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Electronic Supplementary Information

Computational study of Cu-catalyzed 1,2-hydrocarboxylation of 1,3-dienes with CO_2: Pauli repulsion-controlled regioselectivity of Cu–Bpin additions

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Transition States of CO_2 Insertion into Allyl-Cu Intermediates 3a and 5a

The allyl-Cu species **3a** and **5a** are derived from the Cu–Bpin addition across 1,3-diene (**1**) via **TS1-34**. It is a straightforward mechanism for CO_2 insertion into these allyl-Cu intermediates, which competes with the pathway of Cu–C protonation with MeOH (**TS3**, reported in Fig. 2 in the main text). The computed barriers of CO_2 insertion via both 6- and 3-membered transition states (**s-TS1**, **s-TS3** and **s-TS2**, **s-TS4** in Fig. S1) are higher than that of Cu–C protonation (**TS3**, $\Delta G^{\ddagger}$ = 17.9 kcal/mol). This indicates that the process of Cu–C protonation is superior to CO_2 insertion.

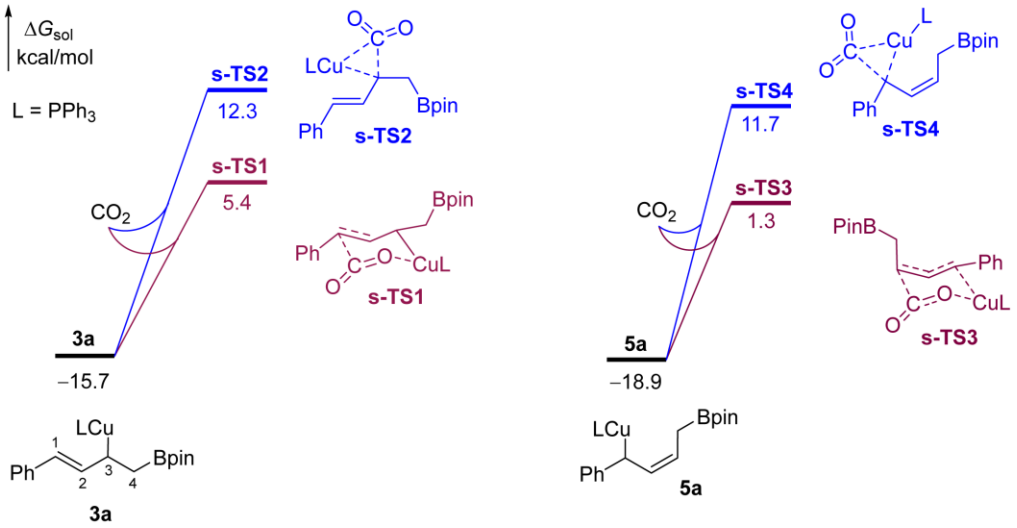

Fig. S1. Energy profiles for the disfavored CO_2 insertion pathways.

Transition States of Cu–C Protonations

As shown in Fig. S2, the low barrier of Cu–C protonation (**TS3**, $\Delta G^{\ddagger}$ = 17.9 kcal/mol) is mostly due to the stabilizing interactions of Cu–O (2.28 Å) and Cu–π (2.33 and 2.54 Å). In contrast, the transition state (**s-TS5**) without these interactions requires a much higher barrier ($\Delta G^{\ddagger}$ = 26.7 kcal/mol).

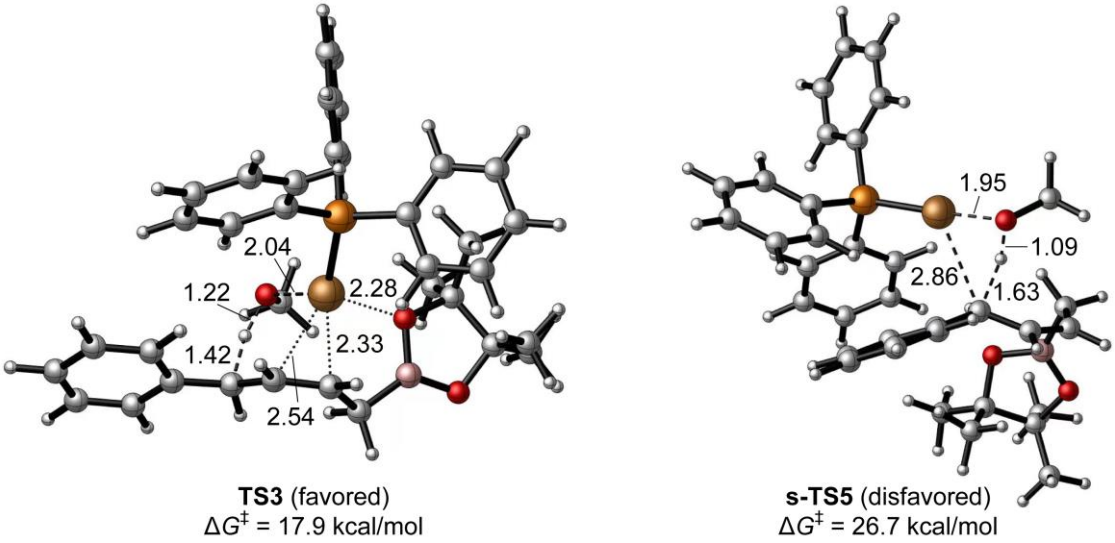

Fig. S2. Optimized transition states of Cu–C protonation with MeOH. Key bond distances are given in Å.

Transition States of CO_2 Insertion and 1,3-Cu Migration of Allyl-Cu 8a

As discussed in the manuscript, after the formation of allyl-Cu **8a**, the CO_2 insertion via 6-membered transition state (**TS8**) can afford the 1,2-hydrocarboxylation product of 1,3-butadienes. The 3-membered transition state (**s-TS6**, Fig. S3), giving the 1,4-hydrocarboxylation product, requires a much higher barrier. In addition, although the allyl-Cu **8a** can isomerize to **8b** via 1,3-Cu migration transition state (**s-TS7**), the subsequent CO_2 insertion is less favorable than **TS8** (see Fig. 3).

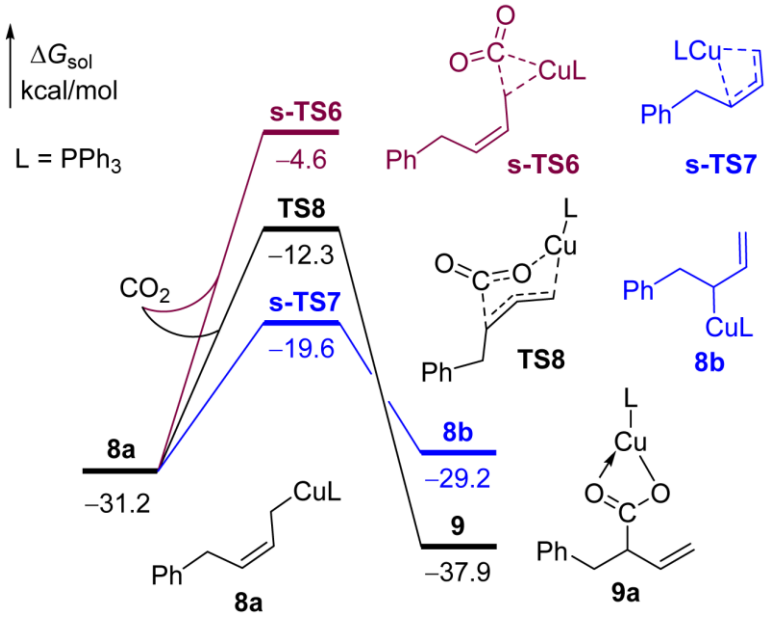

Fig. S3. Energy profiles of CO_2 insertion and 1,3-Cu migration.

EDA Results of Regioselective Cu–Bpin Addition Transition States

The comparison between **TS1-34** and **TS1-21** has been discussed in the main text (Fig. 5). Fig. S4 and S5 show the EDA results of **TS1-12** and **TS1-43** by comparing with the most favorable **TS1-34**, respectively. The results suggest that the difference of Pauli repulsion is the dominant factor for the barrier difference. The closed-shell repulsion between copper d orbital and carbon p orbital of 1,3-butadiene accounts for the difference of Pauli repulsion.

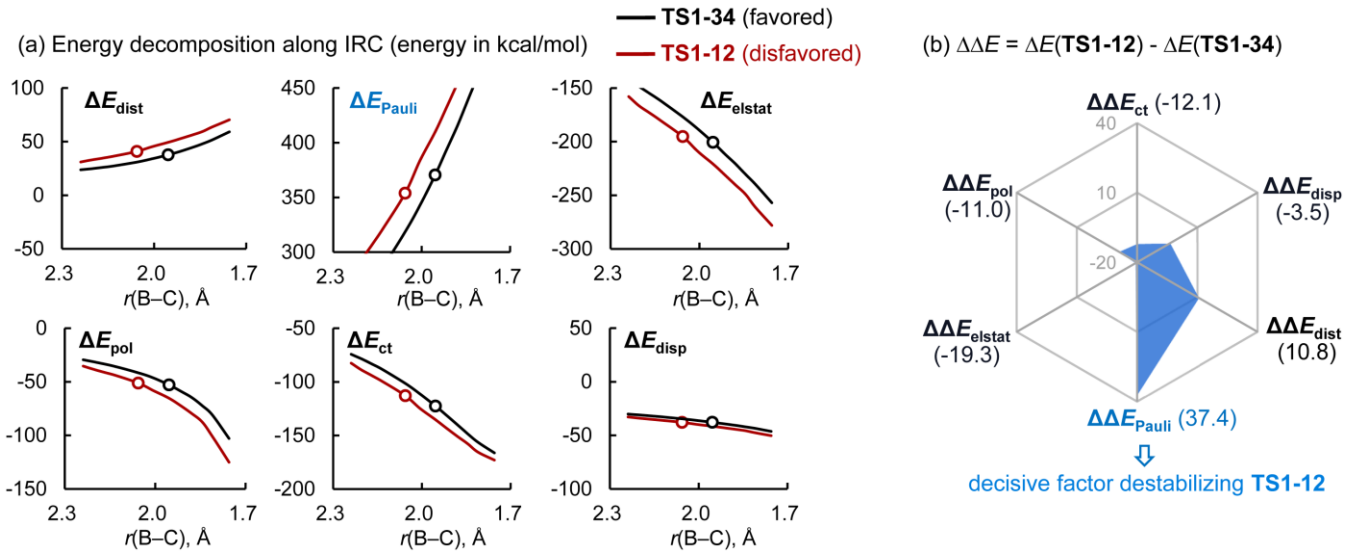

Fig. S4. (a) EDA results along IRC for the regioselective transition states (**TS1-34** and **TS1-12**). (b) Comparison of each energy term between **TS1-34** and **TS1-12**.

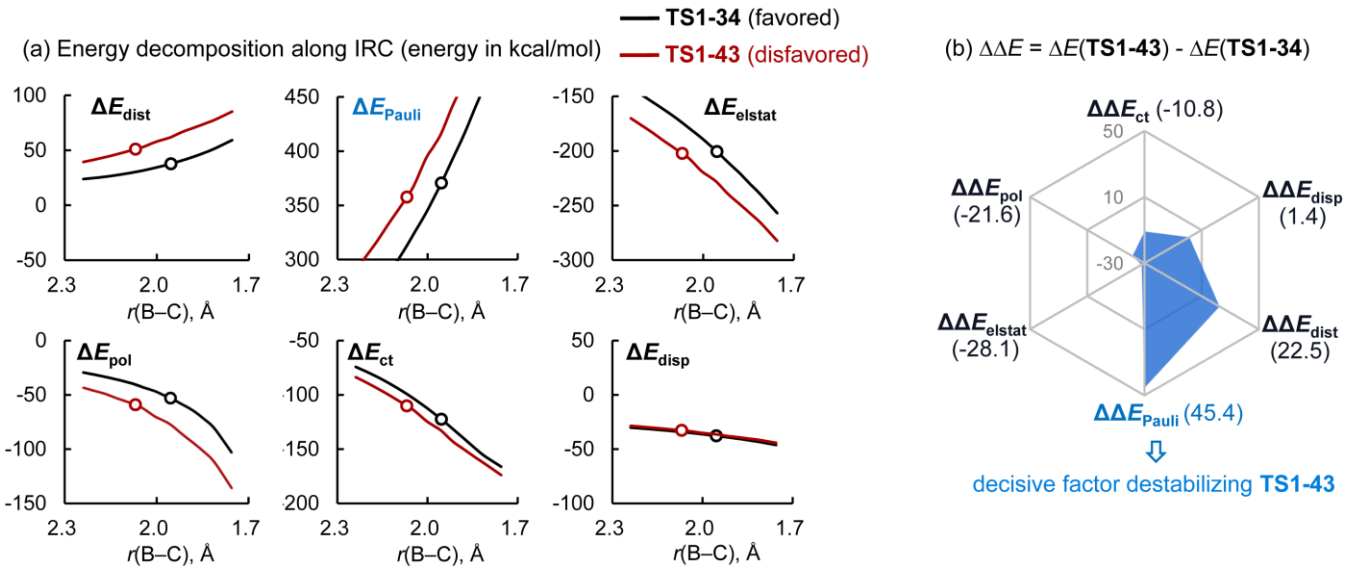

Fig. S5. (a) EDA results along IRC for the regioselective transition states (**TS1-34** and **TS1-43**). (b) Comparison of each energy term between **TS1-34** and **TS1-43**.

Additional Computational Results

Complexes of PPh_3Cu-Bpin with 1-phenyl-1,3-butadiene

We computed the structures of PPh_3Cu-Bpin coordination at different positions of 1-phenyl-1,3-butadiene (Fig. S6). All these structures are less stable than the separated PPh_3Cu-Bpin and 1-phenyl-1,3-butadiene ($\Delta G > 8$ kcal/mol), which do not affect the relative barriers of Cu-Bpin addition transition states.

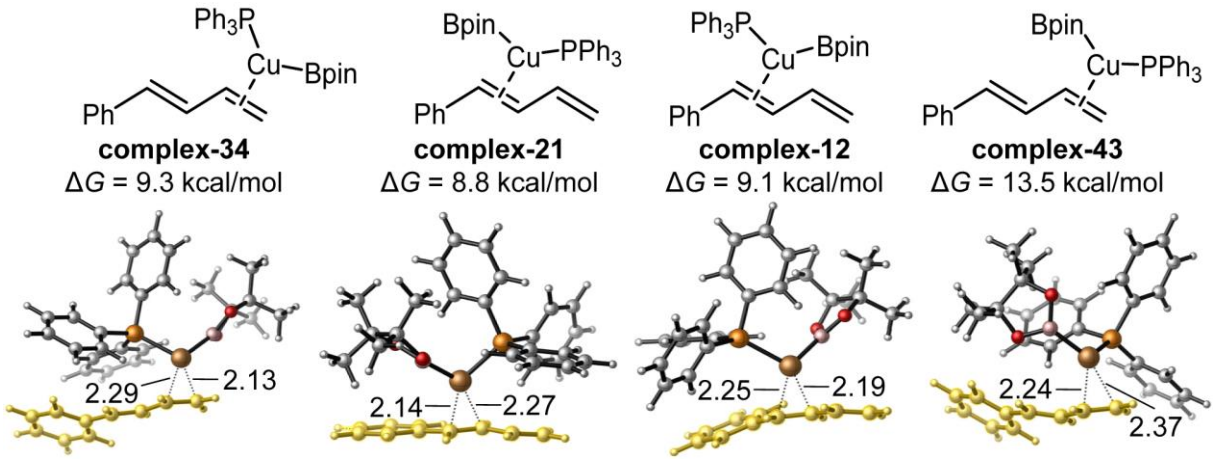

Fig. S6. Computed energies of complexes of PPh_3Cu-Bpin with 1-phenyl-1,3-butadiene.

*Stability difference between cis-**5a** and trans-**5b***

As shown in Fig. S7, the more stable cis-**5a** has much stronger non-covalent interactions than the less stable trans-**5b**. This is because Bpin is proximal to $PhPh_3Cu$ moieties in cis-**5a**.

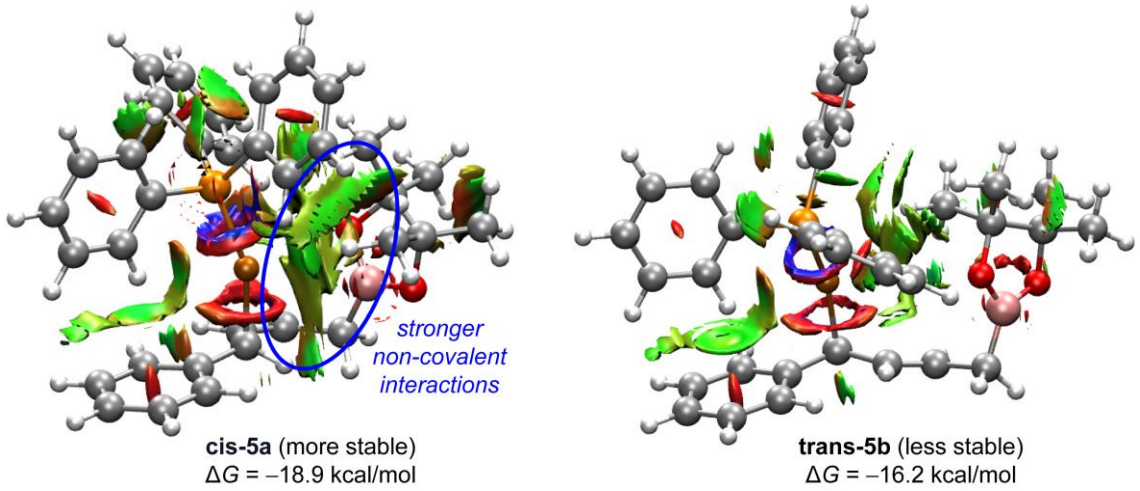

Fig. S7. NCI plots of cis-**5a** and trans-**5b**

*Comparison of Cu–C protonations in **3a** and **5a***

The computed transition state of Cu-C(allyl) bond protonation in **3a** requires a barrier of 27.1 kcal/mol (**S-TS8**, Fig. S8), which is much higher than the barrier of protonation of Cu-C(benzyl and allyl) bond in **5a** (**TS3**, $\Delta G^{\ddagger}$ = 17.9 kcal/mol). The high barrier of **S-TS8** is mostly due to the lack of stabilizing interactions between copper and the double bond.

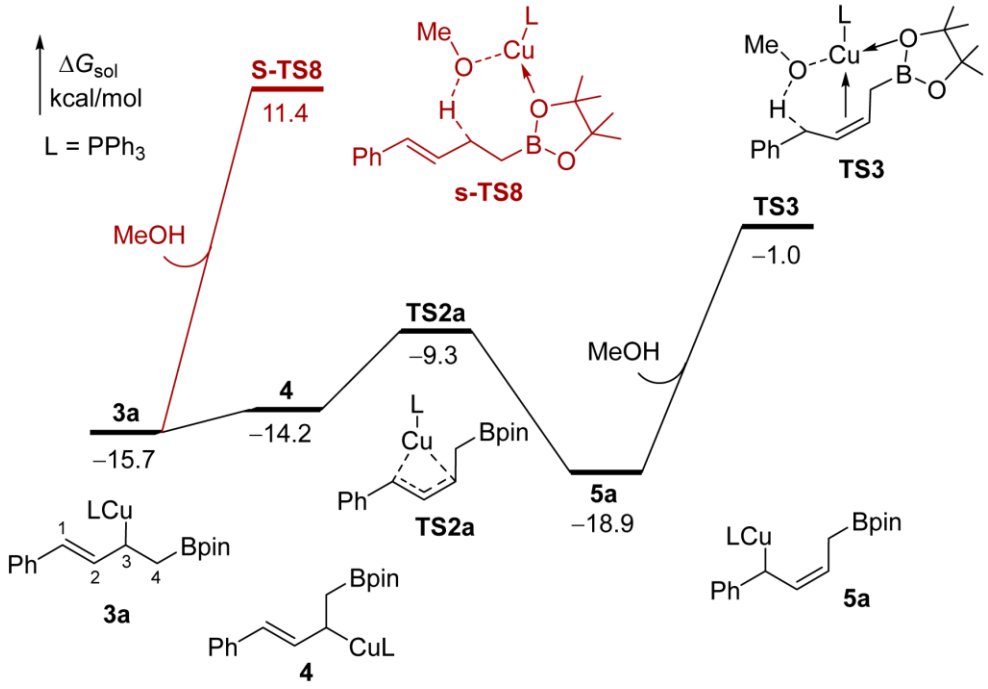

Fig. S8. Energy profiles of Cu–C protonations in **3a** and **5a**.

*Comparison of orbital interactions between **TS1-34** and **TS1-21***

Based on the EDA results along IRC for **TS1-34** and **TS1-21** (Fig. 5 in the main text), we found that the difference of Pauli repulsion is the dominant factor affecting the regioselectivity. The effect of charge transfer (i.e., orbital interaction) is a negative contributor. As shown in Fig. S9, the complementary occupied-virtual pairs calculations indicate that the most significant charge transfer is from σ(Cu-B) to π* orbital. This effect in the disfavored **TS1-21** (ΔE_{ct} = –68.9 kcal/mol) is stronger than that in the favored **TS1-34** (ΔE_{ct} = –60.3 kcal/mol). This is mainly because the HOMO-LUMO gap in **TS1-21** (ΔE_{gap} = 2.23 eV) is smaller than that in **TS1-34** (ΔE_{gap} = 2.45 eV).

The prior studies only considered the difference of LUMO orbital coefficients at different carbon positions (20% at the terminal carbon vs 17% at the benzylic carbon) based on the free optimized 1-phenyl-1,3-butadiene. This is not sufficient because the butadiene can be distorted in transition states and these orbital coefficients will change. In **TS1-34** and **TS1-21**, the computed LUMO orbital coefficients of the distorted butadiene are identical between the terminal carbon (28% in blue) and the benzylic carbon (28% in red). Thus, the regioselectivity of Cu-Bpin additions cannot be controlled by the orbital interaction of σ(Cu-B)→π*.

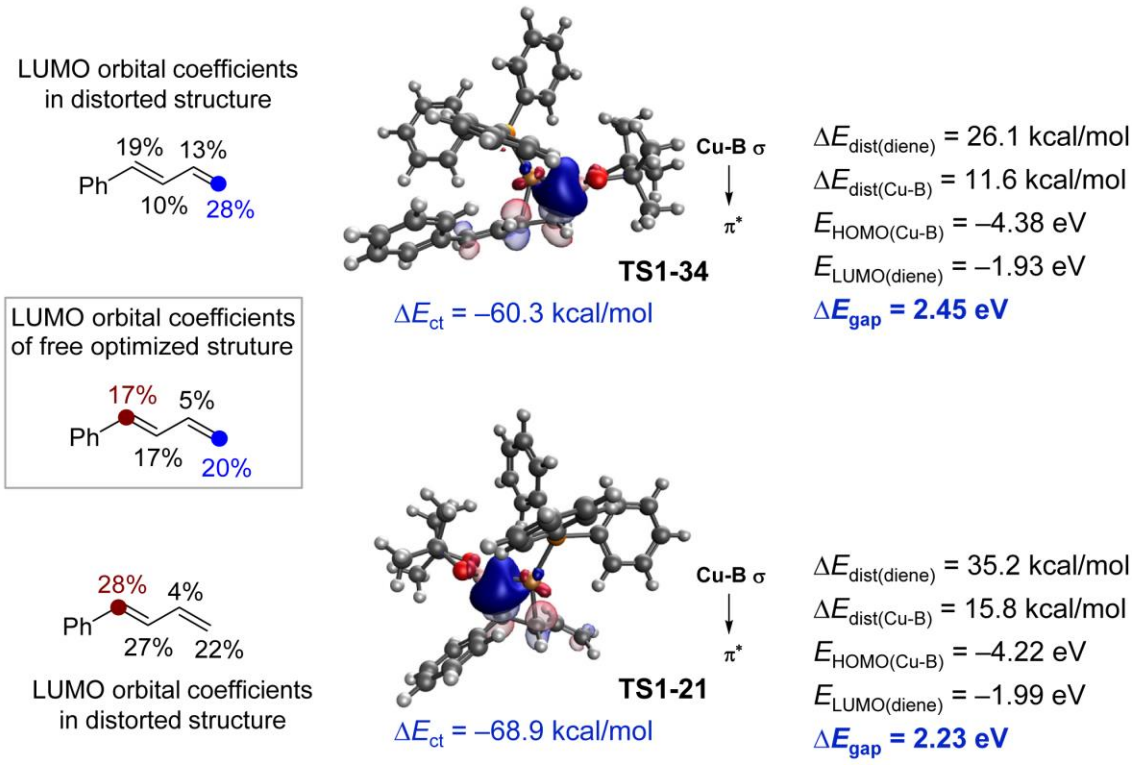

Fig. S9. Difference of orbital interactions between **TS1-34** and **TS1-21**.

Energy Terms of EDA along IRC

Table S1. EDA energy terms of Cu-B insertion transition states (TS1-34) along IRC

Energy terms (in kcal/mol) / *r*(C-B) in **TS1-34** (in Å)	ΔE_{dist}	ΔE_{Pauli}	ΔE_{ct}	ΔE_{elstat}	ΔE_{pol}	ΔE_{disp}
2.24	23.79	246.54	-74.28	-142.41	-29.38	-30.15
2.20	24.77	258.99	-78.57	-148.57	-31.34	-30.88
2.17	25.94	272.30	-83.43	-155.02	-33.45	-31.70
2.13	27.35	286.55	-88.86	-161.82	-35.79	-32.56
2.07	30.27	312.94	-99.21	-174.233	-40.51	-34.20
2.06	30.95	318.57	-101.48	-176.84	-41.59	-34.56
2.01	34.02	342.63	-111.36	-187.92	-46.39	-36.05
1.95(TS)	37.72	370.59	-122.51	-200.55	-52.89	-37.77
1.92	40.84	393.34	-131.38	-210.84	-58.64	-39.14
1.88	44.23	415.22	-140.24	-220.43	-64.60	-40.51
1.84	47.83	438.54	-148.68	-230.41	-72.25	-41.96
1.81	51.58	460.77	-156.17	-239.62	-80.74	-43.40
1.76	59.21	504.17	-166.22	-256.97	-102.85	-46.24

Table S2. EDA energy terms of Cu-B insertion transition states (TS1-21) along IRC

Energy terms (in kcal/mol) / *r*(C-C) in **TS1-21**(in Å)	ΔE_{dist}	ΔE_{Pauli}	ΔE_{ct}	ΔE_{elstat}	ΔE_{pol}	ΔE_{disp}
2.24	32.59	281.64	-83.80	-163.02	-37.67	-31.07
2.20	33.99	294.68	-88.37	-169.24	-40.18	-31.90
2.17	35.62	308.42	-93.47	-175.69	-42.83	-32.83
2.13	37.51	324.78	-99.08	-183.47	-46.51	-33.82
2.07	41.22	351.90	-109.50	-196.01	-52.53	-35.56
2.06	42.06	357.62	-111.73	-198.64	-53.85	-35.94
2.00(TS)	46.68	388.05	-123.75	-212.39	-61.45	-37.92
1.95	50.96	415.87	-134.40	-224.57	-69.43	-39.70
1.92	54.45	438.36	-142.69	-234.33	-76.44	-41.15
1.88	58.04	461.36	-150.68	-244.16	-84.36	-42.61
1.84	61.65	484.64	-158.00	-253.90	-93.39	-44.07
1.81	65.16	505.93	-164.28	-262.53	-102.57	-45.47
1.76	72.42	550.80	-173.81	-279.640	-126.67	-48.45

Table S3. EDA energy terms of Cu-B insertion transition states (TS1-12) along IRC

Energy terms (in kcal/mol) / *r*(C-C) in **TS1-12** (in Å)	ΔE_{dist}	ΔE_{Pauli}	ΔE_{ct}	ΔE_{elstat}	ΔE_{pol}	ΔE_{disp}
2.24	31.04	275.35	-82.54	-157.91	-35.33	-32.81
2.20	32.94	292.78	-88.91	-166.49	-38.41	-33.92
2.17	34.61	306.91	-94.24	-173.19	-41.20	-34.83
2.13	36.50	321.65	-100.05	-180.24	-44.06	-35.76
2.07	40.14	347.74	-110.66	-192.50	-49.43	-37.48
2.06(TS)	40.95	353.92	-112.92	-195.20	-51.14	-37.87
2.01	45.35	383.54	-124.84	-208.85	-58.22	-39.80
1.95	49.38	409.95	-135.31	-220.72	-65.33	-41.48
1.92	52.63	431.99	-143.32	-230.40	-72.17	-42.87
1.88	55.97	453.94	-151.01	-240.00	-79.54	-44.22
1.84	59.32	475.11	-157.96	-249.05	-87.48	-45.57
1.81	63.66	504.30	-165.43	-261.07	-100.65	-47.47
1.76	70.38	547.53	-172.97	-278.03	-125.01	-50.30

Table S4. EDA energy terms of Cu-B insertion transition states (TS1-43) along IRC

Energy terms (in kcal/mol) / *r*(C-C) in **TS1-43** (in Å)	ΔE_{dist}	ΔE_{Pauli}	ΔE_{ct}	ΔE_{elstat}	ΔE_{pol}	ΔE_{disp}
2.24	39.34	290.35	-83.68	-170.09	-43.30	-28.59
2.20	41.43	303.47	-88.60	-176.47	-46.15	-29.39
2.17	43.75	317.00	-93.96	-183.14	-48.95	-30.23
2.13	46.30	332.60	-99.73	-190.52	-52.95	-31.17
2.07(TS)	51.02	357.59	-110.15	-202.21	-59.11	-32.76
2.06	52.03	363.73	-112.34	-205.13	-60.88	-33.10
2.00	57.36	393.00	-123.66	-218.28	-69.78	-34.90
1.96	61.95	416.82	-133.18	-228.80	-77.42	-36.37
1.91	66.79	442.35	-142.98	-239.90	-86.27	-37.93
1.88	70.50	463.26	-150.20	-248.72	-94.43	-39.17
1.84	74.19	483.50	-157.02	-257.21	-102.73	-40.36
1.81	77.76	504.11	-163.18	-265.56	-112.09	-41.58
1.75	85.16	548.33	-173.87	-282.23	-135.80	-44.21

Cartesian Coordinates (Å) and Energies of the Optimized Structures

MeOH
B3LYP-D3 SCF energy: -115.71332581 a.u.
B3LYP-D3 enthalpy: -115.657666 a.u.
B3LYP-D3 free energy: -115.684613 a.u.
wB97XD SCF energy in solution: -115.73075039 a.u.
wB97XD enthalpy in solution: -115.675091 a.u.
wB97XD free energy in solution: -115.702038 a.u.
Three lowest frequencies (cm-1): 350.3507 1067.6046 1100.6272

Cartesian coordinates

ATOM	X	Y	Z
C	0.662272	-0.019658	0.000000
H	1.080094	0.991243	-0.000001
H	1.039140	-0.543472	-0.893373
H	1.039140	-0.543470	0.893374
O	-0.749312	0.122356	0.000000
H	-1.137514	-0.765201	0.000000

CO_2
B3LYP-D3 SCF energy: -188.57776042 a.u.
B3LYP-D3 enthalpy: -188.562560 a.u.
B3LYP-D3 free energy: -188.586861 a.u.
wB97XD SCF energy in solution: -188.58292474 a.u.
wB97XD enthalpy in solution: -188.567724 a.u.
wB97XD free energy in solution: -188.592025 a.u.
Three lowest frequencies (cm-1): 647.2717 647.2717 1369.4400

Cartesian coordinates

ATOM	X	Y	Z
C	0.000000	0.000000	0.000000
O	0.000000	0.000000	1.169724
O	0.000000	0.000000	-1.169724

CO
B3LYP-D3 SCF energy: -113.30691453 a.u.
B3LYP-D3 enthalpy: -113.298574 a.u.
B3LYP-D3 free energy: -113.321017 a.u.
wB97XD SCF energy in solution: -113.30444483 a.u.
wB97XD enthalpy in solution: -113.296103 a.u.
wB97XD free energy in solution: -113.318546 a.u.
The frequency (cm-1): 2210.57

Cartesian coordinates

ATOM	X	Y	Z
O	0.000000	0.000000	0.48760300
C	0.000000	0.000000	-0.65013800

B_2pin_2

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B3LYP-D3 enthalpy: -822.191368 a.u.
B3LYP-D3 free energy: -822.258170 a.u.
wB97XD SCF energy in solution: -822.55189622 a.u.
wB97XD enthalpy in solution: -822.164846 a.u.
wB97XD free energy in solution: -822.231648 a.u.
Three lowest frequencies (cm-1): 30.83 39.74 43.54

Cartesian coordinates

ATOM	X	Y	Z
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H	-3.039089	-2.796678	0.256534
H	-2.605456	-1.973257	-1.249812
C	-2.997485	0.651638	-0.438592
C	-3.256660	1.928089	0.371755
H	-4.298411	1.990545	0.703683
H	-3.037961	2.796777	-0.256599
H	-2.605055	1.973219	1.249874
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H	-3.816865	1.550134	-2.218591
H	-4.952129	0.484019	-1.367405
H	-3.630521	-0.204527	-2.338662
C	-3.905246	-0.609527	1.664742
H	-3.630816	0.204832	2.338491
H	-3.818028	-1.549732	2.218314
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O	-1.613419	0.720825	-0.888565
O	-1.613884	-0.721314	0.888794
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C	2.997728	-0.651599	-0.438540
C	3.257291	-1.927978	0.371784
H	4.299036	-1.990117	0.703765
H	3.038910	-2.796723	-0.256604
H	2.605616	-1.973305	1.249840
C	2.997589	0.651605	0.438569
C	3.256705	1.928024	-0.371837
H	4.298386	1.990374	-0.704007
H	3.038230	2.796725	0.256572
H	2.604908	1.973225	-1.249811
C	3.904977	0.609938	1.664833
H	3.817387	1.550127	2.218369
H	4.952366	0.483804	1.367065
H	3.630838	-0.204500	2.338605
C	3.904923	-0.609560	-1.664931
H	3.630482	0.204909	-2.338545
H	3.817455	-1.549694	-2.218582
H	4.952334	-0.483217	-1.367326
O	1.613587	0.720873	0.888776
O	1.613706	-0.721275	-0.888569

LCu-Bpin

B3LYP-D3 SCF energy: -1643.78356024 a.u.
B3LYP-D3 enthalpy: -1643.295411 a.u.
B3LYP-D3 free energy: -1643.389688 a.u.
wB97XD SCF energy in solution: -1644.91698047 a.u.
wB97XD enthalpy in solution: -1644.428831 a.u.
wB97XD free energy in solution: -1644.523108 a.u.
Three lowest frequencies (cm-1): 12.5051 13.1051 15.3371

Cartesian coordinates

ATOM	X	Y	Z
Cu	0.841424	-0.037048	-0.031764
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C	5.024862	-0.793955	0.030351
C	5.938969	-1.381540	1.103302
H	6.985290	-1.111025	0.916163
H	5.862043	-2.473869	1.094344
H	5.660107	-1.033898	2.100623
C	5.013087	0.770433	-0.052986
C	5.932521	1.372610	-1.113226
H	6.980180	1.117608	-0.912294
H	5.839149	2.463663	-1.104625
H	5.672145	1.021797	-2.114424
C	5.257559	1.448855	1.302561
H	5.025537	2.514578	1.210552
H	6.298234	1.345128	1.629689
H	4.602351	1.024964	2.069654
C	5.299254	-1.467718	-1.321766
H	4.647749	-1.054012	-2.097519
H	5.083736	-2.537183	-1.233411
H	6.342425	-1.346098	-1.634475
O	3.635729	1.047770	-0.417383
O	3.647233	-1.093247	0.375700
P	-1.490845	-0.009542	-0.004139
C	-2.243121	-1.496643	0.761121
C	-3.508643	-1.991793	0.412470
H	-4.086250	-1.503967	-0.367513
C	-4.021935	-3.118086	1.057587
H	-5.001941	-3.497935	0.781345
C	-3.276863	-3.758904	2.050939
H	-3.677986	-4.637571	2.548774
C	-2.175182	1.411930	0.930745
C	-1.431382	2.602968	0.910554
H	-0.480052	2.632490	0.383419
C	-1.901331	3.737487	1.572242
H	-1.318947	4.654411	1.551240
C	-3.110476	3.688305	2.270360
H	-3.473435	4.569749	2.792002
C	-3.847259	2.501867	2.307960
H	-4.782878	2.458810	2.859143
C	-3.383257	1.365903	1.642109
H	-3.954736	0.443071	1.683074
C	-2.255664	0.104969	-1.666956
C	-3.483021	0.737506	-1.914755
H	-4.018199	1.221361	-1.102635
C	-4.012568	0.756593	-3.206186
H	-4.963157	1.249511	-3.391728

C	-3.321500	0.149462	-4.257829
H	-3.735193	0.168984	-5.262438
C	-2.092876	-0.471428	-4.019753
H	-1.546023	-0.932739	-4.837395
C	-1.558499	-0.488530	-2.731283
H	-0.592557	-0.953441	-2.545547
C	-2.011588	-3.277284	2.395114
H	-1.423493	-3.780759	3.157329
C	-1.493351	-2.154388	1.749361
H	-0.499586	-1.789350	2.000011

1
B3LYP-D3 SCF energy: -387.05859240 a.u.
B3LYP-D3 enthalpy: -386.881154 a.u.
B3LYP-D3 free energy: -386.925771 a.u.
wB97XD SCF energy in solution: -387.02911182 a.u.
wB97XD enthalpy in solution: -386.851673 a.u.
wB97XD free energy in solution: -386.896290 a.u.
Three lowest frequencies (cm-1): 38.0052 115.5030 122.2993

Cartesian coordinates

ATOM	X	Y	Z
C	2.294014	1.395567	0.000000
C	0.940001	1.075164	0.000002
C	0.513331	-0.268447	0.000005
C	1.502173	-1.270946	0.000000
C	2.858746	-0.950692	-0.000008
C	3.262194	0.385615	-0.000002
H	2.598252	2.439072	0.000006
H	0.206725	1.876183	0.000010
H	1.195891	-2.314731	-0.000001
H	3.600330	-1.745187	-0.000009
H	4.318510	0.640132	-0.000002
C	-0.896077	-0.665665	0.000008
C	-1.980822	0.139555	0.000005
H	-1.069153	-1.742823	0.000001
H	-1.861303	1.222552	0.000001
C	-3.345717	-0.352624	0.000002
C	-4.435473	0.433083	-0.000009
H	-3.470090	-1.436278	0.000009
H	-5.439252	0.019361	-0.000011
H	-4.354128	1.518059	-0.000016

TS1-34
B3LYP-D3 SCF energy: -2030.85154646 a.u.
B3LYP-D3 enthalpy: -2030.185680 a.u.
B3LYP-D3 free energy: -2030.297702 a.u.
wB97XD SCF energy in solution: -2031.94601209 a.u.
wB97XD enthalpy in solution: -2031.280146 a.u.
wB97XD free energy in solution: -2031.392168 a.u.
Three lowest frequencies (cm-1): -280.6754 10.8142 21.5879
Imaginary frequency: -280.6754 cm-1

Cartesian coordinates

ATOM	X	Y	Z
C	-4.653459	-1.861414	1.725057
C	-3.591331	-1.976290	0.833975
C	-3.808221	-2.241370	-0.540969
C	-5.154229	-2.352479	-0.963075
C	-6.214930	-2.228168	-0.069461
C	-5.976448	-1.986139	1.286740
H	-4.443214	-1.651762	2.771574
H	-2.580666	-1.828384	1.203591
H	-5.357200	-2.546935	-2.014683
H	-7.235790	-2.322553	-0.433741
H	-6.803168	-1.886888	1.985138
C	-2.734509	-2.332817	-1.515577
C	-1.395288	-2.386848	-1.231122
H	-3.032652	-2.277125	-2.563593
H	-1.110154	-2.530904	-0.184585
C	-0.300799	-2.212323	-2.134509
C	1.102770	-2.480446	-1.729743
H	-0.505985	-2.082848	-3.194863
H	1.767169	-2.658263	-2.575590
H	1.213880	-3.250095	-0.961442
Cu	0.577926	-0.542375	-1.236779
B	2.431287	-1.434424	-0.749631
C	4.687217	-1.138928	-0.465706
C	5.944627	-1.694348	-1.127103
H	6.762784	-1.767400	-0.401149
H	6.262686	-1.026442	-1.933998
H	5.768527	-2.682408	-1.557778
C	4.111382	-2.010574	0.707417
C	4.524555	-1.570165	2.107596
H	5.612350	-1.630015	2.228393
H	4.062405	-2.227273	2.851376
H	4.203629	-0.546933	2.314827
C	4.355752	-3.512225	0.520547
H	3.755288	-4.062784	1.251173
H	5.409052	-3.773047	0.668113
H	4.053744	-3.836402	-0.480462
C	4.890031	0.330029	-0.078124
H	3.995831	0.738606	0.399812
H	5.081366	0.912105	-0.985082
H	5.741277	0.454391	0.599432
O	2.674860	-1.803641	0.562930
O	3.599724	-1.174953	-1.437786
P	-0.159591	1.255905	-0.188823
C	-0.754195	0.679526	1.452906
C	-1.948623	1.143079	2.021401
H	-2.552480	1.877082	1.497686
C	-2.383494	0.634155	3.246220
H	-3.317472	0.988119	3.673360
C	-1.634876	-0.341701	3.906939
H	-1.983451	-0.746084	4.853406
C	1.044833	2.590349	0.150043
C	2.204713	2.645003	-0.634774
H	2.373161	1.879853	-1.389210

C	3.150546	3.649544	-0.422838
H	4.049128	3.682691	-1.032570
C	2.947069	4.597838	0.581862
H	3.685983	5.376160	0.752247
C	1.798968	4.539896	1.377945
H	1.646171	5.270709	2.167443
C	0.849727	3.539991	1.165161
H	-0.036373	3.487554	1.792097
C	-1.632349	2.046056	-0.935993
C	-1.827656	3.430024	-1.031255
H	-1.059176	4.117814	-0.691636
C	-3.018878	3.926613	-1.567361
H	-3.166366	5.000584	-1.645313
C	-4.018660	3.049381	-1.993572
H	-4.947533	3.441837	-2.398901
C	-3.823640	1.667915	-1.900467
H	-4.597228	0.975716	-2.220633
C	-2.630040	1.164597	-1.387256
H	-2.477854	0.089885	-1.329173
C	-0.443817	-0.807221	3.342852
H	0.137501	-1.573657	3.848135
C	-0.001751	-0.302472	2.119826
H	0.915751	-0.682140	1.677030

TS1-21
B3LYP-D3 SCF energy: -2030.84168449 a.u.
B3LYP-D3 enthalpy: -2030.175896 a.u.
B3LYP-D3 free energy: -2030.286131 a.u.
wB97XD SCF energy in solution: -2031.93618107 a.u.
wB97XD enthalpy in solution: -2031.270393 a.u.
wB97XD free energy in solution: -2031.380628 a.u.
Three lowest frequencies (cm-1): -260.8216 12.3976 21.9115
Imaginary frequency: -260.8216 cm-1

Cartesian coordinates

ATOM	X	Y	Z
C	-4.112060	-2.055969	2.229395
C	-2.996324	-1.974995	1.401610
C	-3.140473	-1.871071	0.008845
C	-4.433603	-1.844938	-0.529529
C	-5.556006	-1.920419	0.300184
C	-5.399931	-2.024731	1.682610
H	-3.979979	-2.132308	3.305748
H	-1.996002	-1.966086	1.827187
H	-4.560494	-1.764670	-1.606505
H	-6.550940	-1.899994	-0.137495
H	-6.271001	-2.081474	2.329944
C	-1.940661	-1.785569	-0.890477
C	-0.927615	-2.889445	-0.722641
H	-2.222410	-1.635112	-1.934917
H	-1.076230	-3.545934	0.132168
C	-0.272825	-3.450802	-1.887876
C	0.411973	-4.614449	-1.980960
H	-0.326462	-2.830595	-2.789306

H	0.881389	-4.921252	-2.910421
H	0.500738	-5.291792	-1.133574
Cu	-0.039733	-1.113687	-0.341405
B	-1.699010	0.183429	-0.635782
C	-2.506759	2.163845	0.220179
C	-3.712864	2.476946	1.102607
H	-4.139978	3.454156	0.849241
H	-3.399148	2.503101	2.151170
H	-4.486432	1.712573	1.004208
C	-2.818439	2.070052	-1.324481
C	-2.391885	3.287320	-2.140016
H	-2.934901	4.181846	-1.813884
H	-2.620437	3.116609	-3.197100
H	-1.319958	3.473656	-2.049871
C	-4.273516	1.703076	-1.633919
H	-4.362782	1.484876	-2.702883
H	-4.955586	2.524285	-1.389324
H	-4.581780	0.812185	-1.080075
C	-1.342461	3.102664	0.557931
H	-0.457484	2.873714	-0.040106
H	-1.076251	2.974409	1.611882
H	-1.614070	4.151227	0.396645
O	-2.007359	0.930370	-1.748699
O	-2.067836	0.811276	0.537050
P	1.820790	-0.047770	0.113044
C	3.332059	-0.951519	-0.396047
C	3.194693	-2.312797	-0.712938
H	2.213670	-2.783663	-0.687386
C	4.314832	-3.053944	-1.095335
H	4.196900	-4.103599	-1.348814
C	5.569376	-2.445672	-1.166570
H	6.438808	-3.024524	-1.467011
C	1.986405	1.621207	-0.639334
C	1.347821	1.845322	-1.868455
H	0.747720	1.056444	-2.314146
C	1.436279	3.091545	-2.489551
H	0.938605	3.254708	-3.441402
C	2.142632	4.130620	-1.877205
H	2.199557	5.105053	-2.354668
C	2.762729	3.919389	-0.643348
H	3.300778	4.729283	-0.158023
C	2.688717	2.669073	-0.026253
H	3.159533	2.514553	0.940731
C	1.939766	0.247617	1.918811
C	3.139008	0.172997	2.639954
H	4.061425	-0.101448	2.137165
C	3.147034	0.439157	4.011357
H	4.079460	0.376387	4.566014
C	1.962682	0.778560	4.668519
H	1.972812	0.982708	5.735826
C	0.763189	0.845344	3.953932
H	-0.162897	1.098770	4.463010
C	0.746300	0.577124	2.585582
H	-0.188685	0.620598	2.031381
C	5.706664	-1.086144	-0.868878
H	6.679990	-0.607787	-0.938904

C	4.591827	-0.337950	-0.491705
H	4.698145	0.723607	-0.285324

TS1-12

B3LYP-D3 SCF energy: -2030.84418570 a.u.
B3LYP-D3 enthalpy: -2030.178387 a.u.
B3LYP-D3 free energy: -2030.288866 a.u.
wB97XD SCF energy in solution: -2031.93479739 a.u.
wB97XD enthalpy in solution: -2031.268999 a.u.
wB97XD free energy in solution: -2031.379478 a.u.
Three lowest frequencies (cm-1): -234.6069 14.5951 18.5740
Imaginary frequency: -234.6069 cm-1

Cartesian coordinates

ATOM	X	Y	Z
C	-2.133558	-3.325004	1.813407
C	-1.058393	-3.102269	0.951878
C	-1.202874	-3.229441	-0.460351
C	-2.475624	-3.654805	-0.930347
C	-3.531392	-3.891218	-0.061446
C	-3.381490	-3.714801	1.323754
H	-1.986788	-3.195108	2.883541
H	-0.100840	-2.805217	1.373084
H	-2.620234	-3.770948	-2.002332
H	-4.489234	-4.214524	-0.464674
H	-4.213071	-3.893303	1.999217
C	-0.150563	-2.866965	-1.387511
C	1.246289	-2.653966	-0.930572
H	-0.310335	-3.051934	-2.445377
H	1.506949	-3.185908	-0.011621
C	2.277224	-2.816179	-1.991581
C	3.381082	-3.560443	-1.867686
H	2.073268	-2.295718	-2.926669
H	4.086210	-3.673638	-2.686472
H	3.608963	-4.090047	-0.945167
Cu	0.055285	-0.937080	-0.712667
B	2.068752	-0.936103	-0.149919
C	3.772922	0.592221	-0.087632
C	5.046450	0.812596	-0.898299
H	5.836440	1.244530	-0.272917
H	4.840304	1.509028	-1.717467
H	5.410596	-0.121015	-1.332173
C	3.913835	-0.417272	1.113391
C	4.090005	0.230401	2.483490
H	5.016564	0.814703	2.520804
H	4.145692	-0.547414	3.251907
H	3.252422	0.888487	2.726955
C	4.978949	-1.492393	0.882289
H	4.888845	-2.254149	1.663092
H	5.989801	-1.072717	0.920741
H	4.834113	-1.979955	-0.086129
C	3.158181	1.939167	0.313782
H	2.231068	1.799654	0.876375
H	2.912280	2.502913	-0.590236

H	3.852011	2.531112	0.920303
O	2.621556	-1.102983	1.100201
O	2.800435	-0.077361	-0.943106
P	-1.040371	0.911269	-0.195120
C	-1.039312	1.282628	1.606862
C	-2.028387	2.081880	2.201324
H	-2.850536	2.463535	1.602463
C	-1.969347	2.374314	3.564660
H	-2.740195	2.992637	4.016871
C	-0.929547	1.865825	4.347566
H	-0.888741	2.091389	5.409871
C	-0.274169	2.377205	-0.989426
C	0.438015	2.168347	-2.180524
H	0.516151	1.164097	-2.588593
C	1.069353	3.233821	-2.821696
H	1.621655	3.059340	-3.740872
C	1.005580	4.516648	-2.271528
H	1.505449	5.345874	-2.764927
C	0.307013	4.730630	-1.080737
H	0.262898	5.725544	-0.645923
C	-0.331326	3.666770	-0.440796
H	-0.857335	3.837574	0.493725
C	-2.817005	0.932815	-0.639023
C	-3.481578	2.057324	-1.147882
H	-2.936922	2.981349	-1.320706
C	-4.845591	1.985493	-1.440701
H	-5.357640	2.857618	-1.838951
C	-5.548685	0.797525	-1.225241
H	-6.609452	0.745946	-1.456215
C	-4.885952	-0.325674	-0.722046
H	-5.419253	-1.258064	-0.560280
C	-3.523696	-0.263724	-0.434395
H	-3.011511	-1.145467	-0.062150
C	0.046999	1.055374	3.764869
H	0.848978	0.641427	4.370317
C	-0.008070	0.759332	2.401774
H	0.742032	0.110972	1.959812

TS1-43
B3LYP-D3 SCF energy: -2030.83588471 a.u.
B3LYP-D3 enthalpy: -2030.169779 a.u.
B3LYP-D3 free energy: -2030.280802 a.u.
wB97XD SCF energy in solution: -2031.92895998 a.u.
wB97XD enthalpy in solution: -2031.262854 a.u.
wB97XD free energy in solution: -2031.373877 a.u.
Three lowest frequencies (cm-1): -276.6899 9.3234 19.1169
Imaginary frequency: -276.6899 cm-1

Cartesian coordinates

ATOM	X	Y	Z
C	6.680679	1.497257	1.676524
C	5.445903	1.468243	1.034183
C	5.359145	1.308177	-0.363347
C	6.559259	1.155562	-1.081593

C	7.796427	1.182301	-0.438723
C	7.864521	1.356803	0.944703
H	6.720942	1.619886	2.756047
H	4.535990	1.549539	1.621692
H	6.515141	1.020835	-2.160203
H	8.708020	1.065656	-1.019395
H	8.826626	1.375193	1.449525
C	4.079346	1.260562	-1.079778
C	2.876831	1.624300	-0.598957
H	4.127995	0.879929	-2.101137
H	2.786000	2.038532	0.403275
C	1.609962	1.533875	-1.360576
C	0.736313	2.748816	-1.387500
H	1.731440	1.054743	-2.335264
H	0.447727	3.083662	-2.382403
H	1.047058	3.560883	-0.729795
Cu	-0.313560	1.263416	-0.568409
B	1.152335	-0.289326	-0.492854
C	2.200593	-1.999240	0.637769
C	3.714686	-1.823365	0.491594
H	4.226700	-2.791879	0.487610
H	4.092019	-1.233196	1.331528
H	3.969018	-1.285851	-0.423317
C	1.507885	-2.550123	-0.661264
C	0.162667	-3.233246	-0.383707
H	0.300839	-4.195136	0.121104
H	-0.352230	-3.412254	-1.332627
H	-0.482111	-2.603666	0.235473
C	2.385488	-3.444584	-1.531360
H	1.823917	-3.762025	-2.416024
H	2.690692	-4.341431	-0.979919
H	3.281057	-2.919186	-1.869276
C	1.886455	-2.776340	1.912467
H	0.816749	-2.793290	2.125087
H	2.393981	-2.305240	2.760966
H	2.248271	-3.808061	1.831323
O	1.221124	-1.327138	-1.405105
O	1.614771	-0.663260	0.752936
P	-2.277741	0.465365	0.050752
C	-3.517982	1.724625	0.559542
C	-4.607560	1.442386	1.397983
H	-4.733893	0.446989	1.813802
C	-5.526373	2.445030	1.712215
H	-6.366245	2.221488	2.364804
C	-5.364129	3.732956	1.194876
H	-6.079679	4.511991	1.444416
C	-3.046695	-0.428511	-1.359048
C	-2.190530	-1.117274	-2.234823
H	-1.115832	-1.089257	-2.076005
C	-2.718654	-1.839490	-3.305138
H	-2.048641	-2.367987	-3.977983
C	-4.099298	-1.875275	-3.516223
H	-4.508278	-2.434463	-4.353513
C	-4.953181	-1.182693	-2.654909
H	-6.027019	-1.199888	-2.821248
C	-4.431313	-0.458882	-1.580774

H	-5.100508	0.088271	-0.923363
C	-2.260763	-0.753012	1.424437
C	-3.202290	-1.786525	1.544966
H	-3.975682	-1.905686	0.791468
C	-3.135061	-2.674690	2.619699
H	-3.862715	-3.477582	2.702582
C	-2.133276	-2.533946	3.583554
H	-2.082521	-3.226099	4.419740
C	-1.187791	-1.512461	3.462738
H	-0.393673	-1.412964	4.197338
C	-1.241693	-0.633595	2.380316
H	-0.470118	0.118951	2.248230
C	-4.275394	4.021066	0.368622
H	-4.138638	5.024829	-0.024530
C	-3.350799	3.023622	0.056157
H	-2.482133	3.240070	-0.563546

3a

B3LYP-D3 SCF energy: -2030.91221627 a.u.
B3LYP-D3 enthalpy: -2030.244033 a.u.
B3LYP-D3 free energy: -2030.357117 a.u.
wB97XD SCF energy in solution: -2031.99953926 a.u.
wB97XD enthalpy in solution: -2031.331356 a.u.
wB97XD free energy in solution: -2031.444440 a.u.
Three lowest frequencies (cm-1): 10.5001 14.6358 25.0803

Cartesian coordinates

ATOM	X	Y	Z
C	5.500144	2.370272	1.340157
C	4.165971	2.588441	1.009561
C	3.751919	2.730636	-0.336629
C	4.761106	2.644679	-1.322972
C	6.096178	2.426317	-0.991318
C	6.481204	2.283738	0.344952
H	5.778310	2.262927	2.386233
H	3.430161	2.643078	1.807078
H	4.478981	2.745656	-2.368905
H	6.840642	2.363650	-1.781836
H	7.521669	2.112841	0.607310
C	2.365507	2.904333	-0.747922
C	1.263609	2.917332	0.058710
H	2.199317	2.939536	-1.825909
H	1.420716	2.878809	1.139993
C	-0.141639	2.858711	-0.345561
C	-1.188789	3.429052	0.639640
H	-0.310045	3.203071	-1.372999
H	-1.263106	4.525298	0.564661
H	-0.873388	3.192729	1.665769
Cu	-0.120235	0.857092	-0.323277
B	-2.554125	2.714606	0.365696
C	-4.646847	2.245499	-0.435367
C	-5.663119	2.944217	0.476152
H	-6.592709	2.371277	0.559665
H	-5.895640	3.928143	0.057914

H	-5.250316	3.091720	1.479068
C	-4.019384	0.956370	0.213041
C	-3.436381	-0.014796	-0.820985
H	-4.219049	-0.487746	-1.422507
H	-2.881237	-0.803168	-0.306281
H	-2.737353	0.499647	-1.488837
C	-4.925103	0.204298	1.185057
H	-4.389315	-0.661276	1.589121
H	-5.825126	-0.159274	0.676283
H	-5.227304	0.836230	2.023159
C	-5.233365	2.046584	-1.830318
H	-4.473559	1.704924	-2.536711
H	-5.633838	2.996070	-2.199217
H	-6.049620	1.315409	-1.808601
O	-2.900617	1.507688	0.959557
O	-3.500968	3.131305	-0.538917
P	0.290362	-1.343898	-0.042518
C	-0.190367	-1.907812	1.635236
C	0.421922	-2.992421	2.281010
H	1.248072	-3.512396	1.804274
C	-0.017170	-3.394229	3.543556
H	0.463040	-4.233643	4.039277
C	-1.064709	-2.715036	4.171468
H	-1.401980	-3.028535	5.155796
C	-0.614106	-2.446901	-1.196080
C	-0.866782	-1.953519	-2.485940
H	-0.541597	-0.948521	-2.746429
C	-1.542657	-2.736205	-3.421142
H	-1.734050	-2.344918	-4.416507
C	-1.982795	-4.015904	-3.072137
H	-2.515984	-4.624101	-3.797746
C	-1.745696	-4.508667	-1.787035
H	-2.094289	-5.500239	-1.511030
C	-1.064661	-3.728760	-0.849974
H	-0.895664	-4.111993	0.152101
C	2.061531	-1.765176	-0.241957
C	2.513963	-3.045165	-0.599080
H	1.800584	-3.840918	-0.796728
C	3.882648	-3.288412	-0.721777
H	4.230432	-4.279162	-1.002490
C	4.803270	-2.260169	-0.495219
H	5.867387	-2.454775	-0.600209
C	4.359541	-0.981653	-0.149576
H	5.062730	-0.169756	0.010516
C	2.991437	-0.735741	-0.026993
H	2.649735	0.266669	0.212825
C	-1.666348	-1.624209	3.539653
H	-2.469143	-1.080769	4.030598
C	-1.229464	-1.214201	2.278830
H	-1.686180	-0.347691	1.806274

3b
B3LYP-D3 SCF energy: -2030.89506273 a.u.
B3LYP-D3 enthalpy: -2030.226995 a.u.

B3LYP-D3 free energy: -2030.341376 a.u.
wB97XD SCF energy in solution: -2031.99953926 a.u.
wB97XD enthalpy in solution: 0.000000 a.u.
wB97XD free energy in solution: 0.000000 a.u.
Three lowest frequencies (cm-1): 13.3418 15.2980 20.9410

Cartesian coordinates

ATOM	X	Y	Z
C	-6.283073	-1.594341	1.078238
C	-4.989707	-1.098002	0.918296
C	-4.246166	-1.379481	-0.240023
C	-4.844273	-2.170505	-1.230341
C	-6.139372	-2.670248	-1.074264
C	-6.865567	-2.383920	0.082558
H	-6.840597	-1.362374	1.982930
H	-4.546241	-0.477756	1.691836
H	-4.284130	-2.400384	-2.134604
H	-6.579261	-3.284251	-1.856854
H	-7.873578	-2.771151	0.208399
C	-2.823398	-0.866660	-0.402471
C	-1.811649	-1.517124	0.587771
H	-2.488957	-1.098096	-1.423314
H	-2.146417	-1.361988	1.621721
C	-1.510875	-2.943515	0.321729
C	-1.190199	-3.904788	1.211027
H	-1.505313	-3.217262	-0.738091
H	-0.944470	-4.915068	0.895114
H	-1.180105	-3.707219	2.281777
Cu	0.005181	-0.763196	0.422709
B	-2.669807	0.683163	-0.215563
C	-2.411957	2.676570	0.861937
C	-3.314365	3.648813	1.614604
H	-2.961600	4.679672	1.494217
H	-3.305890	3.406436	2.682213
H	-4.346728	3.586043	1.263923
C	-2.339988	2.892586	-0.691039
C	-1.183987	3.765374	-1.167022
H	-1.269454	4.775015	-0.748778
H	-1.206391	3.847097	-2.258712
H	-0.216243	3.348193	-0.884968
C	-3.663444	3.386437	-1.288203
H	-3.612204	3.303156	-2.378103
H	-3.859346	4.431754	-1.026984
H	-4.500846	2.773933	-0.939784
C	-1.024142	2.615898	1.514994
H	-0.369884	1.933316	0.961722
H	-1.129203	2.231319	2.534358
H	-0.550031	3.602160	1.554642
O	-2.147978	1.532861	-1.175248
O	-2.980735	1.346534	0.952898
P	2.179486	-0.281688	0.041926
C	3.025718	-1.745130	-0.672377
C	2.502680	-3.011849	-0.361685
H	1.607122	-3.101304	0.251135
C	3.115586	-4.163166	-0.858497
H	2.701527	-5.137723	-0.615471

C	4.244166	-4.061221	-1.674542
H	4.715652	-4.958576	-2.066064
C	2.432727	1.074497	-1.165410
C	1.382283	1.353876	-2.054264
H	0.435935	0.825224	-1.964566
C	1.534505	2.341318	-3.029365
H	0.714575	2.552340	-3.709681
C	2.724362	3.066780	-3.113145
H	2.838651	3.839161	-3.868905
C	3.763134	2.811410	-2.213201
H	4.683821	3.386269	-2.265959
C	3.619301	1.821057	-1.241123
H	4.423341	1.635999	-0.534110
C	3.163751	0.197186	1.512349
C	4.521411	-0.116639	1.672546
H	5.037512	-0.700671	0.916004
C	5.207923	0.307151	2.811965
H	6.258856	0.057844	2.931319
C	4.546296	1.042438	3.798385
H	5.083043	1.367526	4.685426
C	3.191201	1.348366	3.649722
H	2.669585	1.908622	4.420765
C	2.500607	0.922586	2.515280
H	1.441561	1.143881	2.406691
C	4.758838	-2.803509	-1.999880
H	5.629232	-2.720521	-2.645226
C	4.152106	-1.648830	-1.504210
H	4.546069	-0.674091	-1.776883

3c

B3LYP-D3 SCF energy: -2030.90125341 a.u.
B3LYP-D3 enthalpy: -2030.233389 a.u.
B3LYP-D3 free energy: -2030.347134 a.u.
wB97XD SCF energy in solution: -2031.99953926 a.u.
wB97XD enthalpy in solution: 0.000000 a.u.
wB97XD free energy in solution: 0.000000 a.u.
Three lowest frequencies (cm-1): 15.5852 18.3772 25.8067

Cartesian coordinates

ATOM	X	Y	Z
C	-0.868317	-4.602148	0.901161
C	0.166366	-3.673966	0.778184
C	0.611409	-3.221811	-0.484922
C	-0.025634	-3.786873	-1.615288
C	-1.060239	-4.709779	-1.493238
C	-1.499761	-5.125452	-0.230446
H	-1.183594	-4.918111	1.893403
H	0.625851	-3.274605	1.677741
H	0.293376	-3.465095	-2.605086
H	-1.526006	-5.112334	-2.390331
H	-2.302883	-5.851146	-0.132709
C	1.601301	-2.118243	-0.659436
C	2.740985	-1.971993	0.400531
H	2.042729	-2.154091	-1.662694

H	2.311623	-2.051762	1.407258
C	3.820460	-3.004468	0.228611
C	4.156385	-3.936492	1.123659
H	4.339710	-2.973736	-0.731096
H	4.935612	-4.669109	0.927730
H	3.656540	-4.004603	2.088568
Cu	0.308239	-0.616964	-0.504990
B	3.187614	-0.482416	0.202570
C	3.861204	1.390244	-0.917287
C	5.205155	2.040155	-1.233051
H	5.105318	3.130270	-1.288249
H	5.568343	1.680102	-2.200788
H	5.955857	1.793336	-0.479309
C	3.233621	1.802393	0.469955
C	2.153100	2.878705	0.389946
H	2.562437	3.809099	-0.019579
H	1.762520	3.089765	1.390652
H	1.315021	2.562707	-0.235039
C	4.280309	2.172784	1.526639
H	3.785472	2.257516	2.499273
H	4.765836	3.127518	1.299258
H	5.048259	1.397089	1.604640
C	2.893913	1.570140	-2.095006
H	1.939367	1.072416	-1.892337
H	3.329768	1.104006	-2.983908
H	2.701420	2.626779	-2.307698
O	2.620008	0.563617	0.916691
O	4.061155	-0.039378	-0.761229
P	-1.466463	0.667665	-0.014753
C	-1.566262	1.074855	1.768975
C	-2.779775	1.334172	2.424178
H	-3.717083	1.265925	1.878977
C	-2.785786	1.661638	3.780732
H	-3.728538	1.859355	4.283800
C	-1.584425	1.725602	4.492147
H	-1.592982	1.976487	5.549486
C	-1.536914	2.275647	-0.893355
C	-0.985709	2.318698	-2.184784
H	-0.548059	1.417813	-2.609439
C	-0.982679	3.508222	-2.912298
H	-0.551798	3.530631	-3.909449
C	-1.520716	4.669669	-2.351614
H	-1.511300	5.599661	-2.913486
C	-2.062069	4.636611	-1.064410
H	-2.474046	5.540541	-0.623842
C	-2.070888	3.445695	-0.335208
H	-2.478878	3.430408	0.671102
C	-3.028107	-0.202810	-0.412874
C	-4.212692	0.463187	-0.761580
H	-4.226726	1.547545	-0.832743
C	-5.369743	-0.268899	-1.033296
H	-6.284697	0.250234	-1.306242
C	-5.350315	-1.664795	-0.961278
H	-6.252432	-2.230707	-1.178243
C	-4.170459	-2.331963	-0.623470
H	-4.135631	-3.416488	-0.579793

C	-3.009723	-1.606790	-0.354775
H	-2.093139	-2.138207	-0.109643
C	-0.375905	1.452996	3.847263
H	0.558771	1.485607	4.400601
C	-0.362136	1.122891	2.490877
H	0.578882	0.893425	1.997253

3d

B3LYP-D3 SCF energy: -2030.89932105 a.u.
B3LYP-D3 enthalpy: -2030.230842 a.u.
B3LYP-D3 free energy: -2030.345095 a.u.
wB97XD SCF energy in solution: -2031.99953926 a.u.
wB97XD enthalpy in solution: 0.000000 a.u.
wB97XD free energy in solution: 0.000000 a.u.
Three lowest frequencies (cm-1): 12.6393 17.6761 20.6262

Cartesian coordinates

ATOM	X	Y	Z
C	8.261328	1.259645	1.244422
C	6.902140	1.050630	1.028471
C	6.273036	1.506366	-0.147685
C	7.070424	2.183151	-1.089763
C	8.432264	2.393684	-0.875059
C	9.037767	1.932067	0.294681
H	8.719434	0.897733	2.161892
H	6.319354	0.531019	1.783387
H	6.608471	2.547105	-2.005234
H	9.020350	2.919950	-1.623124
H	10.098444	2.094407	0.467201
C	4.844036	1.309206	-0.430150
C	3.950780	0.630773	0.310092
H	4.492514	1.769129	-1.355809
H	4.264804	0.148941	1.236444
C	2.493545	0.473943	-0.011018
C	1.583939	1.129987	1.091179
H	2.272982	0.956481	-0.973359
H	1.864772	2.190483	1.185595
H	1.812957	0.668921	2.064984
Cu	-0.327155	0.974817	0.683368
B	2.060572	-1.030028	-0.096838
C	2.001571	-3.283211	0.284013
C	3.073519	-3.921903	-0.607909
H	2.778128	-4.921829	-0.943159
H	4.003542	-4.004653	-0.037734
H	3.270972	-3.300068	-1.486665
C	0.719817	-2.838890	-0.511522
C	-0.513540	-2.671170	0.382765
H	-0.859135	-3.626536	0.789861
H	-1.329899	-2.241770	-0.202348
H	-0.303793	-1.987895	1.211652
C	0.377237	-3.689575	-1.730926
H	-0.507251	-3.276539	-2.227378
H	0.152124	-4.720234	-1.433638
H	1.196198	-3.703583	-2.453362

C	1.734164	-4.159497	1.504211
H	1.101831	-3.646030	2.231874
H	2.681672	-4.404526	1.994469
H	1.247375	-5.097003	1.211330
O	1.095070	-1.508352	-0.967797
O	2.537621	-2.013628	0.737200
P	-2.521684	0.721343	0.106365
C	-3.592710	2.176739	0.415474
C	-4.955693	2.074803	0.732062
H	-5.417698	1.096811	0.833679
C	-5.716355	3.228175	0.930708
H	-6.771042	3.142464	1.178121
C	-5.123515	4.488275	0.817893
H	-5.717632	5.384119	0.976576
C	-2.761987	0.312335	-1.666241
C	-1.692189	-0.301992	-2.338686
H	-0.752724	-0.487761	-1.824544
C	-1.831849	-0.677885	-3.676120
H	-0.998564	-1.153041	-4.186536
C	-3.027908	-0.432637	-4.354088
H	-3.132386	-0.720248	-5.396852
C	-4.087699	0.195702	-3.694111
H	-5.015094	0.399432	-4.222751
C	-3.957199	0.569473	-2.355774
H	-4.780184	1.068380	-1.851762
C	-3.321370	-0.649590	1.030146
C	-4.270058	-1.516137	0.469233
H	-4.573276	-1.394403	-0.566302
C	-4.813489	-2.550676	1.234052
H	-5.544662	-3.221036	0.790229
C	-4.416057	-2.727656	2.560956
H	-4.837399	-3.536410	3.151775
C	-3.468696	-1.869035	3.125230
H	-3.148571	-2.008661	4.154038
C	-2.919401	-0.839493	2.362186
H	-2.161246	-0.187658	2.790862
C	-3.764451	4.596038	0.512822
H	-3.297323	5.573932	0.436138
C	-3.000089	3.445374	0.318032
H	-1.937532	3.524597	0.098826

4
B3LYP-D3 SCF energy: -2030.90392489 a.u.
B3LYP-D3 enthalpy: -2030.236162 a.u.
B3LYP-D3 free energy: -2030.346992 a.u.
wB97XD SCF energy in solution: -2031.99487051 a.u.
wB97XD enthalpy in solution: -2031.327108 a.u.
wB97XD free energy in solution: -2031.437938 a.u.
Three lowest frequencies (cm-1): 7.5767 10.4764 15.2540

Cartesian coordinates

ATOM	X	Y	Z
C	1.829652	4.597440	0.858517

C	1.743625	3.222966	1.059368
C	2.087310	2.306796	0.038279
C	2.526179	2.853525	-1.189300
C	2.609494	4.229666	-1.390088
C	2.258563	5.116950	-0.368349
H	1.551723	5.272128	1.665087
H	1.391957	2.852598	2.018091
H	2.795078	2.174566	-1.995904
H	2.947475	4.611635	-2.350725
H	2.320299	6.190786	-0.522228
C	1.971831	0.858886	0.166196
C	1.567957	0.163779	1.273479
H	2.214002	0.299097	-0.733745
H	1.356312	0.729087	2.183134
C	1.313960	-1.271097	1.388343
C	1.949952	-2.201465	0.327935
H	1.487218	-1.633163	2.405523
H	1.496029	-2.051577	-0.662034
H	1.744600	-3.241802	0.608933
Cu	-0.636126	-1.043883	1.021403
B	3.497065	-1.924835	0.213331
C	5.585434	-1.318550	0.896882
C	5.456665	0.073589	1.529593
H	6.348102	0.683362	1.347689
H	5.330300	-0.043988	2.610503
H	4.578087	0.599823	1.145467
C	5.509540	-1.296489	-0.679278
C	6.183474	-2.504982	-1.339457
H	7.273999	-2.460754	-1.249429
H	5.922088	-2.518825	-2.402200
H	5.832121	-3.440218	-0.892287
C	5.986873	0.001155	-1.327980
H	5.887508	-0.074232	-2.415904
H	7.040719	0.190455	-1.093264
H	5.391901	0.853821	-0.993173
C	6.793188	-2.051846	1.474607
H	6.820697	-3.096536	1.156944
H	6.743445	-2.032972	2.567993
H	7.725685	-1.565031	1.166363
O	4.085438	-1.428690	-0.927434
O	4.382462	-2.049796	1.257938
P	-2.635152	-0.412696	0.122810
C	-4.107956	-0.561801	1.208802
C	-4.810680	-1.774631	1.291207
H	-4.544806	-2.602724	0.640545
C	-5.862727	-1.919870	2.196143
H	-6.403090	-2.861377	2.244458
C	-6.221077	-0.861427	3.033881
H	-7.041237	-0.976131	3.737182
C	-2.614638	1.339958	-0.424397
C	-1.376116	1.993083	-0.499096
H	-0.467224	1.477180	-0.204704
C	-1.296551	3.313112	-0.951257
H	-0.328265	3.802436	-0.996625
C	-2.459286	3.986190	-1.326577
H	-2.403421	5.014168	-1.674975

C	-3.700520	3.343354	-1.250335
H	-4.605912	3.870611	-1.539434
C	-3.781289	2.026097	-0.803202
H	-4.749500	1.538502	-0.734720
C	-3.054479	-1.379801	-1.381638
C	-4.327786	-1.344709	-1.972581
H	-5.126024	-0.772555	-1.509005
C	-4.577819	-2.056800	-3.144391
H	-5.566557	-2.026161	-3.594126
C	-3.559843	-2.808396	-3.739867
H	-3.757585	-3.362069	-4.653673
C	-2.292352	-2.850739	-3.157649
H	-1.499426	-3.436830	-3.613661
C	-2.041008	-2.141834	-1.980995
H	-1.054227	-2.180778	-1.524637
C	-5.519554	0.344031	2.965132
H	-5.791652	1.171926	3.614167
C	-4.466954	0.494257	2.061389
H	-3.932404	1.438247	2.010954

TS2a

B3LYP-D3 SCF energy: -2030.89706174 a.u.

B3LYP-D3 enthalpy: -2030.230032 a.u.

B3LYP-D3 free energy: -2030.341364 a.u.

wB97XD SCF energy in solution: -2031.98992076 a.u.

wB97XD enthalpy in solution: -2031.322891 a.u.

wB97XD free energy in solution: -2031.434223 a.u.

Three lowest frequencies (cm-1): -76.2721 12.4874 21.3670

Imaginary frequency: -76.2721 cm-1

Cartesian coordinates

ATOM	X	Y	Z
C	-0.240687	4.934927	-1.027204
C	-0.544488	3.660391	-1.501354
C	-1.188709	2.698104	-0.683688
C	-1.518652	3.111625	0.630695
C	-1.211802	4.383709	1.101199
C	-0.564282	5.314633	0.279942
H	0.260084	5.639866	-1.687776
H	-0.252677	3.393825	-2.514255
H	-2.004266	2.397914	1.294059
H	-1.478989	4.652738	2.121169
H	-0.327856	6.310348	0.644703
C	-1.445771	1.321071	-1.089477
C	-1.425485	0.844840	-2.460582
H	-1.980958	0.721541	-0.356985
H	-1.193466	1.583003	-3.230099
C	-1.583544	-0.450003	-2.913085
C	-1.955512	-1.654649	-2.055996
H	-1.515561	-0.612120	-3.984746
H	-1.091416	-2.026674	-1.481706
H	-2.242912	-2.477566	-2.723454
Cu	0.355952	0.318759	-1.315381
B	-3.128326	-1.407212	-1.033487

C	-4.227971	-1.293395	0.977680
C	-4.624463	-2.705713	1.423874
H	-5.578281	-2.708925	1.961281
H	-3.850438	-3.097978	2.091570
H	-4.703561	-3.379404	0.565005
C	-5.134520	-0.720085	-0.181977
C	-5.180642	0.812632	-0.227288
H	-5.736836	1.221903	0.622657
H	-5.680723	1.119933	-1.150614
H	-4.177079	1.245929	-0.236868
C	-6.551627	-1.287084	-0.226900
H	-7.090832	-0.853996	-1.075015
H	-7.098547	-1.037875	0.689654
H	-6.548007	-2.372412	-0.349400
C	-4.073923	-0.377448	2.189028
H	-3.645412	0.587157	1.908154
H	-3.405593	-0.843623	2.920476
H	-5.042501	-0.203924	2.671219
O	-4.429501	-1.152747	-1.377604
O	-2.930797	-1.417530	0.333164
P	2.078076	-0.372843	-0.108921
C	3.704779	-0.735232	-0.877295
C	3.692223	-1.279266	-2.171305
H	2.741119	-1.432092	-2.677184
C	4.886966	-1.612681	-2.808454
H	4.866109	-2.034479	-3.809573
C	6.107161	-1.390607	-2.164666
H	7.039147	-1.641520	-2.663858
C	2.388311	0.843707	1.229088
C	1.979999	2.171300	1.028788
H	1.482906	2.461376	0.107613
C	2.169455	3.124607	2.030591
H	1.820766	4.139331	1.864339
C	2.767816	2.758519	3.237417
H	2.908718	3.498123	4.021244
C	3.167812	1.435009	3.448441
H	3.619062	1.145765	4.393920
C	2.972988	0.477707	2.452910
H	3.255500	-0.556261	2.633103
C	1.601754	-1.918930	0.761514
C	2.518772	-2.929356	1.085093
H	3.565604	-2.821290	0.815897
C	2.084774	-4.082883	1.742223
H	2.800649	-4.862530	1.988977
C	0.736441	-4.239594	2.073476
H	0.402639	-5.143387	2.576337
C	-0.181541	-3.237848	1.748220
H	-1.236418	-3.351643	1.981035
C	0.246623	-2.081259	1.098394
H	-0.483609	-1.317714	0.845806
C	6.128044	-0.834519	-0.883746
H	7.075797	-0.651009	-0.384732
C	4.932995	-0.508370	-0.239233
H	4.958364	-0.068594	0.752919

TS2b
B3LYP-D3 SCF energy: -2030.90288736 a.u.
B3LYP-D3 enthalpy: -2030.236363 a.u.
B3LYP-D3 free energy: -2030.345120 a.u.
wB97XD SCF energy in solution: -2031.99291329 a.u.
wB97XD enthalpy in solution: -2031.326389 a.u.
wB97XD free energy in solution: -2031.435146 a.u.
Three lowest frequencies (cm-1): -44.5044 19.0077 28.1995
Imaginary frequency: -44.5044 cm-1

Cartesian coordinates

ATOM	X	Y	Z
C	-4.818312	-2.527092	1.402096
C	-3.542805	-2.730521	0.883141
C	-3.289211	-2.680200	-0.512944
C	-4.411480	-2.429773	-1.342441
C	-5.683672	-2.223596	-0.818630
C	-5.907550	-2.265142	0.562827
H	-4.962752	-2.566980	2.480001
H	-2.719900	-2.902285	1.572757
H	-4.262007	-2.382738	-2.419571
H	-6.512054	-2.029496	-1.497236
H	-6.901388	-2.107942	0.972568
C	-1.964990	-2.786018	-1.101525
C	-0.776429	-3.193595	-0.408239
H	-1.919884	-2.746848	-2.191192
H	-0.892684	-3.498108	0.636184
C	0.538171	-3.098267	-0.860008
C	1.753422	-3.460814	-0.043690
H	0.710507	-2.885741	-1.918700
H	2.209355	-4.414368	-0.361910
H	1.457156	-3.630801	1.004649
Cu	-0.651997	-1.104875	-0.517773
B	2.881002	-2.360887	-0.041172
C	4.871889	-1.348727	0.430125
C	4.835831	-0.992501	1.922158
H	5.388443	-0.071203	2.132758
H	5.286347	-1.809920	2.493030
H	3.804817	-0.864514	2.267448
C	3.982684	-0.397234	-0.447547
C	4.355637	-0.419505	-1.934818
H	5.307730	0.089351	-2.118547
H	3.572127	0.095505	-2.498041
H	4.430617	-1.446551	-2.306369
C	3.892836	1.042525	0.048520
H	3.281253	1.636290	-0.634742
H	4.892645	1.490380	0.088592
H	3.441763	1.102723	1.040694
C	6.313159	-1.506793	-0.043601
H	6.357832	-1.915947	-1.055183
H	6.847893	-2.191896	0.621890
H	6.831447	-0.541128	-0.030204
O	2.673693	-1.029947	-0.343402
O	4.190082	-2.624316	0.289594
P	-0.644754	1.054184	-0.069841

C	-0.101155	1.381548	1.655457
C	-0.636446	2.405671	2.448845
H	-1.434696	3.032112	2.061342
C	-0.154527	2.611392	3.743709
H	-0.575618	3.404878	4.355266
C	0.858064	1.796313	4.254400
H	1.227438	1.956499	5.263718
C	0.477267	2.076048	-1.098807
C	0.862991	1.567147	-2.347452
H	0.498047	0.592329	-2.661866
C	1.728132	2.291510	-3.168427
H	2.021810	1.888040	-4.133559
C	2.225438	3.526002	-2.742016
H	2.906577	4.086242	-3.376634
C	1.855482	4.033574	-1.493902
H	2.250482	4.987385	-1.154874
C	0.986910	3.311907	-0.673244
H	0.724604	3.698422	0.307641
C	-2.311435	1.808822	-0.205491
C	-2.533448	3.167622	-0.477801
H	-1.694463	3.834521	-0.654582
C	-3.837534	3.661420	-0.541718
H	-4.005130	4.713117	-0.758991
C	-4.924234	2.806154	-0.335344
H	-5.937402	3.195620	-0.391318
C	-4.709089	1.451501	-0.072167
H	-5.540509	0.768124	0.073856
C	-3.407660	0.952112	-0.013346
H	-3.250559	-0.107601	0.165721
C	1.387450	0.767427	3.470332
H	2.168791	0.125467	3.868561
C	0.907671	0.555025	2.177758
H	1.317036	-0.239430	1.558961

5a

B3LYP-D3 SCF energy: -2030.91393386 a.u.
B3LYP-D3 enthalpy: -2030.245658 a.u.
B3LYP-D3 free energy: -2030.357090 a.u.
wB97XD SCF energy in solution: -2032.00629096 a.u.
wB97XD enthalpy in solution: -2031.338015 a.u.
wB97XD free energy in solution: -2031.449447 a.u.
Three lowest frequencies (cm-1): 14.5165 19.2991 28.6218

Cartesian coordinates

ATOM	X	Y	Z
C	4.229153	3.245669	-0.396206
C	2.887357	3.159068	-0.776200
C	1.842779	3.200054	0.175661
C	2.233411	3.364809	1.527057
C	3.568370	3.447920	1.904927
C	4.587831	3.381837	0.945777
H	4.999677	3.209596	-1.163938
H	2.652747	3.047046	-1.830308
H	1.455599	3.404537	2.287989

H	3.819534	3.568023	2.956632
H	5.631838	3.450677	1.239056
C	0.404244	3.015859	-0.155475
C	-0.066497	3.167087	-1.547213
H	-0.245203	3.499194	0.581185
H	0.673511	3.020968	-2.332931
C	-1.333967	3.403645	-1.944307
C	-2.490805	3.575334	-0.991669
H	-1.553083	3.432255	-3.009317
H	-3.349807	4.021441	-1.516621
H	-2.246686	4.285110	-0.187423
Cu	0.249365	1.034161	0.062027
B	-3.013646	2.250050	-0.319355
C	-3.835302	0.127026	-0.138447
C	-5.146304	0.141851	-0.935259
H	-5.892002	-0.528580	-0.495739
H	-4.940590	-0.188891	-1.957962
H	-5.567590	1.151004	-0.981517
C	-3.943372	0.864499	1.242402
C	-2.821888	0.481459	2.216671
H	-2.939466	-0.537814	2.597451
H	-2.833086	1.178268	3.060440
H	-1.842224	0.558419	1.731662
C	-5.302586	0.755765	1.926612
H	-5.282905	1.301528	2.875254
H	-5.544871	-0.291926	2.138969
H	-6.096450	1.182602	1.309793
C	-3.277493	-1.287239	-0.067001
H	-2.281771	-1.300777	0.371702
H	-3.210053	-1.719191	-1.070301
H	-3.927724	-1.927282	0.540021
O	-3.716842	2.247145	0.863850
O	-2.902615	0.981125	-0.863193
P	0.783470	-1.157340	-0.071416
C	2.575307	-1.426416	0.208882
C	3.434560	-0.323161	0.092820
H	3.041006	0.661973	-0.140742
C	4.806624	-0.477359	0.295810
H	5.451164	0.392940	0.215890
C	5.329053	-1.730738	0.619288
H	6.396732	-1.850184	0.783418
C	-0.022606	-2.328108	1.089899
C	-0.180448	-1.900934	2.418102
H	0.171340	-0.914307	2.710639
C	-0.800211	-2.726161	3.355256
H	-0.919048	-2.385069	4.379951
C	-1.278674	-3.982369	2.971837
H	-1.770289	-4.622339	3.699414
C	-1.129084	-4.411170	1.651261
H	-1.503475	-5.385576	1.349208
C	-0.502345	-3.589549	0.711641
H	-0.400764	-3.922795	-0.316740
C	0.407647	-1.785256	-1.752733
C	1.116305	-2.833873	-2.358796
H	1.952629	-3.295741	-1.842169
C	0.759876	-3.274102	-3.634259

H	1.314662	-4.084492	-4.099455
C	-0.301036	-2.669471	-4.314134
H	-0.573205	-3.011952	-5.308916
C	-1.001518	-1.617327	-3.720191
H	-1.818006	-1.134425	-4.249960
C	-0.648068	-1.168914	-2.446450
H	-1.192800	-0.342053	-1.996193
C	4.476735	-2.831974	0.748362
H	4.880248	-3.805834	1.012672
C	3.104131	-2.682328	0.550365
H	2.443563	-3.535946	0.677122

5b

B3LYP-D3 SCF energy: -2030.91019770 a.u.
B3LYP-D3 enthalpy: -2030.241850 a.u.
B3LYP-D3 free energy: -2030.354115 a.u.
wB97XD SCF energy in solution: -2032.00134968 a.u.
wB97XD enthalpy in solution: -2031.333002 a.u.
wB97XD free energy in solution: -2031.445267 a.u.
Three lowest frequencies (cm-1): 14.2590 21.1888 26.9270

Cartesian coordinates

ATOM	X	Y	Z
C	-3.679399	-3.380281	1.020199
C	-2.318550	-3.271434	0.729764
C	-1.847415	-3.213328	-0.604174
C	-2.828788	-3.313522	-1.621207
C	-4.183507	-3.426947	-1.329639
C	-4.629361	-3.452967	-0.001434
H	-3.997444	-3.412699	2.060133
H	-1.611155	-3.219769	1.551878
H	-2.503713	-3.274333	-2.659342
H	-4.900610	-3.496729	-2.144814
H	-5.687342	-3.546255	0.228329
C	-0.428395	-2.970314	-0.971399
C	0.654361	-3.166168	0.006704
H	-0.181935	-3.328843	-1.975124
H	0.416255	-2.924794	1.045736
C	1.934450	-3.510979	-0.246651
C	3.054405	-3.399818	0.771676
H	2.232435	-3.742501	-1.270894
H	3.769115	-4.227287	0.686132
H	2.641871	-3.404073	1.788849
Cu	-0.517378	-0.971266	-0.867598
B	3.716017	-2.014622	0.442403
C	5.110433	-0.426832	-0.426726
C	6.208851	-0.171640	0.612112
H	6.550294	0.868703	0.591066
H	7.060779	-0.823105	0.395156
H	5.851260	-0.402692	1.620469
C	3.733105	0.215908	-0.032202
C	2.781922	0.359159	-1.227644
H	3.106622	1.146152	-1.915659
H	1.787661	0.624396	-0.861990

H	2.694194	-0.584566	-1.775172
C	3.817475	1.529794	0.738283
H	2.809691	1.889444	0.968353
H	4.323806	2.295315	0.139304
H	4.356128	1.407035	1.680826
C	5.607908	-0.078973	-1.826303
H	4.905899	-0.413204	-2.593261
H	6.568388	-0.570867	-2.010363
H	5.751881	1.003022	-1.927078
O	3.166827	-0.805245	0.835257
O	4.805903	-1.847155	-0.379922
P	-1.095909	1.060378	-0.077036
C	-0.319984	2.520667	-0.868161
C	0.104711	3.649014	-0.152545
H	-0.036472	3.694289	0.923226
C	0.722141	4.709594	-0.819433
H	1.052990	5.578931	-0.257618
C	0.917398	4.652876	-2.200979
H	1.401326	5.478145	-2.716162
C	-2.903737	1.327680	-0.176619
C	-3.725463	0.189033	-0.138048
H	-3.289510	-0.804671	-0.078540
C	-5.112650	0.328239	-0.178739
H	-5.731978	-0.563285	-0.148786
C	-5.686464	1.598486	-0.270476
H	-6.767242	1.705682	-0.310214
C	-4.871837	2.733443	-0.321182
H	-5.317465	3.721425	-0.401047
C	-3.483005	2.602032	-0.274471
H	-2.851666	3.485157	-0.324365
C	-0.662615	1.192452	1.698044
C	-1.409489	1.947511	2.614789
H	-2.313580	2.456348	2.292379
C	-0.996666	2.034697	3.945432
H	-1.580295	2.617204	4.653294
C	0.160000	1.372748	4.367899
H	0.476724	1.443699	5.405049
C	0.901219	0.613818	3.459330
H	1.799640	0.091008	3.774778
C	0.488357	0.514359	2.130264
H	1.070664	-0.089688	1.440409
C	0.497955	3.529542	-2.919576
H	0.655951	3.477369	-3.993262
C	-0.110724	2.465645	-2.255600
H	-0.412378	1.578432	-2.808217

TS3
B3LYP-D3 SCF energy: -2146.64241177 a.u.
B3LYP-D3 enthalpy: -2145.921847 a.u.
B3LYP-D3 free energy: -2146.041801 a.u.
wB97XD SCF energy in solution: -2147.72364006 a.u.
wB97XD enthalpy in solution: -2147.003075 a.u.
wB97XD free energy in solution: -2147.123029 a.u.
Three lowest frequencies (cm-1): -1244.5606 11.2638 19.5175

Imaginary frequency: -1244.5606 cm-1

Cartesian coordinates

ATOM	X	Y	Z
C	6.048960	-0.300321	-0.504277
C	4.717677	-0.681620	-0.666489
C	4.258277	-1.952519	-0.258495
C	5.211294	-2.812160	0.326170
C	6.540197	-2.429026	0.495512
C	6.975104	-1.167026	0.080869
H	6.365098	0.685313	-0.841971
H	4.026972	0.024033	-1.117514
H	4.894021	-3.801184	0.651997
H	7.243249	-3.124132	0.949695
H	8.011806	-0.867537	0.209268
C	2.842979	-2.371108	-0.349923
C	1.968519	-1.795264	-1.347333
H	2.697440	-3.443243	-0.184931
H	2.334510	-0.911007	-1.870508
C	0.666259	-2.139378	-1.648075
C	-0.052655	-3.393018	-1.166240
H	0.202659	-1.628753	-2.492297
H	0.518017	-3.849025	-0.345284
H	-0.108677	-4.152111	-1.959716
Cu	0.198847	-0.638124	0.068585
B	-1.483723	-3.058285	-0.616825
C	-3.037939	-1.963176	0.691885
C	-2.903368	-2.531277	2.107550
H	-2.489366	-3.544049	2.089085
H	-3.868764	-2.554171	2.622815
H	-2.217442	-1.898258	2.678287
C	-3.744149	-2.939786	-0.318602
C	-4.306268	-2.219294	-1.550497
H	-5.192993	-1.627810	-1.301147
H	-4.583726	-2.966855	-2.299608
H	-3.559893	-1.551045	-1.991505
C	-4.800018	-3.847961	0.301725
H	-5.226803	-4.496714	-0.469362
H	-5.610644	-3.252327	0.736574
H	-4.373482	-4.483405	1.080790
C	-3.616378	-0.553877	0.730090
H	-3.547259	-0.061548	-0.240236
H	-3.070000	0.057203	1.453983
H	-4.667702	-0.585858	1.037698
O	-2.639641	-3.765629	-0.793514
O	-1.686470	-1.911804	0.139714
P	-0.323558	1.528747	-0.029826
C	1.073189	2.536148	-0.659820
C	2.360303	2.120303	-0.280272
H	2.480788	1.228741	0.331596
C	3.480799	2.838892	-0.696159
H	4.470229	2.502708	-0.398765
C	3.325259	3.968952	-1.504018
H	4.198429	4.523817	-1.836584
C	-1.745896	1.907872	-1.132408
C	-1.854851	1.119178	-2.291280

H	-1.100639	0.361330	-2.488880
C	-2.930789	1.280811	-3.162790
H	-3.001073	0.664327	-4.054934
C	-3.924744	2.222227	-2.877946
H	-4.771507	2.340783	-3.548489
C	-3.829933	3.002960	-1.724864
H	-4.603397	3.731132	-1.495354
C	-2.745499	2.850584	-0.856187
H	-2.693164	3.452856	0.045120
C	-0.722089	2.307041	1.586707
C	-0.981175	1.453959	2.669827
H	-0.905960	0.379015	2.525245
C	-1.294478	1.979610	3.924580
H	-1.489519	1.310106	4.757923
C	-1.339043	3.362847	4.109509
H	-1.577149	3.773823	5.086882
C	-1.057022	4.220147	3.041663
H	-1.071683	5.296694	3.189418
C	-0.744063	3.696114	1.787117
H	-0.499609	4.365081	0.966153
C	2.047857	4.379470	-1.893625
H	1.926842	5.253528	-2.528222
C	0.921891	3.667312	-1.473199
H	-0.069783	3.984122	-1.785331
C	0.916201	-2.273282	2.500861
H	0.275776	-3.042877	2.036110
H	0.313954	-1.764812	3.268324
H	1.746529	-2.782995	3.013275
O	1.397406	-1.333741	1.568481
H	2.182548	-1.855675	0.796127

LCu-OMe

B3LYP-D3 SCF energy: -1347.64091110 a.u.
B3LYP-D3 enthalpy: -1347.301034 a.u.
B3LYP-D3 free energy: -1347.379416 a.u.
wB97XD SCF energy in solution: -1348.79141752 a.u.
wB97XD enthalpy in solution: -1348.451540 a.u.
wB97XD free energy in solution: -1348.529922 a.u.
Three lowest frequencies (cm-1): 18.9378 28.2650 33.3651

Cartesian coordinates

ATOM	X	Y	Z
Cu	-2.210959	-0.087692	-0.593611
P	-0.063744	-0.005751	-0.068513
C	0.975002	-1.186933	-1.013004
C	2.173560	-1.720967	-0.516018
H	2.507588	-1.468722	0.486429
C	2.930801	-2.590886	-1.302007
H	3.856672	-3.003461	-0.910402
C	2.496892	-2.936554	-2.584358
H	3.086760	-3.617267	-3.192079
C	0.702571	1.638884	-0.344323
C	-0.132376	2.763118	-0.249730
H	-1.195334	2.625593	-0.063363

C	0.392929	4.045613	-0.408553
H	-0.261390	4.909625	-0.334363
C	1.753582	4.214741	-0.675267
H	2.162059	5.213092	-0.806065
C	2.587185	3.099140	-0.787398
H	3.643486	3.228116	-1.007404
C	2.066085	1.814593	-0.624592
H	2.716643	0.951134	-0.728104
C	0.257586	-0.395728	1.695466
C	1.331040	0.144630	2.418927
H	1.998469	0.861365	1.949384
C	1.534659	-0.225507	3.749482
H	2.366269	0.198953	4.305412
C	0.669822	-1.132570	4.366598
H	0.829399	-1.415787	5.403404
C	-0.407061	-1.665876	3.654220
H	-1.089028	-2.362156	4.134133
C	-0.616422	-1.295243	2.325932
H	-1.464385	-1.693820	1.773070
C	1.298374	-2.417640	-3.079733
H	0.950559	-2.694533	-4.070924
C	0.536917	-1.550676	-2.295725
H	-0.407041	-1.161402	-2.671133
O	-3.910990	-0.169692	-1.153747
C	-5.064410	-0.034671	-0.381561
H	-5.161751	0.962811	0.090398
H	-5.960789	-0.172790	-1.012202
H	-5.136722	-0.778704	0.436088

6a

B3LYP-D3 SCF energy: -798.99025816 a.u.
B3LYP-D3 enthalpy: -798.605256 a.u.
B3LYP-D3 free energy: -798.672762 a.u.
wB97XD SCF energy in solution: -798.94912660 a.u.
wB97XD enthalpy in solution: -798.564124 a.u.
wB97XD free energy in solution: -798.631630 a.u.
Three lowest frequencies (cm-1): 17.0634 28.2997 39.7903

Cartesian coordinates

ATOM	X	Y	Z
C	2.260766	-2.027610	-0.397422
C	1.929556	-0.707898	-0.711173
C	2.791093	0.343941	-0.367345
C	3.984083	0.043051	0.301418
C	4.313180	-1.275545	0.623398
C	3.451810	-2.316966	0.273390
H	1.591384	-2.834375	-0.686197
H	0.995927	-0.489119	-1.222318
H	4.663944	0.849527	0.569195
H	5.245086	-1.488941	1.140956
H	3.708811	-3.344880	0.515395
C	2.414945	1.784456	-0.678171
H	3.329995	2.360461	-0.875581
H	1.816122	1.816860	-1.593759

C	1.666508	2.417457	0.472708
C	0.380049	2.787079	0.494773
H	2.252194	2.540968	1.383758
H	-0.016492	3.181788	1.429582
C	-0.639333	2.640016	-0.613358
H	-1.329658	3.493616	-0.592710
H	-0.173860	2.615244	-1.603534
B	-1.425712	1.299688	-0.351866
C	-2.263226	-0.803635	-0.641903
C	-3.553058	-0.674285	-1.460258
H	-4.289336	-1.432006	-1.172961
H	-3.315728	-0.803208	-2.520634
H	-4.001494	0.315750	-1.330290
C	-2.427433	-0.347916	0.853833
C	-1.336006	-0.905210	1.776737
H	-1.471753	-1.976363	1.959117
H	-1.385143	-0.380221	2.735445
H	-0.338854	-0.744721	1.354703
C	-3.808964	-0.584851	1.455234
H	-3.826781	-0.223118	2.488092
H	-4.047541	-1.654563	1.463197
H	-4.585824	-0.055525	0.899069
C	-1.649049	-2.187115	-0.831379
H	-0.666368	-2.256775	-0.362205
H	-1.532982	-2.394802	-1.899986
H	-2.298546	-2.958032	-0.401382
O	-2.197032	1.087009	0.763348
O	-1.338475	0.194763	-1.165914

TS4a

B3LYP-D3 SCF energy: -2170.26090594 a.u.
B3LYP-D3 enthalpy: -2169.533180 a.u.
B3LYP-D3 free energy: -2169.650120 a.u.
wB97XD SCF energy in solution: -2171.35797569 a.u.
wB97XD enthalpy in solution: -2170.630250 a.u.
wB97XD free energy in solution: -2170.747190 a.u.
Three lowest frequencies (cm-1): -33.8111 13.9471 20.4560
Imaginary frequency: -33.8111 cm-1

Cartesian coordinates

ATOM	X	Y	Z
Cu	-0.065039	-0.856400	0.339636
P	2.078450	-0.429615	-0.069147
C	3.180968	-1.803772	-0.565860
C	4.325316	-1.629996	-1.358488
H	4.579591	-0.644771	-1.738236
C	5.129878	-2.725995	-1.673912
H	6.013313	-2.586347	-2.291050
C	4.797734	-3.999211	-1.203804
H	5.424502	-4.850718	-1.454372
C	2.237833	0.855416	-1.370367
C	1.213318	0.952462	-2.325022
H	0.347944	0.298823	-2.260103
C	1.275547	1.926305	-3.323116

H	0.473197	1.998331	-4.051668
C	2.349790	2.817780	-3.366133
H	2.390990	3.582971	-4.136584
C	3.364220	2.736423	-2.408046
H	4.193365	3.438408	-2.430952
C	3.309607	1.760899	-1.412006
H	4.087452	1.717303	-0.654612
C	2.849398	0.329742	1.412849
C	2.018881	1.115954	2.230697
H	0.964723	1.229374	1.987222
C	2.547287	1.753410	3.352899
H	1.899625	2.359813	3.980277
C	3.899308	1.604563	3.674131
H	4.307427	2.097492	4.552372
C	4.723966	0.813344	2.871376
H	5.773477	0.688334	3.124114
C	4.203068	0.175757	1.743060
H	4.846563	-0.445932	1.127022
C	3.653544	-4.179826	-0.422981
H	3.384738	-5.170488	-0.067342
C	2.843660	-3.087865	-0.110097
H	1.940922	-3.226494	0.481221
O	-1.450568	-1.760973	1.770792
C	-1.513193	-1.101060	3.030501
H	-1.209947	-0.048224	2.954526
H	-2.536313	-1.134926	3.423564
H	-0.841091	-1.621713	3.720465
B	-2.218340	-1.156327	0.660653
C	-3.612363	-2.146545	-0.923170
C	-3.684261	-1.257456	-2.173549
H	-4.670272	-1.305038	-2.650401
H	-2.937164	-1.612165	-2.892277
H	-3.445564	-0.221368	-1.929600
C	-4.453497	-1.582841	0.286227
C	-4.796676	-2.664451	1.323461
H	-5.548730	-3.369919	0.952071
H	-5.193358	-2.174870	2.218955
H	-3.897735	-3.218209	1.609229
C	-5.714419	-0.819413	-0.112535
H	-6.223669	-0.453173	0.785617
H	-6.408269	-1.470554	-0.657686
H	-5.476146	0.041875	-0.740339
C	-3.948089	-3.591015	-1.300780
H	-3.754774	-4.273686	-0.470430
H	-3.323823	-3.902874	-2.145153
H	-4.999130	-3.685031	-1.600399
O	-3.540109	-0.664098	0.923236
O	-2.273398	-2.113497	-0.411136
B	-1.560104	0.687422	0.185643
C	-2.327297	2.648767	-0.739444
C	-1.964864	3.507956	-1.946809
H	-2.191424	4.563587	-1.756092
H	-2.551251	3.184938	-2.813386
H	-0.906895	3.414259	-2.200807
C	-1.531538	2.972255	0.573227
C	-2.258250	3.872432	1.568788

H	-2.462508	4.856361	1.130204
H	-1.632508	4.017865	2.455655
H	-3.201522	3.427046	1.891396
C	-0.117056	3.503836	0.309223
H	0.442159	3.521810	1.249957
H	-0.139415	4.521508	-0.095175
H	0.421874	2.860486	-0.391232
C	-3.846551	2.620648	-0.530317
H	-4.107986	1.957359	0.298855
H	-4.319910	2.226975	-1.435483
H	-4.247870	3.621553	-0.338137
O	-1.387801	1.653668	1.174787
O	-1.922445	1.277819	-1.013295

TS4b

B3LYP-D3 SCF energy: -2146.66367028 a.u.
B3LYP-D3 enthalpy: -2145.938718 a.u.
B3LYP-D3 free energy: -2146.055502 a.u.
wB97XD SCF energy in solution: -2147.74074507 a.u.
wB97XD enthalpy in solution: -2147.015793 a.u.
wB97XD free energy in solution: -2147.132577 a.u.
Three lowest frequencies (cm-1): -280.6777 13.8267 15.5043
Imaginary frequency: -280.6777 cm-1

Cartesian coordinates

ATOM	X	Y	Z
C	2.504304	-2.231646	1.479989
C	1.496265	-2.792534	0.688536
C	1.805411	-3.500494	-0.481773
C	3.157416	-3.646579	-0.828491
C	4.167305	-3.090834	-0.040765
C	3.842976	-2.373275	1.114387
H	2.240294	-1.677176	2.375049
H	0.457382	-2.712225	0.991469
H	3.418245	-4.201684	-1.727705
H	5.208104	-3.216600	-0.329210
H	4.624191	-1.928044	1.723938
C	0.717469	-4.058605	-1.395305
H	0.618310	-3.369193	-2.246796
H	1.081505	-5.002146	-1.824572
C	-0.634746	-4.274820	-0.763835
C	-1.646545	-3.385464	-0.774064
H	-0.777651	-5.225791	-0.252430
H	-2.576291	-3.677240	-0.284919
C	-1.654624	-2.007137	-1.320125
H	-0.860521	-1.885158	-2.089015
H	-2.572880	-1.783261	-1.859637
B	-2.605474	-0.803270	0.204077
C	-4.217105	0.769662	-0.189732
C	-4.295413	1.510310	1.155221
H	-3.942941	0.872137	1.970629
H	-5.313530	1.846182	1.381760
H	-3.639160	2.385243	1.106797
C	-4.882828	-0.659536	-0.146545

C	-5.259131	-1.186408	-1.538481
H	-6.146897	-0.679963	-1.933222
H	-5.472906	-2.257153	-1.463318
H	-4.441704	-1.051641	-2.251015
C	-6.088115	-0.771410	0.786925
H	-5.809733	-0.551127	1.820007
H	-6.485319	-1.791504	0.755106
H	-6.885907	-0.083958	0.481585
C	-4.714021	1.677283	-1.312401
H	-4.508786	1.243872	-2.293948
H	-4.203044	2.644279	-1.254590
H	-5.791854	1.856653	-1.223684
O	-3.826708	-1.481541	0.390392
O	-2.833063	0.449322	-0.432296
Cu	-0.301404	-0.622318	-0.487100
P	1.116024	1.086869	-0.180260
C	1.782054	1.071367	1.530709
C	3.140268	1.228410	1.831393
H	3.857807	1.401934	1.035155
C	3.577460	1.135710	3.155336
H	4.634027	1.250751	3.382674
C	2.663064	0.890200	4.181507
H	3.007036	0.812520	5.209412
C	2.592456	1.113154	-1.263582
C	3.216189	2.286005	-1.713131
H	2.806223	3.256998	-1.452521
C	4.361590	2.206305	-2.507848
H	4.836644	3.118201	-2.859791
C	4.895234	0.961222	-2.850917
H	5.787726	0.904695	-3.468490
C	4.276652	-0.209072	-2.404630
H	4.682746	-1.182765	-2.663399
C	3.125075	-0.134425	-1.622563
H	2.641340	-1.044496	-1.283516
C	0.329628	2.734960	-0.330763
C	0.863727	3.872736	0.295942
H	1.755573	3.784087	0.910548
C	0.243332	5.112638	0.144000
H	0.660565	5.989304	0.632198
C	-0.916558	5.224232	-0.628383
H	-1.401111	6.190290	-0.742854
C	-1.459601	4.092705	-1.239974
H	-2.369678	4.173511	-1.827968
C	-0.844535	2.848170	-1.089224
H	-1.297844	1.960583	-1.517749
C	1.304406	0.739705	3.883842
H	0.590318	0.544329	4.679444
C	0.862419	0.823627	2.564066
H	-0.185260	0.665081	2.321435
O	-1.705580	-0.778989	1.325827
C	-1.788841	-1.820482	2.290785
H	-1.620462	-2.803453	1.837255
H	-1.015026	-1.636775	3.043733
H	-2.774825	-1.823177	2.769540

MeOBpin
B3LYP-D3 SCF energy: -526.46930674 a.u.
B3LYP-D3 enthalpy: -526.229668 a.u.
B3LYP-D3 free energy: -526.280546 a.u.
wB97XD SCF energy in solution: -526.45597113 a.u.
wB97XD enthalpy in solution: -526.216332 a.u.
wB97XD free energy in solution: -526.267210 a.u.
Three lowest frequencies (cm-1): 45.5497 78.0827 111.3345

Cartesian coordinates

ATOM	X	Y	Z
C	0.719565	0.842283	0.033605
C	0.879251	1.533630	-1.326040
H	1.933041	1.651705	-1.598690
H	0.419783	2.525536	-1.274935
H	0.376204	0.965466	-2.115015
C	1.067003	-0.694622	-0.012896
C	1.364718	-1.281891	1.372573
H	2.332673	-0.943750	1.757098
H	1.380674	-2.373204	1.296822
H	0.586681	-1.002889	2.090406
C	2.167775	-1.076146	-0.998310
H	2.332704	-2.157757	-0.965142
H	3.108838	-0.577676	-0.738910
H	1.898213	-0.808581	-2.022294
C	1.437714	1.635773	1.120705
H	1.204289	1.252238	2.116209
H	1.125011	2.684202	1.080602
H	2.523014	1.596736	0.973391
O	-0.181907	-1.280880	-0.460844
O	-0.702106	0.823710	0.332052
B	-1.176448	-0.397320	-0.108144
O	-2.488081	-0.722561	-0.202649
C	-3.484759	0.236862	0.132648
H	-3.140470	1.261067	-0.048494
H	-4.366906	0.034705	-0.482185
H	-3.762357	0.141312	1.189665

TS5
B3LYP-D3 SCF energy: -1832.36143712 a.u.
B3LYP-D3 enthalpy: -1831.858067 a.u.
B3LYP-D3 free energy: -1831.956046 a.u.
wB97XD SCF energy in solution: -1833.48637479 a.u.
wB97XD enthalpy in solution: -1832.983005 a.u.
wB97XD free energy in solution: -1833.080984 a.u.
Three lowest frequencies (cm-1): -70.8117 20.3871 21.8983
Imaginary frequency: -70.8117 cm-1

Cartesian coordinates

ATOM	X	Y	Z
Cu	-0.224550	1.679099	-0.101367
B	-2.088016	0.906953	-0.065243
C	-3.528237	-0.711185	0.679281

C	-2.751155	-2.033977	0.645511
H	-3.406211	-2.881433	0.416795
H	-2.296639	-2.203292	1.627018
H	-1.948520	-2.000322	-0.096593
C	-3.966610	-0.211125	-0.742037
C	-5.118042	0.799615	-0.702922
H	-6.061493	0.326772	-0.408832
H	-5.241030	1.231622	-1.700770
H	-4.892862	1.617656	-0.012752
C	-4.249106	-1.317727	-1.753666
H	-4.528804	-0.873182	-2.714310
H	-5.078220	-1.950972	-1.416554
H	-3.369486	-1.945654	-1.913720
C	-4.643590	-0.771911	1.717475
H	-5.097119	0.209199	1.871559
H	-4.236527	-1.111255	2.675695
H	-5.423316	-1.477739	1.407885
O	-2.785983	0.524510	-1.186452
O	-2.575679	0.317692	1.085729
P	1.474023	0.163202	-0.083340
C	1.704051	-0.433479	1.637091
C	2.953239	-0.784852	2.166693
H	3.848527	-0.692093	1.559177
C	3.049092	-1.252496	3.479493
H	4.020782	-1.521502	3.885042
C	1.902835	-1.371937	4.267706
H	1.980972	-1.734361	5.289191
C	0.872110	-1.323993	-0.979403
C	-0.009277	-1.140095	-2.055557
H	-0.338506	-0.140189	-2.322180
C	-0.513628	-2.241941	-2.747988
H	-1.203236	-2.087065	-3.572779
C	-0.152873	-3.535234	-2.363305
H	-0.555541	-4.393177	-2.894858
C	0.713648	-3.726101	-1.283450
H	0.985522	-4.731482	-0.973523
C	1.223424	-2.626557	-0.591853
H	1.877729	-2.780618	0.261668
C	3.155216	0.501720	-0.725322
C	3.987898	-0.488034	-1.269344
H	3.633635	-1.511316	-1.352046
C	5.268014	-0.156935	-1.715545
H	5.907145	-0.926960	-2.139134
C	5.725851	1.160074	-1.621929
H	6.722325	1.414486	-1.972617
C	4.898983	2.151095	-1.087785
H	5.247450	3.178044	-1.023321
C	3.615875	1.825304	-0.647215
H	2.963615	2.598328	-0.246563
C	0.656199	-1.018285	3.743586
H	-0.237840	-1.102720	4.355363
C	0.551272	-0.546247	2.435725
H	-0.422085	-0.268761	2.036769
C	-1.672849	3.332488	0.064951
O	-0.547014	3.822399	0.028792
O	-2.846649	3.536925	0.145582

7
B3LYP-D3 SCF energy: -1832.40946322 a.u.
B3LYP-D3 enthalpy: -1831.903745 a.u.
B3LYP-D3 free energy: -1832.005245 a.u.
wB97XD SCF energy in solution: -1833.54325583 a.u.
wB97XD enthalpy in solution: -1833.037538 a.u.
wB97XD free energy in solution: -1833.139038 a.u.
Three lowest frequencies (cm-1): 11.1715 15.1699 18.7736

Cartesian coordinates

ATOM	X	Y	Z
Cu	-0.074323	0.159739	-0.739162
B	3.952613	0.030322	-0.125220
C	6.081537	-0.763844	-0.133540
C	6.326456	-1.403689	1.238518
H	7.365667	-1.279994	1.561044
H	6.105131	-2.473313	1.174152
H	5.668236	-0.966986	1.995994
C	6.086421	0.809322	-0.093662
C	6.348690	1.447284	-1.463487
H	7.389937	1.316114	-1.776374
H	6.134446	2.518474	-1.401220
H	5.694377	1.015357	-2.227053
C	6.995470	1.427762	0.964236
H	6.914364	2.518692	0.925720
H	8.041450	1.155153	0.781952
H	6.717576	1.104845	1.969803
C	6.996297	-1.388105	-1.183021
H	6.728765	-1.064286	-2.191103
H	6.909039	-2.478570	-1.144526
H	8.042114	-1.120935	-0.991965
O	4.704599	1.113832	0.248535
O	4.700734	-1.059285	-0.488886
P	-2.204168	0.029278	-0.127035
C	-2.402560	-1.139156	1.271898
C	-3.609891	-1.805233	1.535636
H	-4.463873	-1.668266	0.878089
C	-3.710164	-2.659323	2.634103
H	-4.646069	-3.174497	2.833374
C	-2.607607	-2.857688	3.469929
H	-2.687412	-3.526781	4.322592
C	-2.880405	1.629305	0.460177
C	-2.387215	2.800706	-0.134849
H	-1.604897	2.731594	-0.887640
C	-2.884208	4.047314	0.245431
H	-2.494374	4.948548	-0.219267
C	-3.870090	4.134253	1.231204
H	-4.252347	5.105416	1.533418
C	-4.354681	2.973152	1.838420
H	-5.112445	3.039573	2.614390
C	-3.862304	1.723880	1.457633
H	-4.230608	0.825892	1.944763
C	-3.377147	-0.550050	-1.411873

C	-4.724393	-0.161562	-1.452224
H	-5.108549	0.545766	-0.722882
C	-5.570760	-0.672482	-2.437937
H	-6.612668	-0.365116	-2.465494
C	-5.080037	-1.570868	-3.388359
H	-5.740756	-1.964623	-4.155848
C	-3.736795	-1.954016	-3.358908
H	-3.348588	-2.643698	-4.103147
C	-2.887118	-1.441380	-2.378912
H	-1.836919	-1.725114	-2.363538
C	-1.401280	-2.207421	3.201928
H	-0.537669	-2.370918	3.840303
C	-1.290188	-1.352106	2.103970
H	-0.339263	-0.869975	1.884856
C	2.364407	0.031189	-0.113072
O	1.773876	0.248899	-1.247270
O	1.743986	-0.170826	0.954809

TS6
B3LYP-D3 SCF energy: -1832.37990163 a.u.
B3LYP-D3 enthalpy: -1831.877295 a.u.
B3LYP-D3 free energy: -1831.975530 a.u.
wB97XD SCF energy in solution: -1833.50658174 a.u.
wB97XD enthalpy in solution: -1833.003975 a.u.
wB97XD free energy in solution: -1833.102210 a.u.
Three lowest frequencies (cm-1): -218.2912 8.7296 15.5259
Imaginary frequency: -218.2912 cm-1

Cartesian coordinates

ATOM	X	Y	Z
Cu	0.290381	-0.886272	0.860280
B	3.142777	-1.212411	0.541288
C	3.979482	0.496767	-0.764354
C	4.906912	-0.217097	-1.759310
H	5.769340	0.401772	-2.031216
H	4.340422	-0.443504	-2.668488
H	5.270076	-1.159955	-1.339999
C	4.585111	0.566233	0.681878
C	3.847570	1.580625	1.572947
H	4.091622	2.616458	1.310068
H	4.137587	1.406549	2.613558
H	2.763633	1.443242	1.495682
C	6.091231	0.811886	0.738343
H	6.420996	0.842676	1.782129
H	6.351393	1.768291	0.268629
H	6.639813	0.011139	0.237136
C	3.533693	1.839209	-1.338527
H	2.754274	2.298203	-0.726420
H	3.134902	1.694342	-2.349327
H	4.380652	2.531934	-1.405488
O	4.311931	-0.750559	1.185101
O	2.823815	-0.338576	-0.557173
P	-1.600806	-0.019208	0.107975
C	-1.323293	1.547390	-0.797674

C	-2.301967	2.549079	-0.888977
H	-3.252899	2.430388	-0.377509
C	-2.048567	3.707132	-1.624853
H	-2.808144	4.481307	-1.690750
C	-0.819602	3.872312	-2.268727
H	-0.623113	4.776130	-2.838969
C	-2.443340	-1.136022	-1.074193
C	-2.258064	-2.518215	-0.914518
H	-1.604270	-2.888813	-0.127904
C	-2.896319	-3.416048	-1.770386
H	-2.743326	-4.483691	-1.642377
C	-3.715721	-2.939551	-2.796258
H	-4.206747	-3.638358	-3.467807
C	-3.893224	-1.564333	-2.968543
H	-4.520550	-1.192521	-3.774001
C	-3.258479	-0.662624	-2.113396
H	-3.384461	0.405744	-2.262467
C	-2.835969	0.367840	1.403930
C	-4.219603	0.320459	1.178055
H	-4.603484	0.008467	0.211110
C	-5.105906	0.659739	2.201704
H	-6.176741	0.617592	2.022652
C	-4.619577	1.045426	3.453244
H	-5.312715	1.304894	4.248618
C	-3.242665	1.085690	3.686137
H	-2.860995	1.373531	4.661555
C	-2.353883	0.742763	2.667632
H	-1.281656	0.756381	2.851855
C	0.161244	2.883095	-2.168620
H	1.123427	3.016796	-2.653022
C	-0.082005	1.723266	-1.431325
H	0.695606	0.967238	-1.336129
C	2.690113	-2.743812	0.518782
O	1.924548	-1.658397	1.349693
O	2.329640	-3.865147	0.419474

LCu-OBpin

B3LYP-D3 SCF energy: -1719.10989909 a.u.
B3LYP-D3 enthalpy: -1718.615710 a.u.
B3LYP-D3 free energy: -1718.710321 a.u.
wB97XD SCF energy in solution: -1720.24333766 a.u.
wB97XD enthalpy in solution: -1719.749149 a.u.
wB97XD free energy in solution: -1719.843760 a.u.
Three lowest frequencies (cm-1): 9.3188 15.8627 30.1940

Cartesian coordinates

ATOM	X	Y	Z
B	-2.953045	0.301558	-1.381163
C	-4.100859	-0.367418	0.511699
C	-4.145345	-1.901149	0.445548
H	-5.068580	-2.305684	0.874690
H	-3.295107	-2.303202	1.006634
H	-4.061274	-2.242940	-0.590811
C	-5.080181	0.315545	-0.514738

C	-5.375870	1.780715	-0.159244
H	-6.026575	1.868561	0.718109
H	-5.872228	2.254997	-1.011396
H	-4.446404	2.325220	0.037124
C	-6.385151	-0.439849	-0.757607
H	-6.997157	0.106619	-1.482711
H	-6.959902	-0.538057	0.171174
H	-6.196981	-1.436750	-1.162695
C	-4.247631	0.100975	1.958585
H	-4.047012	1.171159	2.050419
H	-3.533767	-0.434831	2.595344
H	-5.256327	-0.102153	2.336597
O	-4.307503	0.316247	-1.727293
O	-2.817881	0.045910	0.012656
P	1.539754	0.047285	-0.201297
C	2.097227	-1.696548	-0.101440
C	2.729294	-2.233194	1.030149
H	2.877007	-1.618846	1.913439
C	3.152639	-3.563196	1.029748
H	3.638347	-3.974087	1.910644
C	2.945896	-4.365999	-0.094841
H	3.272664	-5.402234	-0.089808
C	3.013882	1.004804	-0.720292
C	2.791384	2.221301	-1.383893
H	1.772414	2.535599	-1.599583
C	3.868060	3.018413	-1.772189
H	3.686463	3.958242	-2.285896
C	5.175423	2.601342	-1.510161
H	6.014788	3.218517	-1.818600
C	5.404082	1.385151	-0.861939
H	6.420590	1.054419	-0.666849
C	4.328946	0.586690	-0.468020
H	4.512993	-0.364141	0.023782
C	1.204527	0.559160	1.528334
C	2.214278	1.006708	2.394571
H	3.237286	1.097385	2.040330
C	1.902633	1.354674	3.709544
H	2.687600	1.703080	4.375413
C	0.584521	1.264304	4.165272
H	0.344512	1.541546	5.188294
C	-0.424295	0.831656	3.301911
H	-1.453991	0.775835	3.644420
C	-0.122315	0.482226	1.984763
H	-0.922283	0.171221	1.315591
C	2.307085	-3.840363	-1.220420
H	2.132025	-4.465118	-2.091703
C	1.879106	-2.512736	-1.222119
H	1.361946	-2.106499	-2.088738
Cu	-0.275613	0.307951	-1.437278
O	-1.932539	0.488497	-2.203641

TS7
B3LYP-D3 SCF energy: -2518.12202499 a.u.
B3LYP-D3 enthalpy: -2517.243058 a.u.

B3LYP-D3 free energy: -2517.375647 a.u.
wB97XD SCF energy in solution: -2519.17950463 a.u.
wB97XD enthalpy in solution: -2518.300538 a.u.
wB97XD free energy in solution: -2518.433127 a.u.
Three lowest frequencies (cm-1): -270.6300 18.4888 21.2869
Imaginary frequency: -270.6300 cm-1

Cartesian coordinates

ATOM	X	Y	Z
C	1.094122	-3.367914	0.229522
C	0.337163	-2.769687	-0.782077
C	0.590338	-3.049547	-2.131843
C	1.624057	-3.946912	-2.441063
C	2.389952	-4.538322	-1.434442
C	2.127103	-4.248579	-0.092432
H	0.875338	-3.134473	1.265821
H	-0.468498	-2.094246	-0.516110
H	1.830829	-4.180500	-3.483837
H	3.187248	-5.229373	-1.697663
H	2.721338	-4.704040	0.695093
C	-0.184622	-2.362507	-3.250511
H	0.393165	-1.483417	-3.568784
H	-0.200269	-3.033586	-4.120877
C	-1.591232	-1.946955	-2.902602
C	-1.994719	-0.691957	-2.630068
H	-2.326155	-2.750725	-2.867793
H	-3.046399	-0.551057	-2.382731
C	-1.173490	0.540898	-2.539480
H	-0.234880	0.438264	-3.125692
H	-1.672268	1.395599	-2.991171
B	-1.890240	1.424218	-0.697310
C	-1.993673	3.658504	-0.179164
C	-2.353544	3.635422	1.314503
H	-2.862159	2.703047	1.576642
H	-2.995319	4.478104	1.594799
H	-1.427104	3.690970	1.895018
C	-3.203634	3.272109	-1.107311
C	-3.002020	3.726419	-2.560476
H	-3.145227	4.807365	-2.668067
H	-3.732848	3.213747	-3.193661
H	-2.000733	3.473646	-2.919418
C	-4.567708	3.740446	-0.602318
H	-4.802908	3.291763	0.365243
H	-5.346067	3.438430	-1.310779
H	-4.596041	4.832357	-0.505259
C	-1.305133	4.974821	-0.529009
H	-0.880563	4.946371	-1.535707
H	-0.492864	5.164593	0.179282
H	-2.012129	5.810607	-0.470061
O	-3.182658	1.832927	-1.059845
O	-1.078193	2.567657	-0.420806
Cu	0.322594	0.541999	-1.086098
P	2.154882	0.604214	0.214164
C	1.987105	-0.449128	1.705947
C	3.053542	-1.179465	2.248980
H	4.037504	-1.129110	1.792043

C	2.842183	-1.996517	3.360919
H	3.669591	-2.566404	3.775525
C	1.568893	-2.093386	3.930240
H	1.406163	-2.742539	4.786707
C	3.712541	0.041721	-0.575647
C	4.941966	0.699188	-0.428163
H	5.009311	1.608596	0.160658
C	6.086766	0.187825	-1.044570
H	7.035000	0.706444	-0.930238
C	6.015236	-0.982595	-1.802831
H	6.908858	-1.377653	-2.278753
C	4.791780	-1.641291	-1.950946
H	4.721224	-2.554240	-2.535236
C	3.644451	-1.128759	-1.348443
H	2.698431	-1.644166	-1.471508
C	2.507301	2.281061	0.864293
C	3.266738	2.482121	2.027963
H	3.629282	1.627384	2.592398
C	3.548764	3.776039	2.466177
H	4.135639	3.924762	3.368605
C	3.074337	4.877227	1.747766
H	3.295259	5.884778	2.089907
C	2.305764	4.682098	0.598525
H	1.922969	5.535772	0.046411
C	2.012950	3.388895	0.161037
H	1.371473	3.234929	-0.700965
C	0.504026	-1.369679	3.387279
H	-0.497600	-1.464269	3.794767
C	0.710661	-0.548700	2.278966
H	-0.126566	-0.023386	1.832515
O	-1.761838	0.342262	0.232288
B	-2.604252	-0.660896	0.558443
O	-2.198324	-1.640474	1.451362
O	-3.895308	-0.837973	0.115143
C	-3.221758	-2.667946	1.447971
C	-4.486335	-1.876480	0.933759
C	-2.765666	-3.760924	0.475343
C	-3.339078	-3.232777	2.860882
C	-5.250363	-1.166373	2.058730
C	-5.446420	-2.687054	0.068124
H	-3.468998	-4.600025	0.457049
H	-1.784748	-4.131712	0.785713
H	-2.661270	-3.363124	-0.537968
H	-3.524470	-2.444404	3.594255
H	-2.403797	-3.734355	3.130767
H	-4.150436	-3.966924	2.921056
H	-4.567390	-0.584920	2.686847
H	-5.792499	-1.874875	2.693985
H	-5.969923	-0.473964	1.611739
H	-4.950986	-3.059787	-0.830945
H	-6.282146	-2.053398	-0.245483
H	-5.850846	-3.537863	0.628268

8a
B3LYP-D3 SCF energy: -1620.19728205 a.u.
B3LYP-D3 enthalpy: -1619.711916 a.u.
B3LYP-D3 free energy: -1619.802286 a.u.
wB97XD SCF energy in solution: -1621.30938814 a.u.
wB97XD enthalpy in solution: -1620.824022 a.u.
wB97XD free energy in solution: -1620.914392 a.u.
Three lowest frequencies (cm-1): 16.0207 24.3072 29.1585

Cartesian coordinates

ATOM	X	Y	Z
C	2.302977	-1.870322	-0.915787
C	2.811445	-0.606085	-1.228255
C	3.769260	0.009138	-0.406275
C	4.208240	-0.686284	0.729000
C	3.705152	-1.949532	1.042030
C	2.745507	-2.546031	0.221866
H	1.560383	-2.330389	-1.561453
H	2.473647	-0.089055	-2.123197
H	4.955818	-0.227802	1.373398
H	4.058307	-2.467155	1.930328
H	2.343169	-3.524232	0.469385
C	4.290954	1.403375	-0.711720
H	5.357385	1.450363	-0.452390
H	4.221551	1.586530	-1.790922
C	3.535217	2.476307	0.044712
C	2.455560	3.135797	-0.433035
H	3.882244	2.688707	1.054966
H	1.997612	3.866096	0.239004
C	1.752629	2.957128	-1.722175
H	1.291260	3.884814	-2.077558
H	2.377047	2.533212	-2.518151
P	-0.993392	0.181669	-0.113887
C	-0.196136	-0.643779	1.315695
C	-0.615712	-1.883308	1.821546
H	-1.412468	-2.431834	1.328189
C	-0.000268	-2.423176	2.951275
H	-0.328382	-3.384988	3.336562
C	1.036686	-1.731258	3.582163
H	1.516825	-2.154847	4.460262
C	-2.482856	1.000840	0.582175
C	-3.020721	2.074159	-0.146149
H	-2.526095	2.403744	-1.057418
C	-4.172287	2.722620	0.299571
H	-4.580347	3.552010	-0.271494
C	-4.789759	2.313852	1.484332
H	-5.682798	2.823188	1.836172
C	-4.250725	1.257819	2.222598
H	-4.722485	0.945112	3.150320
C	-3.101322	0.602539	1.776384
H	-2.680548	-0.208979	2.362601
C	-1.673231	-1.153064	-1.173989
C	-2.851167	-1.852139	-0.869439
H	-3.425669	-1.587105	0.013797
C	-3.297941	-2.873872	-1.708429
H	-4.210620	-3.411216	-1.465245

C	-2.579566	-3.199705	-2.862048
H	-2.931395	-3.993996	-3.514724
C	-1.418779	-2.492913	-3.184106
H	-0.866952	-2.730667	-4.089312
C	-0.971322	-1.469938	-2.346997
H	-0.079575	-0.903225	-2.602528
C	1.470304	-0.507303	3.070338
H	2.298356	0.018651	3.536079
C	0.863901	0.033729	1.937095
H	1.238591	0.964560	1.517208
Cu	0.400682	1.634893	-1.158959

8b

B3LYP-D3 SCF energy: -1620.18595334 a.u.
B3LYP-D3 enthalpy: -1619.701298 a.u.
B3LYP-D3 free energy: -1619.796813 a.u.
wB97XD SCF energy in solution: -1621.30122353 a.u.
wB97XD enthalpy in solution: -1620.816568 a.u.
wB97XD free energy in solution: -1620.912083 a.u.
Three lowest frequencies (cm-1): 7.2439 15.3857 19.1153

Cartesian coordinates

ATOM	X	Y	Z
C	4.033241	-1.600914	-1.259379
C	4.135079	-0.258279	-0.888026
C	3.674173	0.183623	0.360328
C	3.121302	-0.767791	1.231625
C	3.013774	-2.111266	0.865767
C	3.466892	-2.532955	-0.386000
H	4.398371	-1.920687	-2.232751
H	4.571799	0.463223	-1.574971
H	2.769853	-0.441322	2.208626
H	2.577266	-2.828313	1.557058
H	3.377616	-3.575568	-0.678045
C	3.690226	1.654338	0.717519
H	3.556232	1.759823	1.802445
H	4.681311	2.078555	0.483663
C	2.567200	2.434069	-0.007636
C	2.313747	3.782241	0.550128
H	2.815892	2.507214	-1.078597
H	2.273172	3.826749	1.643601
C	2.093044	4.922811	-0.127112
H	1.858055	5.854885	0.380158
H	2.124460	4.951518	-1.215595
P	-0.949978	0.052689	-0.030712
C	-0.654064	-1.501526	-0.955944
C	0.426224	-1.538766	-1.848666
H	1.079896	-0.675366	-1.940790
C	0.690025	-2.695213	-2.584017
H	1.537509	-2.717079	-3.262770
C	-0.115721	-3.823591	-2.425712
H	0.093110	-4.725636	-2.994686
C	-1.564498	-0.528731	1.598010
C	-2.908621	-0.473970	1.988857

H	-3.655942	-0.067263	1.314229
C	-3.290125	-0.940973	3.249621
H	-4.334304	-0.893164	3.546941
C	-2.336799	-1.465740	4.123556
H	-2.636823	-1.826654	5.103548
C	-0.993918	-1.521853	3.737800
H	-0.247582	-1.926231	4.416276
C	-0.607362	-1.050627	2.484730
H	0.436772	-1.090527	2.184632
C	-2.381759	0.871907	-0.829969
C	-2.441882	2.272371	-0.747215
H	-1.637714	2.816067	-0.255651
C	-3.518126	2.965610	-1.302312
H	-3.554554	4.049209	-1.233905
C	-4.536407	2.266879	-1.954401
H	-5.371390	2.806387	-2.393140
C	-4.475873	0.874138	-2.053082
H	-5.262290	0.329865	-2.569039
C	-3.403902	0.177071	-1.494255
H	-3.357146	-0.903949	-1.584902
C	-1.180812	-3.801165	-1.519720
H	-1.798372	-4.684754	-1.382406
C	-1.447710	-2.647628	-0.783143
H	-2.260871	-2.640890	-0.062227
Cu	0.896940	1.373074	0.063133

$(Bpin)_2O$

B3LYP-D3 SCF energy: -897.91417901 a.u.
B3LYP-D3 enthalpy: -897.521211 a.u.
B3LYP-D3 free energy: -897.591117 a.u.
wB97XD SCF energy in solution: -897.88660980 a.u.
wB97XD enthalpy in solution: -897.493642 a.u.
wB97XD free energy in solution: -897.563548 a.u.
Three lowest frequencies (cm-1): 20.7377 21.6505 27.8022

Cartesian coordinates

ATOM	X	Y	Z
C	-3.444121	-0.518188	0.217215
C	-4.120011	-1.287055	-0.924421
H	-5.029244	-0.782991	-1.267863
H	-4.387791	-2.286071	-0.567643
H	-3.440257	-1.401736	-1.774789
C	-2.753749	0.817482	-0.261091
C	-2.504498	1.810969	0.880459
H	-3.435231	2.271853	1.227189
H	-1.835835	2.598436	0.520136
H	-2.017696	1.319004	1.728332
C	-3.438556	1.512807	-1.433242
H	-2.884326	2.418576	-1.699341
H	-4.461039	1.803078	-1.166162
H	-3.475108	0.868715	-2.314427
C	-4.401184	-0.362264	1.394835
H	-3.890975	0.036268	2.274414
H	-4.820145	-1.337881	1.660802

H	-5.229282	0.306619	1.133961
O	-1.449494	0.348157	-0.693267
O	-2.308588	-1.317525	0.646192
B	1.209777	-0.820541	0.006928
C	3.444123	-0.518205	-0.217341
C	4.120363	-1.286967	0.924129
H	5.029706	-0.782872	1.267236
H	4.388030	-2.285993	0.567302
H	3.440857	-1.401589	1.774699
C	2.753792	0.817437	0.261108
C	2.504296	1.810969	-0.880334
H	3.434952	2.271800	-1.227331
H	1.835817	2.598490	-0.519771
H	2.017131	1.319133	-1.728072
C	3.438794	1.512743	1.433169
H	2.884258	2.418212	1.699627
H	4.461047	1.803491	1.165714
H	3.476013	0.868531	2.314240
C	4.400786	-0.362155	-1.395279
H	3.890103	0.036106	-2.274703
H	4.819999	-1.337645	-1.661294
H	5.228757	0.307045	-1.134802
O	1.449620	0.348095	0.693516
O	2.308469	-1.317717	-0.645953
B	-1.209754	-0.820482	-0.006592
O	-0.000016	-1.449622	0.000216

TS8

B3LYP-D3 SCF energy: -1808.76983593 a.u.
B3LYP-D3 enthalpy: -1808.269251 a.u.
B3LYP-D3 free energy: -1808.372602 a.u.
wB97XD SCF energy in solution: -1809.87361000 a.u.
wB97XD enthalpy in solution: -1809.373025 a.u.
wB97XD free energy in solution: -1809.476376 a.u.
Three lowest frequencies (cm-1): -223.1149 3.0384 8.9858
Imaginary frequency: -223.1149 cm-1

Cartesian coordinates

ATOM	X	Y	Z
C	6.649557	0.902658	-0.299136
C	5.733889	-0.133774	-0.118571
C	4.436239	0.124340	0.344035
C	4.080751	1.451180	0.615359
C	4.992155	2.494431	0.434788
C	6.282375	2.222792	-0.022567
H	7.651287	0.681000	-0.658947
H	6.021002	-1.157107	-0.347587
H	3.073900	1.670302	0.967109
H	4.691834	3.517618	0.647101
H	6.994481	3.031078	-0.166699
C	3.443340	-1.007328	0.563736
H	3.731000	-1.564045	1.466170
H	2.457874	-0.570296	0.780115
C	3.287180	-1.982236	-0.584933

C	2.754548	-1.588751	-1.805001
H	3.871346	-2.895970	-0.557682
H	2.707888	-2.360790	-2.576190
C	2.157881	-0.324555	-2.113632
H	2.621807	0.541723	-1.632619
H	1.965237	-0.153061	-3.174821
P	-1.581246	0.188433	-0.153670
C	-2.255081	1.797283	-0.721140
C	-3.079354	2.604456	0.078121
H	-3.324435	2.295260	1.090247
C	-3.574279	3.810256	-0.419949
H	-4.209142	4.432159	0.205376
C	-3.250007	4.220366	-1.716103
H	-3.633715	5.161929	-2.099501
C	-2.959155	-1.011468	-0.330870
C	-2.641915	-2.374803	-0.204654
H	-1.613565	-2.672441	-0.018574
C	-3.644778	-3.338072	-0.308202
H	-3.391686	-4.389816	-0.206488
C	-4.966522	-2.953488	-0.550241
H	-5.745207	-3.706370	-0.637995
C	-5.284241	-1.600787	-0.685356
H	-6.309918	-1.297754	-0.878236
C	-4.286032	-0.629901	-0.575336
H	-4.541578	0.419485	-0.684175
C	-1.367008	0.380066	1.657793
C	-2.387660	0.109135	2.580357
H	-3.351529	-0.251405	2.232286
C	-2.161363	0.288349	3.946335
H	-2.955445	0.074115	4.656559
C	-0.917503	0.733751	4.400199
H	-0.743141	0.866177	5.464488
C	0.105890	0.997440	3.486204
H	1.079428	1.330902	3.834710
C	-0.116945	0.817272	2.121806
H	0.683360	1.003726	1.409809
C	-2.424004	3.425641	-2.513998
H	-2.160715	3.746652	-3.518009
C	-1.923937	2.221371	-2.016774
H	-1.263421	1.608086	-2.625941
Cu	0.381173	-0.373319	-1.145485
C	1.462155	-3.134980	-0.017130
O	1.764782	-4.274989	-0.165439
O	0.670301	-2.285670	0.315783

TS9
B3LYP-D3 SCF energy: -1808.77685627 a.u.
B3LYP-D3 enthalpy: -1808.276305 a.u.
B3LYP-D3 free energy: -1808.375132 a.u.
wB97XD SCF energy in solution: -1809.87571429 a.u.
wB97XD enthalpy in solution: -1809.375163 a.u.
wB97XD free energy in solution: -1809.473990 a.u.
Three lowest frequencies (cm-1): -247.5482 19.1983 23.8841
Imaginary frequency: -247.5482 cm-1

Cartesian coordinates

ATOM	X	Y	Z
C	2.614419	-3.712157	-0.378838
C	3.299913	-2.549942	-0.746474
C	3.153891	-1.366482	-0.011583
C	2.301342	-1.380842	1.104748
C	1.611136	-2.536030	1.475731
C	1.766150	-3.708608	0.731645
H	2.744366	-4.621626	-0.960719
H	3.956326	-2.558730	-1.613948
H	2.173131	-0.468791	1.683328
H	0.948349	-2.513162	2.336121
H	1.228709	-4.610235	1.012779
C	3.820685	-0.075342	-0.443208
H	3.972864	0.547648	0.445280
H	4.821006	-0.289716	-0.852488
C	2.966995	0.696172	-1.458478
C	3.195963	2.103880	-1.644862
H	2.833553	0.148724	-2.397900
H	2.730995	2.519680	-2.542968
C	3.812960	3.001067	-0.806427
H	3.930021	4.036195	-1.105645
H	4.441265	2.667859	0.016024
P	-1.017550	0.136682	-0.146259
C	-1.191606	-0.444364	1.587411
C	-1.927880	-1.584808	1.936932
H	-2.444084	-2.154762	1.170610
C	-1.979285	-2.005129	3.267810
H	-2.547032	-2.893888	3.530105
C	-1.296669	-1.292572	4.256172
H	-1.330974	-1.626505	5.289648
C	-2.329437	1.397142	-0.358835
C	-2.110770	2.406553	-1.308804
H	-1.175751	2.422789	-1.865032
C	-3.078291	3.386601	-1.530896
H	-2.899806	4.165919	-2.266528
C	-4.267464	3.371290	-0.797796
H	-5.018292	4.138814	-0.964662
C	-4.486735	2.376200	0.158343
H	-5.407235	2.369057	0.735819
C	-3.522245	1.391979	0.379756
H	-3.689729	0.627001	1.132817
C	-1.535186	-1.302128	-1.159556
C	-2.861213	-1.541838	-1.547806
H	-3.642825	-0.835656	-1.282865
C	-3.177636	-2.686150	-2.283007
H	-4.205914	-2.864511	-2.586135
C	-2.176765	-3.597824	-2.628785
H	-2.427279	-4.487637	-3.200253
C	-0.854178	-3.360613	-2.246264
H	-0.069089	-4.062874	-2.512223
C	-0.530533	-2.213946	-1.522148
H	0.500483	-2.027616	-1.236011
C	-0.564208	-0.152502	3.912569
H	-0.026645	0.401781	4.676998

C	-0.507217	0.269436	2.584470
H	0.082964	1.140788	2.315006
Cu	1.086857	0.753832	-0.689358
C	2.086794	3.493078	0.790859
O	1.583097	2.427473	0.990055
O	2.275331	4.650699	0.928952

9
B3LYP-D3 SCF energy: -1808.80851419 a.u.
B3LYP-D3 enthalpy: -1808.304557 a.u.
B3LYP-D3 free energy: -1808.402298 a.u.
wB97XD SCF energy in solution: -1809.92337979 a.u.
wB97XD enthalpy in solution: -1809.419423 a.u.
wB97XD free energy in solution: -1809.517164 a.u.
Three lowest frequencies (cm-1): 16.3383 29.0681 34.1164

Cartesian coordinates

ATOM	X	Y	Z
C	1.279043	3.057057	0.308090
C	2.331723	3.242754	-0.591423
C	3.444967	2.400520	-0.555263
C	3.530349	1.360139	0.378888
C	2.473541	1.191906	1.284342
C	1.356741	2.028466	1.250101
H	0.403618	3.698689	0.272563
H	2.283113	4.041350	-1.327662
H	4.251551	2.540585	-1.271817
H	2.518638	0.376251	1.999142
H	0.542790	1.870036	1.952232
C	4.668518	0.363572	0.345382
H	4.696229	-0.202016	1.281606
H	5.634298	0.873195	0.234421
C	4.514406	-0.668772	-0.822160
H	4.655727	-0.130151	-1.765871
C	5.568354	-1.744845	-0.710891
C	5.387966	-3.005604	-0.314336
H	6.575056	-1.407526	-0.966118
H	6.223881	-3.698773	-0.258399
H	4.408229	-3.375677	-0.029821
C	3.060887	-1.149321	-0.796772
O	2.617356	-1.762068	0.193074
O	2.344010	-0.750921	-1.798407
P	-1.378344	-0.252375	-0.163614
C	-1.372423	-0.798092	1.584781
C	-2.549232	-0.850215	2.350702
H	-3.503246	-0.585994	1.902436
C	-2.499210	-1.254668	3.683803
H	-3.412128	-1.291342	4.272033
C	-1.277762	-1.621501	4.257944
H	-1.241503	-1.940129	5.296269
C	-1.837088	1.525283	-0.173380
C	-1.724293	2.198747	-1.400369
H	-1.374741	1.661987	-2.279230
C	-2.034271	3.553808	-1.493262

H	-1.941774	4.064374	-2.447671
C	-2.442075	4.256953	-0.355599
H	-2.671914	5.316652	-0.423785
C	-2.542424	3.596602	0.870160
H	-2.849347	4.140768	1.759134
C	-2.245375	2.234109	0.963127
H	-2.317610	1.733188	1.922954
C	-2.818883	-1.098492	-0.919237
C	-4.115037	-0.563179	-0.895390
H	-4.291679	0.413528	-0.453577
C	-5.176251	-1.277087	-1.454355
H	-6.177938	-0.856261	-1.436155
C	-4.951464	-2.525659	-2.039446
H	-5.779241	-3.077684	-2.476076
C	-3.660883	-3.059831	-2.072577
H	-3.480844	-4.025998	-2.535559
C	-2.596911	-2.346863	-1.520092
H	-1.588146	-2.752798	-1.556866
C	-0.110244	-1.594445	3.493784
H	0.837187	-1.898597	3.929597
C	-0.151029	-1.187575	2.157943
H	0.758943	-1.201415	1.562594
Cu	0.577767	-0.619976	-1.129188

s-TS1

B3LYP-D3 SCF energy: -2219.48918298 a.u.
B3LYP-D3 enthalpy: -2218.805425 a.u.
B3LYP-D3 free energy: -2218.924433 a.u.
wB97XD SCF energy in solution: -2220.56750501 a.u.
wB97XD enthalpy in solution: -2219.883747 a.u.
wB97XD free energy in solution: -2220.002755 a.u.
Three lowest frequencies (cm-1): -282.1590 10.1694 18.4122
Imaginary frequency: -282.1590 cm-1

Cartesian coordinates

ATOM	X	Y	Z
C	4.616290	-1.528877	1.750598
C	3.737809	-1.197604	0.721093
C	3.669011	-1.959689	-0.466095
C	4.516874	-3.081181	-0.550865
C	5.391653	-3.417295	0.480105
C	5.452444	-2.643371	1.641294
H	4.646952	-0.910081	2.645279
H	3.093376	-0.332539	0.851590
H	4.476869	-3.700943	-1.443158
H	6.029700	-4.291620	0.375392
H	6.134941	-2.903771	2.445639
C	2.742913	-1.661764	-1.568094
C	2.168645	-0.390009	-1.719198
H	2.879382	-2.253495	-2.473683
H	2.338868	0.295457	-0.890399
C	1.348163	0.136957	-2.740486
C	1.252031	1.663501	-2.917972
H	1.292955	-0.443234	-3.666914

H	0.285739	1.930361	-3.370210
H	2.017619	2.012226	-3.628458
Cu	-0.317495	-0.441193	-1.653675
B	1.432867	2.466061	-1.572041
C	1.111619	3.155849	0.593788
C	-0.073389	4.124525	0.625238
H	0.077782	4.915638	1.367083
H	-0.978996	3.573835	0.884098
H	-0.227459	4.587971	-0.354042
C	2.423839	3.793836	0.001377
C	3.706099	3.083199	0.454019
H	3.919036	3.274645	1.510874
H	4.545177	3.452395	-0.142949
H	3.642406	2.001165	0.303409
C	2.559525	5.300427	0.203888
H	3.487535	5.649459	-0.259608
H	2.596295	5.546855	1.271147
H	1.729613	5.843353	-0.253360
C	1.271115	2.476562	1.950735
H	2.018300	1.680738	1.919084
H	0.319389	2.027230	2.249785
H	1.566709	3.204145	2.715037
O	2.285188	3.530301	-1.423349
O	0.796819	2.131923	-0.393684
P	-1.941748	-0.368380	-0.085494
C	-2.643368	1.297625	0.222518
C	-3.068655	1.739399	1.483568
H	-2.944206	1.100764	2.352999
C	-3.646154	3.003539	1.625822
H	-3.969639	3.340564	2.606938
C	-3.805474	3.832497	0.512778
H	-4.254231	4.815406	0.626699
C	-3.410041	-1.437491	-0.355313
C	-3.192444	-2.678351	-0.977064
H	-2.189738	-2.953023	-1.293968
C	-4.258805	-3.553755	-1.182066
H	-4.081806	-4.512851	-1.661039
C	-5.548833	-3.196038	-0.781415
H	-6.379243	-3.876900	-0.947971
C	-5.771101	-1.959168	-0.172519
H	-6.774005	-1.674823	0.134855
C	-4.706998	-1.080601	0.041803
H	-4.889418	-0.117932	0.509984
C	-1.248954	-0.952204	1.511524
C	-2.048446	-1.467071	2.544086
H	-3.126639	-1.521553	2.420945
C	-1.457506	-1.936602	3.717837
H	-2.081839	-2.335618	4.512805
C	-0.067182	-1.916095	3.862346
H	0.389411	-2.302565	4.769454
C	0.735978	-1.419736	2.833583
H	1.818584	-1.432689	2.917803
C	0.146130	-0.935005	1.666320
H	0.771882	-0.553548	0.865876
C	-3.372196	3.402379	-0.744159
H	-3.477557	4.050884	-1.609432

C	-2.785159	2.145651	-0.886011
H	-2.420796	1.818327	-1.856998
C	1.054608	-3.162627	-1.159113
O	1.589166	-4.023750	-0.544352
O	0.089584	-2.701310	-1.719751

s-TS2

B3LYP-D3 SCF energy: -2219.46775995 a.u.
B3LYP-D3 enthalpy: -2218.784101 a.u.
B3LYP-D3 free energy: -2218.903241 a.u.
wB97XD SCF energy in solution: -2220.55636311 a.u.
wB97XD enthalpy in solution: -2219.872704 a.u.
wB97XD free energy in solution: -2219.991844 a.u.
Three lowest frequencies (cm-1): -194.2549 12.7136 23.3492
Imaginary frequency: -194.2549 cm-1

Cartesian coordinates

ATOM	X	Y	Z
C	1.704981	3.597865	-1.968902
C	1.659082	2.600940	-1.000772
C	1.698571	2.914937	0.376131
C	1.799436	4.277112	0.724645
C	1.842547	5.276803	-0.246418
C	1.793893	4.945564	-1.602033
H	1.663183	3.322870	-3.020048
H	1.572659	1.565971	-1.318799
H	1.834047	4.547299	1.777838
H	1.915458	6.318191	0.058071
H	1.828819	5.722005	-2.361517
C	1.624733	1.910016	1.434633
C	1.397116	0.587412	1.245796
H	1.723442	2.275598	2.455113
H	1.281546	0.236495	0.221678
C	1.245155	-0.434535	2.291648
C	1.540318	-1.917386	1.898700
H	1.804343	-0.179093	3.188728
H	0.712999	-2.411669	1.353286
H	1.678723	-2.494829	2.815940
Cu	-0.784706	-0.790566	1.634254
B	2.794321	-1.898312	0.954271
C	3.976074	-1.742528	-1.005136
C	4.241526	-3.148804	-1.553377
H	5.209642	-3.208718	-2.060829
H	3.457076	-3.405634	-2.272667
H	4.219056	-3.892033	-0.750593
C	4.887280	-1.366206	0.226880
C	5.054439	0.146100	0.420101
H	5.677900	0.584292	-0.366233
H	5.536994	0.324802	1.385714
H	4.087728	0.657788	0.433846
C	6.246635	-2.059195	0.257027
H	6.795249	-1.748594	1.151506
H	6.840535	-1.782420	-0.621562
H	6.145780	-3.146510	0.284835

C	3.966151	-0.720033	-2.138578
H	3.640223	0.262867	-1.791414
H	3.275274	-1.048633	-2.922514
H	4.963420	-0.621980	-2.581874
O	4.100716	-1.842375	1.358701
O	2.648223	-1.775064	-0.412583
P	-2.118110	-0.460683	-0.112791
C	-3.897667	-0.738907	0.209375
C	-4.910200	-0.085050	-0.509673
H	-4.651021	0.641714	-1.274578
C	-6.250163	-0.352994	-0.228382
H	-7.030808	0.157678	-0.785600
C	-6.587822	-1.267453	0.773304
H	-7.632531	-1.469133	0.993657
C	-1.969080	1.283037	-0.653139
C	-2.126091	1.675405	-1.991569
H	-2.323659	0.931294	-2.758080
C	-2.006272	3.020455	-2.341216
H	-2.117254	3.319024	-3.380213
C	-1.727141	3.977855	-1.362883
H	-1.606668	5.020424	-1.641193
C	-1.566337	3.591040	-0.031826
H	-1.312050	4.327025	0.723443
C	-1.679543	2.247779	0.324623
H	-1.505912	1.947388	1.355280
C	-1.694812	-1.462989	-1.588331
C	-2.643761	-1.871513	-2.536838
H	-3.693471	-1.631562	-2.396016
C	-2.241816	-2.599071	-3.658983
H	-2.982622	-2.915380	-4.388377
C	-0.895380	-2.924622	-3.841381
H	-0.588140	-3.494217	-4.714345
C	0.051203	-2.526947	-2.894186
H	1.099450	-2.785585	-3.015178
C	-0.345006	-1.803241	-1.770466
H	0.405633	-1.516615	-1.041538
C	-5.584201	-1.909638	1.501874
H	-5.843451	-2.607444	2.292991
C	-4.242753	-1.642862	1.225232
H	-3.458280	-2.120942	1.807940
C	-0.382927	-0.047227	3.670438
O	-0.985648	-1.098576	3.889919
O	-0.255269	1.098488	4.008028

s-TS3
B3LYP-D3 SCF energy: -2219.48981379 a.u.
B3LYP-D3 enthalpy: -2218.806205 a.u.
B3LYP-D3 free energy: -2218.928435 a.u.
wB97XD SCF energy in solution: -2220.57073114 a.u.
wB97XD enthalpy in solution: -2219.887122 a.u.
wB97XD free energy in solution: -2220.009352 a.u.
Three lowest frequencies (cm-1): -209.2664 6.4581 12.4790
Imaginary frequency: -209.2664 cm-1

Cartesian coordinates

ATOM	X	Y	Z
C	-0.367364	3.214269	2.041565
C	0.132656	1.932791	1.821310
C	1.066160	1.672037	0.791596
C	1.468825	2.770541	0.000874
C	0.965376	4.052196	0.220926
C	0.040660	4.287616	1.243473
H	-1.099681	3.367328	2.830532
H	-0.242807	1.108319	2.421846
H	2.177371	2.600644	-0.807511
H	1.300279	4.873300	-0.409343
H	-0.356320	5.284746	1.412044
C	1.566550	0.312489	0.480847
C	1.815536	-0.645611	1.530836
H	2.275902	0.289589	-0.346943
H	1.469554	-0.385624	2.532228
C	2.404835	-1.883721	1.384795
C	2.987150	-2.349541	0.065156
H	2.690970	-2.421312	2.282573
H	2.224235	-2.261595	-0.724061
H	3.270840	-3.406975	0.135131
Cu	-0.156778	-0.482622	-0.283879
B	4.224761	-1.453532	-0.318079
C	5.533928	0.037151	-1.456805
C	6.383102	-0.740244	-2.469022
H	7.365002	-0.277120	-2.612046
H	5.861787	-0.756911	-3.431056
H	6.527928	-1.774944	-2.142888
C	6.034767	-0.119764	0.026746
C	5.541216	1.001972	0.950696
H	6.048267	1.949675	0.741243
H	5.745712	0.718041	1.987304
H	4.461160	1.149595	0.851728
C	7.538893	-0.318344	0.184607
H	7.784940	-0.432225	1.245071
H	8.086067	0.548805	-0.202632
H	7.882637	-1.213067	-0.339122
C	5.333768	1.476959	-1.922604
H	4.606104	2.001000	-1.298762
H	4.963861	1.482470	-2.953019
H	6.280673	2.028211	-1.895379
O	5.355257	-1.332065	0.454150
O	4.235583	-0.615848	-1.411745
P	-2.388761	-0.204224	-0.464363
C	-2.905967	1.341533	-1.299244
C	-2.013861	2.424545	-1.237098
H	-1.050838	2.311028	-0.749448
C	-2.366394	3.654652	-1.791765
H	-1.670623	4.485659	-1.722172
C	-3.599725	3.807381	-2.429507
H	-3.871199	4.763574	-2.869022
C	-3.427046	-1.549088	-1.138836
C	-2.849185	-2.418873	-2.074635
H	-1.806022	-2.289203	-2.352194
C	-3.601395	-3.455112	-2.629282

H	-3.145833	-4.127286	-3.351025
C	-4.931779	-3.634995	-2.244133
H	-5.515543	-4.446388	-2.670304
C	-5.509811	-2.780367	-1.300949
H	-6.541543	-2.926769	-0.992906
C	-4.761339	-1.741581	-0.747222
H	-5.205282	-1.087519	-0.001697
C	-2.953009	-0.010439	1.275926
C	-3.489326	1.183818	1.773040
H	-3.662417	2.022468	1.106645
C	-3.783773	1.305207	3.133583
H	-4.197513	2.236520	3.511225
C	-3.543007	0.241640	4.004810
H	-3.765272	0.343274	5.063517
C	-3.010569	-0.954221	3.512647
H	-2.814429	-1.785696	4.183706
C	-2.714020	-1.079391	2.156888
H	-2.291201	-2.006715	1.780719
C	-4.483853	2.727829	-2.507340
H	-5.441152	2.842442	-3.008853
C	-4.143520	1.498624	-1.940198
H	-4.836610	0.665026	-2.002952
C	0.289997	-2.967300	1.489796
O	0.276923	-3.395878	2.592680
O	-0.135977	-2.770368	0.387075

s-TS4
B3LYP-D3 SCF energy: -2219.47023368 a.u.
B3LYP-D3 enthalpy: -2218.786451 a.u.
B3LYP-D3 free energy: -2218.907036 a.u.
wB97XD SCF energy in solution: -2220.55598880 a.u.
wB97XD enthalpy in solution: -2219.872206 a.u.
wB97XD free energy in solution: -2219.992791 a.u.
Three lowest frequencies (cm-1): -173.0510 11.7963 12.1135
Imaginary frequency: -173.0510 cm-1

Cartesian coordinates

ATOM	X	Y	Z
C	0.843071	3.309651	0.761185
C	1.078028	1.942995	0.899197
C	1.360494	1.124050	-0.229960
C	1.362624	1.766485	-1.503506
C	1.113288	3.134649	-1.626681
C	0.855988	3.917976	-0.498569
H	0.653255	3.906563	1.650181
H	1.089721	1.499496	1.888622
H	1.569262	1.164559	-2.382872
H	1.129691	3.589247	-2.613893
H	0.670551	4.983542	-0.598127
C	1.602020	-0.340644	-0.144507
C	1.647278	-0.997363	1.165719
H	2.397821	-0.627158	-0.825480
H	0.921538	-0.657747	1.904439
C	2.436151	-2.032748	1.512344

C	3.512549	-2.654579	0.640956
H	2.324445	-2.439234	2.516138
H	3.076132	-3.032396	-0.291818
H	3.961083	-3.506424	1.164788
Cu	-0.548544	0.221807	-0.681921
B	4.596012	-1.553014	0.332975
C	5.910680	0.258591	0.741791
C	4.963480	1.339547	1.279678
H	5.275517	2.342018	0.968792
H	4.964911	1.295403	2.373043
H	3.937810	1.170777	0.939889
C	5.778904	0.039118	-0.812198
C	7.017416	-0.609628	-1.440100
H	7.863524	0.084764	-1.473158
H	6.777186	-0.916689	-2.462548
H	7.316233	-1.500924	-0.879479
C	5.358505	1.273830	-1.606210
H	5.281498	1.017734	-2.667977
H	6.098898	2.075207	-1.500607
H	4.385363	1.647954	-1.279722
C	7.331192	0.499201	1.244090
H	7.989119	-0.339897	1.007111
H	7.319469	0.622084	2.331778
H	7.749469	1.410590	0.801313
O	4.708807	-0.940337	-0.894772
O	5.434453	-1.006967	1.276475
P	-2.655245	-0.016392	-0.025739
C	-3.588046	1.545307	0.191455
C	-2.837173	2.712432	0.404016
H	-1.751199	2.663676	0.403884
C	-3.479347	3.934672	0.602913
H	-2.888183	4.831852	0.764714
C	-4.874058	4.004029	0.579334
H	-5.374599	4.957155	0.727159
C	-3.661044	-1.086769	-1.116879
C	-3.258634	-1.226434	-2.453578
H	-2.346750	-0.744866	-2.796573
C	-4.003194	-2.021073	-3.327031
H	-3.681675	-2.132312	-4.358657
C	-5.143202	-2.685228	-2.870335
H	-5.717774	-3.308619	-3.550096
C	-5.535159	-2.566634	-1.533589
H	-6.411079	-3.099049	-1.172876
C	-4.794575	-1.775286	-0.656071
H	-5.083166	-1.708234	0.389593
C	-2.674370	-0.863970	1.601308
C	-3.566586	-0.541231	2.632686
H	-4.290113	0.257840	2.498274
C	-3.515811	-1.239269	3.841679
H	-4.207038	-0.983502	4.640342
C	-2.577531	-2.257304	4.026053
H	-2.537787	-2.794317	4.969941
C	-1.683895	-2.578617	3.000427
H	-0.943493	-3.361057	3.140346
C	-1.726102	-1.884136	1.792128
H	-1.015793	-2.127876	1.004825

C	-5.626523	2.848550	0.352056
H	-6.711395	2.902283	0.321050
C	-4.988708	1.622463	0.157359
H	-5.579242	0.731948	-0.035763
C	0.517378	-1.667001	-1.523199
O	0.194840	-1.003763	-2.505327
O	0.613484	-2.770135	-1.066805

s-TS5

B3LYP-D3 SCF energy: -2146.61958138 a.u.
B3LYP-D3 enthalpy: -2145.897221 a.u.
B3LYP-D3 free energy: -2146.015638 a.u.
wB97XD SCF energy in solution: -2147.71134312 a.u.
wB97XD enthalpy in solution: -2146.988983 a.u.
wB97XD free energy in solution: -2147.107400 a.u.
Three lowest frequencies (cm-1): -298.2200 20.0898 23.4719
Imaginary frequency: -298.2200 cm-1

Cartesian coordinates

ATOM	X	Y	Z
C	-0.114716	2.983270	1.665718
C	0.492425	1.988936	0.902098
C	0.806859	2.183358	-0.467687
C	0.433587	3.431494	-1.027655
C	-0.165620	4.427686	-0.258144
C	-0.442338	4.219573	1.098665
H	-0.330612	2.790571	2.714585
H	0.758183	1.043801	1.366557
H	0.622255	3.610282	-2.083780
H	-0.424901	5.376254	-0.724365
H	-0.908580	4.998465	1.696042
C	1.448171	1.120456	-1.249092
C	2.576506	1.415297	-2.126433
H	1.581752	0.206963	-0.672764
H	2.697167	2.458290	-2.426088
C	3.439144	0.514085	-2.662217
C	3.437752	-0.971843	-2.331086
H	4.247812	0.868767	-3.296258
H	3.960810	-1.540013	-3.108284
H	2.412806	-1.361843	-2.248474
Cu	-1.206615	0.212454	-1.788870
B	4.185165	-1.013940	-0.953062
C	4.501020	-0.475098	1.234606
C	4.286780	1.043826	1.265866
H	4.465507	1.483124	0.279827
H	4.942806	1.527072	1.997815
H	3.247172	1.254427	1.532581
C	5.869563	-0.895910	0.585893
C	6.290873	-2.325419	0.949066
H	6.619869	-2.399511	1.991134
H	7.119139	-2.625891	0.300040
H	5.464135	-3.025280	0.790797
C	7.020193	0.077205	0.826073
H	7.925275	-0.291462	0.332444
H	7.229174	0.174421	1.897843

H	6.792694	1.065334	0.420858
C	4.231300	-1.075927	2.610411
H	4.207367	-2.168406	2.576958
H	3.266307	-0.722479	2.985749
H	5.007073	-0.766900	3.320371
O	5.552369	-0.895773	-0.828732
O	3.544170	-1.010273	0.275660
P	-2.402849	-0.461076	-0.054173
C	-3.495624	0.836078	0.625524
C	-3.109835	2.171138	0.432847
H	-2.201589	2.406727	-0.114430
C	-3.883575	3.203132	0.964152
H	-3.562840	4.230516	0.822734
C	-5.048944	2.910368	1.674898
H	-5.653623	3.715694	2.083346
C	-3.487140	-1.902149	-0.379496
C	-4.058763	-2.021914	-1.655324
H	-3.820906	-1.285568	-2.420283
C	-4.919664	-3.080458	-1.944772
H	-5.357571	-3.166022	-2.935342
C	-5.207318	-4.033554	-0.964415
H	-5.871969	-4.862608	-1.191195
C	-4.632095	-3.926611	0.304105
H	-4.847928	-4.671965	1.064706
C	-3.773879	-2.865726	0.598611
H	-3.319016	-2.792260	1.582273
C	-1.293561	-0.984661	1.303582
C	-0.072279	-1.575310	0.945209
H	0.185897	-1.695955	-0.103878
C	0.842251	-1.956689	1.924466
H	1.801470	-2.361599	1.622983
C	0.538623	-1.751355	3.272869
H	1.255675	-2.034846	4.038542
C	-0.675392	-1.162598	3.637346
H	-0.905469	-0.992199	4.685597
C	-1.590940	-0.774919	2.657165
H	-2.520150	-0.290819	2.942794
C	-5.442896	1.581347	1.858953
H	-6.353373	1.352950	2.406394
C	-4.670039	0.543885	1.337116
H	-4.984198	-0.487133	1.472480
C	0.269857	-0.168051	-4.341496
H	1.031522	0.308769	-4.967123
H	-0.576424	-0.475057	-4.964476
H	0.709133	-1.057768	-3.869921
O	-0.195059	0.765529	-3.363561
H	0.583348	0.934309	-2.615124

s-TS6
B3LYP-D3 SCF energy: -1808.76782324 a.u.
B3LYP-D3 enthalpy: -1808.266870 a.u.
B3LYP-D3 free energy: -1808.362625 a.u.
wB97XD SCF energy in solution: -1809.86934162 a.u.

wB97XD enthalpy in solution: -1809.368388 a.u.
wB97XD free energy in solution: -1809.464143 a.u.
Three lowest frequencies (cm-1): -202.5497 21.4018 30.8691
Imaginary frequency: -202.5497 cm-1

Cartesian coordinates

ATOM	X	Y	Z
C	2.394458	0.800573	2.056538
C	3.035561	0.037492	1.068842
C	3.378399	0.615345	-0.168649
C	3.071416	1.968414	-0.383256
C	2.440840	2.724459	0.601954
C	2.092133	2.140589	1.824005
H	2.134883	0.331176	3.000484
H	3.287654	-0.995931	1.287570
H	3.320080	2.425175	-1.338241
H	2.190713	3.762837	0.406078
H	1.583932	2.728033	2.583287
C	3.971304	-0.236112	-1.282929
H	4.626163	0.379944	-1.909978
H	4.592283	-1.028003	-0.845771
C	2.878103	-0.849858	-2.139506
C	2.250695	-2.040114	-1.868366
H	2.590558	-0.307769	-3.036724
H	1.505527	-2.372729	-2.593932
C	2.407871	-2.883059	-0.681030
H	2.189401	-3.929558	-0.880119
H	3.333855	-2.747622	-0.125461
P	-0.820121	0.096110	-0.078316
C	-0.703649	1.888324	-0.466211
C	-1.083407	2.902105	0.421264
H	-1.510595	2.649383	1.385981
C	-0.902593	4.244165	0.075122
H	-1.197176	5.022628	0.773898
C	-0.348653	4.584599	-1.159519
H	-0.211229	5.628833	-1.426907
C	-2.073521	-0.534375	-1.264199
C	-2.072673	-1.914015	-1.528086
H	-1.340790	-2.556510	-1.044189
C	-3.021470	-2.455390	-2.396582
H	-3.019087	-3.523961	-2.593682
C	-3.965258	-1.629423	-3.012303
H	-4.698867	-2.053827	-3.692629
C	-3.962773	-0.255995	-2.756908
H	-4.692800	0.389768	-3.237853
C	-3.020568	0.292872	-1.885296
H	-3.014987	1.363047	-1.699117
C	-1.632865	-0.020874	1.557649
C	-2.949330	0.424200	1.760919
H	-3.513914	0.843324	0.932456
C	-3.536763	0.317420	3.020381
H	-4.555670	0.663014	3.173039
C	-2.819361	-0.244943	4.081497
H	-3.281955	-0.333802	5.060882
C	-1.517795	-0.705554	3.879010
H	-0.964459	-1.162352	4.694641

C	-0.922923	-0.595957	2.620144
H	0.078777	-0.980299	2.459068
C	0.031527	3.576252	-2.050974
H	0.468350	3.833230	-3.012255
C	-0.136639	2.238216	-1.702689
H	0.185330	1.456656	-2.386434
Cu	1.136041	-0.986524	-0.330018
C	1.039356	-3.049806	0.945469
O	1.663291	-2.772210	1.947745
O	0.004476	-3.522097	0.528934

s-TS7
B3LYP-D3 SCF energy: -1620.17281048 a.u.
B3LYP-D3 enthalpy: -1619.689969 a.u.
B3LYP-D3 free energy: -1619.777979 a.u.
wB97XD SCF energy in solution: -1621.29078552 a.u.
wB97XD enthalpy in solution: -1620.807944 a.u.
wB97XD free energy in solution: -1620.895954 a.u.
Three lowest frequencies (cm-1): -50.5750 -1.1755 19.2526
Imaginary frequency: -50.5750 cm-1

Cartesian coordinates

ATOM	X	Y	Z
C	6.813506	1.279959	0.190897
C	5.425774	1.386220	0.059721
C	4.620924	0.245581	-0.040018
C	5.240873	-1.013811	-0.009493
C	6.623960	-1.124210	0.125012
C	7.417711	0.023227	0.226418
H	7.419820	2.179722	0.264263
H	4.961120	2.370098	0.032649
H	4.628531	-1.906911	-0.100470
H	7.086005	-2.108260	0.150106
H	8.496263	-0.064068	0.329876
C	3.109913	0.359109	-0.188922
H	2.635521	-0.119176	0.681691
H	2.831897	1.420207	-0.141013
C	2.577001	-0.252035	-1.472858
C	2.226931	-1.610252	-1.602179
H	2.818484	0.284250	-2.385628
H	2.071190	-1.948321	-2.631280
C	1.833115	-2.530352	-0.589794
H	1.580164	-3.541917	-0.887257
H	2.188920	-2.419982	0.432550
P	-1.465136	-0.048922	-0.100516
C	-2.238792	1.307280	-1.068022
C	-3.064718	2.285101	-0.492959
H	-3.249106	2.279504	0.577751
C	-3.637283	3.276791	-1.291443
H	-4.271514	4.034271	-0.838672
C	-3.391147	3.300021	-2.666426
H	-3.835773	4.075032	-3.284850
C	-2.787389	-1.315426	0.073648
C	-2.382732	-2.646538	0.258922

H	-1.320049	-2.883016	0.248643
C	-3.334617	-3.651006	0.438017
H	-3.012826	-4.679010	0.580674
C	-4.695609	-3.337033	0.422757
H	-5.436728	-4.120692	0.555510
C	-5.104640	-2.015707	0.225052
H	-6.163083	-1.770270	0.202145
C	-4.156167	-1.006820	0.049853
H	-4.481765	0.015837	-0.115880
C	-1.248332	0.654447	1.582169
C	-2.218120	0.555958	2.589976
H	-3.143455	0.018400	2.405361
C	-1.990731	1.138385	3.838829
H	-2.745611	1.055982	4.616222
C	-0.797193	1.818169	4.091165
H	-0.622180	2.266092	5.065555
C	0.176140	1.912366	3.092883
H	1.111209	2.430357	3.287172
C	-0.046035	1.329943	1.845727
H	0.714969	1.390967	1.071988
C	-2.562028	2.334799	-3.243482
H	-2.357031	2.357845	-4.310233
C	-1.982165	1.347742	-2.446366
H	-1.311879	0.611567	-2.885069
Cu	0.441898	-0.855383	-0.876157