Electronic Supplementary Information

Computational study of silver-catalyzed stereoselective hydroalkylation of alkynes: Pauli repulsion controlled *Z*/*E* selectivity

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Computational Details

The B3LYP density functional and a mixed basis set of LANL2DZ for Ag and 6-31G(d) for other atoms were used in the gas-phase geometry optimizations. All minima have zero imaginary frequency and all transition states have only one imaginary frequency and confirmed by intrinsic reaction coordinate (IRC) calculations. Single-point energies were calculated by using B3LYP with dispersion corrections (D3BJ)[1] and a mixed basis set of SDD for the transition metals and 6-311+G(d,p) for other atoms. Solvation energy corrections were calculated using the SMD model[2] with the solvent reported in the experimental conditions. The frontier molecular orbitals of fragments were computed at the HF/6-31G(d)-LANL2DZ(Ag) level of theory. All these calculations were carried out with Gaussian 09.[3]

To validate the conclusion based on the method used in the present study, we further computed the barriers of syn/anti-1,2 migration (**9-TS** and **8-TS**) using a few popular modern density functionals and basis sets. As shown in Table S1, although the absolute barriers of **8-TS** and **9-TS** 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 and basis sets in both optimization and single-point energy calculations.

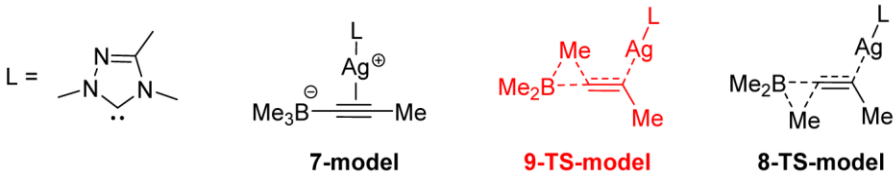
Moreover, we performed DFT calculations using triple ζ basis sets for both geometry optimizations and single-point energy calculations. Because the real catalyst systems are computationally demanding when locating transition states, we used the model transition states (**9-TS-model** and **8-TS-model**) for benchmark calculations. As shown Table S2, the trend of barrier difference ($\Delta\Delta G^{\ddagger}_{sol}$) of syn/anti-to-Ag 1,2-migration is slightly affected by the choice of density functionals and triple ζ basis sets. The results of DFT calculations with triple ζ basis sets are consistent with those of the combination of double ζ basis set for geometry optimization and triple ζ basis set for single-point energy calculations.

Energy decomposition analysis (EDA) calculations at the B3LYP-D3BJ/6-311+G(d,p)–LANL2DZ (Ag) 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 the two stereoselective migration transition states have different bond distances. To minimize the effect of early or late transition states in comparing each energy term between the migration pathways, we performed EDA calculations along the reaction coordinates obtained from IRC calculations. The reported energies in the radar charts are the average of $\Delta\Delta E$ values at the two C–C bond distances that correspond to the syn- and anti-migration transition states. The geometries and orbitals were visualized using CYLview[5] and IQmol, respectively.

Table S1. Comparison of barriers (in kcal/mol) of syn-to-metal (9-TS) and anti-to-metal (8-TS) 1,2-migration using different levels of theories.

Entry	Method for Single-Point Energy Calculation in Solvent Using SMD	Method for Gas-Phase Geometry Optimization	Barrier of **9-TS** ($\Delta G^{\ddagger}_{sol}$) with respect to **7**	Barrier of **8-TS** ($\Delta G^{\ddagger}_{sol}$) with respect to **7**	$\Delta\Delta G^{\ddagger}_{sol}$ (**9-TS** – **8-TS**)
1	B3LYP-D3BJ/ SDD−6-311+G(d,p)	B3LYP/ LANL2DZ−6-31G(d)	26.1	23.3	2.8
2	M06/ SDD−6-311+G(d,p)		26.0	23.1	2.9
3	M06L/ SDD−6-311+G(d,p)		27.9	24.6	3.3
4	ωB97xD/ SDD−6-311+G(d,p)		28.4	25.1	3.3
5	B3LYP/ LANL2DZ−6-31G(d)		21.9	18.9	3.0
6	B3LYP-D3BJ/ SDD−6-311+G(d,p)	B3LYP-D3BJ/ LANL2DZ−6-31G(d)	27.9	22.6	5.3
7	M06/ SDD−6-311+G(d,p)		28.0	23.0	5.0
8	M06L/ SDD−6-311+G(d,p)		29.1	24.6	4.5
9	ωB97xD/ SDD−6-311+G(d,p)		30.0	24.6	5.4
10	B3LYP-D3BJ/ LANL2DZ−6-31G(d)		27.0	22.8	4.2
11	B3LYP-D3BJ/ SDD−6-311+G(d,p)	M06/ LANL2DZ−6-31G(d)	28.6	24.3	4.3
12	M06/ SDD−6-311+G(d,p)		29.3	24.9	4.4
13	M06L/ SDD−6-311+G(d,p)		30.8	26.9	3.9
14	ωB97xD/ SDD−6-311+G(d,p)		31.6	26.3	5.3
15	M06/ LANL2DZ−6-31G(d)		27.5	23.6	3.9

Table S2. Comparison of barriers (in kcal/mol) of syn-to-metal (9-TS-model) and anti-to-metal (8-TS-model) 1,2-migration using higher levels of theories.



7-model **9-TS-model** **8-TS-model**

Entry	Method for Single-Point Energy Calculation in Solvent Using SMD	Method for Gas-Phase Geometry Optimization	Barrier of **9-TS-model** ($\Delta G^{\ddagger}_{sol}$) with respect to **7-model**	Barrier of **8-TS-model** ($\Delta G^{\ddagger}_{sol}$) with respect to **7-model**	$\Delta\Delta G^{\ddagger}_{sol}$ (**9-TS-model** – **8-TS-model**)
1	B3LYP-D3BJ/ SDD−6-311+G(d,p)	B3LYP/ LANL2DZ−6-311+G(d,p)	23.7	20.0	3.7
2	M06/ SDD−6-311+G(d,p)		23.5	20.0	3.5
3	M06L/ SDD−6-311+G(d,p)		25.7	21.7	4.0
4	ωB97xD/ SDD−6-311+G(d,p)		25.9	22.0	3.9
5	B3LYP/ LANL2DZ−6-31G(d)		21.1	17.3	3.8
6	B3LYP-D3BJ/ SDD−6-311+G(d,p)	B3LYP-D3BJ/ LANL2DZ−6-311+G(d,p)	24.4	20.8	3.6
7	M06/ SDD−6-311+G(d,p)		24.2	20.5	3.7
8	M06L/ SDD−6-311+G(d,p)		26.4	22.3	4.1
9	ωB97xD/ SDD−6-311+G(d,p)		26.6	22.8	3.8
10	B3LYP-D3BJ/ LANL2DZ−6-31G(d)		23.3	19.8	3.5
11	B3LYP-D3BJ/ SDD−6-311+G(d,p)	M06/ LANL2DZ−6-311+G(d,p)	22.3	20.4	1.9
12	M06/ SDD−6-311+G(d,p)		22.5	20.2	2.3
13	M06L/ SDD−6-311+G(d,p)		24.7	22.2	2.5
14	ωB97xD/ SDD−6-311+G(d,p)		24.3	21.9	2.4
15	M06/ LANL2DZ−6-31G(d)		20.4	18.3	2.1
16	B3LYP-D3BJ/ SDD−6-311+G(d,p)		23.5	20.1	3.4

17	M06/SDD−6-311+G(d,p)	B3LYP/ def2-TZVP	23.4	20.0	3.4
18	M06L/ SDD−6-311+G(d,p)		25.4	21.6	3.8
19	ωB97xD/ SDD−6-311+G(d,p)		25.7	22.1	3.6
20	B3LYP/ def2-TZVP		22.4	18.8	3.6
21	B3LYP-D3BJ/ SDD−6-311+G(d,p)	B3LYP-D3BJ/ def2-TZVP	22.9	19.9	3.0
22	M06/ SDD−6-311+G(d,p)		22.7	19.6	3.1
23	M06L/ SDD−6-311+G(d,p)		24.8	21.3	3.5
24	ωB97xD/ SDD−6-311+G(d,p)		25.1	21.9	3.2
25	B3LYP-D3BJ/ def2-TZVP		23.3	20.3	3.0
26	B3LYP-D3BJ/ SDD−6-311+G(d,p)	M06/ def2-TZVP	23.5	20.1	3.4
27	M06/ SDD−6-311+G(d,p)		23.4	20.0	3.4
28	M06L/ SDD−6-311+G(d,p)		25.4	21.6	3.8
29	ωB97xD/ SDD−6-311+G(d,p)		25.7	22.1	3.6
30	M06/ def2-TZVP		22.4	18.8	3.6

Alkyne C–H Activation with Possible Ag(I) Species

Under the experimental condition with L-Ag-Cl, LiO^{t}Bu, and MeOH, we computed several possible Ag(I) species as the active catalyst. As shown in Fig. S1, the barriers of alkyne C–H activation by these active Ag(I) complexes are lower than 17 kcal/mol, and thus can be easily surmounted. It should be noted that the interactions with LiO^{t}Bu significantly stabilize the L-Ag-OMe, L-Ag-O^{t}Bu and L-Ag-Cl species, forming the complexes of **1**, **s8** and **s10**, respectively. Based on these complexes, the 6-membered transition states of C–H cleavages require quite low barriers, smaller than 12 kcal/mol. Because the protonation with MeOH is the final step in the overall catalytic cycle, which regenerates the L-Ag-OMe species, the complex **1** was chosen as the energy reference and reported in the main text.

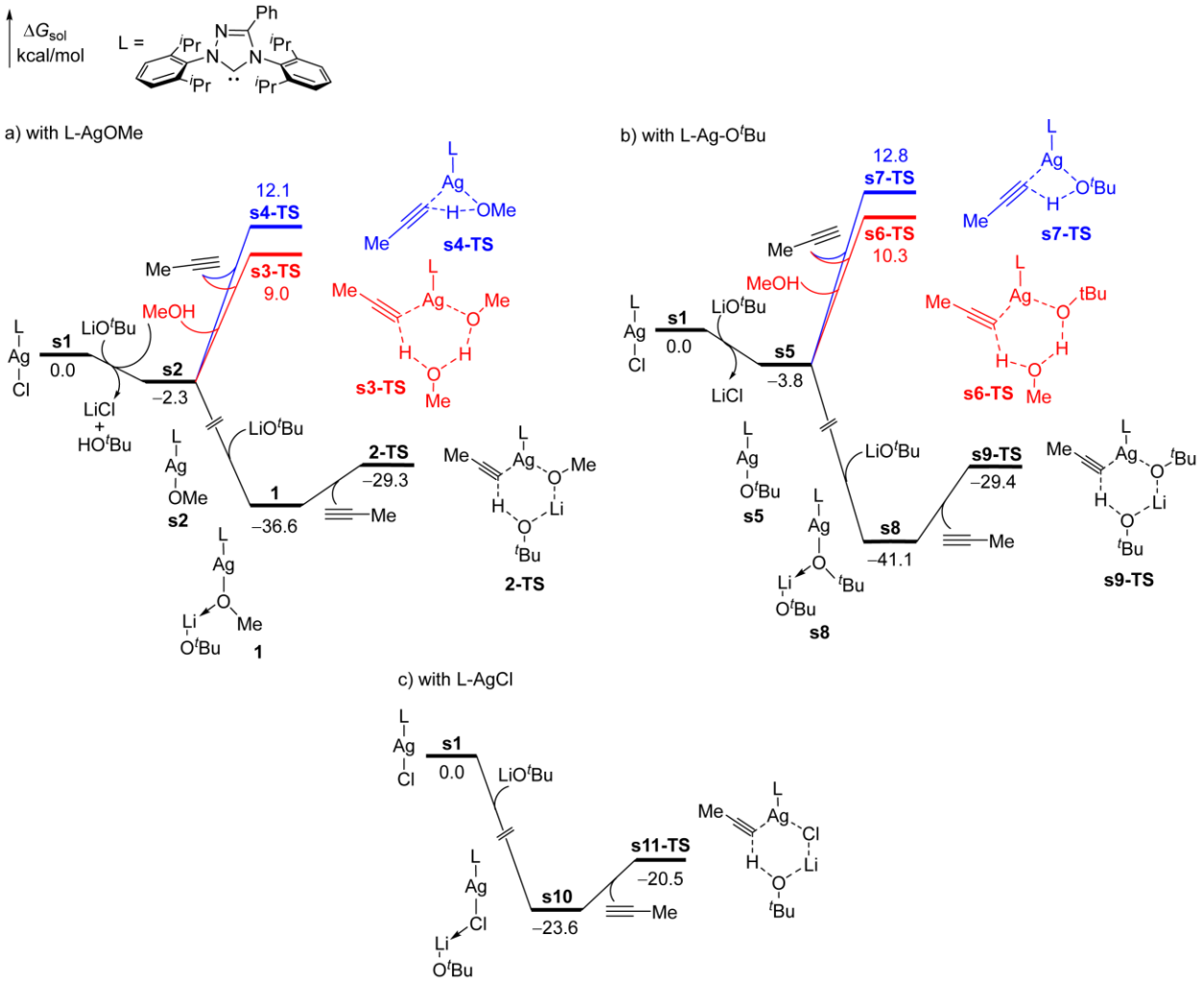


Fig. S1. Energy profile of alkyne C–H activation by possible Ag(I) species.

Competing Pathways

The anti- and syn-to-Ag 1,2-migrations from alkynyl boronate **7** result in the formation of alkenyl Ag(I) intermediates **10** and **11**, respectively. The protonation of Ag–C bond in **10** can also be promoted by an addition trialkylboron via **s13-TS** (Fig. S2), which is slightly less favorable than the boron-assisted protonation transition state **12-TS** (Fig. 3). Further, the protonation with two MeOH is highly disfavored (**s12-TS**).

The protonation of Ag–C bond in **11** with boron assistance also requires a low barrier (**s14-TS**, Fig. S2). This indicates that the pathway for generating minor *E*-olefin can go through with the similar mechanism of forming major *Z*-olefin (the first Ag–C protonation, transmetalation and the second Ag–C protonation). The major difference lies in the 1,2-migration step, which determine the stereoselectivity.

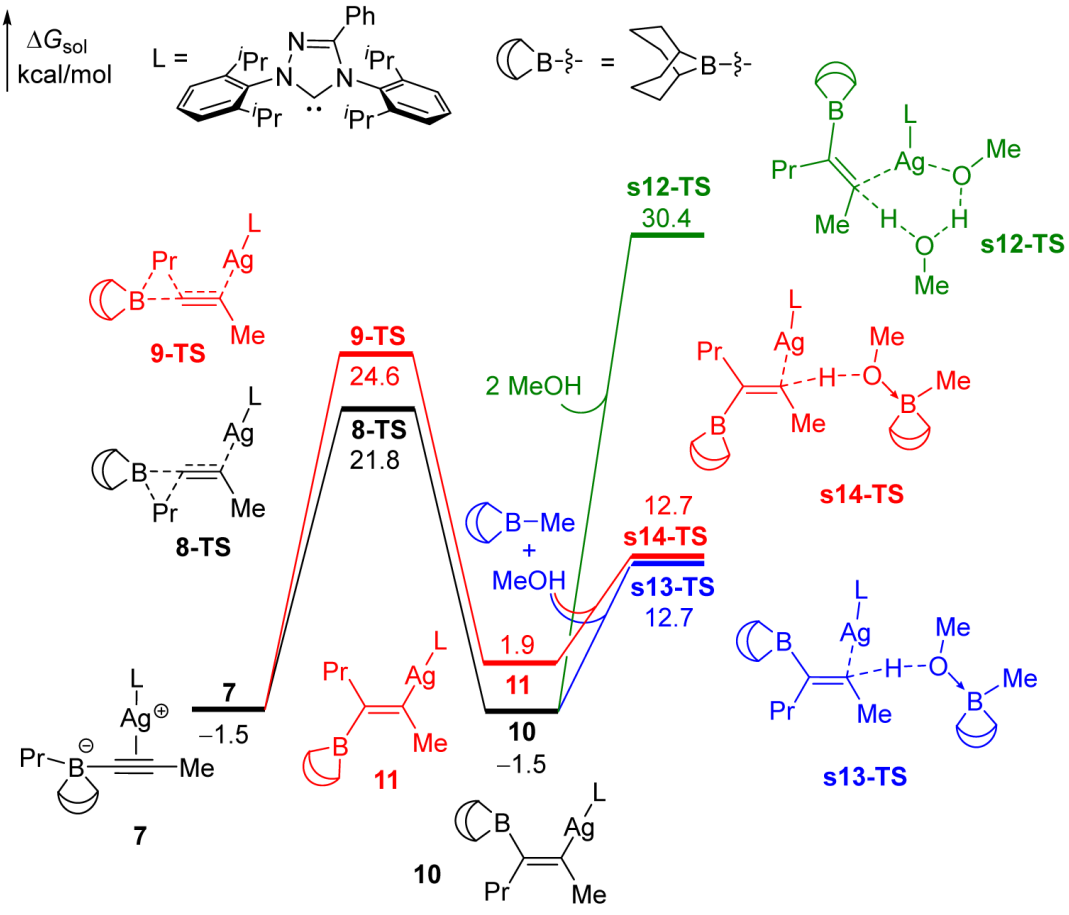


Fig. S2. Energy profiles of competing pathways of alkynyl boronate **7**.

We further computed several unproductive pathways to fully describe the possibilities of reaction mechanisms. During the process of the reaction, the intermediates of alkynyl Ag (**4**), methoxyl Ag (**13**) and alkenyl Ag (**15**) are generated, which could react with the alkylboron reagent via transmetalation mechanism. As shown in Fig. S3, these unproductive pathways (**6a-TS**, **14a-TS** and **16a-TS**) are less favorable than the corresponding productive pathways (**6-TS**, **14-TS** and **16-TS**), respectively.

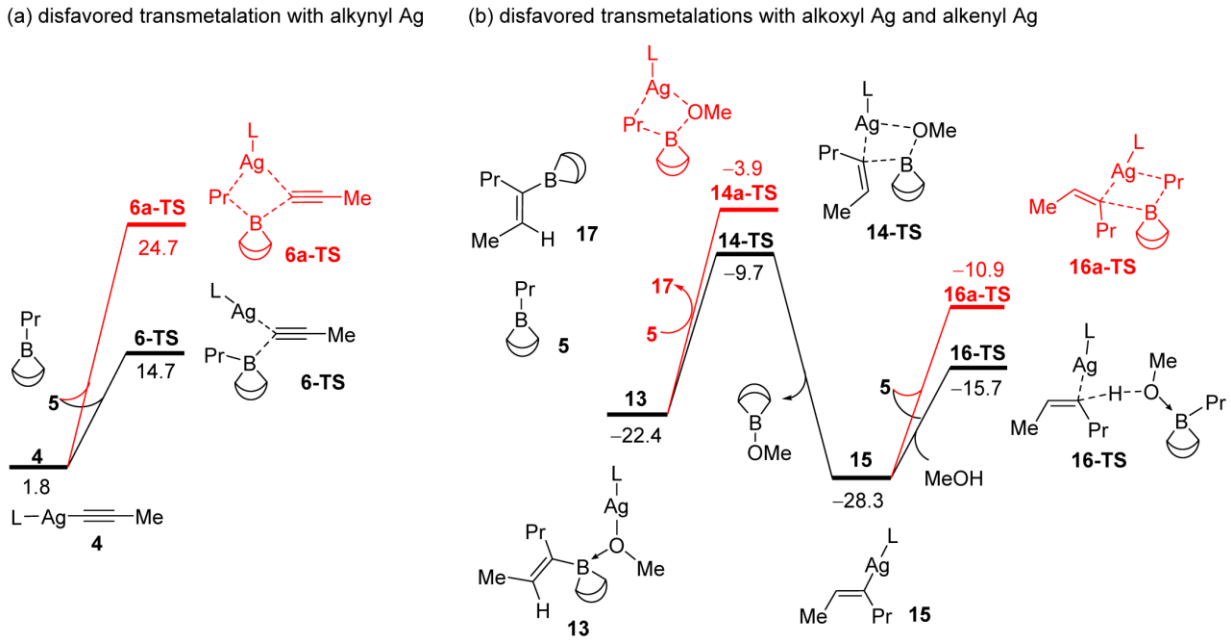


Fig. S3. Energy profiles of disfavored transmetalation pathways.

Charge Density Difference

To understand the change of alkyne π electron density when interacting with cationic silver complexes, we performed calculations of charge density difference to study the areas of electron gain and loss. As shown in Fig. S4, the alkyne π electron of intermediate **7** is depleted (cyan) at the opposite site of Ag and accumulated (yellow) at the same side of Ag. This unequal redistribution of π electron density leads to different σ)(π Pauli repulsion (see detailed discussions in the main text), thus distinguishing the reactivity when the migrated alkyl groups approaching from different sides of silver.

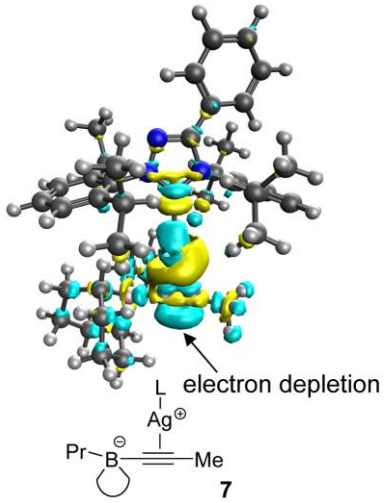


Fig. S4. Charge density difference (yellow: electron gain; cyan: electron loss) in complex **7**.

Energy Terms of EDA along IRC

The computed energy terms of EDA results along the IRC of **8-TS** and **9-TS** were shown in Tables S3 and S4. The change trends of these energy terms shown in Fig. 5a in the manuscript were plotted from these data. Clearly, the disfavored **9-TS** always has stronger interactions of charge transfer (ΔE_{ct}), electrostatics (ΔE_{elstat}), polarization (ΔE_{pol}) and dispersion (ΔE_{disp}) than the favored **8-TS** along the process of 1,2-migration. However, these stabilizing interactions are suppressed by the destabilizing interactions of distortion (ΔE_{dist}) and Pauli repulsion (ΔE_{Pauli}).

The radar chart shown in Fig. S5 quantitatively demonstrates the contribution of each energy term to the barrier difference of the two transition states. Clearly, the difference of Pauli repulsion ($\Delta\Delta E_{Pauli}$ = 26.2 kcal/mol) is the most significant effect on destabilizing **9-TS**. The deformation of two fragements also destabilizes **9-TS** albeit with relatively low importance ($\Delta\Delta E_{dist}$ = 7.0 kcal/mol).

Table S3. EDA energy terms of anti-to-metal 1,2-migration (8-TS) along IRC

Energy terms (in kcal/mol) / *r*(C-C) in **8-TS** (in Å)	ΔE_{dist}	ΔE_{Pauli}	ΔE_{ct}	ΔE_{elstat}	ΔE_{pol}	ΔE_{disp}
2.14	62.72	313.71	-84.27	-168.75	-99.62	-29.54
2.11	64.50	336.88	-88.73	-178.42	-108.34	-30.88
2.08	66.51	362.28	-93.65	-188.42	-118.66	-32.34
2.05	68.75	390.57	-99.04	-199.10	-130.81	-34.01
2.02	71.17	420.52	-104.87	-209.88	-144.31	-35.78
1.98	73.74	453.21	-111.13	-220.90	-159.97	-37.76
1.95 (TS)	76.42	488.17	-117.81	-232.08	-177.54	-39.89
1.92	79.30	525.66	-124.85	-243.51	-197.27	-42.21
1.88	82.25	565.44	-132.19	-254.83	-219.26	-44.68
1.85	85.23	607.26	-139.70	-266.18	-243.28	-47.28

Table S4. EDA energy terms of syn-to-metal 1,2-migration (9-TS) along IRC

Energy terms (in kcal/mol) / *r*(C-C) in **9-TS** (in Å)	ΔE_{dist}	ΔE_{Pauli}	ΔE_{ct}	ΔE_{elstat}	ΔE_{pol}	ΔE_{disp}
2.12	73.05	351.41	-92.98	-183.82	-116.51	-31.53
2.10	74.21	372.15	-97.05	-191.62	-125.09	-32.76
2.07	75.53	394.49	-101.37	-199.76	-134.82	-34.08
2.04 (TS)	77.00	420.34	-106.25	-208.85	-146.54	-35.63
2.00	78.62	457.31	-113.82	-220.41	-162.03	-37.28
1.98	80.38	478.03	-117.05	-227.65	-174.79	-39.14
1.95	82.22	510.97	-123.10	-237.76	-191.77	-41.21

1.91	84.14	546.54	-131.86	-247.91	-211.08	-43.44
1.88	86.11	584.06	-136.12	-258.40	-231.83	-45.83
1.84	88.14	623.91	-142.96	-268.87	-254.81	-48.36

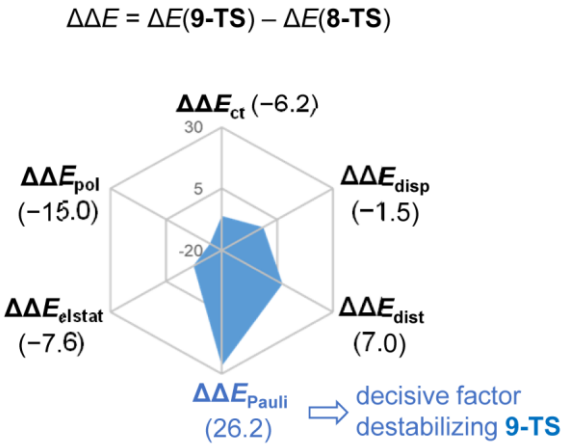


Fig. S5. Radar chart of the difference of energy terms between **9-TS** and **8-TS**.

The in-plane π Orbital along IRC

We computed the in-plane π orbital of L-Ag-alkyne fragment for three representative structures along IRC. The results clearly show that these in-plane π orbitals are accumulated at the same side of Ag 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 approaching to L-Ag-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.

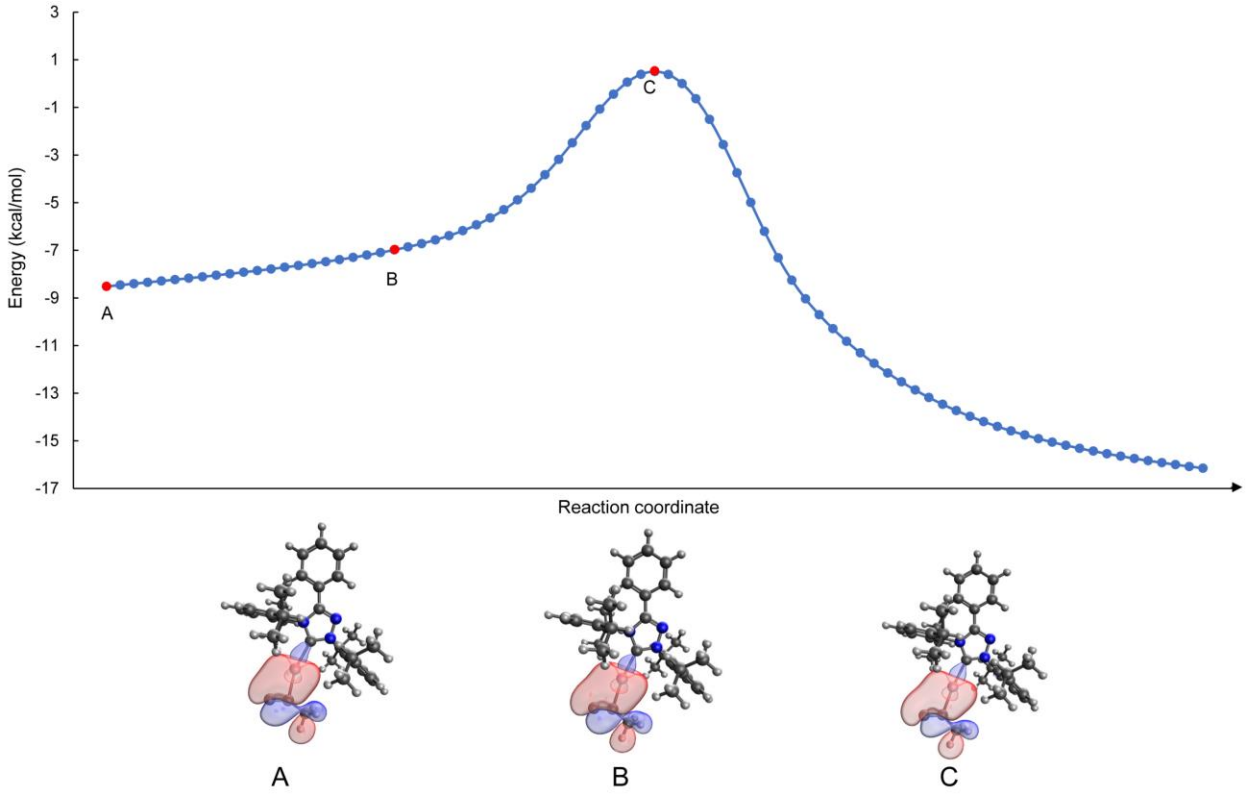


Fig. S6. The in-plane π orbital of L-Ag-alkyne fragment along reaction coordinates.

Cartesian Coordinates (Å) and Energies of the Optimized Structures

```
  1
B3LYP SCF energy:                    -1908.73525678 a.u.
B3LYP enthalpy:                      -1907.871906 a.u.
B3LYP free energy:                   -1908.015699 a.u.
B3LYP-D3BJ SCF energy in solution:      -1910.72784320 a.u.
B3LYP-D3BJ enthalpy in solution:     -1909.864492 a.u.
B3LYP-D3BJ free energy in solution:      -1910.008285 a.u.
Three lowest frequencies (cm-1):       9.2206     13.7256     16.6562

Cartesian coordinates
ATOM       X           Y           Z
N        1.600895   -0.370716   -0.108544
N        0.604746    1.476568   -0.454644
C        0.491572    0.342967    0.254966
C        2.337723    0.380832   -1.026025
C        1.890139   -1.682879    0.434813
C        2.731889   -1.773336    1.561757
C        1.294454   -2.809281   -0.170627
C        2.983373   -3.051903    2.074235
C        1.584071   -4.061449    0.386936
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H        1.142028   -4.951048   -0.051525
H        2.626750   -5.167246    1.909333
C       -0.327309    2.581577   -0.457000
C       -1.367026    2.577766   -1.408036
C       -0.148051    3.607448    0.489292
C       -2.258037    3.657272   -1.377186
C       -1.069170    4.661631    0.470699
C       -2.113851    4.685522   -0.449096
H       -3.077558    3.690186   -2.087464
H       -0.966795    5.471865    1.186707
H       -2.821008    5.510528   -0.443421
C        0.997853    3.615342    1.495696
C        0.486524    3.689279    2.947165
C        1.990911    4.754976    1.192032
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H        2.831988    4.727085    1.895054
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C        4.895958   -0.621344    2.224087
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H        3.068566    0.337114    1.668861
H        5.282823   -0.721053    1.204573
H        5.316966    0.291289    2.661292
H        5.266274   -1.470333    2.810233
```

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C	-0.906735	1.989830	-3.806417
C	-2.947390	0.995579	-2.656999
H	-0.907206	0.629448	-2.153018
H	0.140824	2.287220	-3.688883
H	-0.958419	1.198774	-4.563787
H	-1.465546	2.854337	-4.184437
H	-3.383185	0.602229	-1.731889
H	-3.605838	1.786239	-3.035201
H	-2.961083	0.188111	-3.398213
C	0.369740	-2.721605	-1.382578
C	-1.043705	-3.239774	-1.049578
C	0.958115	-3.463475	-2.599907
H	0.269460	-1.669162	-1.665220
H	-1.484141	-2.696230	-0.207079
H	-1.709569	-3.112017	-1.909611
H	-1.029358	-4.305318	-0.792307
H	1.940262	-3.066222	-2.879626
H	1.071647	-4.535437	-2.401087
H	0.291171	-3.355334	-3.462481
C	-2.810526	-0.850510	3.983124
O	-2.827711	-0.579635	2.605237
Ag	-1.098266	-0.152469	1.537491
H	-2.172173	-1.713571	4.239574
H	-2.455792	0.008954	4.577792
H	-3.828517	-1.085639	4.336066
C	3.619700	0.052786	-1.675824
C	4.181405	-1.234890	-1.700022
C	4.300295	1.102475	-2.323221
C	5.394547	-1.460071	-2.353052
H	3.680513	-2.065485	-1.221348
C	5.507411	0.868659	-2.973118
H	3.868599	2.096890	-2.308791
C	6.062012	-0.414176	-2.989538
H	5.813162	-2.462324	-2.363934
H	6.018093	1.691084	-3.465893
H	7.005959	-0.595550	-3.495709
N	1.723115	1.522346	-1.243685
Li	-4.137679	-0.805205	1.371852
O	-5.027118	-1.038713	-0.022209
C	-5.949035	-1.566581	-0.898740
C	-6.973018	-2.442975	-0.134985
C	-6.711401	-0.428658	-1.622513
C	-5.235427	-2.447952	-1.955362
H	-6.447986	-3.252703	0.387654
H	-7.489511	-1.834610	0.618045
H	-7.729935	-2.891452	-0.794176
H	-6.004919	0.202166	-2.175525
H	-7.465253	-0.802907	-2.329390

H	-7.215580	0.204206	-0.882113
H	-5.930831	-2.895175	-2.679549
H	-4.503530	-1.846239	-2.508341
H	-4.693197	-3.257958	-1.451288

Propyne

B3LYP SCF energy: -116.65327005 a.u.
B3LYP enthalpy: -116.592615 a.u.
B3LYP free energy: -116.620746 a.u.
B3LYP-D3BJ SCF energy in solution: -116.70212004 a.u.
B3LYP-D3BJ enthalpy in solution: -116.641465 a.u.
B3LYP-D3BJ free energy in solution: -116.669596 a.u.
Three lowest frequencies (cm-1): 346.8899 346.8909 600.4941

Cartesian coordinates

ATOM	X	Y	Z
C	0.000000	0.000000	1.426148
C	0.000000	0.000000	0.218947
H	0.000000	0.000000	2.492236
C	0.000000	0.000000	-1.241448
H	0.000000	1.022440	-1.638041
H	0.885459	-0.511220	-1.638041
H	-0.885459	-0.511220	-1.638041

2-TS

B3LYP SCF energy: -2025.38395919 a.u.
B3LYP enthalpy: -2024.462564 a.u.
B3LYP free energy: -2024.616960 a.u.
B3LYP-D3BJ SCF energy in solution: -2027.43203795 a.u.
B3LYP-D3BJ enthalpy in solution: -2026.510643 a.u.
B3LYP-D3BJ free energy in solution: -2026.665039 a.u.
Three lowest frequencies (cm-1): -943.9102 9.6661 11.7859
Imaginary frequency: -943.9102 cm-1

Cartesian coordinates

ATOM	X	Y	Z
N	-1.294789	0.901634	-0.064524
N	-1.781158	-1.163807	-0.052397
C	-0.720855	-0.340260	0.042586
C	-2.675825	0.760581	-0.213792
C	-0.511441	2.119928	-0.024148
C	-0.351746	2.781373	1.210250
C	0.075077	2.582202	-1.222167
C	0.403640	3.961044	1.211984
C	0.821904	3.765030	-1.156193
C	0.982073	4.451341	0.044850
H	0.545339	4.497187	2.145591
H	1.288439	4.149310	-2.058436

H	1.566468	5.367137	0.072070
C	-1.753010	-2.606614	-0.069220
C	-1.741148	-3.254517	-1.319798
C	-1.764513	-3.300104	1.156987
C	-1.721808	-4.654922	-1.316082
C	-1.739325	-4.699112	1.099390
C	-1.715210	-5.369589	-0.121175
H	-1.716611	-5.191564	-2.260007
H	-1.743325	-5.271780	2.020953
H	-1.697819	-6.456147	-0.140627
C	-1.873750	-2.573862	2.494509
C	-1.064338	-3.238160	3.620616
C	-3.357572	-2.427765	2.896480
H	-1.465411	-1.566502	2.363833
H	-0.015914	-3.373819	3.336336
H	-1.090117	-2.605536	4.514720
H	-1.474379	-4.214673	3.903808
H	-3.928309	-1.900097	2.125472
H	-3.818283	-3.412062	3.044657
H	-3.445882	-1.867870	3.835224
C	-0.954793	2.273685	2.516375
C	-2.037908	3.234933	3.046544
C	0.136808	2.021340	3.575625
H	-1.438885	1.312180	2.317504
H	-2.836725	3.390774	2.313658
H	-2.487352	2.829456	3.960631
H	-1.611743	4.214789	3.293417
H	0.917615	1.351583	3.195697
H	0.610060	2.961024	3.887448
H	-0.311559	1.571510	4.469952
C	-1.809575	-2.486805	-2.636745
C	-3.246147	-2.519015	-3.199001
C	-0.794855	-2.986688	-3.680127
H	-1.562518	-1.440647	-2.431078
H	-3.957261	-2.098900	-2.480939
H	-3.307288	-1.936708	-4.126242
H	-3.555370	-3.546728	-3.424703
H	0.228944	-2.944735	-3.294261
H	-0.999397	-4.016575	-3.994636
H	-0.844103	-2.358199	-4.576836
C	-0.079304	1.866501	-2.562768
C	1.283136	1.414118	-3.124920
C	-0.834820	2.739322	-3.585768
H	-0.677190	0.964020	-2.403651
H	1.807652	0.750255	-2.430322
H	1.137277	0.873900	-4.068098
H	1.935326	2.270642	-3.331213
H	-1.827925	3.023579	-3.220900
H	-0.283330	3.659308	-3.812328
H	-0.964576	2.191147	-4.526187
C	2.286147	-1.058548	3.515025
O	2.472518	-0.207967	2.427418

Ag	1.397560	-0.768557	0.392963
H	1.295424	-0.924345	3.991562
H	2.363161	-2.129625	3.244872
H	3.034785	-0.884391	4.312508
C	-3.710737	1.804082	-0.342458
C	-3.436792	3.151210	-0.632938
C	-5.052556	1.406156	-0.181927
C	-4.479963	4.070617	-0.758275
H	-2.418314	3.489909	-0.765611
C	-6.085874	2.328242	-0.309573
H	-5.269401	0.368039	0.043060
C	-5.804798	3.666727	-0.597687
H	-4.248342	5.107590	-0.984395
H	-7.113849	2.001545	-0.179836
H	-6.612216	4.387134	-0.694810
N	-2.983093	-0.515995	-0.209794
Li	3.878422	0.485415	1.654076
O	4.837821	0.703824	0.171436
C	6.087432	1.023823	-0.411272
C	5.862281	1.519149	-1.853224
C	6.732602	2.137325	0.429599
C	6.991219	-0.224954	-0.413868
H	5.385308	0.737151	-2.454631
H	5.202381	2.394164	-1.850249
H	6.806420	1.797500	-2.338327
H	6.888513	1.794115	1.460370
H	7.705402	2.440691	0.022725
H	6.080664	3.018496	0.456184
H	7.973748	-0.013648	-0.854466
H	7.143227	-0.582173	0.611736
H	6.523589	-1.033678	-0.985854
C	3.123535	-2.394914	-1.104819
C	3.421216	-1.254244	-0.740125
H	4.197779	-0.206076	-0.371419
C	2.843364	-3.756399	-1.569999
H	3.233326	-4.508286	-0.872061
H	1.766711	-3.935335	-1.675199
H	3.305161	-3.941307	-2.548499

3
B3LYP SCF energy: -2025.40380334 a.u.
B3LYP enthalpy: -2024.476167 a.u.
B3LYP free energy: -2024.630513 a.u.
B3LYP-D3BJ SCF energy in solution: -2027.45465945 a.u.
B3LYP-D3BJ enthalpy in solution: -2026.527023 a.u.
B3LYP-D3BJ free energy in solution: -2026.681369 a.u.
Three lowest frequencies (cm-1): 6.2130 14.7575 15.2289

Cartesian coordinates

ATOM	X	Y	Z

N	1.344056	-0.884330	-0.057559
N	1.849746	1.163931	0.177620
C	0.783309	0.368079	-0.024048
C	2.725164	-0.775756	0.116809
C	0.553360	-2.075449	-0.289887
C	-0.023653	-2.731975	0.817060
C	0.378612	-2.517891	-1.617575
C	-0.775556	-3.885080	0.556024
C	-0.384051	-3.675515	-1.815271
C	-0.952655	-4.355909	-0.742073
H	-1.231259	-4.417816	1.385218
H	-0.535342	-4.044588	-2.825450
H	-1.539463	-5.253669	-0.918154
C	1.850373	2.604457	0.276093
C	1.843653	3.361319	-0.911095
C	1.889949	3.186797	1.558737
C	1.860092	4.755871	-0.780932
C	1.909935	4.584514	1.626503
C	1.891017	5.362009	0.471109
H	1.854089	5.373127	-1.674288
H	1.939524	5.071360	2.596090
H	1.903790	6.446072	0.548125
C	1.963469	2.348840	2.831347
C	1.048716	2.873918	3.951619
C	3.424609	2.238963	3.316302
H	1.620070	1.337681	2.588379
H	0.011355	2.959282	3.613958
H	1.071995	2.182294	4.801651
H	1.373739	3.852933	4.322776
H	4.064483	1.801838	2.543548
H	3.825027	3.227389	3.572993
H	3.483564	1.608192	4.211605
C	0.147199	-2.257280	2.257355
C	0.953870	-3.275123	3.090381
C	-1.210711	-1.948936	2.918083
H	0.716463	-1.322672	2.244219
H	1.942380	-3.465775	2.657751
H	1.097540	-2.895767	4.108664
H	0.428554	-4.234867	3.165828
H	-1.765075	-1.172698	2.375101
H	-1.835171	-2.849251	2.981924
H	-1.047125	-1.595088	3.943106
C	1.869272	2.730816	-2.299863
C	3.247164	2.937639	-2.961707
C	0.731113	3.247427	-3.199731
H	1.720018	1.652988	-2.188928
H	4.050519	2.523220	-2.342755
H	3.278197	2.443734	-3.940323
H	3.457636	4.002515	-3.117307
H	-0.247898	3.066362	-2.744280
H	0.824818	4.321293	-3.399978
H	0.756388	2.730209	-4.166328

C	0.976771	-1.799058	-2.823765
C	-0.125572	-1.262019	-3.758385
C	1.965872	-2.702180	-3.587869
H	1.541313	-0.933825	-2.463939
H	-0.801609	-0.583738	-3.227202
H	0.324494	-0.713422	-4.594660
H	-0.723589	-2.078449	-4.180465
H	2.770770	-3.057529	-2.935360
H	1.463185	-3.579938	-4.010867
H	2.419353	-2.148120	-4.417963
C	-2.498920	1.424405	2.896134
O	-2.802819	0.789833	1.706490
Ag	-1.262961	0.897305	-0.432150
H	-1.597338	1.004043	3.388989
H	-2.303176	2.512431	2.781093
H	-3.312416	1.343049	3.650036
C	3.752505	-1.835452	0.123766
C	3.468114	-3.211501	0.108490
C	5.100433	-1.425851	0.152437
C	4.505548	-4.146164	0.122764
H	2.446151	-3.564233	0.089362
C	6.127427	-2.363227	0.167749
H	5.326132	-0.365624	0.161590
C	5.835616	-3.730225	0.152260
H	4.264052	-5.205295	0.112125
H	7.159720	-2.025171	0.189267
H	6.638509	-4.462092	0.162703
N	3.042538	0.489647	0.264879
Li	-3.915006	1.016172	0.374769
O	-5.561504	0.040763	-0.021511
C	-5.910334	-1.193804	0.676108
C	-4.849079	-2.256618	0.366974
C	-5.899223	-0.820877	2.159471
C	-7.301891	-1.634226	0.208723
H	-4.810864	-2.473431	-0.708818
H	-3.860516	-1.914905	0.689042
H	-5.079832	-3.194410	0.885508
H	-6.640246	-0.039720	2.363455
H	-6.143720	-1.695186	2.772749
H	-4.906919	-0.450991	2.440512
H	-7.622099	-2.537804	0.739877
H	-8.036070	-0.843721	0.395307
H	-7.303645	-1.859661	-0.865482
C	-3.944315	1.847188	-2.207781
C	-2.984341	1.429990	-1.561147
H	-5.410002	-0.149043	-0.964568
C	-5.045344	2.381407	-3.017713
H	-5.997932	2.370829	-2.471835
H	-4.853969	3.421561	-3.311732
H	-5.189270	1.803585	-3.940272

tBuOH

B3LYP SCF energy: -233.67095826 a.u.
B3LYP enthalpy: -233.527113 a.u.
B3LYP free energy: -233.563784 a.u.
B3LYP-D3BJ SCF energy in solution: -233.77603392 a.u.
B3LYP-D3BJ enthalpy in solution: -233.632189 a.u.
B3LYP-D3BJ free energy in solution: -233.668860 a.u.
Three lowest frequencies (cm-1): 200.5105 257.3467 269.3211

Cartesian coordinates

ATOM	X	Y	Z
C	0.687232	1.267513	-0.509555
C	-0.005452	-0.000021	0.013839
H	0.203462	2.160169	-0.099566
H	1.744108	1.284781	-0.211371
H	0.651626	1.323140	-1.603866
C	0.694170	-1.263471	-0.510169
C	-1.490366	-0.003940	-0.357394
H	0.215546	-2.158992	-0.100393
H	0.658618	-1.318903	-1.604487
H	1.751227	-1.274899	-0.212302
H	-1.622251	-0.003640	-1.444684
H	-1.981239	-0.892009	0.054086
H	-1.986121	0.880910	0.055169
O	0.013422	-0.000300	1.452336
H	0.944147	0.001355	1.728401

MeOLi

B3LYP SCF energy: -122.67689540 a.u.
B3LYP enthalpy: -122.630229 a.u.
B3LYP free energy: -122.659945 a.u.
B3LYP-D3BJ SCF energy in solution: -122.73610585 a.u.
B3LYP-D3BJ enthalpy in solution: -122.689439 a.u.
B3LYP-D3BJ free energy in solution: -122.719155 a.u.
Three lowest frequencies (cm-1): 168.0185 168.1543 839.5774

Cartesian coordinates

ATOM	X	Y	Z
C	-0.931851	-0.000042	0.000110
H	-1.358922	0.082092	-1.019170
H	-1.358517	0.841688	0.581077
H	-1.358415	-0.924008	0.438762
O	0.443480	0.000110	-0.000296
Li	2.039707	-0.000132	0.000346

4

B3LYP SCF energy: -1668.98901753 a.u.

B3LYP enthalpy: -1668.255839 a.u.
B3LYP free energy: -1668.380060 a.u.
B3LYP-D3BJ SCF energy in solution: -1670.87723194 a.u.
B3LYP-D3BJ enthalpy in solution: -1670.144053 a.u.
B3LYP-D3BJ free energy in solution: -1670.268274 a.u.
Three lowest frequencies (cm-1): 14.4997 17.1539 17.4755

Cartesian coordinates

ATOM	X	Y	Z
N	-1.082086	0.039746	-0.045396
N	0.490881	-1.385061	-0.008579
C	0.285459	-0.056594	-0.027279
C	-1.631076	-1.243322	-0.029157
C	-1.765566	1.317191	-0.048014
C	-2.156429	1.874855	1.185479
C	-1.982469	1.963619	-1.282757
C	-2.806861	3.114586	1.152770
C	-2.635392	3.202024	-1.252130
C	-3.047001	3.771778	-0.050340
H	-3.120813	3.574663	2.084980
H	-2.815306	3.730339	-2.183794
H	-3.549225	4.735343	-0.051249
C	1.767964	-2.058288	-0.001949
C	2.322732	-2.448414	-1.235262
C	2.392933	-2.305946	1.234290
C	3.556453	-3.108927	-1.202542
C	3.627941	-2.965275	1.206077
C	4.204413	-3.363370	0.003303
H	4.016547	-3.424855	-2.134135
H	4.143869	-3.168166	2.140050
H	5.163890	-3.873608	0.005325
C	1.784148	-1.890591	2.568944
C	2.679025	-0.873319	3.303600
C	1.481626	-3.117109	3.452012
H	0.829006	-1.395204	2.369952
H	2.862679	0.011992	2.685354
H	2.198212	-0.548500	4.233965
H	3.650398	-1.308662	3.565802
H	0.810858	-3.816876	2.941514
H	2.397303	-3.659661	3.714480
H	1.002439	-2.802849	4.386775
C	-1.884800	1.200048	2.526661
C	-3.188511	0.911912	3.296482
C	-0.905447	2.034388	3.376758
H	-1.403190	0.236364	2.333910
H	-3.874981	0.296915	2.704720
H	-2.967197	0.377231	4.227447
H	-3.710214	1.838142	3.563846
H	0.033208	2.213905	2.841905
H	-1.333870	3.008963	3.638367
H	-0.674502	1.509920	4.311533
C	1.630152	-2.191537	-2.569289

C	1.157808	-3.512832	-3.207557
C	2.521057	-1.384614	-3.532870
H	0.737079	-1.588180	-2.379968
H	0.478118	-4.051043	-2.538386
H	0.629356	-3.315566	-4.147850
H	2.004713	-4.172293	-3.431415
H	2.836322	-0.437544	-3.082067
H	3.422471	-1.940524	-3.815600
H	1.971062	-1.159377	-4.454299
C	-1.532735	1.382187	-2.620348
C	-0.448390	2.264467	-3.271028
C	-2.719941	1.160539	-3.578577
H	-1.082021	0.402469	-2.435048
H	0.411741	2.392572	-2.605169
H	-0.096981	1.806040	-4.202899
H	-0.836603	3.260541	-3.513797
H	-3.474023	0.497393	-3.139946
H	-3.211706	2.105265	-3.837502
H	-2.370220	0.703747	-4.511579
Ag	1.735374	1.503705	0.018951
N	-0.661544	-2.129549	-0.011527
C	-3.049705	-1.644860	0.000552
C	-4.116957	-0.783297	-0.304194
C	-3.333472	-2.982001	0.340438
C	-5.431522	-1.251751	-0.265252
H	-3.933551	0.247266	-0.576989
C	-4.645945	-3.440895	0.374816
H	-2.511653	-3.649040	0.575439
C	-5.702619	-2.576877	0.073858
H	-6.244232	-0.572068	-0.505279
H	-4.844829	-4.475080	0.641486
H	-6.727889	-2.934981	0.103899
C	3.122711	2.998460	0.074132
C	3.954508	3.897614	0.103646
C	4.948417	4.970636	0.138266
H	5.878287	4.649106	0.627191
H	5.215743	5.310288	-0.871843
H	4.581331	5.848624	0.687443

5

B3LYP SCF energy: -456.68461216 a.u.
B3LYP enthalpy: -456.365632 a.u.
B3LYP free energy: -456.419146 a.u.
B3LYP-D3BJ SCF energy in solution: -456.87679839 a.u.
B3LYP-D3BJ enthalpy in solution: -456.557818 a.u.
B3LYP-D3BJ free energy in solution: -456.611332 a.u.
Three lowest frequencies (cm-1): 18.0080 48.7916 94.1315

Cartesian coordinates

ATOM	X	Y	Z

C	2.163177	-1.508768	0.246710
C	1.102487	-1.296170	1.347094
C	1.494027	1.332332	-1.200688
C	0.198424	-0.039427	1.172485
C	1.981472	1.637727	0.231847
C	0.945344	1.321228	1.331255
H	2.555174	-2.531970	0.325140
H	1.597899	-1.266592	2.329085
H	0.809859	2.134909	-1.515370
H	2.252271	2.700458	0.295375
H	3.021450	-0.855956	0.430198
H	0.444832	-2.178091	1.372949
H	2.346692	1.380296	-1.894403
H	-0.566259	-0.078639	1.960189
H	2.907757	1.091390	0.431285
H	0.188369	2.120012	1.339542
H	1.433519	1.364799	2.316271
C	1.636683	-1.284160	-1.186255
H	1.041953	-2.161640	-1.482364
H	2.485794	-1.251727	-1.885191
C	0.743660	-0.023520	-1.374200
H	0.357136	-0.048077	-2.403859
B	-0.404878	-0.056718	-0.287929
C	-1.930928	-0.072821	-0.684617
H	-2.085171	-0.981861	-1.295868
H	-2.094371	0.742236	-1.412623
C	-2.995539	-0.006811	0.421250
C	-4.432098	-0.032567	-0.111951
H	-2.847716	0.904294	1.017845
H	-2.852968	-0.843946	1.118631
H	-5.167009	0.014812	0.700437
H	-4.620203	0.816102	-0.781840
H	-4.624874	-0.949479	-0.683364

6-TS

B3LYP SCF energy: -2125.65881699 a.u.
B3LYP enthalpy: -2124.605944 a.u.
B3LYP free energy: -2124.758166 a.u.
B3LYP-D3BJ SCF energy in solution: -2127.75975559 a.u.
B3LYP-D3BJ enthalpy in solution: -2126.706883 a.u.
B3LYP-D3BJ free energy in solution: -2126.859105 a.u.
Three lowest frequencies (cm-1): -139.9551 11.4653 14.9406
Imaginary frequency: -139.9551 cm-1

Cartesian coordinates

ATOM	X	Y	Z
N	2.063197	1.375451	-0.014200
N	1.898005	-0.741716	-0.021713
C	1.147921	0.399068	-0.138448
C	3.235038	-0.389880	0.171899

C	1.821207	2.798089	-0.059718
C	1.887864	3.450048	-1.305326
C	1.556362	3.470987	1.148029
C	1.666153	4.832367	-1.316536
C	1.343256	4.852905	1.076336
C	1.395378	5.527185	-0.140774
H	1.708790	5.370685	-2.258870
H	1.135884	5.407458	1.986534
H	1.226605	6.600232	-0.172618
C	1.312043	-2.066341	-0.078937
C	0.936795	-2.690850	1.127724
C	1.122737	-2.663882	-1.342644
C	0.362955	-3.965110	1.037429
C	0.543907	-3.938628	-1.368546
C	0.167910	-4.584336	-0.193710
H	0.055858	-4.474148	1.945932
H	0.379643	-4.427412	-2.324257
H	-0.285157	-5.570731	-0.238458
C	1.524314	-1.992175	-2.653884
C	0.299699	-1.742396	-3.555942
C	2.604090	-2.801381	-3.400472
H	1.957968	-1.014628	-2.420687
H	-0.457893	-1.140914	-3.043277
H	0.603430	-1.211492	-4.465904
H	-0.173104	-2.683056	-3.860190
H	3.501084	-2.939212	-2.786937
H	2.235955	-3.793154	-3.687305
H	2.899326	-2.279278	-4.317928
C	2.209088	2.719406	-2.604670
C	3.592422	3.137489	-3.141709
C	1.109237	2.919973	-3.664590
H	2.256404	1.647130	-2.391289
H	4.377440	2.940940	-2.403694
H	3.832259	2.579827	-4.054779
H	3.618137	4.206058	-3.385631
H	0.131634	2.601492	-3.286885
H	1.027020	3.969166	-3.970923
H	1.338451	2.332149	-4.561229
C	1.130906	-2.047450	2.498015
C	2.111440	-2.859224	3.368631
C	-0.213570	-1.844659	3.223885
H	1.571664	-1.055884	2.352978
H	3.082306	-2.979273	2.876557
H	2.274439	-2.351522	4.326363
H	1.717903	-3.858898	3.586822
H	-0.908684	-1.247284	2.625978
H	-0.700359	-2.802057	3.442103
H	-0.051657	-1.329911	4.178221
C	1.525743	2.762005	2.498051
C	0.210184	3.016208	3.257124
C	2.751149	3.154543	3.347902
H	1.588288	1.683951	2.319355

H	-0.657977	2.717615	2.660244
H	0.197001	2.440019	4.189487
H	0.089840	4.072835	3.522101
H	3.684753	2.922039	2.824398
H	2.749818	4.227136	3.575254
H	2.745876	2.610377	4.299762
C	-2.965630	1.111597	-0.823004
C	-3.692793	1.952830	-1.358699
C	-4.631057	2.901840	-1.949481
H	-4.460727	3.922572	-1.584208
H	-4.568785	2.916424	-3.045074
H	-5.659489	2.625004	-1.681848
C	-5.655072	-2.755099	0.859946
C	-4.111059	-2.745201	0.968504
C	-5.668172	-0.771167	-1.682982
C	-3.381050	-1.715444	0.053578
C	-4.849986	-2.020494	-2.079356
C	-3.443717	-2.087368	-1.446141
H	-6.070391	-3.280110	1.732539
H	-3.736792	-3.762437	0.767465
H	-5.308655	0.072325	-2.285190
H	-4.749636	-2.047058	-3.174559
H	-5.954413	-3.355395	-0.004770
H	-3.835418	-2.526221	2.009509
H	-6.718679	-0.930808	-1.977261
H	-2.317203	-1.744514	0.347342
H	-5.409658	-2.926361	-1.822904
H	-2.789204	-1.390671	-1.987600
H	-3.027606	-3.094828	-1.613055
C	-6.307136	-1.356477	0.757255
H	-6.342683	-0.909495	1.760443
H	-7.357138	-1.481075	0.447199
C	-5.581030	-0.356903	-0.193620
H	-6.118974	0.599438	-0.095097
B	-4.063826	-0.280547	0.357460
C	-3.804110	0.384867	1.811702
H	-2.721195	0.476152	2.002729
H	-4.159644	-0.341033	2.564919
Ag	-0.951120	0.670986	-0.454133
N	3.342072	0.919864	0.173613
C	4.407833	-1.261556	0.373560
C	4.412908	-2.645462	0.130286
C	5.595204	-0.647987	0.819001
C	5.576995	-3.390232	0.328810
H	3.520786	-3.149049	-0.216270
C	6.750590	-1.397261	1.013049
H	5.595827	0.419527	1.008062
C	6.747302	-2.773624	0.769714
H	5.562280	-4.458748	0.133867
H	7.655610	-0.905616	1.358509
H	7.649579	-3.358853	0.923362
C	-4.471656	1.733436	2.122804

C	-4.195915	2.249752	3.541053
H	-5.558766	1.645876	1.983482
H	-4.132760	2.479502	1.392255
H	-4.687078	3.213501	3.729700
H	-4.554111	1.540500	4.298941
H	-3.119236	2.388355	3.708703

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B3LYP SCF energy: -2125.67796005 a.u.
B3LYP enthalpy: -2124.624075 a.u.
B3LYP free energy: -2124.776510 a.u.
B3LYP-D3BJ SCF energy in solution: -2127.78636026 a.u.
B3LYP-D3BJ enthalpy in solution: -2126.732475 a.u.
B3LYP-D3BJ free energy in solution: -2126.884910 a.u.
Three lowest frequencies (cm-1): 10.8469 14.0086 16.1779

Cartesian coordinates

ATOM	X	Y	Z
N	-2.273359	-0.163797	0.017123
N	-1.092531	1.600394	0.137564
C	-0.977727	0.276938	-0.054697
C	-2.626110	-1.557083	-0.169043
C	-2.966832	-1.996140	-1.464863
C	-2.585066	-2.418952	0.946634
C	-3.278431	-3.352425	-1.621168
C	-2.906020	-3.764793	0.727609
C	-3.248915	-4.228945	-0.539637
H	-3.545329	-3.726353	-2.605156
H	-2.882950	-4.458400	1.562691
H	-3.493820	-5.277590	-0.684724
C	-0.023452	2.574105	0.160595
C	0.515752	2.942082	1.408136
C	0.402907	3.128598	-1.061546
C	1.534582	3.901619	1.402153
C	1.424443	4.083639	-1.004250
C	1.986267	4.463813	0.211355
H	1.983732	4.208336	2.341073
H	1.787533	4.532177	-1.923227
H	2.784085	5.200907	0.230604
C	-0.240772	2.766267	-2.396389
C	0.788378	2.536591	-3.517608
C	-1.275306	3.838492	-2.799281
H	-0.782731	1.823364	-2.268112
H	1.544022	1.799920	-3.225466
H	0.280632	2.171745	-4.418218
H	1.308679	3.460977	-3.792597
H	-2.045031	3.955279	-2.028849
H	-0.792334	4.812256	-2.943754
H	-1.767458	3.563499	-3.740065
C	-3.004104	-1.068249	-2.675747

C	-4.403755	-1.028864	-3.320855
C	-1.925937	-1.453262	-3.708342
H	-2.776882	-0.052025	-2.339182
H	-5.168866	-0.732059	-2.595707
H	-4.418073	-0.307753	-4.146045
H	-4.687257	-2.005283	-3.730417
H	-0.924728	-1.429308	-3.263989
H	-2.094269	-2.460406	-4.107083
H	-1.941178	-0.753496	-4.551894
C	-0.007619	2.376564	2.724681
C	-0.993000	3.368807	3.377845
C	1.115663	1.985187	3.701072
H	-0.567611	1.461695	2.501238
H	-1.827514	3.596538	2.706761
H	-1.400193	2.948813	4.305492
H	-0.489454	4.310518	3.627183
H	1.827158	1.292685	3.240576
H	1.672816	2.859303	4.056779
H	0.685468	1.496599	4.583065
C	-2.217852	-1.949578	2.351814
C	-0.924012	-2.623873	2.849232
C	-3.374919	-2.172184	3.346629
H	-2.027445	-0.872629	2.315032
H	-0.083777	-2.429539	2.174194
H	-0.655303	-2.241678	3.840326
H	-1.043792	-3.710324	2.932435
H	-4.288697	-1.661445	3.023636
H	-3.606271	-3.237164	3.464045
H	-3.100667	-1.782825	4.333587
C	2.952544	-1.842398	-0.625871
C	2.182230	-2.609633	-1.228217
C	1.623949	-3.728164	-2.011893
H	0.889201	-4.305496	-1.438536
H	1.132288	-3.383173	-2.929159
H	2.430337	-4.411663	-2.304403
C	6.434709	0.925755	0.473345
C	4.997924	1.492817	0.380643
C	5.822913	-1.453346	-1.641976
C	3.993336	0.628161	-0.419237
C	5.574440	-0.109910	-2.363816
C	4.277618	0.617165	-1.940876
H	6.969519	1.439638	1.286160
H	5.052456	2.511475	-0.039954
H	5.185712	-2.218821	-2.108890
H	5.549396	-0.284453	-3.450126
H	6.984876	1.185932	-0.437226
H	4.603921	1.615194	1.398748
H	6.861980	-1.766389	-1.840088
H	3.006398	1.113629	-0.291826
H	6.430077	0.554116	-2.201385
H	3.429714	0.121122	-2.438989
H	4.306987	1.644479	-2.343189

C	6.521385	-0.601595	0.701137
H	6.342861	-0.806721	1.765794
H	7.559085	-0.921225	0.506506
C	5.527946	-1.457195	-0.122744
H	5.662520	-2.497920	0.213855
B	3.990460	-0.915151	0.184961
C	3.548205	-0.996737	1.782751
H	4.159915	-0.303121	2.379866
H	2.508957	-0.623798	1.896657
Ag	0.784037	-0.894523	-0.435816
C	-3.111487	0.928113	0.247913
C	-4.579772	0.961961	0.382493
C	-5.387219	-0.181997	0.501457
C	-5.194006	2.229720	0.407405
C	-6.770578	-0.055561	0.640630
H	-4.950439	-1.171224	0.491480
C	-6.572535	2.346429	0.548108
H	-4.575697	3.115544	0.316473
C	-7.368872	1.203602	0.664470
H	-7.378256	-0.951178	0.733011
H	-7.026916	3.332948	0.564601
H	-8.445862	1.295654	0.772768
N	-2.384108	2.019666	0.324286
C	3.627055	-2.380811	2.446460
H	3.019193	-3.098772	1.875161
H	4.659017	-2.754334	2.385793
C	3.182495	-2.403728	3.915309
H	2.139366	-2.074104	4.019044
H	3.258601	-3.407579	4.354775
H	3.797600	-1.727634	4.523641

8-TS

B3LYP SCF energy: -2125.65179906 a.u.
B3LYP enthalpy: -2124.598367 a.u.
B3LYP free energy: -2124.748416 a.u.
B3LYP-D3BJ SCF energy in solution: -2127.75139373 a.u.
B3LYP-D3BJ enthalpy in solution: -2126.697962 a.u.
B3LYP-D3BJ free energy in solution: -2126.848011 a.u.
Three lowest frequencies (cm-1): -429.6159 10.4376 16.7066
Imaginary frequency: -429.6159 cm-1

Cartesian coordinates

ATOM	X	Y	Z
N	2.421323	1.236124	-0.026367
N	1.956092	-0.828904	0.113958
C	1.365131	0.403148	0.008542
C	2.385488	2.676272	-0.122559
C	2.386417	3.264204	-1.401146
C	2.375541	3.426683	1.068355
C	2.358087	4.662806	-1.462867

C	2.352283	4.821030	0.946395
C	2.339998	5.434101	-0.303947
H	2.353132	5.152929	-2.432149
H	2.345089	5.434149	1.842659
H	2.319830	6.518295	-0.375182
C	1.196034	-2.059892	0.174159
C	0.729633	-2.502939	1.429333
C	0.951362	-2.759172	-1.024380
C	0.011354	-3.704786	1.457446
C	0.228152	-3.954672	-0.933319
C	-0.232783	-4.427231	0.292274
H	-0.367783	-4.075652	2.404957
H	0.016920	-4.518240	-1.836942
H	-0.793213	-5.356707	0.338819
C	1.423213	-2.263349	-2.387938
C	0.226044	-1.862089	-3.273082
C	2.320848	-3.296219	-3.097294
H	2.027320	-1.363267	-2.236800
H	-0.386261	-1.094177	-2.788470
H	0.579751	-1.465457	-4.232188
H	-0.421127	-2.721148	-3.483872
H	3.183280	-3.568894	-2.479603
H	1.771110	-4.214508	-3.333911
H	2.694402	-2.884052	-4.041802
C	2.429881	2.445937	-2.687203
C	3.726125	2.718974	-3.475119
C	1.180511	2.686764	-3.556216
H	2.435217	1.385645	-2.416891
H	4.610998	2.507953	-2.864889
H	3.767803	2.086894	-4.369973
H	3.784388	3.763545	-3.802536
H	0.264405	2.445801	-3.006021
H	1.112681	3.730474	-3.884586
H	1.215593	2.057924	-4.453665
C	0.975034	-1.739633	2.728654
C	1.773697	-2.579900	3.745194
C	-0.348338	-1.240025	3.341218
H	1.577071	-0.855038	2.498758
H	2.736053	-2.903645	3.333596
H	1.973663	-1.989314	4.646668
H	1.219836	-3.474294	4.052805
H	-0.894954	-0.600147	2.640515
H	-1.004333	-2.074470	3.614277
H	-0.148395	-0.660112	4.250042
C	2.418929	2.781150	2.449324
C	1.258898	3.250919	3.346940
C	3.785478	3.021515	3.122078
H	2.307322	1.699849	2.323595
H	0.289223	3.054078	2.877198
H	1.287437	2.720825	4.306157
H	1.318460	4.323777	3.563189
H	4.601557	2.632520	2.503999

H	3.965328	4.090515	3.286920
H	3.824258	2.520915	4.096790
C	-3.616079	0.949055	-0.219364
C	-2.661930	1.843108	-0.246159
C	-2.780532	3.349938	-0.321777
H	-2.432838	3.817590	0.609581
H	-2.145085	3.751116	-1.120858
H	-3.804021	3.702254	-0.506425
C	-6.933312	-2.137081	-0.336578
C	-6.476487	-1.479299	0.986020
C	-3.905795	-2.186154	-1.562273
C	-4.987812	-1.056619	1.042107
C	-3.932036	-3.054913	-0.285668
C	-3.991184	-2.249082	1.031422
H	-8.032366	-2.145232	-0.368972
H	-6.715230	-2.162615	1.816958
H	-2.898633	-1.756565	-1.670406
H	-3.036190	-3.691391	-0.270585
H	-6.640549	-3.191942	-0.335320
H	-7.089548	-0.581845	1.160165
H	-4.056171	-2.837955	-2.438476
H	-4.830663	-0.529856	1.994371
H	-4.778839	-3.747116	-0.331202
H	-2.989330	-1.841587	1.231716
H	-4.210973	-2.941317	1.860905
C	-6.399745	-1.457924	-1.619878
H	-7.017593	-0.570631	-1.827462
H	-6.571738	-2.134102	-2.472804
C	-4.917746	-1.009207	-1.575364
H	-4.722519	-0.432462	-2.492065
B	-4.598261	-0.157239	-0.238262
C	-5.467180	1.558075	-0.220251
H	-5.290312	2.271536	-1.030077
H	-6.346537	0.986728	-0.540920
Ag	-0.706598	1.021278	-0.118896
C	3.343953	-0.673055	0.130019
C	4.394900	-1.706603	0.187585
C	5.707268	-1.307673	-0.133659
C	4.166653	-3.043088	0.556473
C	6.756785	-2.219062	-0.086987
H	5.888028	-0.277322	-0.418618
C	5.225580	-3.951859	0.598593
H	3.173513	-3.382309	0.817390
C	6.520872	-3.547568	0.277726
H	7.761317	-1.892128	-0.340378
H	5.030037	-4.980560	0.887662
H	7.340468	-4.259899	0.311016
N	3.636719	0.604585	0.048103
C	-5.758018	2.250058	1.111078
C	-6.968641	3.192837	1.034828
H	-4.879066	2.814257	1.442151
H	-5.939433	1.493807	1.884393

H	-7.159579	3.677740	2.000474
H	-6.810907	3.984011	0.290614
H	-7.878031	2.649451	0.748864

9-TS

B3LYP SCF energy: -2125.64700874 a.u.
B3LYP enthalpy: -2124.593700 a.u.
B3LYP free energy: -2124.743416 a.u.
B3LYP-D3BJ SCF energy in solution: -2127.74694292 a.u.
B3LYP-D3BJ enthalpy in solution: -2126.693634 a.u.
B3LYP-D3BJ free energy in solution: -2126.843350 a.u.
Three lowest frequencies (cm-1): -306.2576 8.6559 14.5736
Imaginary frequency: -306.2576 cm-1

Cartesian coordinates

ATOM	X	Y	Z
N	1.747227	1.533877	0.235936
N	2.522233	-0.422377	-0.043323
C	1.342837	0.278925	-0.027335
C	0.925022	2.716187	0.342094
C	0.821239	3.554162	-0.785224
C	0.304154	3.001123	1.572261
C	0.050078	4.714376	-0.651432
C	-0.464719	4.169997	1.643960
C	-0.590650	5.018005	0.547702
H	-0.052947	5.386931	-1.497397
H	-0.964993	4.420587	2.574654
H	-1.189950	5.920863	0.627459
C	2.576855	-1.851582	-0.273681
C	2.609023	-2.713945	0.840549
C	2.577861	-2.320755	-1.604314
C	2.660365	-4.090136	0.586394
C	2.630309	-3.707196	-1.795447
C	2.673852	-4.584220	-0.714791
H	2.683784	-4.783603	1.421647
H	2.631248	-4.103579	-2.806380
H	2.712272	-5.656254	-0.887600
C	2.521455	-1.395746	-2.817707
C	1.221971	-1.607788	-3.619939
C	3.760800	-1.556119	-3.720990
H	2.514711	-0.361143	-2.461086
H	0.337588	-1.455130	-2.991844
H	1.173795	-0.900968	-4.456555
H	1.168779	-2.620801	-4.035549
H	4.688735	-1.362609	-3.171573
H	3.824475	-2.564916	-4.144953
H	3.710359	-0.849232	-4.557013
C	1.541592	3.256858	-2.096504
C	2.776384	4.167852	-2.253298
C	0.610834	3.358801	-3.318545

H	1.903921	2.224556	-2.058536
H	3.466764	4.039028	-1.413543
H	3.312688	3.930937	-3.180084
H	2.483336	5.223725	-2.294633
H	-0.267681	2.715073	-3.205112
H	0.258358	4.383444	-3.481757
H	1.147597	3.051208	-4.223528
C	2.573349	-2.214312	2.281952
C	3.816399	-2.663467	3.075105
C	1.273823	-2.651852	2.987448
H	2.578514	-1.119995	2.267556
H	4.741282	-2.337831	2.587500
H	3.793524	-2.236384	4.084312
H	3.855222	-3.753958	3.179499
H	0.389059	-2.299534	2.446192
H	1.208856	-3.743431	3.063667
H	1.239122	-2.243747	4.004344
C	0.466001	2.122707	2.808495
C	-0.887699	1.601329	3.327013
C	1.239935	2.869898	3.913455
H	1.062503	1.248131	2.531518
H	-1.416214	1.029774	2.556339
H	-0.732897	0.944107	4.190731
H	-1.541571	2.420467	3.647956
H	2.217766	3.207634	3.553000
H	0.687796	3.750244	4.262359
H	1.399924	2.212990	4.776522
C	-3.684592	-1.201603	-0.165993
C	-2.465621	-1.655391	-0.233093
C	-2.308969	-3.178990	-0.221312
H	-1.801281	-3.523715	-1.131558
H	-1.688300	-3.501295	0.624819
H	-3.269228	-3.707955	-0.153731
C	-7.840637	0.551092	0.389409
C	-6.827336	0.453773	1.553785
C	-6.826729	-2.216278	-0.965959
C	-5.785149	-0.684555	1.438072
C	-7.328564	-2.553183	0.457541
C	-6.386195	-2.106409	1.598508
H	-8.337744	1.531228	0.429148
H	-7.385868	0.370459	2.500125
H	-6.052840	-2.946275	-1.244762
H	-7.485690	-3.639142	0.530121
H	-8.639904	-0.181421	0.541407
H	-6.283953	1.408901	1.623127
H	-7.656508	-2.366958	-1.675593
H	-5.063837	-0.550968	2.259447
H	-8.318715	-2.110813	0.610195
H	-5.544532	-2.812216	1.655395
H	-6.925028	-2.197444	2.555793
C	-7.229929	0.354425	-1.016889
H	-6.725376	1.287167	-1.313178

H	-8.051261	0.223781	-1.739751
C	-6.208640	-0.801908	-1.144128
H	-5.803313	-0.769337	-2.165945
B	-5.060316	-0.674481	-0.012516
C	-3.963154	0.814662	-0.277225
H	-3.156993	0.979532	0.442204
H	-4.806520	1.428144	0.064824
Ag	-0.636660	-0.579832	-0.211156
C	3.578592	0.450264	0.219580
N	3.105720	1.663136	0.389095
C	5.016796	0.151708	0.346528
C	5.624643	-1.008319	-0.162097
C	5.818455	1.107639	0.999946
C	6.998975	-1.203372	-0.015196
H	5.038691	-1.758254	-0.676779
C	7.187728	0.906535	1.139926
H	5.351714	2.003730	1.393501
C	7.784644	-0.251779	0.634667
H	7.453118	-2.105053	-0.416080
H	7.789564	1.653883	1.649172
H	8.853524	-0.410023	0.747227
C	-3.571197	1.227553	-1.692246
C	-3.306624	2.735114	-1.821437
H	-4.366532	0.942555	-2.391853
H	-2.676151	0.672624	-2.001512
H	-3.019198	3.001935	-2.847013
H	-4.200496	3.318950	-1.566887
H	-2.500103	3.059015	-1.152665

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B3LYP SCF energy: -2125.68991712 a.u.
B3LYP enthalpy: -2124.634037 a.u.
B3LYP free energy: -2124.785017 a.u.
B3LYP-D3BJ SCF energy in solution: -2127.78975042 a.u.
B3LYP-D3BJ enthalpy in solution: -2126.733870 a.u.
B3LYP-D3BJ free energy in solution: -2126.884850 a.u.
Three lowest frequencies (cm-1): 8.0900 15.3136 19.1784

Cartesian coordinates

ATOM	X	Y	Z
N	2.064959	1.431002	-0.261914
N	1.988170	-0.634718	0.211196
C	1.178285	0.453653	0.006684
C	1.768140	2.818014	-0.532134
C	1.486687	3.203109	-1.856164
C	1.799957	3.727383	0.541946
C	1.214772	4.557676	-2.084566
C	1.522371	5.068950	0.254856
C	1.230077	5.481132	-1.042800
H	0.990165	4.892457	-3.092968

H	1.535404	5.799398	1.058454
H	1.015970	6.527478	-1.243518
C	1.483672	-1.960197	0.501744
C	1.121275	-2.269352	1.829732
C	1.381735	-2.888932	-0.553568
C	0.655651	-3.566193	2.082008
C	0.915477	-4.171235	-0.238424
C	0.558725	-4.510192	1.063453
H	0.363826	-3.838040	3.092157
H	0.824366	-4.911365	-1.027648
H	0.195753	-5.510326	1.283741
C	1.737323	-2.552747	-1.999541
C	0.484933	-2.581361	-2.898788
C	2.836769	-3.480907	-2.552726
H	2.130379	-1.531928	-2.029898
H	-0.285150	-1.894729	-2.533173
H	0.747938	-2.290858	-3.922866
H	0.045905	-3.584987	-2.939265
H	3.737139	-3.453207	-1.930382
H	2.495101	-4.521120	-2.606427
H	3.113025	-3.172817	-3.567763
C	1.490234	2.220701	-3.022219
C	2.650896	2.521437	-3.991503
C	0.135801	2.195766	-3.756033
H	1.655590	1.216058	-2.621691
H	3.616347	2.487400	-3.474807
H	2.670216	1.785314	-4.803940
H	2.546256	3.514780	-4.443462
H	-0.681855	1.955504	-3.067974
H	-0.089274	3.160755	-4.224891
H	0.150214	1.438453	-4.548669
C	1.221594	-1.270098	2.980438
C	2.183198	-1.760983	4.081431
C	-0.168087	-0.946810	3.564180
H	1.630554	-0.334271	2.587893
H	3.187833	-1.949365	3.686547
H	2.268005	-1.005729	4.871258
H	1.825372	-2.686690	4.546590
H	-0.836644	-0.542417	2.796384
H	-0.641394	-1.839118	3.990268
H	-0.077939	-0.201994	4.363679
C	2.137923	3.305805	1.967905
C	1.014662	3.671024	2.956513
C	3.492514	3.894444	2.410100
H	2.240332	2.216522	1.986612
H	0.060966	3.226622	2.652249
H	1.260841	3.303261	3.959735
H	0.873495	4.755551	3.028463
H	4.295541	3.583631	1.733495
H	3.465919	4.990495	2.423495
H	3.744319	3.553667	3.421379
C	-4.168222	0.901513	0.067669

C	-2.969831	1.533830	0.285438
C	-2.912479	2.977112	0.770382
H	-2.453506	3.016168	1.769270
H	-2.255365	3.572602	0.121650
H	-3.876635	3.498887	0.835288
C	-5.097198	-2.512807	-2.458007
C	-6.124354	-1.855318	-1.512802
C	-2.837609	-2.737745	-0.130955
C	-5.584690	-1.479533	-0.101257
C	-4.058040	-3.559847	0.332718
C	-5.246884	-2.698088	0.802534
H	-5.486506	-2.485352	-3.485727
H	-7.004365	-2.511269	-1.420487
H	-2.303818	-2.374957	0.759821
H	-3.751097	-4.225186	1.152632
H	-4.997868	-3.575081	-2.214267
H	-6.489458	-0.930834	-1.985440
H	-2.131249	-3.403995	-0.650095
H	-6.393196	-0.934201	0.403360
H	-4.383034	-4.226189	-0.472940
H	-5.021847	-2.312510	1.808824
H	-6.133975	-3.340112	0.920986
C	-3.707364	-1.843372	-2.429235
H	-3.759357	-0.904500	-3.001263
H	-2.988818	-2.482904	-2.966278
C	-3.160639	-1.501197	-1.011068
H	-2.215215	-0.959994	-1.168280
B	-4.263378	-0.600662	-0.303005
C	-5.504376	1.637753	0.275356
H	-5.446059	2.667677	-0.102333
H	-6.288982	1.157352	-0.325048
Ag	-0.976419	0.796135	0.107689
C	3.321980	-0.251937	0.053407
C	4.538283	-1.080108	0.145324
C	5.700666	-0.593042	-0.482625
C	4.604468	-2.297454	0.843458
C	6.893883	-1.305145	-0.413389
H	5.651622	0.347080	-1.020868
C	5.805082	-3.006474	0.906717
H	3.730391	-2.694845	1.342238
C	6.951272	-2.516904	0.280460
H	7.780020	-0.915282	-0.906267
H	5.839649	-3.944886	1.452841
H	7.882406	-3.074296	0.331648
N	3.376466	1.026665	-0.237458
C	-5.983826	1.678893	1.739420
C	-7.334881	2.382037	1.914239
H	-5.224313	2.180071	2.353798
H	-6.051289	0.652148	2.124166
H	-7.652542	2.393230	2.964220
H	-7.287412	3.423200	1.570070
H	-8.120216	1.880382	1.334431

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B3LYP SCF energy: -2125.68957019 a.u.
B3LYP enthalpy: -2124.633531 a.u.
B3LYP free energy: -2124.783419 a.u.
B3LYP-D3BJ SCF energy in solution: -2127.78565219 a.u.
B3LYP-D3BJ enthalpy in solution: -2126.729613 a.u.
B3LYP-D3BJ free energy in solution: -2126.879501 a.u.
Three lowest frequencies (cm-1): 14.0306 15.4348 18.0088

Cartesian coordinates

ATOM	X	Y	Z
N	2.280902	1.483923	0.006243
N	2.314270	-0.627171	-0.195941
C	1.453490	0.423223	-0.005585
C	1.905645	2.868411	0.168776
C	1.636950	3.630666	-0.983361
C	1.844858	3.398285	1.471192
C	1.283027	4.972303	-0.796057
C	1.483497	4.744970	1.598893
C	1.203976	5.524386	0.479668
H	1.065968	5.591715	-1.661390
H	1.420860	5.187967	2.588646
H	0.924857	6.567487	0.602101
C	1.864382	-2.003569	-0.232320
C	1.917041	-2.758520	0.956785
C	1.370128	-2.523344	-1.446839
C	1.464130	-4.082472	0.898789
C	0.933222	-3.854149	-1.443734
C	0.979013	-4.627372	-0.286924
H	1.486495	-4.691504	1.797442
H	0.544868	-4.287096	-2.360793
H	0.630135	-5.656160	-0.308340
C	1.297179	-1.710808	-2.737613
C	-0.157200	-1.561848	-3.226525
C	2.191353	-2.312371	-3.840746
H	1.671750	-0.703885	-2.530063
H	-0.789622	-1.100461	-2.460532
H	-0.190099	-0.931334	-4.122848
H	-0.594521	-2.532877	-3.486735
H	3.238679	-2.373943	-3.524888
H	1.863526	-3.320875	-4.118358
H	2.147142	-1.690098	-4.742011
C	1.729800	3.057419	-2.393281
C	2.869368	3.724441	-3.188642
C	0.385721	3.160277	-3.139335
H	1.973777	1.993711	-2.314210
H	3.830587	3.601068	-2.678337
H	2.950402	3.276371	-4.186029
H	2.691297	4.798372	-3.319027

H	-0.413579	2.656916	-2.584628
H	0.086252	4.203739	-3.291091
H	0.464795	2.691924	-4.127613
C	2.422538	-2.190498	2.279885
C	3.596869	-3.011612	2.847568
C	1.277208	-2.073594	3.305224
H	2.797144	-1.178461	2.098644
H	4.420599	-3.080842	2.129297
H	3.978826	-2.540517	3.760632
H	3.288705	-4.030885	3.107627
H	0.458616	-1.457740	2.918429
H	0.864866	-3.057466	3.556455
H	1.643541	-1.617279	4.232572
C	2.159908	2.574467	2.715021
C	0.944479	2.484590	3.657812
C	3.401019	3.122902	3.446289
H	2.398503	1.554614	2.398563
H	0.075874	2.059750	3.143132
H	1.178112	1.846996	4.518681
H	0.659374	3.470629	4.042724
H	4.271550	3.148505	2.781840
H	3.231366	4.140229	3.817916
H	3.645837	2.490738	4.308096
C	-3.742855	-0.295187	0.244712
C	-2.834695	0.711313	0.081609
C	-3.253870	2.152414	-0.142862
H	-2.811277	2.789554	0.635831
H	-2.861114	2.536440	-1.096266
H	-4.336432	2.328111	-0.122346
C	-7.483711	-1.498414	-1.557136
C	-6.534142	-0.442201	-2.155972
C	-7.409804	-0.089187	1.403568
C	-6.001422	0.627272	-1.151823
C	-8.085205	0.879591	0.411710
C	-7.105000	1.553490	-0.572738
H	-7.618510	-2.312154	-2.283869
H	-7.035326	0.059397	-2.998393
H	-6.889631	0.502450	2.172567
H	-8.615888	1.657950	0.978045
H	-8.478260	-1.062392	-1.422315
H	-5.663529	-0.957492	-2.589891
H	-8.187411	-0.655975	1.938858
H	-5.308956	1.256880	-1.723410
H	-8.862058	0.346766	-0.145162
H	-6.603715	2.380613	-0.047961
H	-7.676600	2.023242	-1.388616
C	-6.985884	-2.092861	-0.222944
H	-6.210354	-2.840860	-0.445906
H	-7.806303	-2.648409	0.258234
C	-6.373717	-1.067895	0.777767
H	-5.951764	-1.652995	1.605764
B	-5.281137	-0.192809	0.010383

C	-3.235292	-1.681627	0.669836
H	-2.273268	-1.881132	0.173692
H	-3.921320	-2.474069	0.334382
Ag	-0.721449	0.483902	0.130150
C	3.620413	-0.140883	-0.284314
N	3.605816	1.166558	-0.163357
C	4.878573	-0.891182	-0.451923
C	4.945829	-2.215606	-0.915613
C	6.077471	-0.217452	-0.148176
C	6.182275	-2.845644	-1.067384
H	4.044328	-2.758968	-1.165716
C	7.305476	-0.851790	-0.304244
H	6.028971	0.805330	0.208579
C	7.364090	-2.170597	-0.763324
H	6.215317	-3.869353	-1.429278
H	8.219323	-0.316164	-0.062991
H	8.323403	-2.666390	-0.882432
C	-3.034031	-1.833979	2.189056
C	-2.592454	-3.242896	2.601426
H	-3.964501	-1.572648	2.710687
H	-2.287715	-1.095316	2.512170
H	-2.436824	-3.317473	3.685041
H	-3.345293	-3.991428	2.322588
H	-1.652783	-3.522500	2.107585

MeOH

B3LYP SCF energy: -115.71440514 a.u.
B3LYP enthalpy: -115.658697 a.u.
B3LYP free energy: -115.685652 a.u.
B3LYP-D3BJ SCF energy in solution: -115.77059205 a.u.
B3LYP-D3BJ enthalpy in solution: -115.714884 a.u.
B3LYP-D3BJ free energy in solution: -115.741839 a.u.
Three lowest frequencies (cm-1): 346.1003 1066.7924 1096.5590

Cartesian coordinates

ATOM	X	Y	Z
C	0.662324	-0.019545	0.000001
H	1.079718	0.991032	-0.000620
H	1.036909	-0.544181	-0.892857
H	1.037007	-0.543133	0.893439
O	-0.749168	0.122497	0.000003
H	-1.134236	-0.766420	0.000010

12-TS

B3LYP SCF energy: -2241.39949946 a.u.
B3LYP enthalpy: -2240.290655 a.u.
B3LYP free energy: -2240.445950 a.u.
B3LYP-D3BJ SCF energy in solution: -2243.56022034 a.u.

B3LYP-D3BJ enthalpy in solution: -2242.451376 a.u.
B3LYP-D3BJ free energy in solution: -2242.606671 a.u.
Three lowest frequencies (cm-1): -1085.2019 9.1517 14.0261
Imaginary frequency: -1085.2019 cm-1

Cartesian coordinates

ATOM	X	Y	Z
N	2.246009	1.462731	-0.114302
N	2.154281	-0.651494	0.060621
C	1.359408	0.464328	0.051085
C	1.954146	2.875087	-0.182214
C	1.620940	3.434400	-1.430113
C	2.042084	3.632944	1.001156
C	1.352246	4.808516	-1.464227
C	1.769960	5.002638	0.905941
C	1.425111	5.585068	-0.311196
H	1.085849	5.274945	-2.408184
H	1.829398	5.620861	1.796694
H	1.214792	6.650028	-0.361336
C	1.642370	-2.003192	0.169188
C	1.338462	-2.515021	1.448478
C	1.484270	-2.756396	-1.011941
C	0.905700	-3.845197	1.519768
C	1.044079	-4.078611	-0.876581
C	0.766844	-4.622901	0.373651
H	0.666407	-4.273587	2.488354
H	0.909292	-4.686908	-1.765960
H	0.425534	-5.651127	0.454037
C	1.746147	-2.192132	-2.405740
C	0.441229	-2.122476	-3.224789
C	2.830393	-2.989830	-3.156451
H	2.113629	-1.166371	-2.300908
H	-0.325516	-1.537710	-2.706829
H	0.631468	-1.658341	-4.199812
H	0.029841	-3.122072	-3.405977
H	3.766736	-3.026040	-2.590210
H	2.510407	-4.020926	-3.345980
H	3.035699	-2.524874	-4.127699
C	1.562727	2.616203	-2.715762
C	2.652003	3.068182	-3.708707
C	0.163026	2.660128	-3.358253
H	1.769816	1.571321	-2.465533
H	3.649287	2.996368	-3.261048
H	2.632739	2.439206	-4.606508
H	2.499935	4.106369	-4.026292
H	-0.604227	2.299534	-2.664378
H	-0.109338	3.677251	-3.662937
H	0.137412	2.027578	-4.253237
C	1.460623	-1.697120	2.732154
C	2.585461	-2.229706	3.642911
C	0.119573	-1.640458	3.491912
H	1.719698	-0.669394	2.460965

H	3.558953	-2.210448	3.140448
H	2.661848	-1.616460	4.548367
H	2.389136	-3.261958	3.955823
H	-0.697523	-1.297108	2.849059
H	-0.159282	-2.624627	3.886459
H	0.202816	-0.955967	4.344475
C	2.445993	3.023296	2.339301
C	1.432065	3.340856	3.454158
C	3.870666	3.464654	2.731341
H	2.465446	1.934883	2.225985
H	0.424216	3.010159	3.180496
H	1.720292	2.829912	4.380297
H	1.386982	4.413890	3.672512
H	4.595032	3.180426	1.960970
H	3.926232	4.551524	2.865258
H	4.170189	2.994037	3.675290
C	-3.885099	0.916399	-0.067864
C	-2.802497	1.540284	0.488926
C	-2.665868	3.061463	0.562450
H	-2.181077	3.485292	-0.331089
H	-3.633170	3.572136	0.670229
H	-2.049179	3.364425	1.417314
C	-5.162571	-2.042555	-2.193914
C	-6.063458	-1.533636	-1.039794
C	-2.877817	-3.063733	-0.139181
C	-5.403983	-1.484677	0.367043
C	-4.187841	-3.795714	0.216576
C	-5.212097	-2.910285	0.954269
H	-5.591593	-1.712764	-3.151334
H	-6.969878	-2.159942	-1.007450
H	-2.272138	-2.978523	0.773061
H	-3.953840	-4.670506	0.841696
H	-5.200049	-3.136178	-2.227893
H	-6.417184	-0.527056	-1.290256
H	-2.296627	-3.694144	-0.832648
H	-6.128022	-0.977076	1.025347
H	-4.642631	-4.206179	-0.690708
H	-4.890396	-2.827356	2.001266
H	-6.179369	-3.437863	0.984380
C	-3.683872	-1.591161	-2.123764
H	-3.612750	-0.555235	-2.486639
H	-3.101854	-2.200360	-2.835087
C	-3.054743	-1.637951	-0.709668
H	-2.036929	-1.212522	-0.806504
B	-3.972589	-0.702575	0.260791
C	-4.958174	1.723000	-0.787085
H	-5.312065	1.166556	-1.664536
H	-4.541552	2.661722	-1.178073
O	-3.195825	-0.657632	1.732739
H	-2.690716	0.371541	1.451533
C	-3.979601	-0.359730	2.890330
H	-4.574346	0.550146	2.736290

H	-4.648758	-1.192269	3.110374
H	-3.303053	-0.209350	3.739536
Ag	-0.759512	0.765776	0.294387
C	3.485890	-0.262695	-0.103175
C	4.691744	-1.106486	-0.195628
C	5.829144	-0.540292	-0.802825
C	4.772368	-2.415845	0.307379
C	7.012130	-1.265317	-0.903972
H	5.769094	0.470282	-1.191311
C	5.962514	-3.136951	0.199972
H	3.917837	-2.876017	0.785244
C	7.083645	-2.568697	-0.404689
H	7.878712	-0.813562	-1.378393
H	6.008539	-4.147575	0.595519
H	8.006488	-3.135998	-0.487244
N	3.549076	1.044447	-0.208847
C	-6.182631	2.069219	0.088012
C	-7.244707	2.874653	-0.669219
H	-5.846718	2.636962	0.966445
H	-6.629134	1.145438	0.473919
H	-8.101123	3.114926	-0.027462
H	-6.833583	3.820361	-1.045023
H	-7.623103	2.313676	-1.532998

12a-TS

B3LYP SCF energy: -2241.37752345 a.u.
B3LYP enthalpy: -2240.269732 a.u.
B3LYP free energy: -2240.424941 a.u.
B3LYP-D3BJ SCF energy in solution: -2243.53532063 a.u.
B3LYP-D3BJ enthalpy in solution: -2242.427529 a.u.
B3LYP-D3BJ free energy in solution: -2242.582738 a.u.
Three lowest frequencies (cm-1): -1250.2534 8.6580 15.6045
Imaginary frequency: -1250.2534 cm-1

Cartesian coordinates

ATOM	X	Y	Z
N	-1.557707	1.566309	0.302012
N	-2.523446	-0.282369	-0.090524
C	-1.276815	0.286377	0.001379
C	-0.628986	2.653614	0.509105
C	-0.072032	2.831391	1.789446
C	-0.373560	3.521755	-0.569192
C	0.768247	3.936676	1.971497
C	0.473340	4.609586	-0.328354
C	1.036581	4.817438	0.927660
H	1.218246	4.108565	2.944388
H	0.694961	5.302146	-1.134814
H	1.692872	5.667666	1.092173
C	-2.713357	-1.688136	-0.381835
C	-2.738232	-2.100769	-1.730237

C	-2.841686	-2.588354	0.695067
C	-2.910104	-3.468187	-1.979928
C	-3.009610	-3.943342	0.383685
C	-3.045631	-4.381204	-0.937322
H	-2.932551	-3.821812	-3.006535
H	-3.107821	-4.664989	1.189281
H	-3.176025	-5.437727	-1.155317
C	-2.791084	-2.149894	2.155686
C	-1.533339	-2.703320	2.855089
C	-4.072325	-2.541583	2.917688
H	-2.721216	-1.058258	2.184913
H	-0.621521	-2.386877	2.336868
H	-1.484385	-2.342533	3.889239
H	-1.542603	-3.799255	2.883176
H	-4.965744	-2.131645	2.434648
H	-4.190224	-3.629756	2.978439
H	-4.032270	-2.156830	3.943238
C	-0.378464	1.903545	2.959901
C	-1.357084	2.575158	3.944980
C	0.898900	1.422830	3.673674
H	-0.874653	1.011357	2.565658
H	-2.289010	2.861635	3.445197
H	-1.603051	1.891138	4.766176
H	-0.918041	3.479819	4.382387
H	1.606173	0.975046	2.967860
H	1.408678	2.244958	4.189910
H	0.640094	0.674254	4.432308
C	-2.587476	-1.133033	-2.901637
C	-3.825184	-1.150727	-3.820502
C	-1.299549	-1.418015	-3.699551
H	-2.498714	-0.119354	-2.499307
H	-4.739298	-0.903140	-3.269686
H	-3.706266	-0.416606	-4.625580
H	-3.967725	-2.132453	-4.286622
H	-0.413937	-1.357067	-3.057601
H	-1.321363	-2.416300	-4.152238
H	-1.186416	-0.686981	-4.508601
C	-1.000974	3.330090	-1.945929
C	0.053807	3.309477	-3.068155
C	-2.080549	4.399028	-2.208911
H	-1.500089	2.355883	-1.959743
H	0.816668	2.545594	-2.885015
H	-0.426054	3.092524	-4.029926
H	0.562884	4.274904	-3.167490
H	-2.858998	4.367551	-1.439554
H	-1.646646	5.405996	-2.212042
H	-2.553034	4.234354	-3.184756
C	3.609783	-1.780479	-0.056717
C	2.293039	-2.085248	-0.335950
C	1.855233	-3.502567	-0.659542
H	1.248237	-3.499535	-1.574824
H	2.660952	-4.236348	-0.791980

H	1.187408	-3.876646	0.130087
C	5.214626	0.521693	-2.768220
C	6.059766	-0.265666	-1.742210
C	3.840655	2.366982	-0.458165
C	5.770113	0.063944	-0.250050
C	5.356998	2.644510	-0.464463
C	6.203678	1.503672	0.139609
H	5.309651	0.038471	-3.751434
H	7.126491	-0.103406	-1.964280
H	3.462725	2.503346	0.563722
H	5.556779	3.571048	0.093901
H	5.637802	1.523019	-2.897453
H	5.880734	-1.337556	-1.899877
H	3.337508	3.130742	-1.071972
H	6.404821	-0.612180	0.344401
H	5.689772	2.848867	-1.487148
H	6.167315	1.590545	1.233439
H	7.259915	1.661226	-0.131575
C	3.717231	0.635138	-2.404161
H	3.226518	-0.319647	-2.640194
H	3.252133	1.390295	-3.059334
C	3.425647	0.945446	-0.914818
H	2.331202	0.897392	-0.793052
B	4.184179	-0.145220	-0.003841
C	4.667657	-2.898252	0.031602
H	5.673577	-2.474484	-0.033666
H	4.583969	-3.575996	-0.829689
O	3.672406	0.080698	1.581694
H	3.419800	-1.062505	1.074814
C	4.552073	-0.008505	2.693148
H	5.403050	-0.675243	2.501890
H	4.942019	0.985167	2.941905
H	3.996426	-0.387704	3.559874
Ag	0.610257	-0.774814	-0.193819
C	-3.492675	0.688134	0.165381
C	-4.960758	0.550825	0.209624
C	-5.690961	1.625558	0.754158
C	-5.662883	-0.568045	-0.269448
C	-7.079453	1.579860	0.816895
H	-5.153397	2.491396	1.123875
C	-7.056872	-0.606517	-0.200806
H	-5.135648	-1.408294	-0.700459
C	-7.770353	0.461928	0.340855
H	-7.623782	2.418439	1.241937
H	-7.582428	-1.479401	-0.577577
H	-8.854930	0.425750	0.392333
N	-2.899840	1.834357	0.406728
C	4.601026	-3.736851	1.324215
C	5.673572	-4.830373	1.384674
H	3.606760	-4.191228	1.422787
H	4.713929	-3.070586	2.191785
H	5.613558	-5.404008	2.317626

H	5.565871	-5.536957	0.551823
H	6.681232	-4.400642	1.321446

12b-TS

B3LYP SCF energy: -2241.38641563 a.u.
B3LYP enthalpy: -2240.278498 a.u.
B3LYP free energy: -2240.438319 a.u.
B3LYP-D3BJ SCF energy in solution: -2243.54147389 a.u.
B3LYP-D3BJ enthalpy in solution: -2242.433556 a.u.
B3LYP-D3BJ free energy in solution: -2242.593377 a.u.
Three lowest frequencies (cm-1): -1219.7721 10.8032 13.0030
Imaginary frequency: -1219.7721 cm-1

Cartesian coordinates

ATOM	X	Y	Z
N	-2.057099	1.479321	-0.167686
N	-2.112367	-0.642242	-0.153116
C	-1.242616	0.413201	-0.082213
C	-3.415609	-0.153625	-0.277459
C	-1.660444	2.867239	-0.124753
C	-1.594485	3.506797	1.127920
C	-1.375336	3.518368	-1.340111
C	-1.205365	4.852377	1.134646
C	-0.993678	4.863235	-1.271398
C	-0.905465	5.522864	-0.047926
H	-1.139340	5.380410	2.080837
H	-0.765756	5.400555	-2.187380
H	-0.605167	6.566871	-0.016763
C	-1.667147	-2.018075	-0.082362
C	-1.328735	-2.675162	-1.283449
C	-1.576011	-2.633435	1.182391
C	-0.896698	-4.003375	-1.187792
C	-1.136022	-3.963294	1.214258
C	-0.802515	-4.642907	0.046196
H	-0.625996	-4.541558	-2.091475
H	-1.050753	-4.470117	2.170638
H	-0.462488	-5.673608	0.097074
C	-1.950987	-1.930580	2.484919
C	-0.737927	-1.780172	3.425221
C	-3.116653	-2.652881	3.191330
H	-2.297531	-0.920826	2.243615
H	0.053734	-1.168153	2.980598
H	-1.050989	-1.294768	4.357262
H	-0.313526	-2.756662	3.687203
H	-3.989988	-2.745517	2.536330
H	-2.828838	-3.660177	3.514447
H	-3.418224	-2.093437	4.084189
C	-1.972529	2.815064	2.434069
C	-3.314784	3.366955	2.958137
C	-0.863634	2.911616	3.499137

H	-2.121551	1.750995	2.225582
H	-4.110968	3.249629	2.214546
H	-3.613381	2.834621	3.868889
H	-3.236878	4.432761	3.204120
H	0.064267	2.435354	3.161091
H	-0.650031	3.953392	3.767653
H	-1.191744	2.402571	4.413784
C	-1.418403	-2.002023	-2.650437
C	-2.346645	-2.770721	-3.611236
C	-0.019019	-1.805980	-3.266429
H	-1.851108	-1.005993	-2.514760
H	-3.352010	-2.884169	-3.191390
H	-2.434955	-2.231106	-4.561189
H	-1.959220	-3.771209	-3.835471
H	0.623044	-1.211858	-2.607373
H	0.478171	-2.766730	-3.443559
H	-0.096421	-1.286188	-4.228766
C	-1.500401	2.826410	-2.693328
C	-0.200258	2.913832	-3.514508
C	-2.701640	3.384603	-3.482803
H	-1.696118	1.764132	-2.517228
H	0.646693	2.492122	-2.962343
H	-0.308452	2.356065	-4.452251
H	0.048681	3.948976	-3.774830
H	-3.632154	3.266889	-2.917407
H	-2.571976	4.451058	-3.701748
H	-2.810639	2.856774	-4.437744
C	3.879624	0.747764	-0.394454
C	3.024940	1.477688	0.406324
C	2.927551	2.991936	0.276685
H	2.492318	3.302733	-0.686035
H	2.297019	3.404166	1.070709
H	3.910122	3.480900	0.347291
C	3.178389	-3.696903	-0.518572
C	2.649109	-2.813659	0.630230
C	6.076385	-2.275119	-0.517013
C	3.560542	-1.629791	1.053176
C	5.866339	-2.867350	0.893614
C	4.878215	-2.067263	1.766966
H	2.349079	-4.298460	-0.916681
H	2.424454	-3.448900	1.501105
H	6.770026	-1.425694	-0.435059
H	6.837979	-2.917729	1.404940
H	3.900972	-4.421674	-0.130370
H	1.682482	-2.389294	0.318524
H	6.587678	-3.015328	-1.152105
H	2.995523	-1.028954	1.772596
H	5.528145	-3.905177	0.814245
H	5.381691	-1.159036	2.130129
H	4.634418	-2.652269	2.667094
C	3.819686	-2.899940	-1.671593
H	3.017565	-2.443251	-2.271750

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H        4.339102   -3.595663   -2.348963
C        4.786787   -1.764941   -1.232843
H        5.120310   -1.263462   -2.151853
B        4.024532   -0.801667   -0.217810
C        4.753793    1.453426   -1.432792
H        4.876157    0.817375   -2.319063
H        4.277776    2.378051   -1.783979
C        2.416099    0.653074    3.914190
H        1.629488    0.627413    4.688541
H        3.133923    1.436568    4.221772
H        2.952667   -0.314402    3.973428
O        1.864850    0.897951    2.655236
H        2.577721    1.092102    1.631808
Ag       0.884532    0.586846    0.273262
C       -4.686713   -0.896699   -0.377569
C       -4.781983   -2.296722   -0.452453
C       -5.873152   -0.136768   -0.403218
C       -6.030995   -2.913390   -0.549834
H       -3.893979   -2.913136   -0.436496
C       -7.112629   -0.759103   -0.501287
H       -5.805638    0.943577   -0.345230
C       -7.198627   -2.152339   -0.574846
H       -6.083571   -3.996961   -0.606240
H       -8.014857   -0.154230   -0.518618
H       -8.167417   -2.638158   -0.650225
N       -3.383758    1.159793   -0.289585
C        6.160578    1.804883   -0.901481
C        7.030496    2.521501   -1.939796
H        6.664142    0.885638   -0.573949
H        6.062948    2.431085   -0.004707
H        8.023916    2.755549   -1.538741
H        7.169461    1.902132   -2.834848
H        6.569525    3.464560   -2.259654


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B3LYP SCF energy:                    -2241.45810126 a.u.
B3LYP enthalpy:                      -2240.343906 a.u.
B3LYP free energy:                   -2240.499978 a.u.
B3LYP-D3BJ SCF energy in solution:      -2243.61789487 a.u.
B3LYP-D3BJ enthalpy in solution:     -2242.503700 a.u.
B3LYP-D3BJ free energy in solution:      -2242.659772 a.u.
Three lowest frequencies (cm-1):       8.7560     10.3371     18.4627

Cartesian coordinates
ATOM       X           Y           Z
N        1.860997    1.645366   -0.029712
N        2.371205   -0.418243    0.007090
C        1.309317    0.434897    0.152471
C        1.184031    2.920774   -0.001718
C        0.677929    3.433265   -1.211324
```

C	1.088633	3.602997	1.225637
C	0.044913	4.681026	-1.159262
C	0.441757	4.844611	1.217495
C	-0.075497	5.378162	0.040124
H	-0.359550	5.111195	-2.070339
H	0.345643	5.401366	2.144968
H	-0.574361	6.343247	0.056816
C	2.231668	-1.859528	0.081350
C	2.260046	-2.474819	1.350749
C	2.051184	-2.581078	-1.116172
C	2.115155	-3.866904	1.390845
C	1.911156	-3.970564	-1.011052
C	1.943794	-4.608897	0.225102
H	2.129846	-4.375014	2.350535
H	1.765832	-4.558130	-1.912396
H	1.827864	-5.687617	0.281529
C	2.002405	-1.922611	-2.492384
C	0.640229	-2.148541	-3.177864
C	3.159712	-2.404578	-3.390524
H	2.122240	-0.842213	-2.362136
H	-0.188192	-1.787202	-2.560606
H	0.610670	-1.618531	-4.137000
H	0.465225	-3.211150	-3.381037
H	4.134001	-2.221215	-2.925565
H	3.082207	-3.477854	-3.599755
H	3.135157	-1.877918	-4.351481
C	0.823434	2.704407	-2.543225
C	1.834445	3.432056	-3.452743
C	-0.529223	2.507174	-3.253603
H	1.228554	1.707084	-2.344624
H	2.812343	3.518773	-2.966833
H	1.964518	2.883789	-4.393221
H	1.489448	4.443034	-3.699637
H	-1.248662	1.983255	-2.615405
H	-0.975905	3.463340	-3.549293
H	-0.388256	1.916326	-4.166199
C	2.442086	-1.699663	2.653681
C	3.735848	-2.110019	3.385792
C	1.216000	-1.853757	3.575815
H	2.531653	-0.635852	2.412509
H	4.620959	-1.950851	2.760197
H	3.856890	-1.516165	4.299020
H	3.714568	-3.166398	3.677234
H	0.295536	-1.536195	3.073842
H	1.079901	-2.893719	3.893602
H	1.343181	-1.243546	4.477652
C	1.678995	3.058007	2.521973
C	0.617569	2.935377	3.631667
C	2.876900	3.912895	2.981681
H	2.058789	2.049816	2.328309
H	-0.220110	2.305592	3.312157
H	1.059513	2.487712	4.529551

H	0.211637	3.912787	3.916093
H	3.650709	3.954866	2.207861
H	2.569058	4.940461	3.207754
H	3.322463	3.489518	3.889704
C	-4.296266	0.691322	-0.389240
C	-3.521869	1.796928	-0.311553
C	-3.796306	3.210380	-0.771494
H	-4.708669	3.308280	-1.366541
H	-3.894433	3.893311	0.086532
H	-2.963318	3.599300	-1.374172
C	-5.159719	-2.899791	-1.535576
C	-5.822382	-2.398643	-0.224737
C	-2.252079	-2.885181	-0.222919
C	-4.865160	-1.819081	0.854922
C	-3.137105	-3.756993	0.696274
C	-4.107413	-2.956134	1.588605
H	-5.913984	-2.910399	-2.336110
H	-6.401235	-3.233621	0.204033
H	-1.414675	-2.508470	0.386255
H	-2.487651	-4.378765	1.331081
H	-4.862320	-3.946839	-1.413539
H	-6.568651	-1.637845	-0.475931
H	-1.786090	-3.532640	-0.985230
H	-5.517431	-1.349066	1.610492
H	-3.706753	-4.468740	0.089327
H	-3.535523	-2.526600	2.421092
H	-4.823138	-3.661511	2.042493
C	-3.931157	-2.090661	-2.015852
H	-4.272853	-1.179207	-2.523604
H	-3.409669	-2.684379	-2.785612
C	-2.957575	-1.674850	-0.890364
H	-2.162501	-1.073582	-1.382463
B	-3.763608	-0.759770	0.215652
C	-5.674027	0.841526	-1.032855
H	-5.959616	-0.073883	-1.559193
H	-5.669491	1.625291	-1.803318
O	-2.693873	-0.433548	1.333758
H	-2.553882	1.711878	0.192208
C	-3.151864	0.202212	2.516542
H	-3.568071	1.195453	2.304517
H	-3.930290	-0.402330	2.997232
H	-2.315762	0.304961	3.220605
Ag	-0.708570	-0.001991	0.613126
C	3.518795	0.330763	-0.257341
C	4.894218	-0.136915	-0.509278
C	5.799449	0.791160	-1.059808
C	5.349511	-1.432745	-0.212472
C	7.120229	0.431227	-1.305806
H	5.451583	1.791980	-1.289662
C	6.676265	-1.785939	-0.464368
H	4.682257	-2.168239	0.216228
C	7.564999	-0.860441	-1.010502

H	7.803089	1.159955	-1.733158
H	7.011709	-2.791660	-0.227956
H	8.595952	-1.141940	-1.205599
N	3.208217	1.607576	-0.277775
C	-6.781807	1.186481	-0.016339
C	-8.167089	1.318371	-0.659300
H	-6.517914	2.125203	0.489797
H	-6.810484	0.417962	0.766023
H	-8.933464	1.576271	0.082107
H	-8.173910	2.099183	-1.431012
H	-8.472103	0.379928	-1.139492

14-TS

B3LYP SCF energy: -2241.43899892 a.u.
B3LYP enthalpy: -2240.326167 a.u.
B3LYP free energy: -2240.481093 a.u.
B3LYP-D3BJ SCF energy in solution: -2243.59776086 a.u.
B3LYP-D3BJ enthalpy in solution: -2242.484929 a.u.
B3LYP-D3BJ free energy in solution: -2242.639855 a.u.
Three lowest frequencies (cm-1): -214.9209 12.7386 14.8852
Imaginary frequency: -214.9209 cm-1

Cartesian coordinates

ATOM	X	Y	Z
N	-2.309538	-0.112863	0.018067
N	-1.271429	1.728311	0.220246
C	-1.043479	0.406189	0.128414
C	-3.236197	0.931157	0.043225
C	-2.567314	-1.531358	-0.120162
C	-2.740216	-2.062998	-1.414401
C	-2.629894	-2.323635	1.046102
C	-2.992038	-3.437031	-1.516567
C	-2.888042	-3.690208	0.880297
C	-3.067891	-4.243465	-0.384669
H	-3.129512	-3.880218	-2.498508
H	-2.944359	-4.329727	1.756247
H	-3.264949	-5.307016	-0.488419
C	-0.287922	2.775954	0.371524
C	0.099912	3.146920	1.673273
C	0.204543	3.403853	-0.787519
C	1.030749	4.185797	1.791181
C	1.131346	4.437874	-0.608296
C	1.542370	4.823841	0.664238
H	1.357380	4.501026	2.777508
H	1.539284	4.943897	-1.477682
H	2.266221	5.626099	0.778701
C	-0.257093	3.023890	-2.189901
C	0.925844	2.757936	-3.139198
C	-1.208935	4.096684	-2.757027
H	-0.824526	2.090264	-2.118452

H	1.602467	2.006662	-2.720050
H	0.552654	2.398102	-4.105915
H	1.502799	3.669504	-3.334594
H	-2.077659	4.240447	-2.105394
H	-0.698937	5.062155	-2.857561
H	-1.568075	3.802241	-3.750535
C	-2.670411	-1.216451	-2.682557
C	-4.006478	-1.236300	-3.452232
C	-1.505511	-1.658331	-3.589405
H	-2.476815	-0.178713	-2.394207
H	-4.837648	-0.902187	-2.822846
H	-3.949449	-0.573444	-4.323300
H	-4.242890	-2.242663	-3.817354
H	-0.548046	-1.604151	-3.062259
H	-1.639357	-2.687589	-3.942103
H	-1.446473	-1.009664	-4.471228
C	-0.487825	2.497667	2.921854
C	-1.520529	3.434148	3.581980
C	0.594245	2.060636	3.925948
H	-1.019996	1.591564	2.615382
H	-2.323194	3.689613	2.882166
H	-1.969063	2.953923	4.460070
H	-1.049671	4.367665	3.912392
H	1.329823	1.399681	3.455142
H	1.132720	2.916638	4.347725
H	0.133956	1.520827	4.761895
C	-2.447567	-1.758913	2.453304
C	-1.268311	-2.429741	3.184544
C	-3.744150	-1.871874	3.281161
H	-2.207800	-0.694877	2.367568
H	-0.339835	-2.332690	2.612736
H	-1.119564	-1.960865	4.164454
H	-1.453977	-3.496963	3.353181
H	-4.577641	-1.345767	2.803093
H	-4.040833	-2.918300	3.418410
H	-3.596002	-1.435402	4.275651
C	2.446215	-0.827490	-2.745279
C	6.230676	-0.109260	1.091002
C	5.002727	0.778958	1.403879
C	5.738466	0.031913	-2.080362
C	4.052217	1.068220	0.214639
C	5.905719	1.486185	-1.577326
C	4.688448	2.054130	-0.812692
H	6.635990	-0.499135	2.036118
H	5.360738	1.729269	1.832675
H	5.133577	0.053615	-2.996640
H	6.120953	2.133766	-2.439781
H	7.032274	0.507091	0.671426
H	4.425925	0.296565	2.199678
H	6.725691	-0.354315	-2.380207
H	3.164596	1.578907	0.620851
H	6.793778	1.551043	-0.941115

H	3.913021	2.334112	-1.535303
H	4.992450	2.984034	-0.305629
C	5.951371	-1.293440	0.140404
H	5.461697	-2.093381	0.709393
H	6.916358	-1.707220	-0.193536
C	5.063749	-0.963317	-1.080690
H	4.928182	-1.904154	-1.633361
B	3.683972	-0.233986	-0.664807
C	2.680857	-1.840837	0.549532
O	2.742318	0.073611	-1.708416
Ag	0.858009	-0.620706	0.203708
H	1.974356	-0.272732	-3.565650
H	3.336990	-1.333923	-3.139673
H	1.737129	-1.601895	-2.407808
C	2.863934	-1.770513	1.897056
C	3.286754	-2.849488	2.869382
H	2.727552	-0.805142	2.387016
H	4.210327	-2.557418	3.389734
H	2.524953	-2.987648	3.650124
H	3.458083	-3.818776	2.395024
C	2.827385	-3.203338	-0.130440
H	3.064437	-3.071818	-1.192423
H	3.677583	-3.766603	0.285703
C	-4.704784	0.874623	-0.083571
C	-5.371671	2.077748	-0.386459
C	-5.466220	-0.292100	0.098602
C	-6.757316	2.110134	-0.503566
H	-4.788008	2.980482	-0.527401
C	-6.856437	-0.251327	-0.022444
H	-4.986999	-1.231760	0.337733
C	-7.507275	0.944512	-0.323961
H	-7.252672	3.047542	-0.740228
H	-7.428612	-1.163142	0.123378
H	-8.589242	0.969652	-0.418645
N	-2.599002	2.071618	0.173191
C	1.570510	-4.088234	-0.032162
C	1.715593	-5.426525	-0.765465
H	0.709634	-3.538950	-0.441122
H	1.334392	-4.269344	1.025241
H	0.801706	-6.028454	-0.688828
H	1.925489	-5.272762	-1.831655
H	2.540889	-6.019579	-0.351596

B-OMe

B3LYP SCF energy: -453.32185876 a.u.
B3LYP enthalpy: -453.055173 a.u.
B3LYP free energy: -453.103725 a.u.
B3LYP-D3BJ SCF energy in solution: -453.50438655 a.u.
B3LYP-D3BJ enthalpy in solution: -453.237701 a.u.
B3LYP-D3BJ free energy in solution: -453.286253 a.u.

Three lowest frequencies (cm-1): 45.4635 57.5354 107.4385

Cartesian coordinates

ATOM	X	Y	Z
C	-1.574084	1.578513	0.279145
C	-0.495499	1.309808	1.351814
C	-1.118864	-1.305646	-1.176205
C	0.320536	-0.005799	1.169834
C	-1.585293	-1.571900	0.272232
C	-0.508313	-1.313061	1.349006
H	-1.899763	2.624330	0.362741
H	-0.965374	1.324153	2.346589
H	-0.487197	-2.145871	-1.500994
H	-1.918260	-2.615706	0.352132
H	-2.464228	0.981407	0.498057
H	0.218634	2.147067	1.346809
H	-1.994160	-1.314318	-1.843114
H	1.096134	-0.009261	1.948224
H	-2.472215	-0.969380	0.489443
H	0.198149	-2.156776	1.346308
H	-0.982087	-1.323449	2.342005
C	-1.113756	1.312839	-1.171424
H	-0.480118	2.151257	-1.496911
H	-1.991198	1.325692	-1.835460
C	-0.300555	0.002395	-1.377428
H	0.081806	0.003527	-2.406968
B	0.868519	-0.002281	-0.316281
O	2.158257	-0.000084	-0.746716
C	3.306973	-0.005646	0.089988
H	3.055795	-0.131019	1.147838
H	3.960454	-0.826699	-0.223070
H	3.848110	0.938099	-0.040272

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B3LYP SCF energy: -1788.15017461 a.u.
B3LYP enthalpy: -1787.304615 a.u.
B3LYP free energy: -1787.439023 a.u.
B3LYP-D3BJ SCF energy in solution: -1790.09436826 a.u.
B3LYP-D3BJ enthalpy in solution: -1789.248809 a.u.
B3LYP-D3BJ free energy in solution: -1789.383217 a.u.
Three lowest frequencies (cm-1): 11.1530 15.8416 17.2208

Cartesian coordinates

ATOM	X	Y	Z
N	-1.430961	0.125510	0.079157
N	-0.163986	-1.573347	0.004838
C	-0.108977	-0.229697	-0.005978
C	-2.215883	-1.028411	0.130231
C	-1.857857	1.509338	0.083439
C	-1.885429	2.203591	1.310694

C	-2.201884	2.112272	-1.142882
C	-2.295699	3.542308	1.281518
C	-2.603364	3.453378	-1.109937
C	-2.653864	4.162002	0.087120
H	-2.327382	4.107935	2.207927
H	-2.872312	3.949833	-2.037714
H	-2.966438	5.202712	0.088695
C	0.956182	-2.481145	-0.058115
C	1.405690	-2.906020	-1.322206
C	1.536572	-2.914774	1.148445
C	2.490599	-3.790593	-1.352608
C	2.616577	-3.801139	1.058233
C	3.091078	-4.233780	-0.177256
H	2.868926	-4.135907	-2.310382
H	3.092624	-4.154926	1.968137
H	3.932746	-4.919627	-0.224167
C	1.026600	-2.471168	2.515359
C	2.129745	-1.782245	3.340815
C	0.401649	-3.653388	3.282327
H	0.233993	-1.732963	2.360872
H	2.541529	-0.919464	2.806601
H	1.723104	-1.431748	4.296907
H	2.955630	-2.467248	3.564352
H	-0.416826	-4.104625	2.711296
H	1.143087	-4.435087	3.485568
H	0.001725	-3.314047	4.245240
C	-1.490552	1.564248	2.639646
C	-2.665606	1.549383	3.637700
C	-0.254328	2.256083	3.248230
H	-1.214626	0.522557	2.449264
H	-3.531634	1.013819	3.233237
H	-2.364600	1.051776	4.566861
H	-2.987733	2.564908	3.895809
H	0.595068	2.233015	2.557291
H	-0.462005	3.304139	3.494132
H	0.042177	1.749315	4.174123
C	0.757163	-2.452280	-2.625644
C	0.116659	-3.640281	-3.370256
C	1.754574	-1.695330	-3.523649
H	-0.048641	-1.753638	-2.381459
H	-0.623417	-4.147125	-2.741476
H	-0.386539	-3.292316	-4.280128
H	0.868849	-4.380098	-3.667986
H	2.169473	-0.824040	-3.005532
H	2.589385	-2.336513	-3.830060
H	1.253506	-1.345501	-4.434090
C	-2.134682	1.377129	-2.478113
C	-1.042123	1.978637	-3.384825
C	-3.502191	1.353541	-3.188730
H	-1.854790	0.337123	-2.284220
H	-0.062497	1.953101	-2.895761
H	-0.974187	1.413423	-4.321947

H	-1.264628	3.021641	-3.638677
H	-4.274213	0.903566	-2.555263
H	-3.833804	2.362689	-3.459495
H	-3.436395	0.769031	-4.113719
C	3.318869	2.307226	-0.384690
C	3.135052	3.644211	-0.436385
C	4.158356	4.751097	-0.593011
H	5.188492	4.387710	-0.640764
H	3.971400	5.334392	-1.507170
H	4.097049	5.462588	0.243793
C	4.697135	1.674334	-0.473562
H	5.490274	2.414129	-0.665789
H	4.719491	0.981411	-1.329650
H	2.114954	4.030431	-0.361814
Ag	1.641142	1.044721	-0.182950
C	-3.684654	-1.151388	0.187287
C	-4.552390	-0.088174	0.488786
C	-4.235249	-2.423343	-0.064924
C	-5.932218	-0.296619	0.532784
H	-4.164185	0.900188	0.694211
C	-5.610808	-2.622670	-0.017307
H	-3.569033	-3.246461	-0.297487
C	-6.467491	-1.558989	0.279972
H	-6.587164	0.537303	0.768918
H	-6.015703	-3.610859	-0.216824
H	-7.542184	-1.714580	0.313898
N	-1.435651	-2.084119	0.088824
C	5.090708	0.878111	0.784418
C	6.452072	0.184443	0.663170
H	4.311422	0.130109	0.989607
H	5.096192	1.557661	1.648262
H	6.704142	-0.373194	1.573787
H	6.460424	-0.524862	-0.174703
H	7.255563	0.910719	0.485843

16-TS

B3LYP SCF energy: -2360.54473682 a.u.
B3LYP enthalpy: -2359.325280 a.u.
B3LYP free energy: -2359.494668 a.u.
B3LYP-D3BJ SCF energy in solution: -2362.76640020 a.u.
B3LYP-D3BJ enthalpy in solution: -2361.546943 a.u.
B3LYP-D3BJ free energy in solution: -2361.716331 a.u.
Three lowest frequencies (cm-1): -1060.8785 9.9489 12.8921
Imaginary frequency: -1060.8785 cm-1

Cartesian coordinates

ATOM	X	Y	Z
N	2.543352	1.285418	-0.599351
N	2.586653	-0.751048	0.004147
C	1.764018	0.343043	-0.043253

C	2.177913	2.652324	-0.889473
C	1.704863	2.957156	-2.181492
C	2.339534	3.619431	0.119951
C	1.370749	4.291426	-2.439952
C	1.985026	4.937567	-0.195067
C	1.504652	5.270613	-1.458022
H	1.001064	4.568907	-3.421858
H	2.091776	5.712364	0.558260
H	1.235807	6.299597	-1.680812
C	2.150723	-2.018478	0.556512
C	2.392850	-2.278052	1.920657
C	1.474196	-2.922320	-0.288893
C	1.940880	-3.502006	2.429417
C	1.043051	-4.128363	0.278058
C	1.273829	-4.417970	1.620302
H	2.108664	-3.736968	3.476423
H	0.511997	-4.845593	-0.340398
H	0.927361	-5.359044	2.038292
C	1.201865	-2.641514	-1.764409
C	-0.310377	-2.555947	-2.048604
C	1.876645	-3.686337	-2.676042
H	1.636441	-1.668464	-2.014652
H	-0.801615	-1.798999	-1.428289
H	-0.482325	-2.299329	-3.100266
H	-0.810245	-3.511567	-1.855883
H	2.959663	-3.724459	-2.514701
H	1.473445	-4.690609	-2.503112
H	1.700139	-3.436394	-3.728369
C	1.607101	1.903910	-3.280801
C	2.855052	1.958133	-4.187590
C	0.316674	2.014937	-4.111793
H	1.592103	0.918756	-2.802119
H	3.771505	1.813146	-3.607046
H	2.804236	1.175586	-4.953945
H	2.923970	2.926390	-4.697722
H	-0.574575	1.997539	-3.475781
H	0.289016	2.932827	-4.709697
H	0.252031	1.172914	-4.810036
C	3.109970	-1.295716	2.842753
C	4.424394	-1.888017	3.388974
C	2.191497	-0.828942	3.989322
H	3.373753	-0.406855	2.260745
H	5.094775	-2.188635	2.576939
H	4.945935	-1.146773	4.005434
H	4.238036	-2.768040	4.015417
H	1.270157	-0.379005	3.603729
H	1.910456	-1.662744	4.642973
H	2.706172	-0.082762	4.606007
C	2.909762	3.293214	1.496633
C	1.967185	3.725796	2.635398
C	4.312358	3.911567	1.665946
H	3.024563	2.207584	1.571717

H	0.979056	3.264639	2.531328
H	2.384272	3.424801	3.603536
H	1.829977	4.812760	2.659989
H	4.994848	3.561687	0.884056
H	4.273473	5.005911	1.614466
H	4.735186	3.636675	2.639411
C	-2.229008	-0.266043	2.575241
C	-2.210525	0.751869	1.669317
C	-2.639142	2.154826	2.091850
H	-3.727988	2.154961	2.250588
H	-2.192986	2.422774	3.063584
C	-2.659846	-0.227511	4.018172
H	-2.737634	0.787913	4.415598
H	-3.645207	-0.705156	4.121605
H	-1.968784	-0.800066	4.650472
Ag	-0.247660	0.527159	0.703360
C	-2.896161	0.670412	-1.691579
H	-1.917554	1.123340	-1.468794
H	-3.618707	1.472695	-1.884111
H	-2.796161	0.059553	-2.594098
O	-3.281975	-0.138114	-0.595483
H	-2.738718	0.265684	0.400430
H	-1.990465	-1.270710	2.219316
C	3.831385	-0.408269	-0.526241
C	-4.150420	-3.472407	-1.154338
C	-4.337226	-2.395083	-2.244695
C	-6.424081	-2.184557	0.778881
C	-5.320925	-1.251227	-1.879606
C	-7.103524	-2.639058	-0.533288
C	-6.782186	-1.769064	-1.773849
H	-3.269952	-4.086047	-1.402525
H	-4.656324	-2.892340	-3.176169
H	-6.986803	-1.335704	1.192409
H	-8.193430	-2.656222	-0.384458
H	-4.995183	-4.168372	-1.181157
H	-3.352787	-1.958986	-2.463101
H	-6.522938	-2.995315	1.520242
H	-5.312378	-0.547082	-2.730451
H	-6.830127	-3.679995	-0.736056
H	-7.453896	-0.904539	-1.774185
H	-7.044181	-2.345266	-2.677090
C	-3.988578	-2.909637	0.275167
H	-2.958440	-2.540177	0.380080
H	-4.088066	-3.741545	0.993693
C	-4.943866	-1.747144	0.638112
H	-4.638355	-1.386200	1.635052
B	-4.884518	-0.545566	-0.465494
C	-5.593840	0.870516	0.019255
H	-5.546835	0.910777	1.122987
H	-4.960810	1.714813	-0.305633
C	5.044139	-1.236138	-0.662791
C	6.242513	-0.572488	-0.991781

C	5.066715	-2.631628	-0.499641
C	7.425933	-1.285182	-1.151376
H	6.229760	0.504071	-1.119057
C	6.259710	-3.338808	-0.659746
H	4.163907	-3.174397	-0.254723
C	7.440983	-2.672813	-0.984275
H	8.340050	-0.755298	-1.403599
H	6.258074	-4.417410	-0.531457
H	8.366252	-3.228686	-1.106711
N	3.808086	0.850655	-0.902570
C	-2.304192	3.267846	1.088903
C	-2.758621	4.653449	1.559252
H	-2.772363	3.038256	0.123608
H	-1.218159	3.281037	0.907547
H	-2.501937	5.429311	0.828319
H	-3.845013	4.681357	1.707487
H	-2.288027	4.924147	2.513327
C	-7.029402	1.254969	-0.386852
C	-7.463216	2.624721	0.154632
H	-7.745630	0.500116	-0.036469
H	-7.116625	1.265577	-1.482733
H	-8.487289	2.881847	-0.147152
H	-7.424620	2.643610	1.251838
H	-6.799167	3.420884	-0.208185

P

B3LYP SCF energy: -235.85204325 a.u.
B3LYP enthalpy: -235.676852 a.u.
B3LYP free energy: -235.718119 a.u.
B3LYP-D3BJ SCF energy in solution: -235.94993962 a.u.
B3LYP-D3BJ enthalpy in solution: -235.774748 a.u.
B3LYP-D3BJ free energy in solution: -235.816015 a.u.
Three lowest frequencies (cm-1): 56.3631 93.4850 140.5396

Cartesian coordinates

ATOM	X	Y	Z
C	-0.770856	0.924012	0.140008
C	-2.003824	0.479290	-0.132407
H	-0.594040	1.997222	0.046172
H	-2.749671	1.220010	-0.424214
C	-2.510204	-0.935617	-0.083213
H	-3.336466	-1.030162	0.634709
H	-2.910181	-1.240994	-1.059722
H	-1.737966	-1.655485	0.201427
C	0.438134	0.125937	0.549561
C	1.603287	0.254174	-0.451327
H	0.187153	-0.933560	0.677955
H	0.786089	0.479167	1.533238
C	2.858148	-0.503933	-0.008186
H	1.272533	-0.112363	-1.432106

H	1.844849	1.317447	-0.589289
H	3.668645	-0.395874	-0.737979
H	3.226369	-0.132795	0.956443
H	2.654573	-1.575799	0.106755

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