Supplementary Material (ESI) for Chemical Communications

Supporting Information

μ-Acetylide and μ-Alkenylidene Ligands in "Click" Triazole Syntheses

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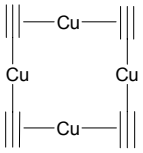
Computational Procedures

The B3LYP/LACV3P**++//B3LYP/LACVP** level of theory as implemented in the Jaguar 6.5 quantum chemistry program package has been utilized throughout this study. For C, N, O, and H, the 6-31G** basis set of Pople and coworkers was used for structure optimizations. For copper, a Hay-Wadt small-core effective potential replaces the 10 innermost core electrons. Full geometry optimizations and vibrational frequency calculations have been performed for all model compounds on the B3LYP/LACVP** level of theory.
Exactly zero imaginary frequencies characterize minima; transition structures are characterized by exactly one imaginary frequency. (In two cases, however, we were unable to remove very soft imaginary frequencies even after several additional structure optimization attempts.) Visual inspection of imaginary frequencies was performed with the Molden program package, and geometry optimizations from slightly distorted transition state structures ensured the assignment of the two corresponding local minima. Single point energies were computed with the LACV3P**++ basis set, which is characterized by the 6-311G**++ basis set for main group elements and by a triple-zeta quality basis set with an additional diffuse d function for copper.
The Gibbs free energies G refer to 298.15 K and 1 atm and are based on unscaled molecular vibrations and ideal gas phase conditions.

1 eV = 96.485 kJ mol^{-1}
1 hartree = 27.2116 eV

Cartesian Coordinates



1

C1	-0.4932348239	-1.9391217807	1.8351310424
C2	-0.8297599075	-1.9202345322	3.0284001410
Cu3	0.0000000000	0.0000000000	2.3070113407
Cu4	0.0000000000	1.9600409540	0.0000000000
C5	-0.4932348239	1.9391217807	-1.8351310424
C6	-0.8297599075	1.9202345322	-3.0284001410
Cu7	0.0000000000	0.0000000000	-2.3070113407
C8	0.8297599075	-1.9202345322	-3.0284001410
C9	0.4932348239	-1.9391217807	-1.8351310424
Cu10	0.0000000000	-1.9600409540	0.0000000000
C11	0.8297599075	1.9202345322	3.0284001410
C12	0.4932348239	1.9391217807	1.8351310424
H13	-1.1743900039	-2.0655748180	4.0304508804
H14	1.1743900039	-2.0655748180	-4.0304508804
H15	1.1743900039	2.0655748180	4.0304508804
H16	-1.1743900039	2.0655748180	-4.0304508804

SCFE: SCF energy: DFT(b3lyp) -1091.78773695681 hartrees

Thermodynamic properties calculated assuming an ideal gas

In the table below, the units for temperature
are kelvins, the units for U, H, and G are
kcal/mol and the units for Cv and S are cal/(mol K)

The zero point energy (ZPE): 47.822 kcal/mol
is not included in U, H, or G in the table below

T = 298.15 K

	U	Cv	S	H	G
trans.	0.889	2.981	43.467	1.481	-11.479
rot.	0.889	2.981	30.444	0.889	-8.188
vib.	9.360	51.773	64.458	9.360	-9.858
elec.	0.000	0.000	0.000	0.000	0.000
total	11.138	57.735	138.370	11.730	-29.525

Total internal energy, Utot (SCFE + ZPE + U): -1091.693778 hartrees
Total enthalpy, Htot (Utot + pV): -1091.692834 hartrees
Total Gibbs free energy, Gtot (Htot - T*S): -1091.758578 hartrees

Single point B3LYP/LACV3P++//B3LYP/LACVP****

Energy components, in hartrees:

(A)	Nuclear repulsion.....	1191.80630603986
(E)	Total one-electron terms.....	-4201.99346259418
(I)	Total two-electron terms.....	1918.23877102159
(J)	Coulomb.....	2038.47002675747

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   (K)    Exchange+Correlation.......    -120.23125573588
   (L)  Electronic energy............   -2283.75469157259  (E+I)
   (N)  Total energy.................   -1091.94838553272  (A+L)

 SCFE: SCF energy: DFT(b3lyp)     -1091.94838553272 hartrees


 HOMO energy:    -0.25107
 LUMO energy:    -0.07643
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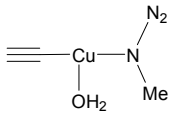
Total Gibbs free energy at the B3LYP/LACV3P**++//B3LYP/LACVP** level of theory: -1091.919227 hartrees



2

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  C1            0.5657065103      2.0853425666      0.4098298314
  Cu2           0.0643543743      0.6455763094     -0.6681195950
  O3            2.2798024153     -0.5107299069      0.5635536653
  H4            1.8317044052     -0.7370552930      1.3916891379
  C5            0.9909715060      2.9563271095      1.1586010180
  N6           -0.2927487977     -0.9146936443     -1.7807144917
  N7           -1.3222935355     -1.0192377465     -2.4814419565
  N8           -2.2824698033     -1.0633000503     -3.0862356686
  C9            0.6995530133     -2.0157905522     -1.9179605901
  H10           1.3384578013      3.7410529323      1.7926783977
  H11           1.4649707599     -1.8034204194     -1.1714142512
  H12           0.2280197298     -2.9824569636     -1.7189398594
  H13           1.1373286979     -2.0089570361     -2.9207672047
  H14           2.2227372015      0.4613868453      0.5608336647

SCFE: SCF energy: DFT(b3lyp)      -553.45097709293 hartrees

  Thermodynamic properties calculated assuming an ideal gas

  In the table below, the units for temperature
  are kelvins, the units for U, H, and G are
  kcal/mol and the units for Cv and S are cal/(mol K)


The zero point energy (ZPE):     59.539 kcal/mol
  is not included in U, H, or G in the table below


  T =   298.15 K

             U         Cv          S          H          G
         ---------  ---------  ---------  ---------  ---------
  trans.     0.889      2.981     41.174      1.481    -10.795
    rot.     0.889      2.981     29.762      0.889     -7.985
    vib.     6.000     33.108     41.278      6.000     -6.307
   elec.     0.000      0.000      0.000      0.000      0.000
   total     7.777     39.069    112.215      8.370    -25.087

  Total internal energy, Utot (SCFE + ZPE + U):    -553.343703 hartrees
             Total enthalpy, Htot (Utot + pV):     -553.342758 hartrees
    Total Gibbs free energy, Gtot (Htot - T*S):    -553.396075 hartrees
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Single point B3LYP/LACV3P++//B3LYP/LACVP****

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 Energy components, in hartrees:
   (A)  Nuclear repulsion.............     433.84071337962
   (E)  Total one-electron terms.....   -1699.42540248520
   (I)  Total two-electron terms.....     711.99808069604
   (J)    Coulomb....................     778.57348915924
   (K)    Exchange+Correlation.......     -66.57540846321
   (L)  Electronic energy............    -987.42732178916  (E+I)
   (N)  Total energy.................    -553.58660840954  (A+L)

 SCFE: SCF energy: DFT(b3lyp)      -553.58660840954 hartrees


 HOMO energy:    -0.23535
 LUMO energy:    -0.09563
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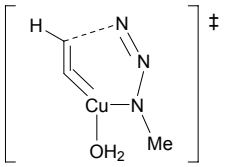
Total Gibbs free energy at the B3LYP/LACV3P**++//B3LYP/LACVP** level of theory: -553.531706 hartrees



3

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  C1           -1.6581089979     -0.9877106671     -0.0169695198
  Cu2          -0.7131713110      0.5960052834     -0.1464673261
  O3           -0.4585693902      2.6551644076      0.0044926048
  H4           -0.6354634093      2.9292180851      0.9154061004
  C5           -1.4365875320     -2.2120865069     -0.2180302372
  N6            1.0483649818     -0.2248355711     -0.7984618792
  N7            1.0925897796     -1.5012092041     -0.9503325532
  N8            0.4074077073     -2.4606069258     -0.8351105348
  C9            2.2968360519      0.4763021112     -1.1178445641
  H10          -1.7463955092     -3.2377446850     -0.2283214964
  H11           2.1118835952      1.5403693378     -0.9565482426
  H12           3.1238238364      0.1659743650     -0.4672439247
  H13           2.5976819135      0.3310009543     -2.1626062742
  H14          -1.1312325157      3.0960804868     -0.5332803957

SCFE: SCF energy: DFT(b3lyp)      -553.42456727858 hartrees

  Thermodynamic properties calculated assuming an ideal gas

  In the table below, the units for temperature
  are kelvins, the units for U, H, and G are
  kcal/mol and the units for Cv and S are cal/(mol K)

  The zero point energy (ZPE):     59.273 kcal/mol
  is not included in U, H, or G in the table below

 T =   298.15 K
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	U	Cv	S	H	G
trans.	0.889	2.981	41.174	1.481	-10.795
rot.	0.889	2.981	29.241	0.889	-7.830
vib.	5.189	29.996	34.880	5.189	-5.210
elec.	0.000	0.000	0.000	0.000	0.000
total	6.967	35.957	105.296	7.559	-23.835

Total internal energy, Utot (SCFE + ZPE + U): -553.319008 hartrees
Total enthalpy, Htot (Utot + pV): -553.318063 hartrees
Total Gibbs free energy, Gtot (Htot - T*S): -553.368093 hartrees

Single point B3LYP/LACV3P++//B3LYP/LACVP****

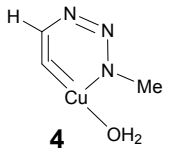
Energy components, in hartrees:

(A)	Nuclear repulsion.....	464.12766111884	
(E)	Total one-electron terms.....	-1761.28073544430	
(I)	Total two-electron terms.....	743.59879330660	
(J)	Coulomb.....	810.16234161532	
(K)	Exchange+Correlation.....	-66.56354830872	
(L)	Electronic energy.....	-1017.68194213770	(E+I)
(N)	Total energy.....	-553.55428101886	(A+L)

SCFE: SCF energy: DFT(b3lyp) -553.55428101886 hartrees

HOMO energy: -0.22657
LUMO energy: -0.06421

Total Gibbs free energy at the B3LYP/LACV3P**++//B3LYP/LACVP** level of theory: -553.497807 hartrees



4

C1	1.3982049417	-0.8892967022	0.0973102265
C2	2.4092983498	-0.2163358983	-0.4002393100
N3	2.2580551010	0.9436177822	-1.2908853935
N4	1.1297151655	1.3598405008	-1.6300430246
N5	-0.0233214836	0.8690968184	-1.2755064056
C6	-1.1572294743	1.6037958161	-1.8572279967
Cu7	-0.3908029498	-0.6814673116	-0.0948431719
O8	-2.3988318819	-1.1018394375	0.1898035533
H9	-2.6271160955	-1.9903039037	-0.1171549233
H10	3.4585041595	-0.4264703520	-0.2209609475
H11	-2.6416363563	-1.0729611477	1.1257148811
H12	-1.1626763192	2.6520191510	-1.5363376488
H13	-1.1344307163	1.5740721128	-2.9528310814
H14	-2.0805862125	1.1304271595	-1.5151422237

SCFE: SCF energy: DFT(b3lyp) -553.43417204920 hartrees

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  Thermodynamic properties calculated assuming an ideal gas

  In the table below, the units for temperature
  are kelvins, the units for U, H, and G are
  kcal/mol and the units for Cv and S are cal/(mol K)

  The zero point energy (ZPE):     60.618 kcal/mol
  is not included in U, H, or G in the table below


  T =   298.15 K

             U         Cv          S          H          G
         ---------  ---------  ---------  ---------  ---------
  trans.      0.889      2.981     41.174      1.481    -10.795
    rot.      0.889      2.981     29.068      0.889     -7.778
    vib.      5.001     29.304     34.745      5.001     -5.358
   elec.      0.000      0.000      0.000      0.000      0.000
   total      6.779     35.266    104.988      7.371    -23.931

  Total internal energy, Utot (SCFE + ZPE + U):    -553.326769 hartrees
             Total enthalpy, Htot (Utot + pV):    -553.325825 hartrees
    Total Gibbs free energy, Gtot (Htot - T*S):    -553.375708 hartrees
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Single point B3LYP/LACV3P++//B3LYP/LACVP****

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 Energy components, in hartrees:
   (A)  Nuclear repulsion.............     474.64889983264
   (E)  Total one-electron terms.....   -1781.95635347924
   (I)  Total two-electron terms.....     753.74561754967
   (J)    Coulomb....................     820.35690385113
   (K)    Exchange+Correlation.......     -66.61128630147
   (L)  Electronic energy............   -1028.21073592957  (E+I)
   (N)  Total energy.................    -553.56183609693  (A+L)

 SCFE: SCF energy: DFT(b3lyp)      -553.56183609693 hartrees


 HOMO energy:    -0.21347
 LUMO energy:    -0.07465

Total Gibbs free energy at the B3LYP/LACV3P**++//B3LYP/LACVP** level of
theory: -553.503372 hartrees
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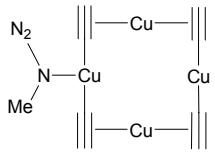

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C1	-0.7830590661000	-1.9432950281000	1.7400855828000
C2	-1.1238553554000	-1.8049514696000	2.9240006964000
Cu3	0.2695483525000	-0.2398611995000	2.2325923007000
C4	1.7006677091000	1.2231697181000	3.1265748868000
C5	1.3613226604000	1.4605736982000	1.9559447674000
Cu6	0.8409596191000	1.8445860155000	0.1486299570000
C7	0.1281793092000	1.8446011736000	-1.6407744236000
C8	-0.3088788110000	1.9590916943000	-2.7973021100000
Cu9	-0.2928038306000	-2.0995276371000	-0.0874353663000
Cu10	0.1413183024000	-0.1172838525000	-2.1955358877000
C11	0.1847104142000	-2.1445917191000	-1.9259806070000
C12	0.4962672141000	-2.1203261935000	-3.1249802837000
H13	-1.5193569910000	-1.8257702631000	3.9158267288000
H14	0.7731213570000	-2.2598595648000	-4.1489302702000
H15	2.0888086474000	1.1458287036000	4.1228450313000
H16	-0.6989660954000	2.2220206878000	-3.7585780325000
N17	1.7975357268000	4.0330257371000	-0.0688047024000
C18	2.6323936214000	4.7173989838000	0.9379392263000
N19	1.7067752684000	4.5848306652000	-1.1756571350000
N20	1.5297522849000	4.9594804783000	-2.2375044548000
H21	2.2325622532000	5.7075491096000	1.1819642729000
H22	2.6023036674000	4.0870385574000	1.8277450995000
H23	3.6712308808000	4.8140472350000	0.5980428582000

SCFE: SCF energy: DFT(b3lyp) -1295.88638240715 hartrees

Thermodynamic properties calculated assuming an ideal gas

In the table below, the units for temperature
are kelvins, the units for U, H, and G are
kcal/mol and the units for Cv and S are cal/(mol K)

The zero point energy (ZPE): 79.943 kcal/mol
is not included in U, H, or G in the table below

T = 298.15 K

	U	Cv	S	H	G
trans.	0.889	2.981	43.915	1.481	-11.612
rot.	0.889	2.981	34.603	0.889	-9.428
vib.	12.861	68.655	92.297	12.861	-14.657
elec.	0.000	0.000	0.000	0.000	0.000
total	14.639	74.617	170.815	15.231	-35.697

Total internal energy, Utot (SCFE + ZPE + U): -1295.735657 hartrees
Total enthalpy, Htot (Utot + pV): -1295.734712 hartrees
Total Gibbs free energy, Gtot (Htot - T*S): -1295.815872 hartrees

Single point B3LYP/LACV3P++//B3LYP/LACVP****

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Energy components, in hartrees:
   (A)  Nuclear repulsion.............    1696.55985651158
   (E)  Total one-electron terms.....   -5485.09139192894
   (I)  Total two-electron terms.....    2492.42452683920
   (J)    Coulomb.....................    2639.84717318063
   (K)    Exchange+Correlation.......    -147.42264634143
   (L)  Electronic energy............   -2992.66686508974  (E+I)
   (N)  Total energy.................   -1296.10700857816  (A+L)

 SCFE: SCF energy: DFT(b3lyp)     -1296.10700857816 hartrees


 HOMO energy:    -0.23006
 LUMO energy:    -0.06512

Total Gibbs free energy at the B3LYP/LACV3P**++//B3LYP/LACVP** level of
theory: -1296.036499 hartrees
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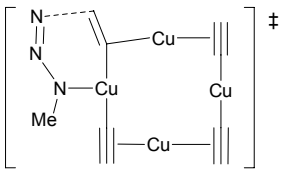

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  C1           -1.1019483611     -1.6098338817      1.8938179866
  C2           -1.3719601745     -1.3414701708      3.0733644877
  Cu3           0.3306738239     -0.1782794212      2.1873524804
  C4            2.1770291862      0.8445143753      2.6838192030
  C5            1.7445405955      1.2163428943      1.5801341716
  Cu6           1.2025269478      1.8718346292     -0.1764874649
  C7            0.5549252902      1.9216529438     -1.9834229960
  C8            0.3275962001      2.8001025707     -2.8591307755
  Cu9          -0.6137502323     -1.9115680215      0.0833896753
  Cu10          0.4411338594     -0.0193403306     -1.9021961388
  C11          -0.0052589925     -2.0265992073     -1.7111008576
  C12           0.4365318821     -2.0417370244     -2.8682678817
  H13          -1.7257293617     -1.2200014423      4.0752915594
  H14           0.7914858796     -2.2017377639     -3.8644138979
  H15           2.6980917939      0.6337077919      3.5945953404
  H16          -0.0543812343      3.0709077025     -3.8236476907
  N17           1.5777206382      3.9049611313     -0.2261009939
  C18           2.1512698196      4.6152292714      0.9281188510
  N19           1.2947067339      4.6162059783     -1.2392223282
  N20           0.8483314804      4.5422939070     -2.3313805846
  H21           1.4771305961      5.3982607520      1.2920404493
  H22           2.2916460999      3.8739671421      1.7137500126
  H23           3.1214641018      5.0598127559      0.6797212387

SCFE: SCF energy: DFT(b3lyp)     -1295.86893932256 hartrees
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  Thermodynamic properties calculated assuming an ideal gas

  In the table below, the units for temperature
  are kelvins, the units for U, H, and G are
  kcal/mol and the units for Cv and S are cal/(mol K)

  The zero point energy (ZPE):     80.478 kcal/mol
  is not included in U, H, or G in the table below


  T =   298.15 K

             U         Cv          S          H          G
         ---------  ---------  ---------  ---------  ---------
  trans.      0.889      2.981     43.915      1.481    -11.612
    rot.      0.889      2.981     34.378      0.889     -9.361
    vib.     12.309     67.230     87.630     12.309    -13.818
   elec.      0.000      0.000      0.000      0.000      0.000
   total     14.086     73.192    165.924     14.679    -34.791

  Total internal energy, Utot (SCFE + ZPE + U):   -1295.718241 hartrees
             Total enthalpy, Htot (Utot + pV):   -1295.717297 hartrees
    Total Gibbs free energy, Gtot (Htot - T*S):   -1295.796133 hartrees
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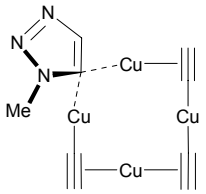
Single point B3LYP/LACV3P++//B3LYP/LACVP****

```
 Energy components, in hartrees:
   (A)  Nuclear repulsion.............    1744.73759183378
   (E)  Total one-electron terms.....   -5580.80662162025
   (I)  Total two-electron terms.....    2539.98091326216
   (J)    Coulomb....................    2687.39762903265
   (K)    Exchange+Correlation.......    -147.41671577049
   (L)  Electronic energy............   -3040.82570835810  (E+I)
   (N)  Total energy.................   -1296.08811652431  (A+L)

 SCFE: SCF energy: DFT(b3lyp)     -1296.08811652431 hartrees


 HOMO energy:    -0.24707
 LUMO energy:    -0.09870

Total Gibbs free energy at the B3LYP/LACV3P**++//B3LYP/LACVP** level of
theory: -1296.015311 hartrees
```



7

C1	-0.6432478529	-1.0825100552	1.9958891164
Cu2	-1.1343385340	-1.3418432277	0.1816322336
C3	-1.5710001385	-1.5101154863	-1.6608948715
C4	-1.8397800360	-1.5924078103	-2.8673693190
Cu5	0.1450019109	-0.6434280114	-2.3335332951
C6	2.0647818834	-0.0931394302	-3.2213896371
C7	1.9065282899	0.4275802826	-2.1060004419
Cu8	1.7187267705	1.2330595575	-0.3860423484
N9	0.9413991036	3.4549496917	1.3622794788
N10	1.5896718555	4.3587869757	2.1068646122
N11	2.6740985562	3.7930963976	2.5816660276
C12	-0.3029563669	-0.8767656389	3.1718090829
Cu13	0.6125161036	0.5787331481	1.8483026667
C14	1.6044688404	2.2375531445	1.3116854232
C15	2.7156782339	2.5161450060	2.1222691298
C16	-0.2872995757	3.8516501535	0.6878517044
H17	-0.1247398947	-0.8529490670	4.2268657046
H18	-2.2028890466	-1.7275341361	-3.8642821222
H19	3.5337454584	1.8584553199	2.3819709116
H20	2.3708659269	-0.4582289863	-4.1796706760
H21	-0.5468740036	4.8489146521	1.0426271660
H22	-0.1400709446	3.8765901598	-0.3954412007
H23	-1.0929616217	3.1532765054	0.9259189976

SCFE: SCF energy: DFT(b3lyp) -1295.97492466019 hartrees

Thermodynamic properties calculated assuming an ideal gas

In the table below, the units for temperature
are kelvins, the units for U, H, and G are
kcal/mol and the units for Cv and S are cal/(mol K)

The zero point energy (ZPE): 84.327 kcal/mol
is not included in U, H, or G in the table below

T = 298.15 K

	U	Cv	S	H	G
trans.	0.889	2.981	43.915	1.481	-11.612
rot.	0.889	2.981	34.266	0.889	-9.328
vib.	11.616	63.609	83.233	11.616	-13.200
elec.	0.000	0.000	0.000	0.000	0.000
total	13.394	69.570	161.414	13.986	-34.140

Total internal energy, Utot (SCFE + ZPE + U): -1295.819196 hartrees
Total enthalpy, Htot (Utot + pV): -1295.818252 hartrees
Total Gibbs free energy, Gtot (Htot - T*S): -1295.894945 hartrees

Single point B3LYP/LACV3P++//B3LYP/LACVP****

```
 Energy components, in hartrees:
   (A)  Nuclear repulsion.............    1768.74029022006
   (E)  Total one-electron terms.....   -5628.11265326556
   (I)  Total two-electron terms.....    2563.18535338770
   (J)    Coulomb....................    2710.77669997155
   (K)    Exchange+Correlation.......    -147.59134658385
   (L)  Electronic energy............   -3064.92729987786  (E+I)
   (N)  Total energy.................   -1296.18700965780  (A+L)

 SCFE: SCF energy: DFT(b3lyp)     -1296.18700965780 hartrees


 HOMO energy:    -0.25611
 LUMO energy:    -0.07828
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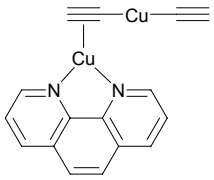
Total Gibbs free energy at the B3LYP/LACV3P**++//B3LYP/LACVP** level of theory: -1296.107030 hartrees



8

C1	-0.4859948274	3.2738155663	-0.0012826108
C2	0.8757847940	3.2324210220	0.0001216649
C3	1.5802341050	1.9824783373	0.0010931794
C4	0.8501422002	0.7697587039	0.0007534493
C5	-0.5928919900	0.8128241902	-0.0005648965
C6	-1.2583254632	2.0649036829	-0.0017543592
N7	1.4478917799	-0.4500010962	0.0013310217
C8	2.7774991772	-0.5098017488	0.0020380684
C9	3.5851389253	0.6463439237	0.0024607503
C10	2.9911314910	1.8896248173	0.0021193529
C11	-2.6708643143	2.0484600879	-0.0034412696
C12	-3.3380161972	0.8398600554	-0.0039888191
C13	-2.5892836257	-0.3515531991	-0.0026303703
N14	-1.2612294431	-0.3698726782	-0.0009339746
Cu15	0.0379391789	-2.0566761890	0.0019266069
C16	-0.6981302704	-3.9977621900	0.0066445097
C17	0.5497233553	-4.0883862502	0.0039106389
H18	3.2367822534	-1.4977045948	0.0021560240
H19	4.6636521403	0.5308987797	0.0030553535
H20	3.5875289419	2.7981948598	0.0024652950
H21	-3.0842607306	-1.3183378846	-0.0029486763
H22	-4.4217459463	0.7936773721	-0.0054156298
H23	-3.2174357821	2.9878288348	-0.0043844775
H24	1.4545064116	4.1518166506	0.0004382174
H25	-1.0101750658	4.2252188590	-0.0021069402
H26	-1.7358847594	-4.2632502520	0.0092438804
Cu27	2.4416010555	-4.0326898876	-0.0006687747
C28	4.2880972812	-3.6683138077	-0.0043555645
C29	5.4748908401	-3.3559442318	-0.0075751285
H30	6.5129274951	-3.1096372118	-0.0097442877

```
SCFE: SCF energy: DFT(b3lyp)     -1117.51221879951 hartrees

  Thermodynamic properties calculated assuming an ideal gas
```

In the table below, the units for temperature
are kelvins, the units for U, H, and G are
kcal/mol and the units for Cv and S are cal/(mol K)

The zero point energy (ZPE): 132.135 kcal/mol
is not included in U, H, or G in the table below

T = 298.15 K

	U	Cv	S	H	G
trans.	0.889	2.981	43.503	1.481	-11.489
rot.	0.889	2.981	34.602	0.889	-9.428
vib.	10.057	63.931	67.421	10.057	-10.045
elec.	0.000	0.000	0.000	0.000	0.000
total	11.835	69.892	145.527	12.427	-30.962

Total internal energy, Utot (SCFE + ZPE + U): -1117.282788 hartrees
Total enthalpy, Htot (Utot + pV): -1117.281844 hartrees
Total Gibbs free energy, Gtot (Htot - T*S): -1117.350988 hartrees

Single point B3LYP/LACV3P++//B3LYP/LACVP****

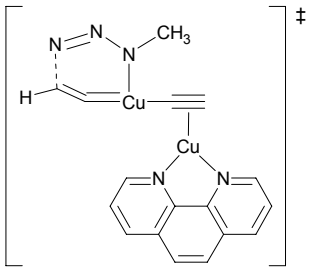
Energy components, in hartrees:

(A)	Nuclear repulsion.....	1751.42255698652	
(E)	Total one-electron terms.....	-5170.56285760099	
(I)	Total two-electron terms.....	2301.41011833581	
(J)	Coulomb.....	2443.56529990516	
(K)	Exchange+Correlation.....	-142.15518156936	
(L)	Electronic energy.....	-2869.15273926519	(E+I)
(N)	Total energy.....	-1117.73018227866	(A+L)

SCFE: SCF energy: DFT(b3lyp) -1117.73018227866 hartrees

HOMO energy: -0.20571
LUMO energy: -0.10842

Total Gibbs free energy at the B3LYP/LACV3P**++//B3LYP/LACVP** level of theory: -1117.568951 hartrees



9

one additional soft vibration -11.4 cm^{-1}

N1	2.0059423834	2.1426438338	0.0000000000
C2	1.0202983071	3.0773651005	0.0000000000
C3	1.2867742770	4.4698389295	0.0000000000
C4	2.6416562267	4.8693053341	0.0000000000
C5	3.6345178815	3.9100687376	0.0000000000
C6	3.2696176966	2.5509180157	0.0000000000
C7	0.1920076071	5.3973732482	0.0000000000
C8	-1.0971905047	4.9564586330	0.0000000000
C9	-1.4017633608	3.5543736261	0.0000000000
C10	-0.3457170047	2.6116340797	0.0000000000
N11	-0.5562151087	1.2700916013	0.0000000000
C12	-1.8073852335	0.8193204114	0.0000000000
C13	-2.9211527355	1.6847356685	0.0000000000
C14	-2.7222064484	3.0482824303	0.0000000000
Cu15	1.2503660422	0.1411471708	0.0000000000
Cu16	-0.4824177759	-2.6163907576	0.0000000000
N17	-0.6426934736	-4.7261977005	0.0000000000
N18	-1.7680066620	-5.3385726567	0.0000000000
N19	-2.9305826470	-5.0933304488	0.0000000000
C20	2.5001195616	-1.4988276145	0.0000000000
C21	1.3337005416	-1.9560373528	0.0000000000
C22	-2.3606656284	-2.5220517645	0.0000000000
C23	-3.4059372468	-3.2264694670	0.0000000000
C24	0.5329515670	-5.6038724575	0.0000000000
H25	-1.9380994474	-0.2638969759	0.0000000000
H26	-3.9184134680	1.2576519516	0.0000000000
H27	-3.5612608246	3.7393232393	0.0000000000
H28	4.0269894885	1.7722965885	0.0000000000
H29	4.6837730082	4.1850269563	0.0000000000
H30	2.8879778398	5.9278042193	0.0000000000
H31	-1.9213543396	5.6646112521	0.0000000000
H32	0.4118562828	6.4612770173	0.0000000000
H33	3.5710156636	-1.4588285017	0.0000000000
H34	-4.4719023521	-3.3338800575	0.0000000000
H35	0.5705794378	-6.2425644126	0.8918537558
H36	0.5705794378	-6.2425644126	-0.8918537558
H37	1.4091039757	-4.9543451233	0.0000000000

SCFE: SCF energy: DFT(b3lyp) -1321.59001548526 hartrees

Thermodynamic properties calculated assuming an ideal gas

In the table below, the units for temperature
are kelvins, the units for U, H, and G are
kcal/mol and the units for Cv and S are cal/(mol K)

The zero point energy (ZPE): 164.312 kcal/mol
is not included in U, H, or G in the table below

T = 298.15 K

	U	Cv	S	H	G
trans.	0.889	2.981	43.946	1.481	-11.621
rot.	0.889	2.981	35.671	0.889	-9.747
vib.	12.441	77.541	84.335	12.441	-12.704
elec.	0.000	0.000	0.000	0.000	0.000
total	14.218	83.503	163.952	14.811	-34.072

Total internal energy, Utot (SCFE + ZPE + U): -1321.305510 hartrees
Total enthalpy, Htot (Utot + pV): -1321.304566 hartrees
Total Gibbs free energy, Gtot (Htot - T*S): -1321.382465 hartrees

Single point B3LYP/LACV3P++//B3LYP/LACVP****

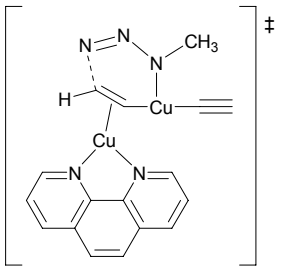
Energy components, in hartrees:

(A)	Nuclear repulsion.....	2289.25716372205	
(E)	Total one-electron terms.....	-6520.58067674699	
(I)	Total two-electron terms.....	2909.46039232884	
(J)	Coulomb.....	3078.80514409766	
(K)	Exchange+Correlation.....	-169.34475176883	
(L)	Electronic energy.....	-3611.12028441816	(E+I)
(N)	Total energy.....	-1321.86312069610	(A+L)

SCFE: SCF energy: DFT(b3lyp) -1321.86312069610 hartrees

HOMO energy: -0.19229
LUMO energy: -0.10711

Total Gibbs free energy at the B3LYP/LACV3P**++//B3LYP/LACVP** level of theory: -1321.655571 hartrees



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N1	-0.9373908345	-0.4586321496	-0.0008325939
C2	-0.4140816154	0.7911562888	-0.0112591268
C3	-1.2178432130	1.9573769469	-0.0211564353
C4	-2.6191231732	1.7717850009	-0.0194242516
C5	-3.1390550848	0.4925854113	-0.0088150660
C6	-2.2547006488	-0.6034846208	0.0002800460
C7	-0.5857443154	3.2459112658	-0.0328235586
C8	0.7726617876	3.3592448328	-0.0344070146
C9	1.6156917681	2.1970791557	-0.0244742955
C10	1.0249454353	0.9119505928	-0.0127651717
N11	1.7568575528	-0.2324153542	-0.0039733316
C12	3.0849878406	-0.1520879442	-0.0063509874
C13	3.7576946664	1.0871455557	-0.0175719187
C14	3.0284871841	2.2577241409	-0.0265990636
Cu15	0.6344254819	-1.9696819481	0.0132383007
C16	0.0990981043	-3.8434725422	0.0365070430
Cu17	2.0238746098	-4.0354956771	0.0065747164
N18	1.9025149585	-6.0818968661	-0.0017501180
N19	0.7920974401	-6.7002259294	0.0187352216
N20	-0.3762539089	-6.5336289284	0.0427224733
C21	-0.8937021654	-4.6162759421	0.0567018809
C22	3.8912775783	-3.5448825603	-0.0146102514
C23	5.0866105095	-3.2634734894	-0.0266231353
C24	3.1153532714	-6.9110210536	-0.0261957440
H25	3.6268973613	-1.0981354572	-0.0007227097
H26	4.8424478865	1.0995696331	-0.0194424416
H27	3.5229526926	3.2256712055	-0.0357317363
H28	-2.6231213952	-1.6260994197	0.0082703828
H29	-4.2100734967	0.3198897677	-0.0076246631
H30	-3.2742609632	2.6385854711	-0.0266431177
H31	1.2425531111	4.3388935344	-0.0434641814
H32	-1.2130897149	4.1329617422	-0.0406187754
H33	-1.9450021275	-4.8179715704	0.0829579921
H34	6.1298992903	-3.0388591549	-0.0375236309
H35	3.1887306006	-7.5436375765	0.8664963771
H36	3.1516850863	-7.5449383487	-0.9202217026
H37	3.9567386093	-6.2183303476	-0.0437588386

SCFE: SCF energy: DFT(b3lyp) -1321.59830235671 hartrees

Thermodynamic properties calculated assuming an ideal gas

In the table below, the units for temperature
are kelvins, the units for U, H, and G are
kcal/mol and the units for Cv and S are cal/(mol K)

The zero point energy (ZPE): 164.956 kcal/mol
is not included in U, H, or G in the table below

T = 298.15 K

	U	Cv	S	H	G
trans.	0.889	2.981	43.946	1.481	-11.621
rot.	0.889	2.981	35.503	0.889	-9.697
vib.	12.902	79.447	89.207	12.902	-13.696
elec.	0.000	0.000	0.000	0.000	0.000
total	14.679	85.408	168.656	15.272	-35.013

Total internal energy, Utot (SCFE + ZPE + U): -1321.312037 hartrees
Total enthalpy, Htot (Utot + pV): -1321.311092 hartrees
Total Gibbs free energy, Gtot (Htot - T*S): -1321.391226 hartrees

Single point B3LYP/LACV3P++//B3LYP/LACVP****

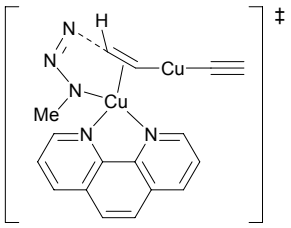
Energy components, in hartrees:

(A)	Nuclear repulsion.....	2338.86558323791	
(E)	Total one-electron terms.....	-6619.44424570881	
(I)	Total two-electron terms.....	2958.70313345078	
(J)	Coulomb.....	3128.05306994389	
(K)	Exchange+Correlation.....	-169.34993649311	
(L)	Electronic energy.....	-3660.74111225803	(E+I)
(N)	Total energy.....	-1321.87552902012	(A+L)

SCFE: SCF energy: DFT(b3lyp) -1321.87552902012 hartrees

HOMO energy: -0.20487
LUMO energy: -0.10513

Total Gibbs free energy at the B3LYP/LACV3P**++//B3LYP/LACVP** level of theory: -1321.668453 hartrees



one additional soft vibration −6.7 cm^{-1}

N1	-0.6559382556	-0.9424127768	-0.0051572817
C2	0.0962742015	0.0385163622	-0.5583226201
C3	-0.4453604807	1.2920411680	-0.9399705886
C4	-1.8287810537	1.4888091083	-0.7290801207
C5	-2.5835803645	0.4788050849	-0.1663535189
C6	-1.9503566935	-0.7288743378	0.1844179474
C7	0.4172908400	2.2911978123	-1.5024264559
C8	1.7503141989	2.0566368523	-1.6577570163
C9	2.3341343269	0.8031563891	-1.2727835003
C10	1.5082800890	-0.2164019338	-0.7389111113
N11	1.9919072744	-1.4285328771	-0.3624395276
C12	3.3001904896	-1.6542864704	-0.4551774868
C13	4.1974830632	-0.6978967797	-0.9697090510
C14	3.7148697332	0.5244303717	-1.3887792477
Cu15	0.5155495527	-2.8062961051	0.3588870098
Cu16	1.9302426830	-3.7419170189	2.2321606233
C17	3.7645301150	-3.4405093578	2.5420328977
C18	4.9609918778	-3.2153628212	2.6917879240
C19	-0.8827198814	-4.9125150560	1.8566238708
C20	0.0915048236	-4.1155810488	1.7749846114
N21	-0.1988120550	-4.1091203128	-1.1010195354
N22	-1.0548765845	-5.0072704751	-0.8029993843
N23	-1.5401234531	-5.5315037970	0.1428821235
C24	-0.0035459832	-3.8762514913	-2.5365117319
H25	3.6572664847	-2.6054407024	-0.0715153588
H26	5.2546596578	-0.9350425823	-1.0210439817
H27	4.3818333441	1.2813334816	-1.7934555459
H28	-2.5095967108	-1.5445097048	0.6359231666
H29	-3.6466028359	0.6013482105	0.0124557160
H30	-2.2836886669	2.4354758531	-1.0081992906
H31	2.3987038374	2.8223071277	-2.0743680617
H32	-0.0129669576	3.2451453442	-1.7948094155
H33	-1.5631390440	-5.4767929608	2.4626853070
H34	6.0005830532	-3.0263526213	2.8400860001
H35	0.3063390404	-4.7888526874	-3.0584004914
H36	-0.9057532768	-3.4802260065	-3.0205521310
H37	0.7946752874	-3.1382253854	-2.6329630369

SCFE: SCF energy: DFT(b3lyp) -1321.59092379970 hartrees

Thermodynamic properties calculated assuming an ideal gas

In the table below, the units for temperature
are kelvins, the units for U, H, and G are
kcal/mol and the units for Cv and S are cal/(mol K)

The zero point energy (ZPE): 164.314 kcal/mol
is not included in U, H, or G in the table below

T = 298.15 K

	U	Cv	S	H	G
trans.	0.889	2.981	43.946	1.481	-11.621
rot.	0.889	2.981	35.240	0.889	-9.618
vib.	12.633	77.936	85.662	12.633	-12.907
elec.	0.000	0.000	0.000	0.000	0.000
total	14.411	83.898	164.848	15.003	-34.146

Total internal energy, Utot (SCFE + ZPE + U): -1321.306108 hartrees
Total enthalpy, Htot (Utot + pV): -1321.305163 hartrees
Total Gibbs free energy, Gtot (Htot - T*S): -1321.383488 hartrees

Single point B3LYP/LACV3P++//B3LYP/LACVP****

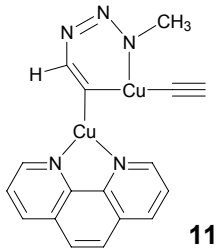
Energy components, in hartrees:

(A)	Nuclear repulsion.....	2418.81319835522	
(E)	Total one-electron terms.....	-6778.94983740645	
(I)	Total two-electron terms.....	3038.27099322524	
(J)	Coulomb.....	3207.61694072512	
(K)	Exchange+Correlation.....	-169.34594749988	
(L)	Electronic energy.....	-3740.67884418121	(E+I)
(N)	Total energy.....	-1321.86564582599	(A+L)

SCFE: SCF energy: DFT(b3lyp) -1321.86564582599 hartrees

HOMO energy: -0.21054
LUMO energy: -0.10091

Total Gibbs free energy at the B3LYP/LACV3P**++//B3LYP/LACVP** level of theory: -1321.658210 hartrees



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N1	-0.9380828625	-0.5278847088	0.0048426151
C2	-0.4338850506	0.7318833108	0.0095872503
C3	-1.2559345023	1.8853447488	0.0171719350
C4	-2.6543123141	1.6800804930	0.0194860228
C5	-3.1547356456	0.3931468131	0.0148065780
C6	-2.2548638210	-0.6897896416	0.0075746818
C7	-0.6439425546	3.1835127591	0.0224508907
C8	0.7122970761	3.3192325754	0.0209591153
C9	1.5732505578	2.1702538565	0.0134704403
C10	1.0018788522	0.8767685980	0.0071023785
N11	1.7520494596	-0.2565769778	-0.0015488366
C12	3.0794167844	-0.1567299801	-0.0032396065
C13	3.7324422818	1.0925435468	0.0037788675
C14	2.9851135615	2.2518863390	0.0118682079
Cu15	0.6565002502	-1.9882649180	-0.0072272885
C16	0.2461372526	-3.8545524332	-0.0035776442
Cu17	2.1061367688	-4.0452659955	-0.0210683748
N18	1.6651425188	-5.9762646750	0.0039231540
N19	0.5626548047	-6.6458639089	0.0143809201
N20	-0.6031122244	-6.1592955842	0.0067080279
C21	-0.7405807746	-4.7302790058	0.0007625639
C22	3.9716919394	-3.5447225836	-0.0483780853
C23	5.1603447094	-3.2412290584	-0.0658899578
C24	2.8652695673	-6.8326812545	0.0648557533
H25	3.6367407147	-1.0937193513	-0.0116006385
H26	4.8167367838	1.1210490089	0.0022731130
H27	3.4649725532	3.2270394883	0.0168968550
H28	-2.6147923310	-1.7147759998	0.0041707143
H29	-4.2228833129	0.2038728586	0.0167813877
H30	-3.3222318623	2.5373338991	0.0251283715
H31	1.1662487712	4.3059294027	0.0252727550
H32	-1.2859289451	4.0596244623	0.0279510814
H33	-1.7911110755	-4.4474132683	-0.0019638473
H34	6.2002561469	-3.0030469623	-0.0821159443
H35	2.9821497371	-7.2613129357	1.0675050197
H36	2.7878044913	-7.6468535723	-0.6626417787
H37	3.7349837060	-6.2167435919	-0.1590668341

SCFE: SCF energy: DFT(b3lyp) -1321.61473141725 hartrees

Thermodynamic properties calculated assuming an ideal gas

In the table below, the units for temperature
are kelvins, the units for U, H, and G are
kcal/mol and the units for Cv and S are cal/(mol K)

The zero point energy (ZPE): 166.737 kcal/mol
is not included in U, H, or G in the table below
T = 298.15 K

	U	Cv	S	H	G
trans.	0.889	2.981	43.946	1.481	-11.621
rot.	0.889	2.981	35.463	0.889	-9.684
vib.	12.014	76.089	80.611	12.014	-12.020
elec.	0.000	0.000	0.000	0.000	0.000
total	13.792	82.051	160.020	14.384	-33.326

Total internal energy, Utot (SCFE + ZPE + U): -1321.327040 hartrees
Total enthalpy, Htot (Utot + pV): -1321.326096 hartrees
Total Gibbs free energy, Gtot (Htot - T*S): -1321.402126 hartrees

Single point B3LYP/LACV3P++//B3LYP/LACVP****

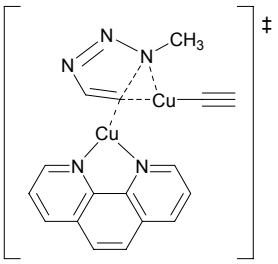
Energy components, in hartrees:

(A)	Nuclear repulsion.....	2359.34781954227	
(E)	Total one-electron terms.....	-6658.97806669920	
(I)	Total two-electron terms.....	2977.74033061589	
(J)	Coulomb.....	3147.12508690682	
(K)	Exchange+Correlation.....	-169.38475629093	
(L)	Electronic energy.....	-3681.23773608331	(E+I)
(N)	Total energy.....	-1321.88991654104	(A+L)

SCFE: SCF energy: DFT(b3lyp) -1321.88991654104 hartrees

HOMO energy: -0.19819
LUMO energy: -0.11349

Total Gibbs free energy at the B3LYP/LACV3P**++//B3LYP/LACVP** level of theory: -1321.677312 hartrees



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N1	-0.9909224437	-0.4284104602	-0.0283730124
C2	-0.4477634458	0.8148681097	-0.0488848573
C3	-1.2337646356	1.9920678652	-0.0980735605
C4	-2.6372675958	1.8287080265	-0.1230532160
C5	-3.1775132078	0.5583339219	-0.0978728322
C6	-2.3118325480	-0.5507598319	-0.0495388351
C7	-0.5827134335	3.2709779172	-0.1200770768
C8	0.7767571858	3.3650397726	-0.0955195020
C9	1.6019668773	2.1915971480	-0.0455641039
C10	0.9917757493	0.9160936743	-0.0193711978
N11	1.7061378706	-0.2383824688	0.0296821843
C12	3.0356475321	-0.1777121461	0.0451090946
C13	3.7266096263	1.0508851090	0.0209406940
C14	3.0152830502	2.2315786127	-0.0218251103
Cu15	0.5370967813	-1.9424442907	0.0635015526
C16	0.1629861402	-3.8279421576	0.1438201439
C17	-0.8175940219	-4.7187346041	0.0255867006
N18	-0.7766298998	-6.0595184458	0.4615059976
N19	0.3107521634	-6.3863084653	1.0466905712
N20	1.2987543318	-5.5623313659	1.1548146734
C21	2.3942682535	-6.0301673314	2.0234587849
Cu22	2.0421370339	-3.9545834051	0.1187356017
C23	3.9097389556	-3.5643276478	-0.0755072261
C24	5.1017130894	-3.2985100273	-0.1924007120
H25	3.5672816858	-1.1290956458	0.0681801682
H26	4.8112377578	1.0466197618	0.0357934681
H27	3.5243854361	3.1916707267	-0.0399898848
H28	-2.7019579014	-1.5644442928	-0.0247478848
H29	-4.2507139223	0.4015639159	-0.1145184645
H30	-3.2780514660	2.7052639517	-0.1610956198
H31	1.2610503398	4.3371536831	-0.1138769523
H32	-1.1968720128	4.1663267998	-0.1576442081
H33	-1.7686359585	-4.4528065851	-0.4317609385
H34	6.1428474998	-3.0917977618	-0.3013567528
H35	2.4193552046	-5.4350529854	2.9433187875
H36	2.2287000939	-7.0799635906	2.2789121692
H37	3.3509174051	-5.9086262227	1.5105870168

SCFE: SCF energy: DFT(b3lyp) -1321.61159264631 hartrees

Thermodynamic properties calculated assuming an ideal gas

In the table below, the units for temperature
are kelvins, the units for U, H, and G are
kcal/mol and the units for Cv and S are cal/(mol K)

The zero point energy (ZPE): 166.545 kcal/mol
is not included in U, H, or G in the table below

T = 298.15 K

	U	Cv	S	H	G
trans.	0.889	2.981	43.946	1.481	-11.621
rot.	0.889	2.981	35.445	0.889	-9.679
vib.	12.166	76.096	84.050	12.166	-12.894
elec.	0.000	0.000	0.000	0.000	0.000
total	13.943	82.057	163.441	14.536	-34.194

Total internal energy, Utot (SCFE + ZPE + U): -1321.323966 hartrees
Total enthalpy, Htot (Utot + pV): -1321.323022 hartrees
Total Gibbs free energy, Gtot (Htot - T*S): -1321.400678 hartrees

Single point B3LYP/LACV3P++//B3LYP/LACVP****

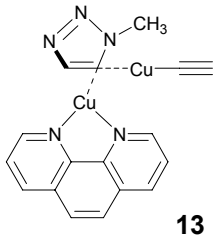
Energy components, in hartrees:

(A)	Nuclear repulsion.....	2366.84239660204	
(E)	Total one-electron terms.....	-6674.14882907819	
(I)	Total two-electron terms.....	2985.42075852222	
(J)	Coulomb.....	3154.82392700087	
(K)	Exchange+Correlation.....	-169.40316847865	
(L)	Electronic energy.....	-3688.72807055597	(E+I)
(N)	Total energy.....	-1321.88567395393	(A+L)

SCFE: SCF energy: DFT(b3lyp) -1321.88567395393 hartrees

HOMO energy: -0.19998
LUMO energy: -0.11277

Total Gibbs free energy at the B3LYP/LACV3P**++//B3LYP/LACVP** level of theory: -1321.674759 hartrees



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C1	2.9435614379	2.2132778264	-0.0162264492
C2	1.5416732248	2.0780665890	0.1107969714
C3	1.0161609755	0.7639251952	0.0928906573
N4	1.7979676869	-0.3377463454	-0.0425614830
C5	3.1145898850	-0.1862608374	-0.1660397074
C6	3.7251357954	1.0850577360	-0.1548200742
C7	-0.4105848764	0.5679170543	0.2171065713
C8	-1.2645388244	1.6905718630	0.3476133614
C9	-0.6970429817	3.0088977740	0.3630488611
C10	0.6487089816	3.1934623556	0.2509501172
C11	-2.6509962114	1.4367616963	0.4553964259
C12	-3.1121738174	0.1356645104	0.4301761671
C13	-2.1837733410	-0.9147948789	0.3003321302
N14	-0.8771628571	-0.7056831631	0.1988275194
Cu15	0.6987101823	-2.1510815668	0.0180871328
Cu16	2.4027315202	-3.8730634118	-0.3072764394
C17	4.2408306874	-3.5611655721	-0.5895233569
C18	5.4287782894	-3.2922927111	-0.7401484880
C19	0.4733917804	-4.1670533830	0.0985537655
C20	-0.4576288488	-4.7636101734	-0.7625303132
N21	-1.2574876884	-5.6361060266	-0.0921498067
N22	-0.8895773493	-5.6398208652	1.1657480590
N23	0.1311667131	-4.7725890025	1.2944755957
C24	0.7532321894	-4.6099568643	2.5994682547
H25	3.7017844898	-1.0971569998	-0.2817311435
H26	4.8028438816	1.1561398380	-0.2568814082
H27	3.3889457754	3.2047773285	-0.0052915113
H28	-2.5077311377	-1.9520093584	0.2766135959
H29	-4.1702561977	-0.0898005031	0.5090848576
H30	-3.3413014056	2.2697587161	0.5559026817
H31	1.0692955322	4.1952307965	0.2637421160
H32	-1.3639551788	3.8603908805	0.4660376882
H33	-0.5727416646	-4.6097233277	-1.8269064964
H34	6.4659744536	-3.0811366472	-0.8760141003
H35	0.6452851984	-3.5803453538	2.9534544223
H36	0.2500872431	-5.2883324632	3.2890037094
H37	1.8166284194	-4.8576840167	2.5483213478

SCFE: SCF energy: DFT(b3lyp) -1321.70004994811 hartrees

Thermodynamic properties calculated assuming an ideal gas

In the table below, the units for temperature
are kelvins, the units for U, H, and G are
kcal/mol and the units for Cv and S are cal/(mol K)

The zero point energy (ZPE): 168.575 kcal/mol
is not included in U, H, or G in the table below

T = 298.15 K

	U	Cv	S	H	G
trans.	0.889	2.981	43.946	1.481	-11.621
rot.	0.889	2.981	35.374	0.889	-9.658
vib.	12.440	75.931	88.455	12.440	-13.933
elec.	0.000	0.000	0.000	0.000	0.000
total	14.218	81.893	167.775	14.810	-35.212

Total internal energy, Utot (SCFE + ZPE + U): -1321.408750 hartrees
Total enthalpy, Htot (Utot + pV): -1321.407806 hartrees
Total Gibbs free energy, Gtot (Htot - T*S): -1321.487522 hartrees

Single point B3LYP/LACV3P++//B3LYP/LACVP****

Energy components, in hartrees:

(A)	Nuclear repulsion.....	2394.72247115924	
(E)	Total one-electron terms.....	-6730.34545926369	
(I)	Total two-electron terms.....	3013.65323034797	
(J)	Coulomb.....	3183.18512590045	
(K)	Exchange+Correlation.....	-169.53189555248	
(L)	Electronic energy.....	-3716.69222891572	(E+I)
(N)	Total energy.....	-1321.96975775648	(A+L)

SCFE: SCF energy: DFT(b3lyp) -1321.96975775648 hartrees

HOMO energy: -0.20455
LUMO energy: -0.11001

Total Gibbs free energy at the B3LYP/LACV3P**++//B3LYP/LACVP** level of theory: -1321.757230 hartrees

Phenanthroline

N1	0.0000000000	1.3792503950	1.5425677347
C2	0.0000000000	2.7016169153	1.5286747241
C3	0.0000000000	3.4803930276	0.3527994603
C4	0.0000000000	2.8282364626	-0.8616764155
C5	0.0000000000	1.4159510676	-0.8911340946
C6	0.0000000000	0.7286642068	0.3565398350
H7	0.0000000000	3.1921597837	2.5016917737
H8	0.0000000000	4.5642509836	0.4140235739
H9	0.0000000000	3.3817685481	-1.7975186410
C10	0.0000000000	0.6801748887	-2.1223599950
C11	0.0000000000	-0.7286642068	0.3565398350
N12	0.0000000000	-1.3792503950	1.5425677347
C13	0.0000000000	-2.7016169153	1.5286747241
C14	0.0000000000	-3.4803930276	0.3527994603
C15	0.0000000000	-2.8282364626	-0.8616764155
C16	0.0000000000	-1.4159510676	-0.8911340946
H17	0.0000000000	-3.1921597837	2.5016917737
H18	0.0000000000	-4.5642509836	0.4140235739
H19	0.0000000000	-3.3817685481	-1.7975186410
C20	0.0000000000	-0.6801748887	-2.1223599950
H21	0.0000000000	1.2340409097	-3.0578313218
H22	0.0000000000	-1.2340409097	-3.0578313218

SCFE: SCF energy: DFT(b3lyp) -571.60975232189 hartrees

Thermodynamic properties calculated assuming an ideal gas

In the table below, the units for temperature
are kelvins, the units for U, H, and G are
kcal/mol and the units for Cv and S are cal/(mol K)
The zero point energy (ZPE): 107.262 kcal/mol
is not included in U, H, or G in the table below

T = 298.15 K

	U	Cv	S	H	G
trans.	0.889	2.981	41.471	1.481	-10.884
rot.	0.889	2.981	29.685	0.889	-7.962
vib.	3.963	32.501	21.665	3.963	-2.496
elec.	0.000	0.000	0.000	0.000	0.000
total	5.741	38.463	92.822	6.333	-21.342

Total internal energy, Utot (SCFE + ZPE + U): -571.429672 hartrees
Total enthalpy, Htot (Utot + pV): -571.428728 hartrees
Total Gibbs free energy, Gtot (Htot - T*S): -571.472830 hartrees

Single point B3LYP/LACV3P**++//B3LYP/LACVP**

Energy components, in hartrees:

(A)	Nuclear repulsion.....	785.99156597207	
(E)	Total one-electron terms.....	-2331.02081263245	
(I)	Total two-electron terms.....	973.28278753366	
(J)	Coulomb.....	1055.31705292381	
(K)	Exchange+Correlation.....	-82.03426539015	
(L)	Electronic energy.....	-1357.73802509878	(E+I)
(N)	Total energy.....	-571.74645912671	(A+L)

SCFE: SCF energy: DFT(b3lyp) -571.74645912671 hartrees

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 HOMO energy:    -0.24251
 LUMO energy:    -0.06697

Total Gibbs free energy at the B3LYP/LACV3P**++//B3LYP/LACVP** level of
theory: -571.609537 hartrees
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Water

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  O1           -0.0543064429     -0.0383998832      0.0000000000
  H2           -0.0079437643      0.9254034739      0.0000000000
  H3            0.8698264229     -0.3159694604      0.0000000000

SCFE: SCF energy: DFT(b3lyp)       -76.41813458182 hartrees

  Thermodynamic properties calculated assuming an ideal gas

  In the table below, the units for temperature
  are kelvins, the units for U, H, and G are
  kcal/mol and the units for Cv and S are cal/(mol K)

  The zero point energy (ZPE):     13.413 kcal/mol
  is not included in U, H, or G in the table below


  T =   298.15 K

             U         Cv          S          H          G
         ---------  ---------  ---------  ---------  ---------
  trans.      0.889      2.981     34.609      1.481     -8.837
    rot.      0.889      2.981     10.498      0.889     -2.241
    vib.      0.002      0.042      0.006      0.002      0.000
   elec.      0.000      0.000      0.000      0.000      0.000
   total      1.779      6.004     45.113      2.372    -11.079

  Total internal energy, Utot (SCFE + ZPE + U):     -76.393924 hartrees
             Total enthalpy, Htot (Utot + pV):     -76.392980 hartrees
    Total Gibbs free energy, Gtot (Htot - T*S):     -76.414414 hartrees
```

Single point B3LYP/LACV3P**++//B3LYP/LACVP**

```
 Energy components, in hartrees:
   (A)  Nuclear repulsion.............       9.12273151382
   (E)  Total one-electron terms.....    -122.90349122497
   (I)  Total two-electron terms.....      37.32227170169
   (J)    Coulomb....................      46.65436804918
   (K)    Exchange+Correlation.......      -9.33209634749
   (L)  Electronic energy............     -85.58121952328  (E+I)
   (N)  Total energy.................     -76.45848800946  (A+L)

 SCFE: SCF energy: DFT(b3lyp)       -76.45848800946 hartrees


 HOMO energy:    -0.32304
 LUMO energy:    -0.02366

Total Gibbs free energy at the B3LYP/LACV3P**++//B3LYP/LACVP** level of
theory: -76.454767 hartrees
```

Acetylene

H1	0.0000000000	0.0000000000	1.6682700682
C2	0.0000000000	0.0000000000	0.6026559375
C3	0.0000000000	0.0000000000	-0.6026559375
H4	0.0000000000	0.0000000000	-1.6682700682

SCFE: SCF energy: DFT(b3lyp) -77.32785505378 hartrees

Thermodynamic properties calculated assuming an ideal gas

In the table below, the units for temperature
are kelvins, the units for U, H, and G are
kcal/mol and the units for Cv and S are cal/(mol K)

The zero point energy (ZPE): 16.823 kcal/mol
is not included in U, H, or G in the table below

T = 298.15 K

	U	Cv	S	H	G
trans.	0.889	2.981	35.705	1.481	-9.164
rot.	0.592	1.987	10.886	0.592	-2.653
vib.	0.327	3.563	1.449	0.327	-0.105
elec.	0.000	0.000	0.000	0.000	0.000
total	1.808	8.531	48.040	2.401	-11.922

Total internal energy, Utot (SCFE + ZPE + U): -77.298165 hartrees
Total enthalpy, Htot (Utot + pV): -77.297221 hartrees
Total Gibbs free energy, Gtot (Htot - T*S): -77.320046 hartrees

Single point B3LYP/LACV3P**++//B3LYP/LACVP**

Energy components, in hartrees:

(A)	Nuclear repulsion.....	24.71935098966	
(E)	Total one-electron terms.....	-151.82531060121	
(I)	Total two-electron terms.....	49.74956231116	
(J)	Coulomb.....	61.25095446930	
(K)	Exchange+Correlation.....	-11.50139215814	
(L)	Electronic energy.....	-102.07574829004	(E+I)
(N)	Total energy.....	-77.35639730038	(A+L)

SCFE: SCF energy: DFT(b3lyp) -77.35639730038 hartrees

HOMO energy: -0.30074
LUMO energy: 0.00380

Total Gibbs free energy at the B3LYP/LACV3P**++//B3LYP/LACVP** level of theory: -77.348588 hartrees

Methyl azide

N1	-0.3142177005	-0.5397902912	0.0000000000
N2	-0.4148140858	-1.6785638529	0.0000000000
N3	-0.3564115962	0.6942584838	0.0000000000
C4	0.9469692964	1.3814168407	0.0000000000
H5	0.7339304113	2.4502254343	0.0000000000
H6	1.5360994802	1.1388999252	0.8926675981
H7	1.5360994802	1.1388999252	-0.8926675981

SCFE: SCF energy: DFT(b3lyp) -204.09199301919 hartrees

Thermodynamic properties calculated assuming an ideal gas

In the table below, the units for temperature
are kelvins, the units for U, H, and G are
kcal/mol and the units for Cv and S are cal/(mol K)

The zero point energy (ZPE): 31.672 kcal/mol
is not included in U, H, or G in the table below

T = 298.15 K

	U	Cv	S	H	G
trans.	0.889	2.981	38.044	1.481	-9.862
rot.	0.889	2.981	23.126	0.889	-6.006
vib.	1.023	7.038	6.187	1.023	-0.822
elec.	0.000	0.000	0.000	0.000	0.000
total	2.801	12.999	67.357	3.393	-16.690

Total internal energy, Utot (SCFE + ZPE + U): -204.037058 hartrees
Total enthalpy, Htot (Utot + pV): -204.036114 hartrees
Total Gibbs free energy, Gtot (Htot - T*S): -204.068117 hartrees

Single point B3LYP/LACV3P**++//B3LYP/LACVP**

Energy components, in hartrees:

(A)	Nuclear repulsion.....	107.76510459429	
(E)	Total one-electron terms.....	-488.24018441900	
(I)	Total two-electron terms.....	176.32203321066	
(J)	Coulomb.....	203.50191908918	
(K)	Exchange+Correlation.....	-27.17988587852	
(L)	Electronic energy.....	-311.91815120834	(E+I)
(N)	Total energy.....	-204.15304661405	(A+L)

SCFE: SCF energy: DFT(b3lyp) -204.15304661405 hartrees

HOMO energy: -0.26653
LUMO energy: -0.04718

Total Gibbs free energy at the B3LYP/LACV3P**++//B3LYP/LACVP** level of theory: -204.129171 hartrees

N-Methyl triazole

N1	0.4462100953	0.4682273847	0.0000000000
N2	-0.9021448022	0.5919794960	0.0000000000
C3	0.8065222084	-0.8405832800	0.0000000000
C4	1.2825831922	1.6546852073	0.0000000000
H5	1.8359001569	-1.1641563816	0.0000000000
C6	-0.3918753929	-1.5185025651	0.0000000000
N7	-1.4087116199	-0.6101822539	0.0000000000
H8	-0.5780951902	-2.5821860177	0.0000000000
H9	0.6143437101	2.5158837719	0.0000000000
H10	1.9136367891	1.6824182761	0.8927958067
H11	1.9136367891	1.6824182761	-0.8927958067

SCFE: SCF energy: DFT(b3lyp) -281.53889733519 hartrees

Thermodynamic properties calculated assuming an ideal gas

In the table below, the units for temperature
are kelvins, the units for U, H, and G are
kcal/mol and the units for Cv and S are cal/(mol K)

The zero point energy (ZPE): 54.572 kcal/mol
is not included in U, H, or G in the table below

T = 298.15 K

	U	Cv	S	H	G
trans.	0.889	2.981	39.165	1.481	-10.196
rot.	0.889	2.981	25.615	0.889	-6.748
vib.	1.488	11.829	8.706	1.488	-1.107
elec.	0.000	0.000	0.000	0.000	0.000
total	3.266	17.790	73.485	3.858	-18.051

Total internal energy, Utot (SCFE + ZPE + U): -281.446726 hartrees
Total enthalpy, Htot (Utot + pV): -281.445782 hartrees
Total Gibbs free energy, Gtot (Htot - T*S): -281.480697 hartrees

Single point B3LYP/LACV3P**++//B3LYP/LACVP**

Energy components, in hartrees:

(A)	Nuclear repulsion.....	228.29013424554	
(E)	Total one-electron terms.....	-831.93097817865	
(I)	Total two-electron terms.....	322.02528452580	
(J)	Coulomb.....	360.89839671754	
(K)	Exchange+Correlation.....	-38.87311219174	
(L)	Electronic energy.....	-509.90569365285	(E+I)
(N)	Total energy.....	-281.61555940731	(A+L)

SCFE: SCF energy: DFT(b3lyp) -281.61555940731 hartrees

HOMO energy: -0.27223
LUMO energy: -0.02258

Total Gibbs free energy at the B3LYP/LACV3P**++//B3LYP/LACVP** level of theory: -281.557359 hartrees

[3+2] cycloaddition transition state

C1	0.8824981705	-1.4298464945	-0.3090970430
C2	-0.2483630018	-1.9176419840	-0.2698074542
N3	-1.5687681524	-0.2722846575	0.2014193435
N4	-0.7548903712	0.5682886223	0.2594269251
N5	0.4988516198	0.6845612132	0.2358122409
C6	1.0994459633	1.9640339681	-0.1325609097
H7	1.9373279975	-1.2915760198	-0.3794235886
H8	0.9035575636	2.7367814682	0.6197948254
H9	2.1783405394	1.7999076726	-0.1726850735
H10	0.7636056899	2.3232304084	-1.1130234615
H11	-1.0283392066	-2.6435803897	-0.3262178874

SCFE: SCF energy: DFT(b3lyp) -281.39421898890 hartrees

Thermodynamic properties calculated assuming an ideal gas

In the table below, the units for temperature
are kelvins, the units for U, H, and G are
kcal/mol and the units for Cv and S are cal/(mol K)

The zero point energy (ZPE): 49.659 kcal/mol
is not included in U, H, or G in the table below

T = 298.15 K

	U	Cv	S	H	G
trans.	0.889	2.981	39.165	1.481	-10.196
rot.	0.889	2.981	26.425	0.889	-6.990
vib.	2.469	16.854	14.993	2.469	-2.001
elec.	0.000	0.000	0.000	0.000	0.000
total	4.246	22.815	80.582	4.839	-19.187

Total internal energy, Utot (SCFE + ZPE + U): -281.308314 hartrees
Total enthalpy, Htot (Utot + pV): -281.307370 hartrees
Total Gibbs free energy, Gtot (Htot - T*S): -281.345657 hartrees

Single point B3LYP/LACV3P**++//B3LYP/LACVP**

Energy components, in hartrees:

(A)	Nuclear repulsion.....	208.72077718009	
(E)	Total one-electron terms.....	-793.01525105918	
(I)	Total two-electron terms.....	302.81579427823	
(J)	Coulomb.....	341.49754389339	
(K)	Exchange+Correlation.....	-38.68174961516	
(L)	Electronic energy.....	-490.19945678095	(E+I)
(N)	Total energy.....	-281.47867960086	(A+L)

SCFE: SCF energy: DFT(b3lyp) -281.47867960086 hartrees

HOMO energy: -0.25528
LUMO energy: -0.06555

Total Gibbs free energy at the B3LYP/LACV3P**++//B3LYP/LACVP** level of theory: -281.430118 hartrees

Total Gibbs free energy at the B3LYP/LACV3P**++//B3LYP/LACVP** level of theory for ¼ of **1** plus MeN_3 plus H_2O: -553.563745 hartrees

Total Gibbs free energy at the B3LYP/LACV3P**++//B3LYP/LACVP** level of theory for **1** plus MeN_3: -1296.048398 hartrees

Total Gibbs free energy at the B3LYP/LACV3P**++//B3LYP/LACVP** level of theory for ½ of **1** plus MeN_3 plus phenanthroline: -1321.698322 hartrees