Electronic Supplementary Information

Origins of regio- and stereoselectivity in Cu-catalyzed alkyne difunctionalization with CO_2 and organoboranes

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Comparison of 1,2-Migration Barriers Using Different Levels of Theories

To validate the conclusion based on the method used in the present study, we computed the barriers of syn/anti-1,2 migration (**TS9** and **TS8**) using a few popular modern density functionals and basis sets (Table S1). Although the absolute barriers of **TS8** and **TS9** differ by a few kcal/mol among the methods tested, the trend of barrier difference ($\Delta\Delta G^{\ddagger}_{sol}$), i.e., the stereoselectivity of 1,2-migration, is only minimally affected by the choice of density functionals in both optimization and single-point energy calculations.

Table S1. Comparison of barriers (in kcal/mol) of syn-to-metal (TS8) and anti-to-metal (TS9) 1,2-migration using different levels of theories.

Method for Single-Point Energy Calculation in Solvent Using SMD	Method for Gas-Phase Geometry Optimization	Barrier of **TS8** ($\Delta G^{\ddagger}_{sol}$) with respect to **15**	Barrier of **TS9** ($\Delta G^{\ddagger}_{sol}$) with respect to **15**	$\Delta\Delta G^{\ddagger}_{sol}$ (**TS9** –**TS8**)
B3LYP-D3BJ/ SDD−6-311+G(d,p)	B3LYP/ LANL2DZ−6-31G(d)	20.2	22.2	2.0
M06/ SDD−6-311+G(d,p)		21.0	22.5	1.5
M06L/ SDD−6-311+G(d,p)		22.3	23.6	1.3
ωB97xD/ SDD−6-311+G(d,p)		21.9	23.9	2.0
B3LYP-D3BJ/ SDD−6-311+G(d,p)	B3LYP-D3BJ/ LANL2DZ−6-31G(d)	21.6	24.0	2.4
M06/ SDD−6-311+G(d,p)		21.7	23.5	1.8
M06L/ SDD−6-311+G(d,p)		24.0	25.6	1.6
ωB97xD/ SDD−6-311+G(d,p)		24.6	26.3	1.7
B3LYP-D3BJ/ SDD−6-311+G(d,p)	M06/ LANL2DZ−6-31G(d)	18.5	21.4	1.9
M06/ SDD−6-311+G(d,p)		19.4	21.6	2.2
M06L/ SDD−6-311+G(d,p)		21.2	22.9	1.7
ωB97xD/ SDD−6-311+G(d,p)		20.9	23.8	2.9
B3LYP-D3BJ/ SDD−6-311+G(d,p)	ωB97xD/ LANL2DZ−6-31G(d)	17.1	20.8	3.7
M06/ SDD−6-311+G(d,p)		18.0	20.7	2.7
M06L/ SDD−6-311+G(d,p)		19.9	22.4	2.5
ωB97xD/ SDD−6-311+G(d,p)		19.5	23.3	2.8

Formation of Alkynyl-Cu Intermediate

Under the experimental condition, LCu-OMe (**5**) is expected to be formed from the reaction of LCuCl with KOMe. The acidic alkyne C(sp)–H can be cleaved via **TS13** with a quite low barrier (Fig. S1). The release of alkynyl-Cu intermediate **14** is endothermic by 13 kcal/mol. This result indicates the formation of alkynyl-Cu species is accessible. The following reaction steps based on alkynyl-Cu are discussed in Fig. 2 of the main text.

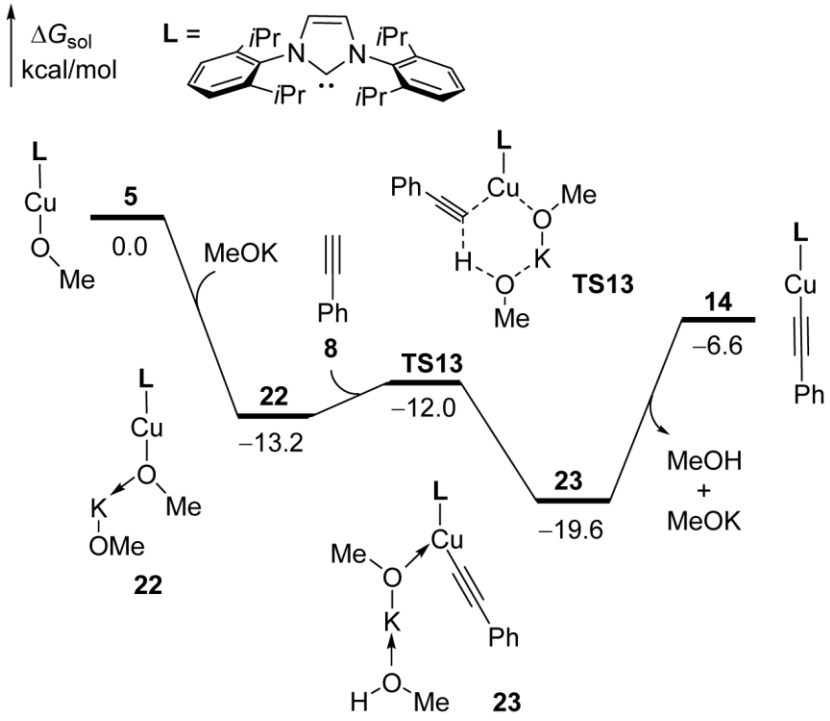

Fig. S1. Energy profile for the formation of alkynyl-Cu species.

Interactions of K^+–π and Cu^+–π

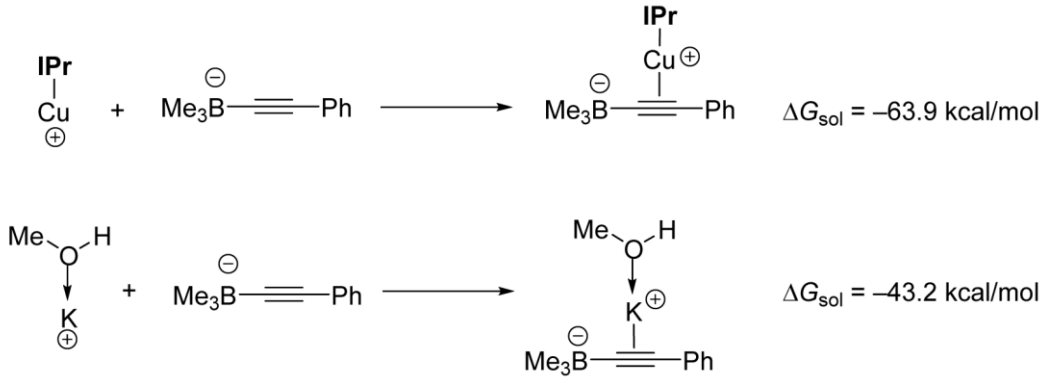

Fig. S2. Energetics of K^+–π and Cu^+–π interactions.

Competing Pathways

The transition states of concerted protonation and 1,2-migration (**S-TS5** and **S-TS6**, Fig. S3) were computed. These transition states require high barriers ($\Delta G^{\ddagger}$ > 35 kcal/mol), which are comparable with the K^+-mediated 1,2-migration transition states (**TS5** and **TS6**, $\Delta G^{\ddagger}$ > 36 kcal/mol, Fig. 1 in the manuscript). Compared to the Cu^+-mediated 1,2-migrations with much lower barriers (**TS8** and **TS9**, $\Delta G^{\ddagger}$ ≈ 20 kcal/mol, Fig. 2), the proton-mediated 1,2-migration pathways (**S-TS5** and **S-TS6**) can also be ruled out.

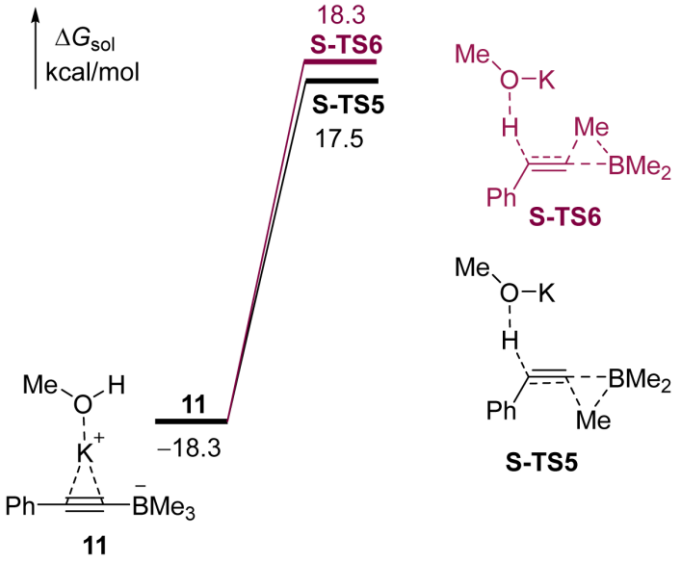

Fig. S3. Energy profile of proton-mediated 1,2-migration.

After the formation of alkenyl-Cu intermediate **17**, the Cu–C(sp^2) protonation has several possible pathways (Fig. S4). The only use of in situ formed MeOH requires the highest barrier (**TS11-b**, $\Delta G^{\ddagger}$ = 24.4 kcal/mol). The addition of external BMe_3 can lower the barrier (**TS11-a**, $\Delta G^{\ddagger}$ = 16.0 kcal/mol). The most favorable pathway is the intramolecular boron-assisted Cu–C protonation with a barrier of 9.9 kcal/mol (**TS11**), which is reported in the main text (Fig. 2).

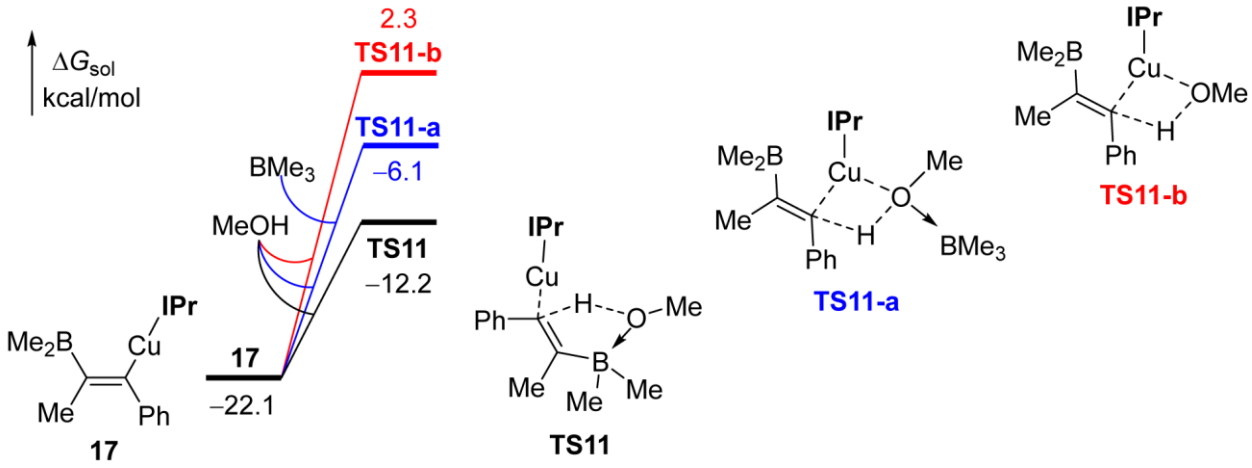

Fig. S4. Energy profile of competing Cu–C(sp^2) protonation pathways.

The competing pathway of CO_2 insertion into alkynyl copper (**14**) was also computed. The transition state (**S-TS7a**) requires a barrier of 12.6 kcal/mol (Fig. S5), which is much higher than the barrierless boron addition (**TS7**, $\Delta G^{\ddagger}$ = 0.8 kcal/mol). This indicates that CO_2 insertion with alkynyl copper **14** is a less favorable pathway.

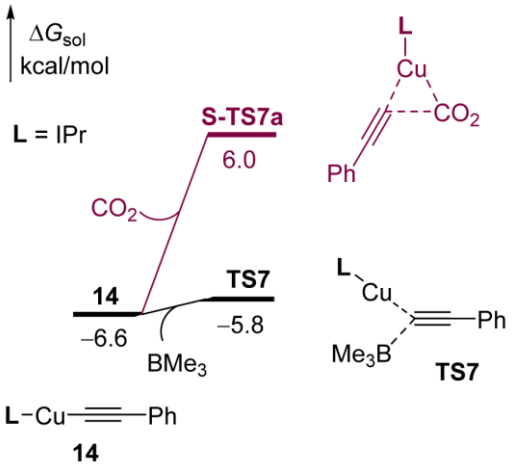

Fig. S5. Energy profile of CO_2 insertion into alkynyl copper.

Since BMe_3 can react with Cu–C bond via transmetalation, although it may be unproductive pathways, the transition states of transmetalations between BMe_3 and intermediates **14**, **17**, **19** were computed. As shown in Fig. S6, all these transition states (**S-TS7b**, **S-TS11**, **S-TS13**) are less favorable than their competing pathways (**TS7**, **TS11**, **TS13**) reported in Fig. 2 in the manuscript.

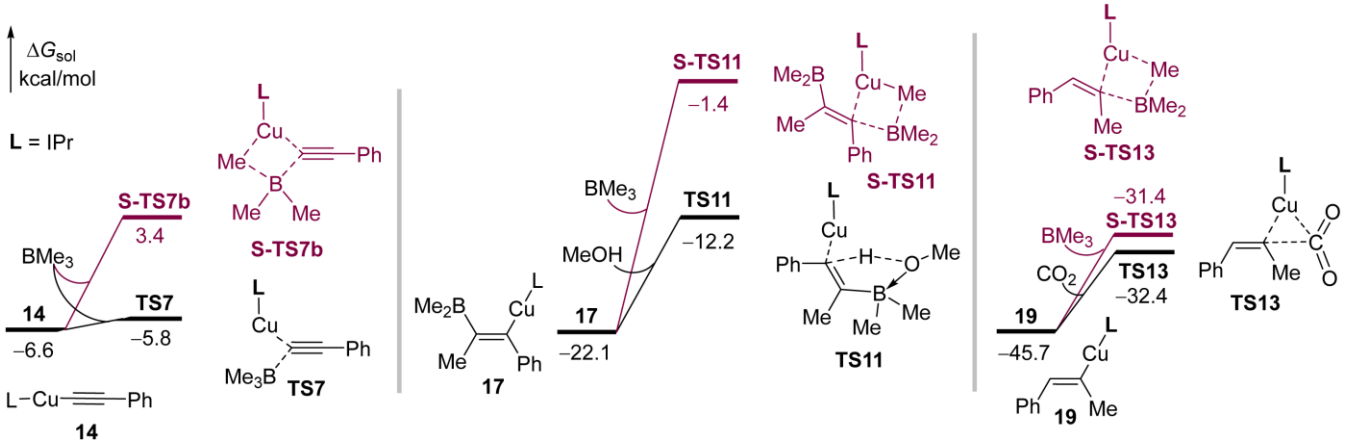

Fig. S6. Energy profiles of Cu–C transmetalation with BMe_3 and their competing pathways.

Comparison of CO_2 Insertion Transition States

Both **TS13** and **TS10** are the transition states for CO_2 insertion into alkenyl copper, but the barriers are not comparable. Although having B···O interactions, **TS10** is higher than **TS13**. The barrier difference for the two CO_2 insertion transition states is mostly due to steric effects. As shown in Fig. S7, **TS10** has shorter O···H distances (2.44 and 2.37 Å) than those in **TS13** (2.53 and 2.45 Å), respectively. Thus, the steric repulsion is much stronger in **TS10**, leading to a higher barrier.

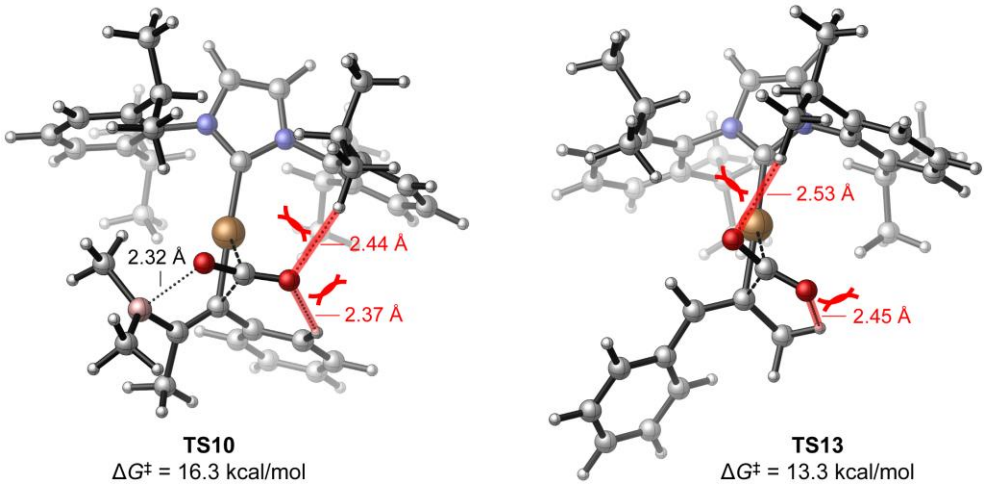

Fig. S7. Optimized transition states of CO_2 insertion.

Charge Density Difference

To understand the change of alkyne π electron density when interacting with the cationic IPrCu, we performed calculations for charge density difference to study the areas of electron gain and loss. As shown in Fig. S8, for the complex **15**, the alkyne π electron is depleted (cyan) at the opposite site of Cu and accumulated (yellow) at the same side of Cu. This unequal redistribution of π electron density leads to different σ)(π Pauli repulsion when the migrated alkyl groups approach from different sides of Cu (see the detailed discussions in the main text).

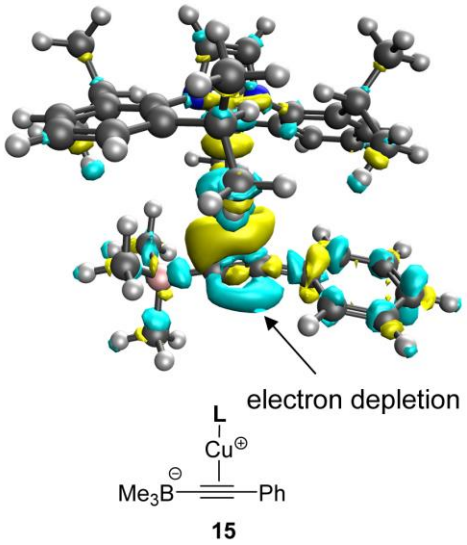

Fig. S8. Charge density difference plot (yellow: electron gain; cyan: electron loss) of the complex **15**.

The in-plane π Orbital of L-Cu-alkyne along IRC

To study whether the change of the in-plane π orbital of L-Cu-alkyne fragment has a consistent trend during the reaction process, we computed this orbital for three representative structures along IRC (Fig. S9). The results show that these in-plane π orbitals are accumulated at the same side of Cu and depleted at the opposite side. This indicates the σ)(π Pauli repulsion can distinguish the syn- and anti-1,2-migration when the migrated group gradually approaches L-Cu-alkyne from different sides. Thus, the insight of the unequal redistribution of alkyne in-plane π orbitals is solid for explaining the difference of Pauli repulsion.

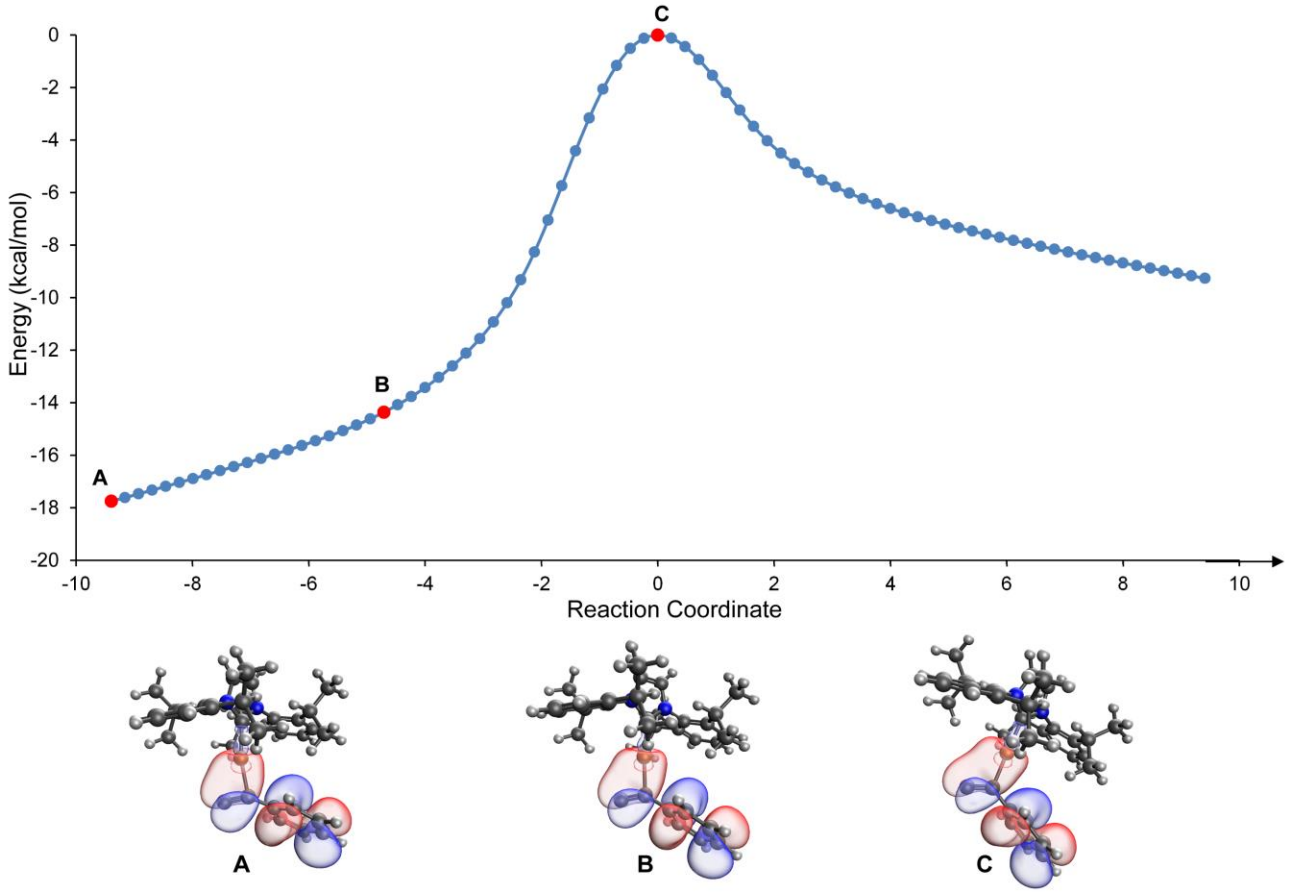

Fig. S9. The in-plane π orbital of L-Cu-alkyne fragment along reaction coordinates.

Energy Terms of EDA along IRC

Table S2. EDA energy terms of anti-to-metal 1,2-migration (TS8) along IRC

Energy terms (in kcal/mol) / *r*(C-C) in **TS8** (in Å)	ΔE_{dist}	ΔE_{Pauli}	ΔE_{ct}	ΔE_{elstat}	ΔE_{pol}	ΔE_{disp}
2.13	60.59	294.84	-83.29	-158.15	-89.40	-23.21
2.1	62.49	316.99	-87.83	-167.66	-97.47	-24.47
2.07	64.66	341.28	-92.83	-177.88	-106.67	-25.86
2.03	67.07	367.87	-98.28	-188.45	-117.54	-27.41
2.0	69.70	396.69	-104.18	-199.32	-130.09	-29.12
1.97	72.47	428.11	-110.51	-210.58	-144.49	-31.03
1.94(TS)	75.35	461.73	-117.28	-222.0	-160.72	-33.09
1.91	78.43	497.67	-124.46	-233.50	-179.09	-35.30
1.87	81.5	536.17	-131.98	-245.03	-199.79	-37.67
1.84	84.73	576.82	-139.76	-256.59	-222.49	-40.17

Table S3. EDA energy terms of syn-to-metal 1,2-migration (TS9) along IRC

Energy terms (in kcal/mol) / *r*(C-C) in **TS9** (in Å)	ΔE_{dist}	ΔE_{Pauli}	ΔE_{ct}	ΔE_{elstat}	ΔE_{pol}	ΔE_{disp}
2.12	71.31	327.67	-91.18	-173.53	-104.04	-24.97
2.09	72.63	345.75	-94.94	-180.71	-111.18	-26.02
2.06	74.14	367.45	-99.31	-189.01	-120.23	-27.30
2.03	75.85	390.79	-103.99	-197.75	-130.35	-28.69
2.0(TS)	77.70	417.86	-109.26	-207.22	-142.88	-30.35
1.97	79.73	447.00	-114.85	-217.00	-157.00	-32.15
1.94	81.88	478.90	-120.90	-227.29	-173.00	-34.15
1.91	84.09	513.79	-127.37	-237.82	-191.37	-36.35
1.87	86.35	551.33	-134.18	-248.60	-211.88	-38.72
1.84	88.67	591.27	-141.27	-259.48	-234.50	-41.23

Cartesian Coordinates (Å) and Energies of the Optimized Structures

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 5
B3LYP SCF energy:     -1471.36267339 a.u.
B3LYP enthalpy:     -1470.710613 a.u.
B3LYP free energy:     -1470.820964 a.u.
B3LYP-D3BJ SCF energy in solution:     -1473.10854763 a.u.
B3LYP-D3BJ enthalpy in solution:     -1472.456487 a.u.
B3LYP-D3BJ free energy in solution:     -1472.566838 a.u.
Three lowest frequencies (cm-1):       9.3191     16.1521     24.9771

Cartesian coordinates
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BMe3

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B3LYP free energy: -144.527559 a.u.
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Three lowest frequencies (cm-1): 17.9541 35.2057 111.5987

Cartesian coordinates

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6
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B3LYP-D3BJ free energy in solution: -1617.166186 a.u.
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C	2.923540	-0.078312	4.018879
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H	1.567595	2.314203	3.651752
H	3.158469	2.503234	2.901146
H	2.974743	-1.173098	3.994237
H	3.940770	0.299392	4.174509
H	2.323034	0.214729	4.887857
C	0.816856	2.790255	-2.857553
C	-1.467430	3.299895	0.248268
H	-0.774108	2.873145	0.997153
C	-1.775117	4.482963	-2.162472
H	-1.313558	4.889824	-3.075909
B	-0.709346	3.897141	-1.074774
C	0.463550	4.960167	-0.673284
H	1.229451	4.521224	-0.011185
H	0.997263	5.388475	-1.535960
H	0.037083	5.816178	-0.128789
Cu	0.005914	1.028168	-0.687125
O	-0.007852	2.598273	-1.723440
H	1.072308	1.819430	-3.301293
H	0.290010	3.385643	-3.612759
H	1.748396	3.310401	-2.594842
H	-2.215577	2.524747	0.007080
H	-2.013938	4.099038	0.771347
H	-2.350777	5.312810	-1.725328
H	-2.509291	3.726104	-2.482874

TS1
B3LYP SCF energy: -1615.97521013 a.u.
B3LYP enthalpy: -1615.199908 a.u.
B3LYP free energy: -1615.319311 a.u.
B3LYP-D3BJ SCF energy in solution: -1617.79013027 a.u.
B3LYP-D3BJ enthalpy in solution: -1617.014828 a.u.
B3LYP-D3BJ free energy in solution: -1617.134231 a.u.
Three lowest frequencies (cm-1): -256.3473 17.5128 25.8374
Imaginary frequency: -256.3473 cm-1

Cartesian coordinates

ATOM	X	Y	Z

N	-1.324224	0.606047	-1.084122
N	0.810353	0.750197	-1.301104
C	-0.154367	0.331375	-0.426260
C	-1.088647	1.182321	-2.328635
H	-1.893253	1.468294	-2.987233
C	0.257044	1.273194	-2.464899
H	0.869388	1.655271	-3.266409
C	-2.651688	0.351130	-0.571919
C	-3.295293	-0.851456	-0.930041
C	-3.270344	1.335741	0.225789
C	-4.600450	-1.049450	-0.462575
C	-4.574954	1.082318	0.666962
C	-5.234866	-0.095455	0.327980
H	-5.126857	-1.963111	-0.721329
H	-5.081417	1.819293	1.282662
H	-6.247710	-0.270370	0.680928
C	2.234740	0.683542	-1.064288
C	2.863063	1.770348	-0.423570
C	2.942532	-0.449399	-1.512484
C	4.247777	1.692382	-0.231278
C	4.326286	-0.469893	-1.298548
C	4.973769	0.586484	-0.664626
H	4.762927	2.508229	0.267451
H	4.901703	-1.330022	-1.627768
H	6.047736	0.546113	-0.503793
C	2.267090	-1.623349	-2.214270
C	2.511539	-2.949865	-1.469044
C	2.708803	-1.716689	-3.688732
H	1.187154	-1.446951	-2.207487
H	2.176781	-2.883280	-0.428931
H	1.962546	-3.761040	-1.963405
H	3.573318	-3.224107	-1.473609
H	2.490521	-0.791521	-4.235350
H	3.785803	-1.904993	-3.771449
H	2.187260	-2.539403	-4.192088
C	-2.637263	-1.898415	-1.824780
C	-3.200196	-1.826507	-3.259636
C	-2.770263	-3.325426	-1.262396
H	-1.567460	-1.673676	-1.876916
H	-3.054233	-0.834801	-3.702209
H	-2.702630	-2.560738	-3.904209
H	-4.275363	-2.041716	-3.270905
H	-2.393025	-3.385601	-0.237207
H	-3.810187	-3.671788	-1.263285
H	-2.194152	-4.024600	-1.879576
C	2.097965	2.996404	0.066150
C	2.625083	4.292872	-0.579300
C	2.119497	3.090331	1.604737
H	1.051911	2.888578	-0.236380
H	2.585987	4.240687	-1.673459
H	2.021050	5.149470	-0.257783
H	3.663413	4.494865	-0.292205
H	1.701129	2.187146	2.060845
H	3.140868	3.216304	1.982568
H	1.529514	3.951706	1.940817
C	-2.591978	2.657764	0.573385

C	-2.691231	2.999754	2.071339
C	-3.159603	3.803714	-0.290043
H	-1.527758	2.562844	0.339305
H	-2.300617	2.186754	2.691417
H	-2.108507	3.903049	2.286283
H	-3.724079	3.197468	2.380844
H	-3.036313	3.600908	-1.359992
H	-4.229676	3.948624	-0.099006
H	-2.646554	4.745699	-0.062657
C	-0.027550	-3.587758	1.631034
C	2.624565	-1.037123	2.737078
H	2.715688	-0.484969	1.791627
C	1.120243	-2.755592	4.236190
H	0.114725	-3.150832	4.430945
B	1.259323	-1.876736	2.894756
C	-0.279034	-0.460791	3.398758
H	-0.740010	0.523200	3.177023
H	-1.105033	-1.109852	3.712783
H	0.342600	-0.256200	4.273760
Cu	0.069909	-0.409182	1.358186
O	0.934146	-2.554980	1.641752
H	-0.113724	-3.964223	0.605090
H	0.264465	-4.421858	2.282437
H	-1.017300	-3.230809	1.957886
H	3.478866	-1.732653	2.770105
H	2.766497	-0.317040	3.553251
H	1.423798	-2.194396	5.128471
H	1.796547	-3.622915	4.167053

BMe2-OMe

B3LYP SCF energy: -219.87217783 a.u.
B3LYP enthalpy: -219.742695 a.u.
B3LYP free energy: -219.783379 a.u.
B3LYP-D3BJ SCF energy in solution: -219.95741005 a.u.
B3LYP-D3BJ enthalpy in solution: -219.827927 a.u.
B3LYP-D3BJ free energy in solution: -219.868611 a.u.
Three lowest frequencies (cm-1): 28.4436 97.7070 120.6810

Cartesian coordinates

ATOM	X	Y	Z
B	-0.485156	-0.001381	-0.000011
C	-1.870300	0.758600	0.000007
H	-2.470492	0.469464	-0.874849
H	-2.470211	0.469763	0.875162
H	-1.764445	1.848241	-0.000178
C	-0.382803	-1.586295	0.000002
H	0.169909	-1.954129	-0.876924
H	0.170258	-1.954188	0.876679
H	-1.362180	-2.075749	0.000171
O	0.631745	0.784740	-0.000036
C	1.949952	0.252726	0.000020
H	2.646833	1.095377	-0.000399
H	2.135628	-0.359627	0.890700
H	2.135426	-0.360354	-0.890201

7
B3LYP SCF energy: -1396.12798418 a.u.
B3LYP enthalpy: -1395.483137 a.u.
B3LYP free energy: -1395.590878 a.u.
B3LYP-D3BJ SCF energy in solution: -1397.84323263 a.u.
B3LYP-D3BJ enthalpy in solution: -1397.198385 a.u.
B3LYP-D3BJ free energy in solution: -1397.306126 a.u.
Three lowest frequencies (cm-1): 8.6707 19.1829 20.3393

Cartesian coordinates

ATOM	X	Y	Z
N	-1.074226	0.001755	-0.939305
N	1.074173	0.001978	-0.939384
C	0.000005	-0.000581	-0.093393
C	-0.678443	0.005387	-2.273163
H	-1.391802	0.007519	-3.082502
C	0.678297	0.005564	-2.273213
H	1.391597	0.007861	-3.082603
C	-2.453818	0.002279	-0.508877
C	-3.101578	-1.233357	-0.312342
C	-3.098985	1.238736	-0.308606
C	-4.439637	-1.202809	0.099221
C	-4.437058	1.209814	0.102942
C	-5.102675	0.003884	0.304855
H	-4.965772	-2.137935	0.268066
H	-4.961200	2.145520	0.274745
H	-6.140293	0.004490	0.627933
C	2.453769	0.002690	-0.508966
C	3.098531	1.239222	-0.307886
C	3.101911	-1.232867	-0.313185
C	4.436588	1.210460	0.103730
C	4.439936	-1.202161	0.098465
C	5.102576	0.004615	0.304914
H	4.960424	2.146225	0.276151
H	4.966371	-2.137221	0.266743
H	6.140171	0.005346	0.628061
C	2.395003	-2.571834	-0.498692
C	2.204539	-3.284127	0.855611
C	3.125790	-3.475941	-1.509769
H	1.397375	-2.376159	-0.903433
H	1.644265	-2.654079	1.554794
H	1.653066	-4.222140	0.718214
H	3.169266	-3.526710	1.316907
H	3.234350	-2.983771	-2.483142
H	4.128255	-3.748883	-1.160739
H	2.565082	-4.405963	-1.659611
C	-2.394292	-2.572226	-0.497051
C	-3.124580	-3.476927	-1.507955
C	-2.204055	-3.283909	0.857612
H	-1.396581	-2.376492	-0.901555
H	-3.232933	-2.985215	-2.481583
H	-2.563649	-4.406909	-1.657206
H	-4.127105	-3.749892	-1.159113

H	-1.644190	-2.653403	1.556709
H	-3.168852	-3.526612	1.318694
H	-1.652244	-4.221806	0.720767
C	2.387813	2.576979	-0.487786
C	3.118601	3.489503	-1.491253
C	2.190664	3.280707	0.870045
H	1.392108	2.380484	-0.896831
H	3.232581	3.003076	-2.466884
H	2.554690	4.418074	-1.638023
H	4.118707	3.764619	-1.137220
H	1.629132	2.645301	1.563358
H	3.153149	3.522614	1.336361
H	1.637630	4.218316	0.736208
C	-2.388618	2.576589	-0.489177
C	-2.191360	3.280824	0.868383
C	-3.119779	3.488632	-1.492798
H	-1.392949	2.380173	-0.898354
H	-1.629543	2.645784	1.561796
H	-1.638577	4.218521	0.734124
H	-3.153817	3.522644	1.334801
H	-3.233924	3.001839	-2.468228
H	-4.119835	3.763756	-1.138635
H	-2.556027	4.417224	-1.640035
C	0.000364	-0.028141	3.806267
Cu	0.000108	-0.011739	1.868266
H	0.888951	0.473724	4.219029
H	-0.883195	0.482254	4.219366
H	-0.004517	-1.053912	4.206371

8

B3LYP SCF energy: -308.39359568 a.u.
B3LYP enthalpy: -308.276663 a.u.
B3LYP free energy: -308.314525 a.u.
B3LYP-D3BJ SCF energy in solution: -308.50579102 a.u.
B3LYP-D3BJ enthalpy in solution: -308.388858 a.u.
B3LYP-D3BJ free energy in solution: -308.426720 a.u.
Three lowest frequencies (cm-1): 145.6993 158.5995 377.5968

Cartesian coordinates

ATOM	X	Y	Z
C	-1.512560	-1.208565	-0.000007
C	-0.119960	-1.213090	0.000004
C	0.594248	-0.000023	0.000017
C	-0.119937	1.213079	0.000006
C	-1.512522	1.208589	-0.000008
C	-2.213021	0.000015	-0.000011
H	-2.053007	-2.151281	-0.000011
H	0.428540	-2.149975	0.000009
H	0.428609	2.149937	0.000011
H	-2.052964	2.151309	-0.000013
H	-3.299617	0.000039	-0.000020
C	2.024188	-0.000018	0.000038
C	3.234231	0.000000	0.000001
H	4.300438	0.000054	-0.000220

TS2
B3LYP SCF energy: -1704.47142912 a.u.
B3LYP enthalpy: -1703.708660 a.u.
B3LYP free energy: -1703.829524 a.u.
B3LYP-D3BJ SCF energy in solution: -1706.31547727 a.u.
B3LYP-D3BJ enthalpy in solution: -1705.552708 a.u.
B3LYP-D3BJ free energy in solution: -1705.673572 a.u.
Three lowest frequencies (cm-1): -347.4256 12.5959 15.8115
Imaginary frequency: -347.4256 cm-1

Cartesian coordinates

ATOM	X	Y	Z
C	-0.805726	0.615138	-0.050844
C	-1.739182	2.679664	-0.353226
H	-1.739545	3.752221	-0.467646
C	-2.751316	1.778356	-0.342697
H	-3.818018	1.903321	-0.442314
C	-2.918640	-0.705391	-0.095122
C	-3.309201	-1.192963	1.168310
C	-4.049694	-2.381779	1.198959
H	-4.364693	-2.786518	2.156292
C	-4.390875	-3.050258	0.027130
H	-4.966156	-3.971065	0.075753
C	-3.999393	-2.540425	-1.208172
H	-4.275940	-3.068425	-2.115784
C	-3.253641	-1.358934	-1.299782
C	-2.871391	-0.801122	-2.668814
H	-2.129666	-0.011219	-2.515213
C	-4.095342	-0.162722	-3.358183
H	-3.809568	0.272539	-4.323228
H	-4.534420	0.632355	-2.744979
H	-4.876826	-0.909178	-3.544025
C	-2.221770	-1.856509	-3.583197
H	-1.342330	-2.306072	-3.111695
H	-1.904338	-1.389988	-4.523306
H	-2.919679	-2.662015	-3.838863
C	-2.995595	-0.462370	2.470550
H	-2.340424	0.381527	2.236250
C	-2.236065	-1.352173	3.472258
H	-2.827437	-2.226427	3.770429
H	-2.014800	-0.779868	4.381529
H	-1.287127	-1.694707	3.046713
C	-4.283745	0.112201	3.095267
H	-4.804391	0.781987	2.400651
H	-4.046342	0.681108	4.002003
H	-4.982753	-0.684969	3.375339
C	0.748843	2.558241	-0.126590
C	1.468064	2.710851	-1.329473
C	2.733260	3.306490	-1.256029
H	3.315267	3.434932	-2.164370
C	3.257669	3.734392	-0.039448
H	4.242734	4.192153	-0.004279
C	2.522471	3.576833	1.132052

H	2.941647	3.914616	2.075441
C	1.252221	2.986826	1.118275
C	0.469555	2.844144	2.420162
H	-0.467928	2.326308	2.198427
C	0.107755	4.224013	3.005370
H	-0.495373	4.105786	3.913251
H	-0.467174	4.825493	2.291540
H	1.004999	4.794037	3.273624
C	1.225094	1.979771	3.447265
H	1.416998	0.981117	3.043518
H	0.626291	1.871403	4.359623
H	2.183190	2.431467	3.730569
C	0.918210	2.264289	-2.680745
H	-0.067065	1.818452	-2.516117
C	1.803215	1.178417	-3.322066
H	2.813318	1.550895	-3.529274
H	1.369285	0.846891	-4.272936
H	1.889813	0.307632	-2.664024
C	0.726544	3.461366	-3.633130
H	0.065055	4.218343	-3.196346
H	0.283965	3.128676	-4.579499
H	1.681065	3.947914	-3.865342
N	-0.562169	1.957273	-0.175917
N	-2.168283	0.526496	-0.162972
Cu	0.474374	-0.798766	0.337118
C	0.860306	-2.448385	-1.000285
H	-0.233234	-2.499294	-1.086785
H	1.303635	-2.047610	-1.914900
H	1.228885	-3.456265	-0.819728
C	1.367670	-1.659443	1.956333
C	1.983528	-2.035034	0.874937
C	3.275346	-2.573708	0.443201
C	3.998760	-2.030930	-0.632549
C	3.848397	-3.637705	1.163161
C	5.255769	-2.528338	-0.970840
H	3.567152	-1.208801	-1.195815
C	5.104477	-4.137920	0.820537
H	3.293398	-4.067311	1.992399
C	5.814343	-3.585886	-0.247862
H	5.802534	-2.089175	-1.801862
H	5.527588	-4.963421	1.387775
H	6.792253	-3.976949	-0.516472
H	1.802939	-1.578043	2.951197

TS3
B3LYP SCF energy: -1704.47768746 a.u.
B3LYP enthalpy: -1703.714292 a.u.
B3LYP free energy: -1703.835420 a.u.
B3LYP-D3BJ SCF energy in solution: -1706.32096997 a.u.
B3LYP-D3BJ enthalpy in solution: -1705.557575 a.u.
B3LYP-D3BJ free energy in solution: -1705.678703 a.u.
Three lowest frequencies (cm-1): -338.3927 13.1908 19.0667
Imaginary frequency: -338.3927 cm-1

Cartesian coordinates

ATOM	X	Y	Z
C	-0.742111	0.478058	0.286419
C	-1.172489	1.879895	2.038394
H	-0.993689	2.714258	2.697890
C	-2.165071	0.957884	2.008709
H	-3.026617	0.817230	2.641822
C	-2.725015	-1.008033	0.568744
C	-2.353673	-2.295925	1.004955
C	-3.180774	-3.365002	0.635288
H	-2.918927	-4.371256	0.949454
C	-4.331640	-3.159968	-0.119079
H	-4.959237	-4.004130	-0.392251
C	-4.684008	-1.873969	-0.520951
H	-5.588226	-1.726426	-1.103639
C	-3.889588	-0.769168	-0.192354
C	-4.317784	0.632900	-0.621134
H	-3.466813	1.305273	-0.473000
C	-5.476225	1.144372	0.261187
H	-5.756585	2.164666	-0.026299
H	-5.204403	1.154870	1.322507
H	-6.362624	0.508169	0.152340
C	-4.702278	0.715154	-2.110547
H	-3.892865	0.356852	-2.754304
H	-4.918534	1.755387	-2.380890
H	-5.599712	0.127657	-2.335684
C	-1.130150	-2.558660	1.878940
H	-0.613345	-1.608223	2.039298
C	-0.125393	-3.506557	1.196949
H	-0.571371	-4.486546	0.988794
H	0.740989	-3.666853	1.849174
H	0.237811	-3.082331	0.255433
C	-1.549904	-3.091333	3.264203
H	-2.233983	-2.400304	3.770571
H	-0.668163	-3.225000	3.901730
H	-2.054035	-4.061699	3.186147
C	0.908545	2.293893	0.716500
C	0.903222	3.293845	-0.276047
C	2.102658	3.978795	-0.509492
H	2.133269	4.752722	-1.271198
C	3.251919	3.687370	0.219352
H	4.171818	4.231553	0.022432
C	3.224938	2.701590	1.202816
H	4.126800	2.485603	1.767737
C	2.056428	1.979339	1.473758
C	2.049101	0.925834	2.578855
H	1.114774	0.361850	2.501115
C	2.074475	1.595225	3.968956
H	2.030993	0.836953	4.759692
H	1.227638	2.277397	4.106797
H	2.994230	2.175244	4.110385
C	3.197045	-0.089958	2.440013
H	3.182312	-0.582525	1.463805
H	3.105160	-0.860880	3.214285
H	4.178583	0.381835	2.566412
C	-0.344670	3.662212	-1.072496

H	-1.158285	3.004374	-0.753115
C	-0.144044	3.434247	-2.582954
H	0.648115	4.076013	-2.986273
H	-1.067872	3.664418	-3.126974
H	0.123919	2.393029	-2.789627
C	-0.784877	5.110549	-0.779894
H	-0.964817	5.265137	0.290197
H	-1.711684	5.343470	-1.317532
H	-0.025362	5.834403	-1.097639
N	-0.312235	1.572716	0.988408
N	-1.894052	0.115183	0.933989
Cu	0.110929	-0.360136	-1.249588
C	-0.948234	-0.645148	-3.128159
H	-1.878607	-0.555953	-2.554568
H	-0.845310	0.201979	-3.810532
H	-0.988641	-1.582169	-3.683793
C	1.776395	-1.447979	-1.765087
C	1.115097	-1.111395	-2.818781
H	1.237480	-1.048190	-3.894488
C	3.082397	-1.973870	-1.432330
C	3.318107	-3.366131	-1.425490
C	4.158580	-1.125502	-1.091147
C	4.572290	-3.880393	-1.102683
H	2.502980	-4.037927	-1.681027
C	5.410754	-1.648565	-0.772489
H	3.999402	-0.050381	-1.083386
C	5.630336	-3.028727	-0.773823
H	4.724140	-4.957611	-1.111161
H	6.223411	-0.969515	-0.523096
H	6.606772	-3.433069	-0.520892

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B3LYP SCF energy: -1704.57792271 a.u.
B3LYP enthalpy: -1703.810041 a.u.
B3LYP free energy: -1703.932446 a.u.
B3LYP-D3BJ SCF energy in solution: -1706.41676868 a.u.
B3LYP-D3BJ enthalpy in solution: -1705.648887 a.u.
B3LYP-D3BJ free energy in solution: -1705.771292 a.u.
Three lowest frequencies (cm-1): 9.4054 14.7346 15.2659

Cartesian coordinates

ATOM	X	Y	Z
C	1.298356	-0.227157	0.005615
C	3.578193	-0.201308	0.063972
H	4.557334	0.250006	0.100166
C	3.189948	-1.500995	0.020538
H	3.760466	-2.416497	0.011270
C	0.989837	-2.694227	-0.064991
C	0.624686	-3.210501	-1.324221
C	-0.157544	-4.371957	-1.342355
H	-0.464620	-4.792375	-2.295565
C	-0.555825	-4.991165	-0.160803
H	-1.166559	-5.889189	-0.198595
C	-0.178346	-4.458862	1.068962

H	-0.501107	-4.945834	1.984522
C	0.603220	-3.299621	1.147294
C	0.977103	-2.726776	2.510919
H	1.656063	-1.883360	2.351896
C	1.726777	-3.753779	3.381221
H	2.032946	-3.294978	4.328579
H	2.626106	-4.126237	2.877308
H	1.097681	-4.618242	3.622384
C	-0.266677	-2.177374	3.238020
H	-0.771070	-1.415230	2.634678
H	0.020942	-1.724468	4.194502
H	-0.989979	-2.973966	3.448817
C	1.027264	-2.545872	-2.636858
H	1.671646	-1.692855	-2.402774
C	-0.205538	-1.991565	-3.378302
H	-0.894765	-2.794347	-3.665595
H	0.103291	-1.472725	-4.293717
H	-0.755895	-1.283030	-2.750406
C	1.841020	-3.497463	-3.534980
H	2.734374	-3.869170	-3.019995
H	2.164348	-2.976194	-4.443578
H	1.249753	-4.366373	-3.846243
C	2.393973	2.005088	0.086669
C	2.350940	2.652859	1.337194
C	2.339022	4.053190	1.337875
H	2.297814	4.584623	2.284289
C	2.369229	4.774628	0.147674
H	2.356017	5.861001	0.171616
C	2.410482	4.107045	-1.073302
H	2.424958	4.679949	-1.995987
C	2.424858	2.708130	-1.134027
C	2.438594	2.007646	-2.489413
H	2.541394	0.931960	-2.316264
C	3.637555	2.443802	-3.353065
H	3.653773	1.876706	-4.291072
H	4.588343	2.272053	-2.835484
H	3.586658	3.507329	-3.612901
C	1.104194	2.223594	-3.231289
H	0.259429	1.866221	-2.632598
H	1.105010	1.680419	-4.183949
H	0.938138	3.284999	-3.450312
C	2.286033	1.892602	2.658223
H	2.386983	0.824678	2.441946
C	0.916675	2.090600	3.338576
H	0.749078	3.142402	3.598686
H	0.862248	1.503407	4.263097
H	0.101685	1.771656	2.680043
C	3.442678	2.276398	3.600860
H	4.417540	2.109211	3.128380
H	3.400525	1.674497	4.516109
H	3.392433	3.330281	3.897509
N	2.414211	0.560146	0.054269
N	1.799550	-1.498049	-0.014487
Cu	-0.571245	0.339752	-0.019748
C	-2.387314	0.949218	-0.035878
C	-3.542117	0.236412	-0.006600

C	-4.892619	0.875944	-0.025191
C	-6.016912	0.244582	0.542555
C	-5.105301	2.133005	-0.627182
C	-7.275387	0.848630	0.540419
H	-5.906240	-0.729317	1.009453
C	-6.359790	2.737231	-0.634990
H	-4.270398	2.629884	-1.112168
C	-7.456742	2.100857	-0.046641
H	-8.117226	0.334966	0.999651
H	-6.485564	3.705652	-1.114323
H	-8.437317	2.570124	-0.055608
H	-2.541736	2.035978	-0.041160
C	-3.533651	-1.280818	0.074840
H	-4.183804	-1.738486	-0.684438
H	-2.516662	-1.657685	-0.066603
H	-3.885490	-1.647054	1.050617

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B3LYP SCF energy: -1704.58002369 a.u.
B3LYP enthalpy: -1703.812555 a.u.
B3LYP free energy: -1703.935946 a.u.
B3LYP-D3BJ SCF energy in solution: -1706.42236273 a.u.
B3LYP-D3BJ enthalpy in solution: -1705.654894 a.u.
B3LYP-D3BJ free energy in solution: -1705.778285 a.u.
Three lowest frequencies (cm-1): 7.8994 17.2614 20.0841

Cartesian coordinates

ATOM	X	Y	Z
C	-0.620524	0.682225	0.319357
C	-0.838709	2.617377	1.505766
H	-0.508751	3.546207	1.943888
C	-2.048308	2.002308	1.510934
H	-2.989922	2.283381	1.955910
C	-2.966708	-0.117558	0.548792
C	-3.117784	-1.202966	1.434494
C	-4.168142	-2.095422	1.186534
H	-4.308028	-2.947467	1.845343
C	-5.030895	-1.912673	0.109515
H	-5.838470	-2.618726	-0.064413
C	-4.858961	-0.828988	-0.747392
H	-5.534738	-0.698623	-1.587765
C	-3.823961	0.093443	-0.549916
C	-3.657651	1.264090	-1.514297
H	-2.800123	1.858285	-1.184358
C	-4.889097	2.191044	-1.497063
H	-4.727534	3.050159	-2.158629
H	-5.091173	2.571355	-0.489097
H	-5.789715	1.670650	-1.842947
C	-3.347339	0.777392	-2.943345
H	-2.447177	0.154467	-2.961869
H	-3.186185	1.634195	-3.608441
H	-4.173805	0.187042	-3.355722
C	-2.187119	-1.440260	2.619749
H	-1.477752	-0.608579	2.668032

C	-1.363673	-2.729916	2.430555
H	-2.010848	-3.613907	2.387060
H	-0.670206	-2.864001	3.269341
H	-0.779504	-2.692743	1.504760
C	-2.957802	-1.458666	3.954292
H	-3.521766	-0.530912	4.105210
H	-2.260402	-1.572962	4.792300
H	-3.668354	-2.292000	4.000266
C	1.410802	2.108412	0.538626
C	1.753282	2.832960	-0.620448
C	3.105783	3.141563	-0.811652
H	3.405786	3.692428	-1.698357
C	4.071290	2.751890	0.112652
H	5.114989	3.004211	-0.054665
C	3.703538	2.033258	1.246851
H	4.466098	1.725370	1.955998
C	2.367271	1.688956	1.484954
C	1.997688	0.891703	2.731665
H	0.940647	0.619322	2.656789
C	2.166339	1.742258	4.006868
H	1.863567	1.169776	4.891563
H	1.557137	2.652910	3.967672
H	3.210411	2.046461	4.146734
C	2.795548	-0.422970	2.829269
H	2.693544	-1.020050	1.917721
H	2.434299	-1.018491	3.676061
H	3.863948	-0.238152	2.990347
C	0.723473	3.259129	-1.662247
H	-0.268959	2.984422	-1.292089
C	0.938806	2.505418	-2.990126
H	1.914972	2.742749	-3.429097
H	0.167258	2.785846	-3.717242
H	0.891391	1.421611	-2.839619
C	0.721982	4.784629	-1.878987
H	0.544394	5.323184	-0.941011
H	-0.066380	5.065325	-2.587145
H	1.674935	5.136566	-2.290473
N	0.018300	1.800375	0.776384
N	-1.897782	0.826811	0.783102
Cu	0.155774	-0.807198	-0.679398
C	-1.046181	-3.045337	-2.894056
H	-1.583488	-3.984072	-2.689102
H	-1.576499	-2.235332	-2.379833
H	-1.128404	-2.873916	-3.978387
C	1.003809	-2.303412	-1.571074
C	0.390080	-3.124346	-2.450221
H	0.958243	-3.933938	-2.928366
C	2.426336	-2.582121	-1.237736
C	2.891684	-3.886519	-0.967759
C	3.370347	-1.537882	-1.149401
C	4.226666	-4.134930	-0.646790
H	2.182278	-4.709559	-0.998937
C	4.707961	-1.783487	-0.839297
H	3.039208	-0.519420	-1.341076
C	5.146597	-3.085601	-0.583657
H	4.549474	-5.153416	-0.440078

H	5.409586	-0.953143	-0.791871
H	6.186383	-3.278073	-0.330710

MeOK

B3LYP SCF energy: -143.25464514 a.u.
B3LYP enthalpy: -143.210208 a.u.
B3LYP free energy: -143.243522 a.u.
B3LYP-D3BJ SCF energy in solution: -143.51225879 a.u.
B3LYP-D3BJ enthalpy in solution: -143.467822 a.u.
B3LYP-D3BJ free energy in solution: -143.501136 a.u.
Three lowest frequencies (cm-1): 95.1828 95.6288 340.5410

Cartesian coordinates

ATOM	X	Y	Z
C	2.199719	-0.000291	-0.000002
H	2.660890	1.021177	0.001303
H	2.659931	-0.510542	-0.885329
H	2.659940	-0.512810	0.884008
O	0.838964	0.000781	0.000006
K	-1.467936	-0.000122	-0.000001

TS4

B3LYP SCF energy: -596.27053861 a.u.
B3LYP enthalpy: -595.985032 a.u.
B3LYP free energy: -596.057022 a.u.
B3LYP-D3BJ SCF energy in solution: -596.71034904 a.u.
B3LYP-D3BJ enthalpy in solution: -596.424842 a.u.
B3LYP-D3BJ free energy in solution: -596.496832 a.u.
Three lowest frequencies (cm-1): -171.4810 9.3423 17.1551
Imaginary frequency: -171.4810 cm-1

Cartesian coordinates

ATOM	X	Y	Z
H	-1.414611	1.020001	-0.120186
C	-2.462009	3.014773	0.204784
O	-2.732926	1.689941	-0.099007
C	-0.331474	0.533741	-0.070568
C	0.896947	0.507051	-0.097597
C	-1.921566	-1.181378	1.555087
H	-2.384972	-0.188275	1.500026
C	0.329685	-2.425334	0.670198
H	1.060915	-2.511521	-0.143066
B	-0.941855	-1.525281	0.311527
C	-1.582378	-1.808799	-1.153492
H	-2.037692	-0.940168	-1.649306
H	-0.828792	-2.176981	-1.859903
H	-2.343275	-2.610204	-1.083050
H	-1.388145	-1.213655	2.512793
H	-2.716470	-1.949890	1.632441
H	-0.024881	-3.449122	0.881665
H	0.862616	-2.092558	1.569612
K	-4.205304	-0.213966	-0.370887

H	-1.380074	3.192467	0.381059
H	-2.756276	3.720039	-0.600495
H	-2.980349	3.366826	1.122560
C	2.318359	0.402804	-0.104397
C	3.055677	0.582190	1.084267
C	3.013178	0.121206	-1.298753
C	4.444333	0.480432	1.075163
H	2.522603	0.800512	2.004324
C	4.401988	0.020315	-1.300223
H	2.447691	-0.015218	-2.215372
C	5.121084	0.199251	-0.115066
H	5.001277	0.620115	1.997819
H	4.925973	-0.197925	-2.226965
H	6.204988	0.120263	-0.119090

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B3LYP SCF energy: -596.32665710 a.u.
B3LYP enthalpy: -596.035891 a.u.
B3LYP free energy: -596.106682 a.u.
B3LYP-D3BJ SCF energy in solution: -596.76472000 a.u.
B3LYP-D3BJ enthalpy in solution: -596.473954 a.u.
B3LYP-D3BJ free energy in solution: -596.544745 a.u.
Three lowest frequencies (cm-1): 22.9132 36.1875 41.6024

Cartesian coordinates

ATOM	X	Y	Z
H	-0.483806	1.445057	0.743113
C	-0.939037	3.247961	1.403341
O	-0.632348	2.332995	0.352511
C	-0.793374	-0.856454	0.299181
C	0.412753	-0.619655	0.222325
C	-3.301766	0.075889	0.757204
H	-3.395176	0.882111	0.000979
C	-2.525868	-2.377682	1.536909
H	-1.930638	-3.280173	1.336019
B	-2.362995	-1.233316	0.364642
C	-2.839982	-1.887697	-1.087424
H	-2.202465	-2.724209	-1.407455
H	-3.859760	-2.286385	-0.988595
H	-2.898633	-1.200072	-1.959699
H	-2.980220	0.571421	1.685707
H	-4.333278	-0.263281	0.928604
H	-3.575930	-2.698170	1.618994
H	-2.224677	-2.013641	2.530081
K	-1.469541	0.962954	-1.792590
H	-0.117093	3.318868	2.127451
H	-1.083834	4.230364	0.945945
H	-1.858896	2.963705	1.929991
C	1.838931	-0.487253	0.133940
C	2.653807	-1.638065	0.077009
C	2.464539	0.776809	0.088934
C	4.038146	-1.524842	-0.024713
H	2.182101	-2.615123	0.116918
C	3.850787	0.881476	-0.013562

H	1.849773	1.671448	0.142107
C	4.644631	-0.266272	-0.072300
H	4.647623	-2.424070	-0.064939
H	4.313386	1.865031	-0.043881
H	5.725165	-0.181670	-0.150489

TS5

B3LYP SCF energy: -596.25928509 a.u.
B3LYP enthalpy: -595.970446 a.u.
B3LYP free energy: -596.047460 a.u.
B3LYP-D3BJ SCF energy in solution: -596.69823926 a.u.
B3LYP-D3BJ enthalpy in solution: -596.409400 a.u.
B3LYP-D3BJ free energy in solution: -596.486414 a.u.
Three lowest frequencies (cm-1): -444.9912 12.1912 15.4008
Imaginary frequency: -444.9912 cm-1

Cartesian coordinates

ATOM	X	Y	Z
H	-5.138069	-1.561235	1.201507
C	-5.404009	-1.984772	-0.693508
O	-4.571951	-1.625569	0.417382
C	0.121212	1.003293	0.006317
C	0.682092	-0.178133	0.092366
C	-1.413898	2.803020	1.309905
H	-0.784730	2.605948	2.186422
C	-1.596013	2.526376	-1.418695
H	-1.080647	2.157003	-2.313647
B	-0.866885	2.122474	-0.042004
C	1.096758	2.495069	-0.202693
H	1.655186	2.251864	-1.107002
H	0.715534	3.518227	-0.307561
H	1.737035	2.462434	0.679279
H	-2.419900	2.409649	1.544466
H	-1.542209	3.891648	1.221664
H	-1.734278	3.611743	-1.529736
H	-2.615011	2.098951	-1.439418
K	-1.945996	-0.934524	0.371177
H	-4.753212	-2.053179	-1.568372
H	-5.884948	-2.958290	-0.538039
H	-6.170720	-1.224301	-0.885853
C	2.095272	-0.514649	0.023354
C	2.877210	-0.671654	1.191191
C	2.740956	-0.748847	-1.213142
C	4.222391	-1.028295	1.124415
H	2.407171	-0.509806	2.159002
C	4.085697	-1.108699	-1.276112
H	2.164266	-0.646420	-2.129954
C	4.841767	-1.252473	-0.108981
H	4.793606	-1.133015	2.045111
H	4.548939	-1.276475	-2.246778
H	5.889330	-1.538022	-0.158988

TS6
B3LYP SCF energy: -596.25439349 a.u.
B3LYP enthalpy: -595.965440 a.u.
B3LYP free energy: -596.040183 a.u.
B3LYP-D3BJ SCF energy in solution: -596.69300586 a.u.
B3LYP-D3BJ enthalpy in solution: -596.404052 a.u.
B3LYP-D3BJ free energy in solution: -596.478795 a.u.
Three lowest frequencies (cm-1): -436.7426 13.2018 20.1148
Imaginary frequency: -436.7426 cm-1

Cartesian coordinates

ATOM	X	Y	Z
H	4.657934	-2.505827	0.000137
C	4.673900	-0.543851	0.000031
O	3.986893	-1.807540	-0.000017
C	-2.283322	-0.202362	0.000044
C	-0.991393	-0.316671	0.000034
C	-4.534432	0.328376	-1.375713
H	-4.001090	-0.021178	-2.268630
C	-4.534410	0.328151	1.375931
H	-4.001073	-0.021592	2.268776
B	-3.749278	0.055856	0.000081
C	-3.196397	-1.848113	-0.000122
H	-2.765847	-2.278697	0.903664
H	-4.276789	-2.036630	-0.000038
H	-2.766019	-2.278468	-0.904099
H	-4.683151	1.411583	-1.497657
H	-5.538543	-0.121476	-1.382221
H	-5.538540	-0.121659	1.382365
H	-4.683081	1.411342	1.498079
K	1.299655	-1.901612	-0.000206
H	3.913856	0.241056	-0.000062
H	5.297318	-0.431480	0.895744
H	5.297514	-0.431519	-0.895552
C	-0.014107	0.756879	0.000063
C	0.558716	1.245764	1.206837
C	0.558296	1.246215	-1.206726
C	1.621836	2.147198	1.203288
H	0.134870	0.910462	2.151595
C	1.621424	2.147637	-1.203208
H	0.134127	0.911258	-2.151460
C	2.177075	2.602006	0.000028
H	2.016681	2.507614	2.151778
H	2.015949	2.508398	-2.151701
H	3.000573	3.311098	0.000016

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B3LYP SCF energy: -453.06275761 a.u.
B3LYP enthalpy: -452.818037 a.u.
B3LYP free energy: -452.872430 a.u.
B3LYP-D3BJ SCF energy in solution: -453.23646774 a.u.
B3LYP-D3BJ enthalpy in solution: -452.991747 a.u.
B3LYP-D3BJ free energy in solution: -453.046140 a.u.
Three lowest frequencies (cm-1): 29.8161 46.7325 75.4949

Cartesian coordinates

ATOM	X	Y	Z
C	-1.434404	0.308212	0.149643
C	-0.372773	-0.513839	-0.068162
C	-3.203887	-1.807497	-0.224900
H	-2.392976	-2.517653	-0.033991
C	-4.113133	0.731418	-0.086844
H	-3.904792	1.681871	-0.594096
B	-2.879429	-0.266558	-0.054411
C	-1.272305	1.765713	0.542529
H	-2.090532	2.084622	1.197105
H	-0.331198	1.957508	1.067295
H	-1.303172	2.433255	-0.330891
H	-0.601384	-1.559697	-0.267004
C	1.074982	-0.248362	-0.060765
C	1.657354	0.988156	-0.401214
C	1.939718	-1.313044	0.264274
C	3.041310	1.155416	-0.386359
H	1.027743	1.813320	-0.712843
C	3.320785	-1.142586	0.293680
H	1.511116	-2.282729	0.507180
C	3.878517	0.096691	-0.029789
H	3.467695	2.116546	-0.661743
H	3.963227	-1.977637	0.560447
H	4.956616	0.232279	-0.015945
H	-3.567346	-1.986273	-1.249130
H	-4.047820	-2.080864	0.425107
H	-4.368111	1.001084	0.952204
H	-5.018899	0.295480	-0.524205

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B3LYP SCF energy: -453.06023846 a.u.
B3LYP enthalpy: -452.816221 a.u.
B3LYP free energy: -452.871382 a.u.
B3LYP-D3BJ SCF energy in solution: -453.23572525 a.u.
B3LYP-D3BJ enthalpy in solution: -452.991708 a.u.
B3LYP-D3BJ free energy in solution: -453.046869 a.u.
Three lowest frequencies (cm-1): 28.7990 41.0558 62.2699

Cartesian coordinates

ATOM	X	Y	Z
H	0.292657	-2.446872	-0.288486
C	1.636799	-0.847888	-0.048572
C	0.393366	-1.365415	-0.165503
C	1.556571	1.353461	1.571216
H	2.351552	1.121104	2.301440
C	2.927003	1.459758	-0.778493
H	3.296011	0.897452	-1.642648
B	1.987565	0.660401	0.217136
C	2.832403	-1.779640	-0.162400
H	3.470616	-1.504241	-1.012682
H	3.472695	-1.734800	0.729873
H	2.522464	-2.822410	-0.295806

H	0.625343	0.969471	1.998738
H	1.507177	2.447927	1.517138
H	3.792527	1.877094	-0.242410
H	2.382841	2.337577	-1.159248
C	-0.883063	-0.636089	-0.161942
C	-1.001176	0.699188	-0.588838
C	-2.053047	-1.292161	0.266607
C	-2.223948	1.366803	-0.540096
H	-0.133289	1.207638	-1.001561
C	-3.276905	-0.629607	0.311452
H	-1.989329	-2.331161	0.582092
C	-3.367268	0.707166	-0.085725
H	-2.287536	2.398388	-0.876717
H	-4.163263	-1.156579	0.655360
H	-4.322708	1.223951	-0.056993

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B3LYP SCF energy: -1664.04550863 a.u.
B3LYP enthalpy: -1663.329987 a.u.
B3LYP free energy: -1663.450591 a.u.
B3LYP-D3BJ SCF energy in solution: -1665.85987607 a.u.
B3LYP-D3BJ enthalpy in solution: -1665.144354 a.u.
B3LYP-D3BJ free energy in solution: -1665.264958 a.u.
Three lowest frequencies (cm-1): 8.8476 9.5577 11.2502

Cartesian coordinates

ATOM	X	Y	Z
N	2.090396	1.073722	0.083719
N	2.088541	-1.076661	0.083654
C	1.249196	-0.000742	0.032714
C	3.420130	0.676091	0.165791
C	3.418957	-0.681337	0.165721
H	4.225898	-1.395553	0.214115
C	1.656479	2.452705	0.051367
C	1.541130	3.094355	-1.197711
C	1.367566	3.098849	1.269578
C	1.120247	4.429829	-1.199481
C	0.951653	4.434415	1.207507
C	0.829101	5.094903	-0.011690
H	1.011399	4.952302	-2.145300
H	0.711978	4.960054	2.127287
H	0.499759	6.130145	-0.036666
C	1.652240	-2.454891	0.051332
C	1.362484	-3.100589	1.269580
C	1.535449	-3.096259	-1.197760
C	0.944255	-4.435436	1.207542
C	1.112254	-4.430999	-1.199494
C	0.820281	-5.095642	-0.011662
H	0.703898	-4.960727	2.127347
H	1.002225	-4.953238	-2.145309
H	0.489166	-6.130320	-0.036618
C	1.814236	-2.386269	-2.519241
C	0.509453	-2.174167	-3.313236
C	2.868600	-3.127991	-3.363063

H	2.221479	-1.395557	-2.294526
H	-0.220599	-1.604748	-2.728310
H	0.712155	-1.624498	-4.240280
H	0.049156	-3.131550	-3.584033
H	3.806104	-3.258348	-2.810364
H	2.520234	-4.121422	-3.667695
H	3.087941	-2.562388	-4.276142
C	1.819047	2.383975	-2.519163
C	2.874839	3.123981	-3.362712
C	0.514093	2.174084	-3.313472
H	2.224584	1.392569	-2.294417
H	3.812422	3.252775	-2.809783
H	3.093463	2.558040	-4.275753
H	2.528188	4.117993	-3.667401
H	-0.217037	1.605860	-2.728731
H	0.055438	3.132236	-3.584340
H	0.716087	1.624109	-4.240490
C	1.458800	-2.397316	2.619680
C	2.418867	-3.125677	3.579796
C	0.062305	-2.220102	3.249167
H	1.866772	-1.395409	2.454263
H	3.419837	-3.228056	3.145008
H	2.511271	-2.567369	4.518656
H	2.059114	-4.130714	3.828210
H	-0.603978	-1.664438	2.580712
H	-0.405541	-3.188632	3.461537
H	0.138477	-1.670068	4.194858
C	1.462425	2.395367	2.619662
C	0.065526	2.220610	3.248959
C	2.423655	3.121969	3.579953
H	1.868605	1.392726	2.454281
H	-0.601670	1.666213	2.580361
H	0.140598	1.670331	4.194597
H	-0.400625	3.189947	3.461392
H	3.424895	3.222496	3.145353
H	2.065712	4.127671	3.828290
H	2.514848	2.563501	4.518836
C	-2.554460	0.002026	-0.100419
C	-3.785302	0.002639	-0.120452
Cu	-0.679323	0.000803	-0.050574
H	4.228301	1.388913	0.214213
C	-5.212068	0.003300	-0.140023
C	-5.923926	0.003485	-1.358954
C	-5.955268	0.003763	1.060161
C	-7.316765	0.004100	-1.373556
H	-5.364657	0.003135	-2.289956
C	-7.347942	0.004376	1.039123
H	-5.420113	0.003628	2.005257
C	-8.037723	0.004546	-0.176340
H	-7.843414	0.004228	-2.325057
H	-7.898844	0.004722	1.976804
H	-9.124606	0.005022	-0.190381

TS7

B3LYP SCF energy: -1808.64300236 a.u.
B3LYP enthalpy: -1807.805014 a.u.
B3LYP free energy: -1807.939185 a.u.
B3LYP-D3BJ SCF energy in solution: -1810.53359969 a.u.
B3LYP-D3BJ enthalpy in solution: -1809.695611 a.u.
B3LYP-D3BJ free energy in solution: -1809.829782 a.u.
Three lowest frequencies (cm-1): -147.6535 7.7785 17.2120
Imaginary frequency: -147.6535 cm-1

Cartesian coordinates

ATOM	X	Y	Z
N	-1.624622	1.529144	0.852687
N	-2.211658	-0.538416	0.949108
C	-1.258919	0.285449	0.421299
C	-2.773393	1.478465	1.633608
H	-3.210672	2.365260	2.064522
C	-3.143812	0.174345	1.694321
H	-3.970412	-0.310867	2.188825
C	-0.910656	2.750331	0.551346
C	0.170321	3.123221	1.375284
C	-1.341137	3.530149	-0.541638
C	0.827783	4.321693	1.070504
C	-0.649802	4.721261	-0.794313
C	0.424252	5.113678	-0.000320
H	1.668077	4.637291	1.681961
H	-0.954565	5.347772	-1.627302
H	0.949018	6.040093	-0.217816
C	-2.255267	-1.972530	0.767279
C	-3.057776	-2.495901	-0.266935
C	-1.512019	-2.789526	1.642631
C	-3.101140	-3.888376	-0.406687
C	-1.589296	-4.174658	1.451233
C	-2.374308	-4.720552	0.439976
H	-3.707755	-4.325358	-1.194292
H	-1.023864	-4.833382	2.103868
H	-2.417646	-5.798371	0.309027
C	-0.651032	-2.230850	2.771582
C	0.835977	-2.590176	2.581697
C	-1.164379	-2.694093	4.149597
H	-0.724291	-1.139424	2.749410
H	1.217411	-2.215901	1.625894
H	1.436096	-2.147721	3.385830
H	0.992305	-3.674965	2.608165
H	-2.212027	-2.411040	4.304008
H	-1.093407	-3.782373	4.260397
H	-0.568043	-2.239707	4.949469
C	0.625533	2.297279	2.574783
C	0.357513	3.047663	3.895168
C	2.105152	1.883485	2.459078
H	0.036893	1.375315	2.598001
H	-0.702909	3.303109	4.004508
H	0.648086	2.428016	4.751643
H	0.931721	3.980016	3.947775
H	2.288671	1.321238	1.538068
H	2.770857	2.754449	2.465108
H	2.384698	1.249086	3.308590

C	-3.876047	-1.614128	-1.206347
C	-5.386438	-1.774167	-0.938155
C	-3.546841	-1.882496	-2.687259
H	-3.617486	-0.569814	-1.005574
H	-5.638707	-1.537980	0.102199
H	-5.963513	-1.105533	-1.587671
H	-5.718002	-2.800417	-1.135462
H	-2.479273	-1.751758	-2.888438
H	-3.823781	-2.899671	-2.987428
H	-4.104017	-1.187516	-3.326462
C	-2.526272	3.138814	-1.420048
C	-2.168749	3.136471	-2.918279
C	-3.738961	4.051500	-1.143919
H	-2.818861	2.116599	-1.160393
H	-1.321000	2.476237	-3.124521
H	-3.025057	2.784299	-3.505366
H	-1.916054	4.140236	-3.278948
H	-4.040645	4.014756	-0.090685
H	-3.511238	5.095926	-1.387625
H	-4.596817	3.743756	-1.753279
C	2.117791	-0.595758	-1.171322
C	3.305929	-0.630819	-0.832143
C	0.743501	-2.595486	-2.724709
H	-0.139065	-2.566871	-2.068519
C	2.761670	-1.183086	-3.895607
H	3.264893	-0.208769	-3.949810
B	1.400280	-1.153750	-3.035223
C	0.370181	0.013151	-3.487345
H	0.825010	1.013556	-3.488466
H	0.059781	-0.190837	-4.526132
H	-0.562274	0.073161	-2.902134
Cu	0.342208	-0.192233	-0.557602
H	2.512678	-1.466151	-4.932843
H	3.493125	-1.916543	-3.533148
H	1.455737	-3.303671	-2.280916
H	0.409151	-3.039751	-3.677862
C	4.686023	-0.678576	-0.480409
C	5.518358	0.445096	-0.671952
C	5.252811	-1.850522	0.064733
C	6.866761	0.395590	-0.328240
H	5.088930	1.347559	-1.096266
C	6.601926	-1.892970	0.406703
H	4.618769	-2.720098	0.208876
C	7.413567	-0.771630	0.212530
H	7.494932	1.268876	-0.484206
H	7.023649	-2.803865	0.823809
H	8.466573	-0.807887	0.479248

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B3LYP SCF energy: -1808.65600974 a.u.
B3LYP enthalpy: -1807.816805 a.u.
B3LYP free energy: -1807.950270 a.u.
B3LYP-D3BJ SCF energy in solution: -1810.55478296 a.u.
B3LYP-D3BJ enthalpy in solution: -1809.715578 a.u.

B3LYP-D3BJ free energy in solution: -1809.849043 a.u.
Three lowest frequencies (cm-1): 9.9164 15.7078 18.9959

Cartesian coordinates

ATOM	X	Y	Z
N	-0.201581	-2.000462	0.474814
N	1.711170	-1.133614	0.947623
C	0.524831	-0.852577	0.334177
C	-1.557918	-2.186413	0.008621
C	-2.613628	-1.983313	0.921244
C	-1.767666	-2.591260	-1.325175
C	-3.916736	-2.195313	0.454806
C	-3.093199	-2.780817	-1.737137
C	-4.156599	-2.587183	-0.859588
H	-4.753662	-2.048580	1.130998
H	-3.292205	-3.090788	-2.758733
H	-5.176163	-2.745482	-1.200916
C	2.830616	-0.224574	1.082667
C	3.928212	-0.374250	0.209778
C	2.797043	0.740293	2.109286
C	5.018027	0.483977	0.397135
C	3.911198	1.578221	2.239896
C	5.010782	1.452232	1.396957
H	5.879609	0.399694	-0.257800
H	3.914517	2.340011	3.013911
H	5.863816	2.114504	1.515763
C	1.622810	0.895559	3.071276
C	0.962555	2.281257	2.934445
C	2.048774	0.621615	4.527373
H	0.865111	0.150156	2.811493
H	0.631922	2.462084	1.906292
H	0.089825	2.353146	3.594468
H	1.655922	3.084959	3.207647
H	2.487656	-0.376955	4.635081
H	2.790156	1.350493	4.874172
H	1.182137	0.686455	5.195730
C	-2.387277	-1.567439	2.372570
C	-2.795577	-2.694980	3.342395
C	-3.111977	-0.252297	2.716540
H	-1.316836	-1.390296	2.514783
H	-2.250329	-3.622762	3.133933
H	-2.584664	-2.402572	4.377640
H	-3.866834	-2.915968	3.269686
H	-2.807319	0.558991	2.048711
H	-4.199993	-0.355246	2.636946
H	-2.882276	0.043102	3.747189
C	3.974018	-1.431352	-0.890609
C	4.938362	-2.575954	-0.515384
C	4.343692	-0.835093	-2.262070
H	2.972724	-1.863401	-0.989010
H	4.657349	-3.052354	0.431096
H	4.939138	-3.346309	-1.295339
H	5.964835	-2.206224	-0.407795
H	3.667057	-0.022938	-2.542243
H	5.367540	-0.444087	-2.272805
H	4.283387	-1.612424	-3.032914

C	-0.626920	-2.855544	-2.303234
C	-0.740899	-1.989711	-3.572117
C	-0.543923	-4.354470	-2.657646
H	0.313631	-2.584626	-1.814243
H	-0.752376	-0.922948	-3.328747
H	0.116721	-2.172139	-4.229166
H	-1.649203	-2.220268	-4.141234
H	-0.414622	-4.973509	-1.762199
H	-1.451411	-4.694954	-3.169876
H	0.305524	-4.540079	-3.325086
C	-0.322492	2.567128	-1.674234
C	-1.383129	2.385149	-1.045704
C	2.273290	3.141426	-1.557452
H	2.547062	2.277404	-0.929864
C	0.640146	4.211755	-3.442929
H	-0.223147	4.079141	-4.111604
B	0.995374	2.864181	-2.559769
C	1.270556	1.571901	-3.547657
H	0.438770	1.376853	-4.242264
H	2.163448	1.750876	-4.166418
H	1.453685	0.627844	-3.004533
C	0.515648	-2.973087	1.159582
H	0.103694	-3.948650	1.364077
C	1.719549	-2.424660	1.460766
H	2.573332	-2.822401	1.985755
Cu	-0.069008	0.788050	-0.534317
H	2.103059	3.987859	-0.874275
H	3.167553	3.388667	-2.149952
H	1.501700	4.464782	-4.080143
H	0.434708	5.095619	-2.821072
C	-2.702081	2.509212	-0.473042
C	-3.012868	3.606668	0.354902
C	-3.709394	1.563381	-0.745087
C	-4.293011	3.753374	0.885098
H	-2.241837	4.342024	0.563521
C	-4.988420	1.717864	-0.212625
H	-3.480029	0.714588	-1.382107
C	-5.286193	2.810974	0.604515
H	-4.517011	4.609188	1.516610
H	-5.755113	0.981495	-0.439337
H	-6.284504	2.930006	1.017131

TS8
B3LYP SCF energy: -1808.63210878 a.u.
B3LYP enthalpy: -1807.793623 a.u.
B3LYP free energy: -1807.927351 a.u.
B3LYP-D3BJ SCF energy in solution: -1810.52163463 a.u.
B3LYP-D3BJ enthalpy in solution: -1809.683149 a.u.
B3LYP-D3BJ free energy in solution: -1809.816877 a.u.
Three lowest frequencies (cm-1): -430.5702 10.4160 18.3724
Imaginary frequency: -430.5702 cm-1

Cartesian coordinates

ATOM	X	Y	Z

N	0.310665	-2.332722	0.169583
N	-1.668153	-1.694556	-0.379618
C	-0.435202	-1.210033	-0.049427
C	1.706525	-2.328509	0.546490
C	2.680152	-2.373498	-0.471231
C	2.036203	-2.290774	1.916014
C	4.023915	-2.384713	-0.077443
C	3.395803	-2.299477	2.250903
C	4.380188	-2.347707	1.267686
H	4.800648	-2.414928	-0.836062
H	3.686612	-2.262756	3.296830
H	5.429289	-2.351831	1.550880
C	-2.813175	-0.872207	-0.702348
C	-3.693951	-0.506805	0.334741
C	-3.007050	-0.478326	-2.041308
C	-4.796451	0.286589	-0.006312
C	-4.126361	0.314057	-2.323931
C	-5.011963	0.694423	-1.319571
H	-5.491092	0.595112	0.769518
H	-4.301584	0.642742	-3.344153
H	-5.870939	1.314712	-1.560395
C	-2.046408	-0.859508	-3.163497
C	-1.310761	0.381340	-3.707195
C	-2.760521	-1.625836	-4.293987
H	-1.286390	-1.529623	-2.750138
H	-0.768614	0.897269	-2.907557
H	-0.589960	0.088320	-4.480053
H	-2.010826	1.096567	-4.154573
H	-3.263710	-2.522617	-3.914671
H	-3.514843	-1.005016	-4.790758
H	-2.036581	-1.938181	-5.055600
C	2.324514	-2.404819	-1.954412
C	2.775319	-3.724317	-2.611878
C	2.900341	-1.185084	-2.699901
H	1.235182	-2.352420	-2.044774
H	2.332439	-4.593618	-2.112026
H	2.473849	-3.747785	-3.665636
H	3.864924	-3.838659	-2.574893
H	2.562381	-0.245340	-2.251208
H	3.996311	-1.185192	-2.686347
H	2.581861	-1.200292	-3.749229
C	-3.479617	-0.922525	1.786684
C	-4.665808	-1.746872	2.324017
C	-3.199015	0.301740	2.679970
H	-2.594480	-1.564626	1.830888
H	-4.846041	-2.637846	1.711369
H	-4.465462	-2.074790	3.350693
H	-5.591524	-1.160325	2.339205
H	-2.333276	0.866488	2.319571
H	-4.055920	0.984668	2.703828
H	-2.997480	-0.017314	3.709583
C	0.983754	-2.219704	3.018102
C	1.046393	-0.868016	3.757331
C	1.102893	-3.400230	4.001281
H	-0.003759	-2.286775	2.551377
H	0.912849	-0.031714	3.062919

H	0.257458	-0.812524	4.516781
H	2.009358	-0.735053	4.264311
H	1.030502	-4.363390	3.483109
H	2.056342	-3.382976	4.541592
H	0.300497	-3.353814	4.746691
C	-0.089507	3.237929	0.723198
C	0.800001	2.470537	0.150259
C	-1.314691	4.059991	2.967181
H	-0.378834	3.841492	3.497462
C	-2.460010	4.469555	0.493832
H	-2.252079	4.576691	-0.578532
B	-1.176077	4.025192	1.360918
C	0.291533	5.132901	0.870427
H	1.224305	5.068033	1.430673
H	0.482853	5.324987	-0.185858
H	-0.294652	5.965287	1.273726
C	-1.688998	-3.084629	-0.365716
H	-2.580053	-3.645388	-0.600621
C	-0.440009	-3.487417	-0.018787
H	-0.017923	-4.471543	0.111419
Cu	0.158114	0.638301	0.061290
C	2.130385	2.837985	-0.381072
C	3.207966	3.127545	0.477518
C	2.372818	2.870464	-1.767662
C	4.468421	3.446506	-0.028899
H	3.044684	3.097902	1.551732
C	3.631242	3.198234	-2.273725
H	1.555381	2.644127	-2.448155
C	4.688844	3.486252	-1.407709
H	5.281692	3.668643	0.658526
H	3.785989	3.227314	-3.350097
H	5.670562	3.736462	-1.801495
H	-2.051920	3.312618	3.296403
H	-1.682935	5.032039	3.327030
H	-2.892047	5.417386	0.847394
H	-3.251793	3.711483	0.589818

TS9

B3LYP SCF energy: -1808.62839012 a.u.
B3LYP enthalpy: -1807.789988 a.u.
B3LYP free energy: -1807.923381 a.u.
B3LYP-D3BJ SCF energy in solution: -1810.51862535 a.u.
B3LYP-D3BJ enthalpy in solution: -1809.680223 a.u.
B3LYP-D3BJ free energy in solution: -1809.813616 a.u.
Three lowest frequencies (cm-1): -313.5435 5.9764 15.2216
Imaginary frequency: -313.5435 cm-1

Cartesian coordinates

ATOM	X	Y	Z
N	-0.321268	-2.299863	0.014729
N	1.655696	-1.631564	0.535257
C	0.440204	-1.170202	0.116006
C	-1.708106	-2.325722	-0.394407
C	-2.705277	-2.306095	0.601860

C	-2.006648	-2.387495	-1.770448
C	-4.039161	-2.362734	0.179396
C	-3.358371	-2.430478	-2.134698
C	-4.364856	-2.422805	-1.172846
H	-4.832446	-2.351096	0.920932
H	-3.624862	-2.469954	-3.186884
H	-5.406971	-2.459806	-1.478592
C	2.812986	-0.801262	0.786548
C	3.786682	-0.679010	-0.226285
C	2.933647	-0.167370	2.039395
C	4.911950	0.105618	0.052703
C	4.075277	0.614424	2.257541
C	5.055737	0.748978	1.279103
H	5.682386	0.220008	-0.703881
H	4.196126	1.123634	3.209159
H	5.933840	1.359406	1.471480
C	1.889903	-0.300613	3.144286
C	1.240705	1.058430	3.472332
C	2.488033	-0.952905	4.406668
H	1.094197	-0.960043	2.785138
H	0.778400	1.501371	2.583736
H	0.463272	0.933016	4.235217
H	1.977133	1.771535	3.860743
H	2.919923	-1.935611	4.184709
H	3.278364	-0.332556	4.844737
H	1.711542	-1.087072	5.168747
C	-2.383864	-2.228941	2.091325
C	-2.708637	-3.559706	2.799601
C	-3.102372	-1.049024	2.774324
H	-1.308649	-2.054624	2.197609
H	-2.157174	-4.397597	2.357516
H	-2.444033	-3.502290	3.861949
H	-3.777697	-3.793359	2.732827
H	-2.897374	-0.103474	2.262526
H	-4.189238	-1.190704	2.790325
H	-2.768676	-0.959248	3.814775
C	3.661293	-1.375220	-1.578786
C	4.647135	-2.556848	-1.685764
C	3.844732	-0.399792	-2.756746
H	2.648791	-1.783483	-1.657284
H	4.488788	-3.289196	-0.885753
H	4.525579	-3.072588	-2.645618
H	5.685749	-2.212047	-1.619046
H	3.156634	0.448025	-2.681937
H	4.864756	-0.001447	-2.801914
H	3.653395	-0.916639	-3.704378
C	-0.931024	-2.394770	-2.852424
C	-0.992127	-1.111548	-3.704589
C	-1.016950	-3.656400	-3.733253
H	0.046812	-2.410154	-2.361360
H	-0.889434	-0.217837	-3.079662
H	-0.183450	-1.107678	-4.444983
H	-1.942113	-1.035786	-4.246354
H	-0.944226	-4.570393	-3.132687
H	-1.959640	-3.697733	-4.290687
H	-0.200269	-3.663675	-4.464384

C	-0.102922	3.485072	-0.894462
C	-0.781216	2.486331	-0.392075
C	1.425016	5.658529	-0.531225
H	1.686364	5.260737	0.458354
C	0.412673	5.040798	-3.018070
H	0.013403	4.238752	-3.652533
B	0.693100	4.587663	-1.494240
C	1.742133	3.045122	-1.535451
H	1.435412	2.254251	-2.220718
H	2.550526	3.622933	-1.999111
H	2.099604	2.638951	-0.588967
C	1.648493	-3.012802	0.694082
H	2.520548	-3.554962	1.024030
C	0.401870	-3.434693	0.363305
H	-0.035559	-4.420358	0.341533
Cu	-0.125013	0.665454	-0.195098
C	-2.153064	2.774367	0.120482
C	-3.211931	1.878519	-0.125017
C	-2.440615	3.928593	0.875734
C	-4.501443	2.133273	0.343969
H	-3.014680	0.978428	-0.702636
C	-3.727179	4.178782	1.352650
H	-1.636449	4.627628	1.087781
C	-4.767594	3.284415	1.088836
H	-5.299249	1.425710	0.129119
H	-3.917908	5.078515	1.933482
H	-5.769734	3.479750	1.461990
H	1.321813	5.428728	-3.501297
H	-0.321682	5.858548	-3.037186
H	0.769728	6.525809	-0.366294
H	2.346661	6.050298	-0.986730

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B3LYP SCF energy: -1808.67023277 a.u.
B3LYP enthalpy: -1807.829681 a.u.
B3LYP free energy: -1807.963590 a.u.
B3LYP-D3BJ SCF energy in solution: -1810.56082394 a.u.
B3LYP-D3BJ enthalpy in solution: -1809.720272 a.u.
B3LYP-D3BJ free energy in solution: -1809.854181 a.u.
Three lowest frequencies (cm-1): 6.0866 15.3474 19.4230

Cartesian coordinates

ATOM	X	Y	Z
N	0.927918	-2.135130	0.003429
N	2.379186	-0.608362	0.429928
C	1.070071	-0.778005	0.077792
C	-0.300118	-2.817348	-0.337874
C	-1.138457	-3.258805	0.705755
C	-0.599067	-3.033637	-1.698078
C	-2.302470	-3.950396	0.348666
C	-1.781635	-3.722586	-1.996193
C	-2.622989	-4.181007	-0.986280
H	-2.969937	-4.306401	1.127757
H	-2.046412	-3.901060	-3.034349

H	-3.534044	-4.716005	-1.240673
C	3.019741	0.672427	0.625669
C	3.742557	1.234354	-0.446301
C	2.914784	1.297518	1.884028
C	4.374548	2.463839	-0.223837
C	3.561559	2.529202	2.046862
C	4.284945	3.107134	1.007620
H	4.939917	2.925564	-1.028165
H	3.495635	3.042269	3.001936
H	4.779384	4.063231	1.157051
C	2.134976	0.692774	3.047514
C	0.936268	1.578463	3.440547
C	3.048478	0.418767	4.258466
H	1.730442	-0.270494	2.722535
H	0.264159	1.732436	2.589649
H	0.364631	1.104987	4.247459
H	1.264123	2.562281	3.796425
H	3.881953	-0.241315	3.991655
H	3.472962	1.345256	4.662102
H	2.477936	-0.061317	5.062076
C	-0.822203	-3.015376	2.178503
C	-0.439004	-4.328899	2.889926
C	-1.982370	-2.309219	2.906437
H	0.043682	-2.348473	2.234122
H	0.422284	-4.810761	2.412541
H	-0.181272	-4.135395	3.937880
H	-1.269913	-5.044101	2.876338
H	-2.276857	-1.389341	2.391797
H	-2.868212	-2.951280	2.975975
H	-1.682071	-2.053942	3.929553
C	3.863919	0.553297	-1.806628
C	5.306499	0.070950	-2.060436
C	3.375945	1.460915	-2.952036
H	3.219854	-0.331423	-1.802500
H	5.644355	-0.616971	-1.276802
H	5.371660	-0.451787	-3.021956
H	6.008535	0.912479	-2.088849
H	2.344895	1.789247	-2.786679
H	4.001702	2.354686	-3.056281
H	3.414785	0.918629	-3.904179
C	0.295758	-2.541827	-2.831680
C	-0.416458	-1.465550	-3.674830
C	0.791210	-3.706119	-3.711398
H	1.179270	-2.071872	-2.389208
H	-0.730144	-0.620645	-3.052215
H	0.255677	-1.086966	-4.454283
H	-1.307371	-1.869743	-4.169752
H	1.324919	-4.457701	-3.118314
H	-0.038600	-4.210288	-4.219894
H	1.474538	-3.333809	-4.483526
C	-1.679560	3.041677	-1.108535
C	-1.767816	1.840011	-0.461109
C	-2.621267	5.601873	-1.269042
H	-1.904144	5.897697	-0.492603
C	-4.291871	3.566256	-1.894322
H	-4.444417	2.484773	-1.944481

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B       -2.871878    4.029731   -1.359588
C       -0.329447    3.512288   -1.641192
H       -0.360053    3.743745   -2.717058
H        0.001736    4.433504   -1.140209
H        0.444818    2.750388   -1.484483
C        3.032597   -1.827689    0.573734
H        4.072806   -1.889764    0.852293
C        2.116740   -2.791459    0.302307
H        2.194724   -3.867228    0.291978
Cu      -0.313731    0.572759   -0.212391
C       -3.031958    1.443784    0.205897
C       -3.592946    0.163099    0.004365
C       -3.695610    2.295464    1.114396
C       -4.774862   -0.222625    0.633511
H       -3.092981   -0.524474   -0.674555
C       -4.870703    1.904294    1.759979
H       -3.263718    3.270767    1.325768
C       -5.423003    0.645610    1.519308
H       -5.190330   -1.208891    0.437479
H       -5.355627    2.587426    2.454254
H       -6.337708    0.339314    2.020594
H       -4.411599    3.973241   -2.913186
H       -5.113350    4.005636   -1.311285
H       -3.542235    6.183087   -1.133958
H       -2.183226    5.935886   -2.225036



 17
B3LYP SCF energy:     -1808.67005934 a.u.
B3LYP enthalpy:     -1807.829479 a.u.
B3LYP free energy:     -1807.961765 a.u.
B3LYP-D3BJ SCF energy in solution:     -1810.56391556 a.u.
B3LYP-D3BJ enthalpy in solution:     -1809.723335 a.u.
B3LYP-D3BJ free energy in solution:     -1809.855621 a.u.
Three lowest frequencies (cm-1):      14.9390     20.1154     24.1065

Cartesian coordinates
ATOM       X           Y           Z
N        0.196455   -2.135298    0.385240
N       -1.734555   -1.294474    0.816445
C       -0.526922   -0.982618    0.255624
C        1.560517   -2.305593   -0.062764
C        1.790846   -2.662078   -1.406863
C        2.603331   -2.128190    0.868151
C        3.121201   -2.834897   -1.808092
C        3.913254   -2.320985    0.412273
C        4.172201   -2.669486   -0.910034
H        3.335631   -3.102810   -2.838652
H        4.740857   -2.187050    1.102389
H        5.197048   -2.810285   -1.243137
C       -2.866445   -0.399704    0.905304
C       -2.894144    0.565560    1.931918
C       -3.916464   -0.552006   -0.024376
C       -4.017258    1.399880    2.001265
C       -5.018619    0.302367    0.100927
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C	-5.069185	1.271775	1.099135
H	-4.067497	2.157664	2.777661
H	-5.844681	0.210917	-0.597994
H	-5.931414	1.928931	1.173989
C	-3.899926	-1.610185	-1.125223
C	-4.157062	-1.008801	-2.520036
C	-4.907829	-2.738194	-0.822651
H	-2.902131	-2.058923	-1.150288
H	-3.447594	-0.206579	-2.743321
H	-4.053623	-1.785905	-3.286630
H	-5.169517	-0.597766	-2.606145
H	-4.704047	-3.216233	0.142339
H	-5.933775	-2.352853	-0.791063
H	-4.863016	-3.510426	-1.599589
C	0.664499	-2.849194	-2.418588
C	0.684701	-4.257635	-3.043808
C	0.705481	-1.754570	-3.503449
H	-0.288623	-2.744461	-1.891372
H	0.633399	-5.037813	-2.275673
H	-0.171489	-4.385502	-3.716401
H	1.593843	-4.427883	-3.631873
H	0.637998	-0.756443	-3.057236
H	1.634272	-1.802681	-4.084264
H	-0.132287	-1.876202	-4.200603
C	-1.781687	0.713243	2.965604
C	-2.286357	0.352231	4.377354
C	-1.157379	2.121707	2.938754
H	-0.986335	0.006111	2.714181
H	-2.695067	-0.664440	4.409276
H	-1.465041	0.411288	5.101107
H	-3.073655	1.038407	4.710862
H	-0.757677	2.357557	1.946670
H	-1.889197	2.893651	3.204996
H	-0.333944	2.181714	3.660121
C	2.358159	-1.738484	2.322922
C	3.022347	-0.392221	2.670350
C	2.817428	-2.851866	3.285611
H	1.280534	-1.612080	2.465362
H	2.675347	0.408495	2.010695
H	2.787730	-0.115281	3.705406
H	4.113004	-0.444079	2.579719
H	2.316790	-3.803136	3.070070
H	3.898172	-3.021956	3.215621
H	2.591148	-2.575929	4.322232
C	0.457363	3.481670	-1.590758
C	0.994778	2.399572	-0.939733
C	-1.779444	4.926059	-2.153063
H	-1.490808	5.663900	-1.392878
C	-1.931680	2.236355	-2.289379
H	-1.394016	1.281092	-2.257507
B	-1.050038	3.518433	-1.977467
C	1.270501	4.745373	-1.881388
H	0.956633	5.587773	-1.247787
H	2.343976	4.604152	-1.727361
H	1.123749	5.078829	-2.918099
C	-1.755559	-2.602659	1.288565

H	-2.624634	-3.022707	1.769649
C	-0.538490	-3.134314	1.012794
H	-0.128663	-4.114308	1.200441
Cu	0.136618	0.725285	-0.437445
C	2.382753	2.449355	-0.398698
C	2.737882	3.301409	0.667639
C	3.386893	1.597283	-0.902649
C	4.029092	3.306155	1.197481
H	1.983629	3.969114	1.077211
C	4.683499	1.616869	-0.388847
H	3.137247	0.916467	-1.713180
C	5.014231	2.467878	0.669415
H	4.269062	3.976158	2.020568
H	5.437496	0.956883	-0.812494
H	6.022333	2.477263	1.076171
H	-2.365225	2.346953	-3.297114
H	-2.793638	2.171741	-1.608940
H	-2.874662	4.860689	-2.172858
H	-1.471706	5.364569	-3.116961

TS10

B3LYP SCF energy: -1997.23509196 a.u.
B3LYP enthalpy: -1996.379217 a.u.
B3LYP free energy: -1996.516879 a.u.
B3LYP-D3BJ SCF energy in solution: -1999.20600353 a.u.
B3LYP-D3BJ enthalpy in solution: -1998.350129 a.u.
B3LYP-D3BJ free energy in solution: -1998.487791 a.u.
Three lowest frequencies (cm-1): -210.8395 10.1445 16.9415
Imaginary frequency: -210.8395 cm-1

Cartesian coordinates

ATOM	X	Y	Z
N	0.514889	2.212232	-0.307571
N	-1.497688	1.655147	-0.821402
C	-0.338189	1.143512	-0.309275
C	1.889722	2.192160	0.146239
C	2.159970	2.489548	1.498796
C	2.902595	1.924035	-0.795445
C	3.501882	2.495294	1.896422
C	4.226577	1.943691	-0.339026
C	4.524230	2.222361	0.991023
H	3.750010	2.713535	2.929860
H	5.032742	1.736713	-1.036232
H	5.558379	2.229074	1.324989
C	-2.731494	0.924569	-1.007665
C	-2.916221	0.199222	-2.201847
C	-3.718801	1.008698	-0.005027
C	-4.137222	-0.465837	-2.368274
C	-4.922130	0.328728	-0.229272
C	-5.130648	-0.402350	-1.395302
H	-4.310395	-1.040753	-3.273444
H	-5.703264	0.368418	0.524223
H	-6.070628	-0.926424	-1.545499
C	-3.529017	1.809852	1.280304

C	-3.659294	0.925134	2.535237
C	-4.502659	3.004367	1.338374
H	-2.514033	2.218841	1.281237
H	-2.931652	0.108263	2.526916
H	-3.487167	1.526905	3.435696
H	-4.660971	0.487668	2.618257
H	-4.384412	3.663773	0.470560
H	-5.546259	2.669460	1.361163
H	-4.323284	3.597492	2.242636
C	1.059481	2.855489	2.492590
C	0.907271	4.389224	2.588015
C	1.275794	2.250226	3.891140
H	0.115463	2.451486	2.111738
H	0.671651	4.837960	1.616695
H	0.102103	4.651231	3.284652
H	1.832914	4.849878	2.953294
H	1.424036	1.168401	3.839154
H	2.139018	2.694800	4.400376
H	0.397286	2.448258	4.516226
C	-1.853474	0.117491	-3.293126
C	-2.366184	0.692151	-4.628190
C	-1.339314	-1.325034	-3.466976
H	-0.999725	0.728089	-2.984398
H	-2.704271	1.728528	-4.514816
H	-1.568366	0.674721	-5.379809
H	-3.205966	0.108649	-5.022797
H	-0.942411	-1.717042	-2.524562
H	-2.137729	-1.997357	-3.802553
H	-0.538952	-1.355382	-4.215725
C	2.611915	1.665209	-2.270976
C	3.266994	0.369295	-2.781496
C	3.037997	2.874836	-3.128877
H	1.530557	1.545185	-2.390157
H	2.967348	-0.496370	-2.184628
H	2.971284	0.187904	-3.821922
H	4.361123	0.429047	-2.758894
H	2.533799	3.794576	-2.809954
H	4.118521	3.047243	-3.059116
H	2.793172	2.701741	-4.183526
C	-0.237978	-3.643754	0.852272
C	0.564500	-2.585590	0.546631
C	-2.860550	-2.841698	0.817958
H	-2.569806	-1.989094	0.193066
C	-1.929052	-4.377589	2.877844
H	-2.677943	-3.916453	3.532448
B	-1.638641	-3.495957	1.585985
C	0.157323	-5.091993	0.583459
H	-0.549893	-5.571228	-0.110151
H	1.158263	-5.190704	0.155549
H	0.117273	-5.679505	1.510145
C	-1.366166	3.001809	-1.137310
H	-2.180810	3.571687	-1.555433
C	-0.097085	3.352606	-0.812616
H	0.426721	4.291443	-0.895005
Cu	0.046556	-0.704551	0.230550
C	1.911584	-2.761909	-0.073312

C	2.031655	-3.241734	-1.395747
C	3.103424	-2.439670	0.607982
C	3.278032	-3.416123	-1.998829
H	1.127428	-3.490323	-1.946279
C	4.349012	-2.613202	0.002685
H	3.042545	-2.056878	1.620642
C	4.447530	-3.104552	-1.301433
H	3.334389	-3.798908	-3.015605
H	5.250671	-2.366811	0.559138
H	5.420002	-3.242114	-1.767372
H	-1.040816	-4.607393	3.478554
H	-2.353007	-5.342807	2.555016
H	-3.686778	-2.537941	1.472066
H	-3.266399	-3.600356	0.127268
C	0.235450	-1.456768	2.585149
O	1.316600	-1.099206	2.937301
O	-0.934580	-1.642947	2.799031

TS11

B3LYP SCF energy: -1924.38770845 a.u.
B3LYP enthalpy: -1923.493946 a.u.
B3LYP free energy: -1923.630893 a.u.
B3LYP-D3BJ SCF energy in solution: -1926.33843140 a.u.
B3LYP-D3BJ enthalpy in solution: -1925.444669 a.u.
B3LYP-D3BJ free energy in solution: -1925.581616 a.u.
Three lowest frequencies (cm-1): -1077.0263 13.0344 16.5849
Imaginary frequency: -1077.0263 cm-1

Cartesian coordinates

ATOM	X	Y	Z
N	-1.171615	-2.036837	-0.358858
N	0.899909	-2.132492	0.212645
C	-0.106427	-1.242364	-0.042428
C	-0.836162	-3.384262	-0.302448
H	-1.553080	-4.159055	-0.523655
C	0.469484	-3.445015	0.059885
H	1.126918	-4.284285	0.222912
C	-2.497081	-1.575541	-0.710722
C	-3.477722	-1.512433	0.299285
C	-2.767465	-1.259662	-2.057116
C	-4.769574	-1.130603	-0.081841
C	-4.075110	-0.875805	-2.377755
C	-5.067939	-0.816674	-1.404315
H	-5.549072	-1.067312	0.671607
H	-4.316542	-0.616905	-3.404597
H	-6.075869	-0.515101	-1.675678
C	2.249307	-1.781074	0.596090
C	3.235666	-1.701309	-0.407507
C	2.531698	-1.570398	1.960502
C	4.540239	-1.391288	-0.004876
C	3.853499	-1.261343	2.304417
C	4.847840	-1.170978	1.334633
H	5.324037	-1.317199	-0.752661
H	4.105871	-1.090717	3.347084

H	5.866968	-0.928804	1.623836
C	1.472212	-1.681760	3.052518
C	1.314873	-0.359568	3.826998
C	1.773357	-2.854604	4.006731
H	0.510063	-1.889516	2.575112
H	1.068976	0.463564	3.148145
H	0.509835	-0.446805	4.566296
H	2.232404	-0.093044	4.364442
H	1.845353	-3.803838	3.463548
H	2.718474	-2.704604	4.541519
H	0.978458	-2.951216	4.755597
C	-3.183998	-1.836034	1.761111
C	-3.936018	-3.102755	2.216174
C	-3.497686	-0.640066	2.681828
H	-2.113083	-2.041214	1.856384
H	-3.676466	-3.970488	1.598230
H	-3.688113	-3.341044	3.257253
H	-5.021867	-2.964753	2.155448
H	-2.957819	0.258650	2.367376
H	-4.568750	-0.406312	2.685666
H	-3.210123	-0.878717	3.713315
C	2.936475	-1.965506	-1.880050
C	3.557543	-3.302383	-2.334854
C	3.395315	-0.807298	-2.784956
H	1.851630	-2.052437	-1.996026
H	3.198277	-4.141904	-1.728340
H	3.302942	-3.506359	-3.381546
H	4.650698	-3.278538	-2.254264
H	2.953728	0.144111	-2.474060
H	4.484827	-0.688501	-2.772407
H	3.098725	-1.004816	-3.822135
C	-1.704115	-1.308754	-3.149744
C	-1.431461	0.096125	-3.722785
C	-2.077544	-2.304201	-4.265579
H	-0.769957	-1.661192	-2.702032
H	-1.129685	0.792261	-2.933096
H	-0.629861	0.052579	-4.469925
H	-2.322368	0.508754	-4.210246
H	-2.235625	-3.312796	-3.866523
H	-2.995011	-2.003738	-4.784519
H	-1.276377	-2.355183	-5.012137
C	-0.750883	3.616345	-0.206147
C	0.224955	2.679080	0.008827
C	-2.669123	4.821973	1.334768
H	-1.912538	5.431279	1.851116
C	-3.282177	2.596544	-0.079863
H	-2.933927	1.609932	-0.416911
B	-2.120593	3.442347	0.673286
C	-0.581960	4.850515	-1.061541
H	-0.856252	5.750754	-0.497435
H	0.428527	4.985338	-1.460068
H	-1.276117	4.810898	-1.914657
O	-1.536267	2.433671	1.845157
H	-0.501898	2.281972	1.276990
C	-1.297682	2.934903	3.156197
H	-0.597159	3.779877	3.146017

H	-2.241324	3.265187	3.597070
H	-0.879390	2.127948	3.769158
Cu	-0.027196	0.698832	0.059340
C	1.627174	2.800229	-0.484117
C	2.707195	2.765391	0.422308
C	1.945577	2.939200	-1.852215
C	4.027562	2.894552	-0.007188
H	2.492851	2.648186	1.482266
C	3.267088	3.067118	-2.285317
H	1.138199	2.947817	-2.579855
C	4.317947	3.048920	-1.365496
H	4.833894	2.876970	0.722763
H	3.475074	3.182598	-3.346997
H	5.346652	3.151230	-1.701564
H	-3.636205	3.129957	-0.975391
H	-4.163628	2.431966	0.557814
H	-3.488237	4.647123	2.048081
H	-3.092590	5.460240	0.546149

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B3LYP SCF energy: -1924.45011553 a.u.
B3LYP enthalpy: -1923.550648 a.u.
B3LYP free energy: -1923.690438 a.u.
B3LYP-D3BJ SCF energy in solution: -1926.39082967 a.u.
B3LYP-D3BJ enthalpy in solution: -1925.491362 a.u.
B3LYP-D3BJ free energy in solution: -1925.631152 a.u.
Three lowest frequencies (cm-1): 10.9097 14.1454 18.6301

Cartesian coordinates

ATOM	X	Y	Z
N	2.879754	-0.877144	-0.409760
N	2.693983	1.268325	-0.409112
C	1.988529	0.125807	-0.160223
C	4.112401	-0.368931	-0.802142
H	4.944718	-1.012754	-1.038531
C	3.995340	0.983240	-0.803835
H	4.703070	1.760695	-1.044836
C	2.599326	-2.291545	-0.285398
C	2.711016	-2.894039	0.983688
C	2.253700	-3.013221	-1.446038
C	2.455053	-4.268312	1.067387
C	2.020466	-4.386176	-1.302918
C	2.115772	-5.008331	-0.061307
H	2.523723	-4.764304	2.031153
H	1.751695	-4.974122	-2.175195
H	1.921627	-6.073686	0.027226
C	2.158972	2.605029	-0.275753
C	1.498824	3.182705	-1.378837
C	2.327545	3.278333	0.951074
C	0.990800	4.478069	-1.218004
C	1.800500	4.571619	1.053405
C	1.138015	5.166492	-0.017046
H	0.470673	4.951694	-2.045387
H	1.908319	5.118523	1.985710

H	0.734486	6.170166	0.085427
C	3.044521	2.655788	2.145546
C	2.092396	2.480289	3.345031
C	4.293023	3.468205	2.541585
H	3.386175	1.657072	1.856658
H	1.229388	1.861100	3.078130
H	2.616059	1.996303	4.177818
H	1.715624	3.444922	3.704151
H	4.990405	3.566064	1.701838
H	4.027569	4.478575	2.873152
H	4.820652	2.975998	3.366726
C	3.097303	-2.120505	2.240681
C	4.411697	-2.651198	2.846566
C	1.959188	-2.131480	3.279908
H	3.269426	-1.076719	1.960614
H	5.232475	-2.609908	2.121333
H	4.697513	-2.051682	3.718809
H	4.311812	-3.691151	3.177700
H	1.034541	-1.721515	2.859804
H	1.743893	-3.147672	3.629334
H	2.236843	-1.530023	4.153754
C	1.318980	2.458887	-2.709771
C	2.006085	3.217625	-3.862374
C	-0.170652	2.208836	-3.016773
H	1.802054	1.479819	-2.634906
H	3.072749	3.371211	-3.662481
H	1.912950	2.652008	-4.796608
H	1.552094	4.201883	-4.024867
H	-0.650813	1.634198	-2.217783
H	-0.721018	3.149962	-3.130009
H	-0.275729	1.646423	-3.951816
C	2.144391	-2.364269	-2.822976
C	0.792052	-2.659965	-3.499534
C	3.318727	-2.789357	-3.728321
H	2.206565	-1.278905	-2.693642
H	-0.045683	-2.373409	-2.856477
H	0.715229	-2.101216	-4.439686
H	0.682407	-3.723287	-3.741529
H	4.287058	-2.531381	-3.283788
H	3.311628	-3.871702	-3.902248
H	3.250202	-2.292739	-4.703303
C	-3.965347	-0.393384	0.215884
C	-5.180700	-0.784887	0.666547
C	-2.748452	-2.035140	2.076577
H	-3.272287	-1.551037	2.913871
C	-1.833578	-1.924505	-0.453790
H	-1.621862	-1.318689	-1.350789
B	-2.592852	-1.106382	0.745298
C	-3.815407	0.675905	-0.852757
H	-2.936011	0.475841	-1.476006
H	-4.686131	0.755307	-1.513860
H	-3.652261	1.671542	-0.411830
O	-1.588312	0.093377	1.096955
C	-1.965439	0.949578	2.164302
H	-3.037787	1.169359	2.099295
H	-1.769330	0.485580	3.141006

H	-1.405871	1.890965	2.100098
H	-5.192408	-1.601517	1.389172
Cu	0.175029	0.027319	0.437651
C	-6.539484	-0.337618	0.298379
C	-6.871923	0.981883	-0.069468
C	-7.596172	-1.270228	0.362529
C	-8.183189	1.336930	-0.389981
H	-6.101909	1.745378	-0.074598
C	-8.904842	-0.919781	0.039980
H	-7.371277	-2.291005	0.664584
C	-9.207189	0.389345	-0.345307
H	-8.406649	2.365250	-0.665987
H	-9.692368	-1.668322	0.091940
H	-10.227714	0.668515	-0.595222
H	-1.761790	-2.349631	2.453963
H	-3.301773	-2.960667	1.861160
H	-2.450821	-2.768785	-0.793029
H	-0.876847	-2.364322	-0.120991

TS12

B3LYP SCF energy: -1924.42504091 a.u.
B3LYP enthalpy: -1923.526786 a.u.
B3LYP free energy: -1923.664292 a.u.
B3LYP-D3BJ SCF energy in solution: -1926.36881791 a.u.
B3LYP-D3BJ enthalpy in solution: -1925.470563 a.u.
B3LYP-D3BJ free energy in solution: -1925.608069 a.u.
Three lowest frequencies (cm-1): -197.5948 10.5358 18.7465
Imaginary frequency: -197.5948 cm-1

Cartesian coordinates

ATOM	X	Y	Z
N	2.429821	1.029638	-0.222158
N	0.623496	2.162512	0.047146
C	1.078281	0.877440	-0.077737
C	2.801643	2.368965	-0.189792
H	3.830409	2.677744	-0.288320
C	1.661894	3.083843	-0.019795
H	1.489452	4.145464	0.061755
C	3.385299	-0.043582	-0.379261
C	4.010553	-0.561784	0.772640
C	3.681717	-0.500289	-1.678848
C	4.961363	-1.573073	0.587763
C	4.638125	-1.515322	-1.802515
C	5.272901	-2.046639	-0.683471
H	5.459683	-1.998801	1.453655
H	4.886018	-1.895723	-2.789289
H	6.010845	-2.835438	-0.802343
C	-0.759299	2.539609	0.233823
C	-1.558689	2.768128	-0.903669
C	-1.245418	2.689869	1.547724
C	-2.891389	3.141011	-0.691099
C	-2.586672	3.062341	1.700499
C	-3.403703	3.282791	0.595330
H	-3.537951	3.316543	-1.545904

H	-2.996287	3.178209	2.699857
H	-4.443200	3.565784	0.736661
C	-0.377471	2.463020	2.781944
C	-0.881992	1.266381	3.610796
C	-0.275287	3.736708	3.643762
H	0.635012	2.216415	2.448228
H	-0.890309	0.351273	3.010965
H	-0.227999	1.101945	4.475538
H	-1.897418	1.437442	3.987317
H	0.116439	4.581586	3.065684
H	-1.251402	4.032651	4.045147
H	0.395060	3.566505	4.494387
C	3.701114	-0.059994	2.180074
C	4.919313	0.663504	2.789224
C	3.204940	-1.192550	3.099918
H	2.889668	0.670921	2.109448
H	5.249981	1.498498	2.160161
H	4.669643	1.062751	3.779364
H	5.769413	-0.018228	2.910068
H	2.308268	-1.671787	2.694073
H	3.973065	-1.962099	3.243021
H	2.961651	-0.785409	4.089217
C	-1.029469	2.628253	-2.327415
C	-1.050345	3.979631	-3.068970
C	-1.798910	1.548347	-3.112018
H	0.014004	2.303358	-2.272930
H	-0.466403	4.738736	-2.535670
H	-0.627113	3.869586	-4.074388
H	-2.071958	4.361821	-3.178094
H	-1.767044	0.588696	-2.586680
H	-2.851090	1.822802	-3.250373
H	-1.355942	1.415133	-4.106414
C	3.004597	0.058388	-2.926543
C	2.168135	-1.019857	-3.642456
C	4.025849	0.701414	-3.885478
H	2.312630	0.846745	-2.615282
H	1.422122	-1.451247	-2.967527
H	1.644082	-0.584312	-4.501789
H	2.797991	-1.836329	-4.014680
H	4.596430	1.494922	-3.389268
H	4.742501	-0.035832	-4.265728
H	3.512566	1.140638	-4.748963
C	-1.525859	-2.007289	-0.538500
C	-2.611750	-1.557779	0.155756
C	-1.103386	-4.491732	0.801552
H	-2.075236	-4.342679	1.285442
C	1.212164	-3.370098	-0.077956
H	1.884956	-2.503614	-0.054007
B	-0.167644	-3.183134	0.736659
C	-1.668991	-2.646971	-1.908039
H	-2.576031	-3.258689	-2.011999
H	-1.697595	-1.887399	-2.704809
H	-0.811962	-3.290564	-2.130275
O	0.026851	-2.421438	1.941366
C	-0.776177	-2.648090	3.079891
H	-0.671657	-3.677182	3.451446

H	-0.448389	-1.964023	3.871252
H	-1.842920	-2.469491	2.885153
H	-2.423819	-1.180446	1.163808
Cu	-0.030659	-0.730389	-0.122785
C	-4.055340	-1.543686	-0.162534
C	-4.972048	-1.509068	0.909852
C	-4.590817	-1.526582	-1.466779
C	-6.348009	-1.495230	0.698104
H	-4.585430	-1.503134	1.926949
C	-5.969148	-1.504948	-1.681198
H	-3.925063	-1.504008	-2.320415
C	-6.856677	-1.497258	-0.603515
H	-7.025473	-1.480808	1.548657
H	-6.351120	-1.489383	-2.699339
H	-7.929975	-1.484759	-0.774708
H	1.070042	-3.651601	-1.128738
H	1.768097	-4.198803	0.391648
H	-0.572533	-5.276429	1.367168
H	-1.295654	-4.911481	-0.192898

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B3LYP SCF energy: -1704.57335183 a.u.
B3LYP enthalpy: -1703.805221 a.u.
B3LYP free energy: -1703.927568 a.u.
B3LYP-D3BJ SCF energy in solution: -1706.41225951 a.u.
B3LYP-D3BJ enthalpy in solution: -1705.644129 a.u.
B3LYP-D3BJ free energy in solution: -1705.766476 a.u.
Three lowest frequencies (cm-1): 9.9317 11.1453 18.5502

Cartesian coordinates

ATOM	X	Y	Z
N	2.499198	0.088467	0.031232
N	1.292839	1.866307	-0.029884
C	1.197826	0.503551	-0.003002
C	3.380239	1.164867	0.025901
H	4.450206	1.029442	0.049755
C	2.618369	2.287243	-0.012726
H	2.888013	3.331654	-0.029296
C	2.912633	-1.296219	0.068473
C	3.082026	-1.917491	1.321654
C	3.134177	-1.967848	-1.150381
C	3.482400	-3.259374	1.327179
C	3.533299	-3.308358	-1.084662
C	3.706404	-3.949383	0.139006
H	3.614098	-3.771461	2.275798
H	3.704297	-3.858474	-2.005403
H	4.013682	-4.991375	0.166616
C	0.160030	2.763632	-0.069890
C	-0.343246	3.160867	-1.324640
C	-0.391105	3.210485	1.147593
C	-1.438277	4.033668	-1.333111
C	-1.485294	4.081627	1.078866
C	-2.004379	4.490880	-0.146311
H	-1.857836	4.352413	-2.282800

H	-1.940580	4.437434	1.998533
H	-2.856668	5.164374	-0.176437
C	0.138114	2.762768	2.506377
C	-0.890897	1.875230	3.235226
C	0.563296	3.958645	3.380175
H	1.030782	2.152055	2.339654
H	-1.157650	1.001366	2.631345
H	-0.480537	1.522015	4.188922
H	-1.811801	2.429241	3.452016
H	1.311564	4.579580	2.874223
H	-0.288371	4.601362	3.631446
H	0.996852	3.603484	4.322325
C	2.820664	-1.197592	2.641184
C	4.049613	-1.231924	3.569825
C	1.571915	-1.769517	3.341915
H	2.613805	-0.146080	2.419523
H	4.933883	-0.807212	3.080910
H	3.852438	-0.652268	4.479074
H	4.297948	-2.253744	3.878750
H	0.689461	-1.691254	2.697831
H	1.709414	-2.825998	3.600864
H	1.369363	-1.220523	4.269413
C	0.236807	2.657163	-2.642408
C	0.692973	3.814550	-3.551254
C	-0.764020	1.735694	-3.368391
H	1.123197	2.056549	-2.415937
H	1.420706	4.459479	-3.045370
H	1.162388	3.419467	-4.459722
H	-0.149343	4.442767	-3.862961
H	-1.051526	0.889089	-2.735860
H	-1.677347	2.276662	-3.642449
H	-0.318950	1.341791	-4.290088
C	2.926904	-1.302184	-2.507272
C	1.702190	-1.897839	-3.230366
C	4.188968	-1.379225	-3.387871
H	2.717796	-0.241492	-2.337428
H	0.796956	-1.791062	-2.623047
H	1.536960	-1.386184	-4.186182
H	1.844788	-2.964408	-3.440632
H	5.057415	-0.939920	-2.883753
H	4.442044	-2.413505	-3.647690
H	4.028522	-0.834760	-4.325649
C	-2.031948	-1.649338	-0.000040
C	-3.234409	-1.014542	-0.007100
C	-1.932145	-3.166423	0.041543
H	-2.829849	-3.666146	0.432154
H	-1.741215	-3.577642	-0.962293
H	-1.081947	-3.482595	0.659344
H	-3.229928	0.078118	0.037282
Cu	-0.418248	-0.592767	-0.005744
C	-4.613023	-1.558371	-0.010358
C	-5.627030	-0.844234	0.660942
C	-4.998116	-2.730518	-0.691354
C	-6.945491	-1.292684	0.687907
H	-5.361077	0.076801	1.176421
C	-6.318719	-3.181437	-0.668798

H	-4.260391	-3.276622	-1.269018
C	-7.299893	-2.471625	0.025960
H	-7.699884	-0.720909	1.223996
H	-6.583885	-4.088518	-1.207602
H	-8.327983	-2.824624	0.041821

CO2

B3LYP SCF energy: -188.58094022 a.u.
B3LYP enthalpy: -188.565756 a.u.
B3LYP free energy: -188.590066 a.u.
B3LYP-D3BJ SCF energy in solution: -188.64897299 a.u.
B3LYP-D3BJ enthalpy in solution: -188.633789 a.u.
B3LYP-D3BJ free energy in solution: -188.658099 a.u.
Three lowest frequencies (cm-1): 640.0427 640.0427 1372.1017

Cartesian coordinates

ATOM	X	Y	Z
C	0.000000	0.000000	0.000000
O	0.000000	0.000000	1.169156
O	0.000000	0.000000	-1.169156

TS13

B3LYP SCF energy: -1893.14323062 a.u.
B3LYP enthalpy: -1892.359807 a.u.
B3LYP free energy: -1892.487921 a.u.
B3LYP-D3BJ SCF energy in solution: -1895.05867504 a.u.
B3LYP-D3BJ enthalpy in solution: -1894.275251 a.u.
B3LYP-D3BJ free energy in solution: -1894.403365 a.u.
Three lowest frequencies (cm-1): -197.2587 13.2202 14.8612
Imaginary frequency: -197.2587 cm-1

Cartesian coordinates

ATOM	X	Y	Z
N	-2.477010	0.626233	0.261439
N	-0.876463	2.062258	0.238538
C	-1.119458	0.721585	0.164043
C	-3.064665	1.878644	0.396413
H	-4.132393	2.001665	0.487070
C	-2.054530	2.785659	0.381203
H	-2.059682	3.861764	0.455032
C	-3.218609	-0.614692	0.207285
C	-3.720075	-1.044810	-1.038173
C	-3.420790	-1.333662	1.401868
C	-4.440836	-2.245074	-1.059100
C	-4.146699	-2.528103	1.319004
C	-4.650128	-2.981640	0.103297
H	-4.838463	-2.609611	-2.001338
H	-4.316868	-3.111239	2.219425
H	-5.206808	-3.913825	0.061024
C	0.440466	2.652850	0.160717
C	1.167192	2.841083	1.353329
C	0.942424	3.015459	-1.105176

C	2.442182	3.409757	1.247350
C	2.224241	3.578350	-1.150239
C	2.967676	3.773344	0.010351
H	3.033903	3.562664	2.145317
H	2.646495	3.862136	-2.109784
H	3.962056	4.207444	-0.049390
C	0.154143	2.822180	-2.397742
C	0.853590	1.831959	-3.350324
C	-0.113793	4.171171	-3.094843
H	-0.819212	2.391118	-2.143902
H	0.953162	0.839684	-2.899485
H	0.269653	1.722699	-4.271838
H	1.853057	2.185389	-3.630290
H	-0.637852	4.869872	-2.432264
H	0.817993	4.651458	-3.415166
H	-0.731995	4.019485	-3.987219
C	-3.538029	-0.244671	-2.325300
C	-4.875155	0.388217	-2.763817
C	-2.922578	-1.082631	-3.461894
H	-2.840389	0.573737	-2.121341
H	-5.298423	1.026127	-1.978839
H	-4.730833	1.002944	-3.660047
H	-5.618506	-0.381690	-3.002159
H	-1.943591	-1.481958	-3.181248
H	-3.569242	-1.920549	-3.747416
H	-2.789727	-0.455160	-4.351529
C	0.624332	2.443913	2.722707
C	0.502522	3.661791	3.659405
C	1.476983	1.330640	3.362634
H	-0.383007	2.038768	2.585781
H	-0.130766	4.441965	3.221720
H	0.060393	3.362426	4.616925
H	1.481235	4.107436	3.871375
H	1.521939	0.449178	2.714266
H	2.504347	1.666421	3.545227
H	1.047389	1.029283	4.325490
C	-2.893774	-0.861332	2.753566
C	-1.894278	-1.867619	3.355381
C	-4.047449	-0.567189	3.733276
H	-2.351635	0.076708	2.600749
H	-1.058810	-2.049254	2.671584
H	-1.488866	-1.481837	4.298521
H	-2.370699	-2.831677	3.567435
H	-4.738800	0.179101	3.325235
H	-4.626773	-1.470995	3.954893
H	-3.653795	-0.183424	4.681872
C	1.701186	-1.996916	0.030834
C	2.819439	-1.551982	-0.606841
C	1.720520	-2.988811	1.172947
H	2.569336	-3.685249	1.128183
H	1.761529	-2.480079	2.147612
H	0.804007	-3.586323	1.151785
H	2.654216	-0.970706	-1.515850
Cu	0.205593	-0.687834	-0.018777
C	4.249485	-1.778718	-0.328214
C	5.164674	-1.647915	-1.393132

C	4.770399	-2.086849	0.944438
C	6.529673	-1.851091	-1.208503
H	4.784964	-1.394650	-2.380490
C	6.138302	-2.282608	1.132295
H	4.103429	-2.148311	1.796101
C	7.024120	-2.173712	0.058150
H	7.209514	-1.755068	-2.051466
H	6.514760	-2.516191	2.125250
H	8.089325	-2.329516	0.207908
C	0.423531	-2.620572	-1.548816
O	0.461209	-1.810671	-2.451319
O	0.027435	-3.686884	-1.168720

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B3LYP SCF energy: -1893.20453221 a.u.
B3LYP enthalpy: -1892.418126 a.u.
B3LYP free energy: -1892.546828 a.u.
B3LYP-D3BJ SCF energy in solution: -1895.10777247 a.u.
B3LYP-D3BJ enthalpy in solution: -1894.321366 a.u.
B3LYP-D3BJ free energy in solution: -1894.450068 a.u.
Three lowest frequencies (cm-1): 8.3444 12.4457 17.2986

Cartesian coordinates

ATOM	X	Y	Z
Cu	0.126129	-0.036561	0.620223
N	2.680570	-1.001650	-0.498820
N	2.561554	1.146530	-0.559480
C	1.872478	0.041642	-0.153369
C	3.848161	-0.556256	-1.108230
C	3.773055	0.798897	-1.146319
H	4.609751	-1.238685	-1.451375
H	4.455846	1.540641	-1.529914
C	-3.898779	-0.159771	1.023474
C	-4.862379	-0.119837	0.078014
C	-4.111817	-0.253753	2.512677
H	-4.497120	-0.133688	-0.947294
C	-2.467152	-0.132477	0.535236
O	-2.197030	-0.126940	-0.684083
O	-1.566124	-0.106292	1.468191
C	-6.324761	-0.096553	0.220141
C	-7.003505	0.496581	1.302788
C	-7.104472	-0.659633	-0.810426
C	-8.396891	0.494677	1.364464
H	-6.437672	0.991725	2.084043
C	-8.495520	-0.670069	-0.745126
H	-6.600043	-1.101713	-1.666464
C	-9.150145	-0.095181	0.347402
H	-8.896352	0.965137	2.207865
H	-9.070512	-1.121371	-1.549899
H	-10.235797	-0.095928	0.398960
H	-3.340736	-0.888341	2.956647
H	-4.018928	0.727627	2.998453
H	-5.097378	-0.660240	2.757331
C	2.348555	-2.391730	-0.278764
C	2.748309	-2.997138	0.929676

C	1.637576	-3.082355	-1.280494
C	2.412302	-4.343029	1.118039
C	1.330978	-4.427496	-1.037608
C	1.712246	-5.052675	0.145913
H	2.697540	-4.839199	2.041060
H	0.780013	-4.989187	-1.786126
H	1.459316	-6.096171	0.313573
C	2.079683	2.502630	-0.417796
C	2.403544	3.214189	0.754970
C	1.304801	3.055094	-1.457196
C	1.923520	4.524517	0.866601
C	0.854045	4.371028	-1.291114
C	1.157861	5.098995	-0.144583
H	2.146814	5.099936	1.760352
H	0.250302	4.826774	-2.070323
H	0.793258	6.116995	-0.036295
C	3.487757	-2.237669	2.026906
C	4.807219	-2.927652	2.422668
C	2.579162	-2.024528	3.254672
H	3.746635	-1.246931	1.640740
H	5.463438	-3.065356	1.555767
H	5.343221	-2.321803	3.162547
H	4.633155	-3.913147	2.869397
H	1.664517	-1.488704	2.979077
H	2.285994	-2.980970	3.703144
H	3.102799	-1.440284	4.020926
C	1.201863	-2.432610	-2.590759
C	-0.332917	-2.419190	-2.740417
C	1.876724	-3.114372	-3.798260
H	1.532749	-1.389619	-2.582349
H	-0.818005	-1.852674	-1.938626
H	-0.608172	-1.950557	-3.692937
H	-0.742907	-3.436356	-2.742901
H	2.969732	-3.096994	-3.712941
H	1.567059	-4.161641	-3.893435
H	1.599478	-2.601308	-4.726383
C	0.949398	2.290313	-2.728698
C	1.576035	2.958391	-3.969412
C	-0.575301	2.126417	-2.889448
H	1.374150	1.284493	-2.653578
H	2.665005	3.045495	-3.874981
H	1.358317	2.368813	-4.867519
H	1.174298	3.965893	-4.128722
H	-1.016561	1.570742	-2.055564
H	-1.076362	3.099254	-2.961371
H	-0.793576	1.574822	-3.811870
C	3.215364	2.603275	1.893383
C	2.336278	2.387114	3.141770
C	4.463550	3.442042	2.227808
H	3.566323	1.617990	1.571485
H	1.476404	1.748608	2.912350
H	2.916950	1.908348	3.939446
H	1.954064	3.338667	3.529354
H	5.101634	3.579355	1.347389
H	4.196314	4.436009	2.604312
H	5.056704	2.944543	3.003921