Three lowest frequencies (cm-1): -346.7103 39.7655 47.4999
Imaginary frequency: -346.7103 cm-1

Cartesian coordinates

ATOM	X	Y	Z
B	-0.636526	-0.126004	0.209677
C	-2.008708	-1.669424	-0.826753
C	-1.895694	-1.942692	0.720561
C	-0.856163	-3.017117	1.049698
H	-0.686622	-3.013064	2.135335

H	-1.194524	-4.018581	0.748292
H	0.103170	-2.805491	0.556997
C	-3.215975	-2.274413	1.398587
H	-3.918828	-1.437116	1.313788
H	-3.670266	-3.174018	0.956796
H	-3.038532	-2.464338	2.466400
C	-3.364923	-1.087579	-1.220057
H	-4.152524	-1.853690	-1.179555
H	-3.646163	-0.255581	-0.563883
H	-3.297094	-0.703235	-2.247259
C	-1.703078	-2.879991	-1.698948
H	-2.399678	-3.703961	-1.482828
H	-1.815839	-2.603570	-2.756905
H	-0.676324	-3.234522	-1.545000
O	-1.420920	-0.696519	1.226529
O	-1.002552	-0.675764	-1.048443
C	0.180131	2.000155	-0.812718
C	1.546198	2.055039	-0.713871
H	2.150881	2.247201	-1.601828
H	2.028936	2.223442	0.249653
H	-0.267109	1.997864	-1.812396
C	1.660878	-0.092480	-0.490132
O	0.850200	-0.318672	0.468966
H	1.314162	-0.308319	-1.510425
C	5.848010	-0.398839	0.257008
C	4.951877	-0.367494	1.327699
C	3.584617	-0.262382	1.091896
C	3.111375	-0.186288	-0.223338
C	4.009594	-0.225155	-1.295171
C	5.376541	-0.330241	-1.054634
H	6.919210	-0.481914	0.446160
H	5.322977	-0.430236	2.351435
H	2.867275	-0.249971	1.914159
H	3.631558	-0.174144	-2.319172
H	6.076271	-0.362186	-1.890558
C	-0.702427	1.662911	0.275412
C	-0.309638	2.070251	1.692985
C	-2.119873	2.107068	-0.025458
H	0.693825	1.704767	1.939918
H	-0.333994	3.163708	1.811336
H	-1.007515	1.613988	2.406924
F	-2.232134	3.443210	0.091264
F	-3.017952	1.584234	0.808987
F	-2.504458	1.807294	-1.270116

IM5
M06-2X-D3 SCF energy: -2344.92973309 a.u.
M06-2X-D3 enthalpy: -2344.328218 a.u.
M06-2X-D3 free energy: -2344.453606 a.u.
M06-2X-D3 SCF energy in solution: -2347.65100472 a.u.
M06-2X-D3 enthalpy in solution: -2347.049490 a.u.
M06-2X-D3 free energy in solution: -2347.174878 a.u.
Three lowest frequencies (cm-1): 9.4567 14.7617 16.5972

Cartesian coordinates

ATOM	X	Y	Z
B	0.596529	0.384991	-1.181826
C	-3.034353	-0.409983	-0.916731
C	-1.604890	-0.588319	-0.295771
C	-1.267404	-2.075407	-0.144906
H	-0.341932	-2.198481	0.432900
H	-2.075378	-2.602533	0.380349
H	-1.114672	-2.538036	-1.129578
C	-1.544387	0.102673	1.071557
H	-1.536273	1.195167	0.960190
H	-2.408395	-0.190962	1.682856
H	-0.638250	-0.199565	1.610747
C	-3.153027	-1.101129	-2.269626
H	-2.362395	-0.717561	-2.927507
H	-3.032570	-2.187627	-2.167909
H	-4.131708	-0.895951	-2.719686
C	-3.414672	1.064370	-1.016256
H	-2.604014	1.590899	-1.537524
H	-4.349159	1.187214	-1.575940
H	-3.542578	1.505572	-0.018241
O	-0.762238	0.026780	-1.243536
C	2.501610	1.320587	-2.783232
C	2.828404	2.534334	-3.236794
H	3.869830	2.858070	-3.296114
H	2.062237	3.237122	-3.575899
H	3.308470	0.651344	-2.452718
C	1.310455	2.791569	0.018627
O	0.543844	1.923628	-0.402652
C	-0.486561	6.527181	1.052655
C	-1.238110	5.532479	0.422902
C	-0.643854	4.321895	0.088300
C	0.711457	4.101114	0.377688
C	1.461511	5.104327	1.006575
C	0.860327	6.312914	1.345802
H	-0.954561	7.476764	1.316630
H	-2.290177	5.704134	0.193403
H	-1.211810	3.531431	-0.404055
H	2.514101	4.945104	1.242043
H	1.444013	7.090078	1.839864
C	1.122088	0.779057	-2.657581
C	0.083403	1.234382	-3.644815
C	0.646670	-0.149503	-3.758347
H	0.379251	1.953361	-4.410772
H	-0.940849	1.333069	-3.281781
H	0.008639	-0.988062	-3.468780
H	1.333107	-0.344602	-4.585551
O	-3.902313	-1.074730	0.047279
C	-5.208209	-1.113889	-0.093411
C	-5.799892	-1.867886	1.115404
O	-5.883963	-0.663326	-0.968275
F	-5.488054	-1.236020	2.244807
F	-5.304675	-3.100021	1.180605
F	-7.113511	-1.941652	1.019928
C	1.600186	-0.527992	-0.300795
C	1.866351	-0.332124	1.058034

C	2.241235	-1.610850	-0.918666
C	2.722061	-1.170566	1.770084
H	1.400796	0.500887	1.591677
C	3.093450	-2.456558	-0.207748
H	2.068720	-1.800656	-1.982193
C	3.343973	-2.247887	1.146467
H	4.012554	-2.906179	1.700332
C	2.948987	-0.870180	3.225377
C	3.764950	-3.584924	-0.944818
F	3.381957	0.388639	3.392816
F	3.848721	-1.679795	3.777932
F	1.819101	-0.977637	3.928850
F	4.435734	-4.391301	-0.121750
F	2.877943	-4.329375	-1.607675
F	4.633974	-3.123124	-1.848362
C	2.777991	2.568827	0.229193
H	2.975167	2.529276	1.313410
H	3.105253	1.633349	-0.227889
H	3.348074	3.405127	-0.195028

TS5

M06-2X-D3 SCF energy: -2344.91209215 a.u.

M06-2X-D3 enthalpy: -2344.311686 a.u.

M06-2X-D3 free energy: -2344.431983 a.u.

M06-2X-D3 SCF energy in solution: -3424.32899098 a.u.

M06-2X-D3 enthalpy in solution: -3423.728585 a.u.

M06-2X-D3 free energy in solution: -3423.848882 a.u.

Three lowest frequencies (cm-1): -408.0889 13.0195 14.9393

Imaginary frequency: -408.0889 cm-1

Cartesian coordinates

ATOM	X	Y	Z
B	0.636955	0.579159	-0.880593
C	-3.056547	0.036496	-0.833529
C	-1.662115	-0.330739	-0.216812
C	-1.458746	-1.850358	-0.236564
H	-0.577581	-2.129073	0.355531
H	-2.334176	-2.358994	0.189762
H	-1.300488	-2.205634	-1.264312
C	-1.570944	0.196992	1.218806
H	-1.458064	1.289223	1.226365
H	-2.468409	-0.081785	1.787141
H	-0.704609	-0.241859	1.729121
C	-3.204772	-0.504866	-2.251203
H	-2.351201	-0.161172	-2.849649
H	-3.214110	-1.602841	-2.251674
H	-4.135828	-0.145689	-2.705387
C	-3.310880	1.539552	-0.781595
H	-2.454149	2.051068	-1.239456
H	-4.226452	1.796374	-1.327201
H	-3.411493	1.883897	0.256538
O	-0.744669	0.322252	-1.068697
C	2.432760	1.688370	-2.312696
C	2.501424	3.004009	-1.892909

H	3.466187	3.483530	-1.716731
H	1.669070	3.663412	-2.145909
H	3.326119	1.053422	-2.243223
C	1.861497	2.619676	0.028969
O	0.819744	1.857524	-0.119233
C	0.721587	6.627412	1.117280
C	-0.214188	5.737897	0.586339
C	0.167197	4.446787	0.237789
C	1.492769	4.026098	0.415801
C	2.425992	4.922425	0.949212
C	2.040122	6.215795	1.298511
H	0.421723	7.639752	1.391491
H	-1.249263	6.052238	0.446143
H	-0.556538	3.741680	-0.172594
H	3.462376	4.622546	1.103700
H	2.776156	6.903144	1.717357
C	1.169445	1.069989	-2.496623
C	0.100755	1.567091	-3.407957
C	0.692692	0.186723	-3.601666
H	0.375629	2.336014	-4.134095
H	-0.918082	1.617941	-3.022842
H	0.054776	-0.656911	-3.326926
H	1.345230	0.020911	-4.461789
O	-3.999900	-0.644568	0.044672
C	-5.300056	-0.571752	-0.131397
C	-5.983427	-1.389010	0.984391
O	-5.912676	0.008124	-0.976159
F	-5.672512	-0.884272	2.175725
F	-5.572370	-2.653226	0.950349
F	-7.294651	-1.364171	0.842321
C	1.524534	-0.641041	-0.287248
C	1.769005	-0.738605	1.088617
C	2.028331	-1.670748	-1.090020
C	2.463203	-1.812574	1.639723
H	1.413394	0.052412	1.754103
C	2.725025	-2.749412	-0.541040
H	1.876312	-1.640357	-2.171838
C	2.947070	-2.837198	0.830158
H	3.491361	-3.678945	1.257055
C	2.679706	-1.822321	3.127805
C	3.228299	-3.820566	-1.471091
F	3.351077	-0.732969	3.522670
F	3.368749	-2.887181	3.533047
F	1.518869	-1.814434	3.787689
F	3.933315	-4.752975	-0.830849
F	2.221718	-4.435467	-2.096516
F	4.013295	-3.304282	-2.422005
C	3.131777	2.051997	0.631672
H	2.975399	1.907379	1.712844
H	3.387252	1.084683	0.190808
H	3.978201	2.733256	0.495773

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