Electronic Supplementary Material (ESI) for RSC Advances.

Supplementary information

DFT and AFIR Study on the Copper (I)-Catalyzed Mechanism of 5-Enamine-Trisubstituted-1, 2, 3-Triazole Synthesis via C-N Cross-Coupling and the Origin of Ring-Opening of *2H*-Azirines

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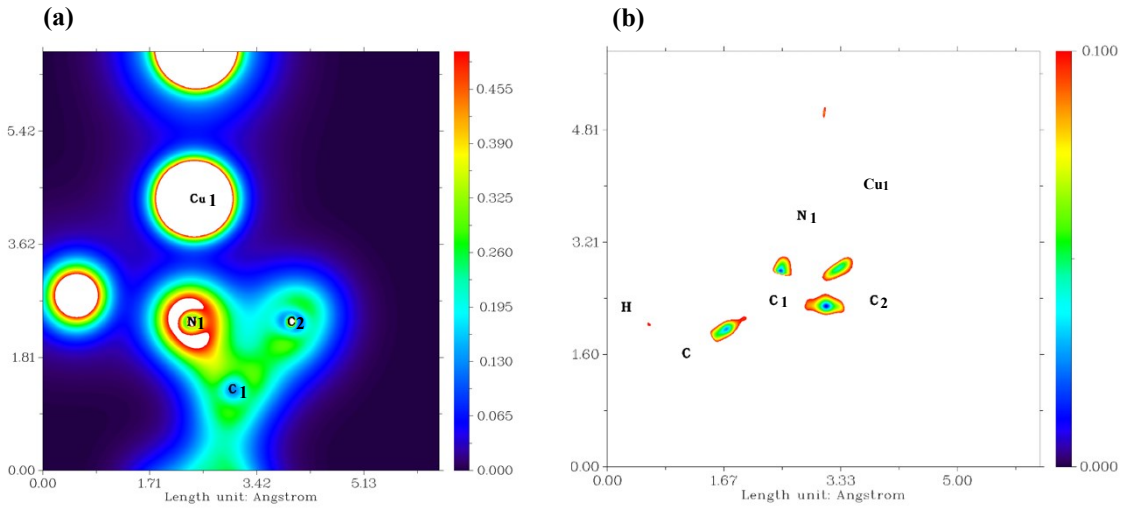


Figure S1. (a) Color-filled plots of the valence electron density and (b) reduced density gradient (RDG) on the C1-C2-Cu1 plane for P2-3s.

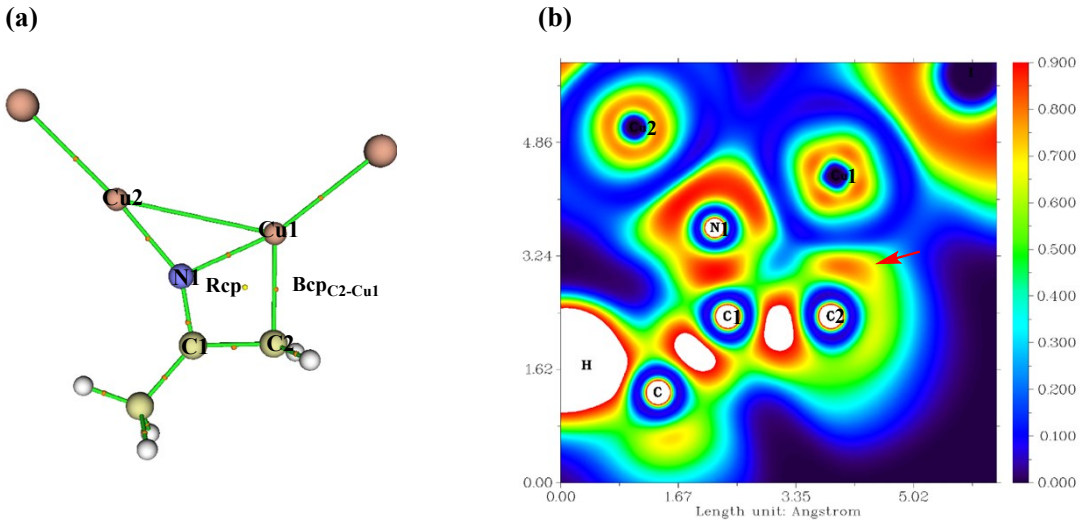


Figure S2. (a) The molecular graph of P2-3s with AIM analysis. (b) Color-filled map of electron localization fuction (ELF) for P2-3s.

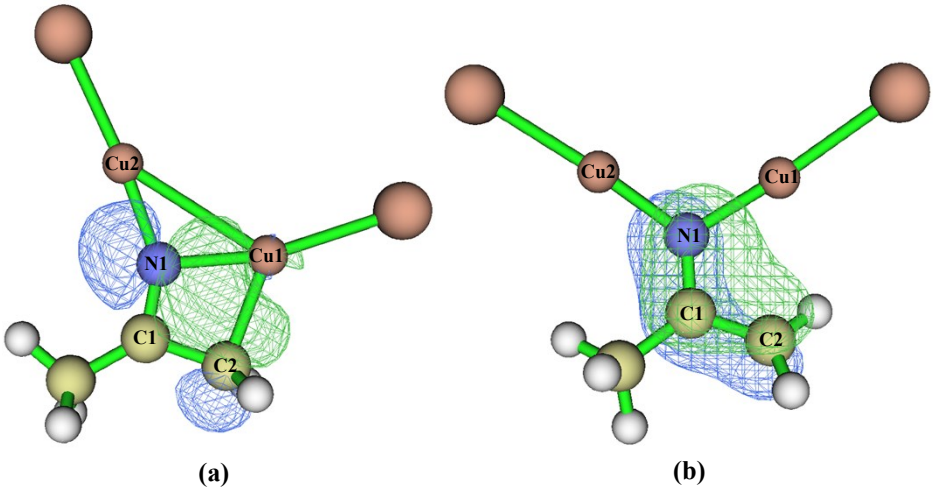


Figure S3. Map of localized molecular orbital (LMO) of (a) P2-TS2s and (b) P2-3s

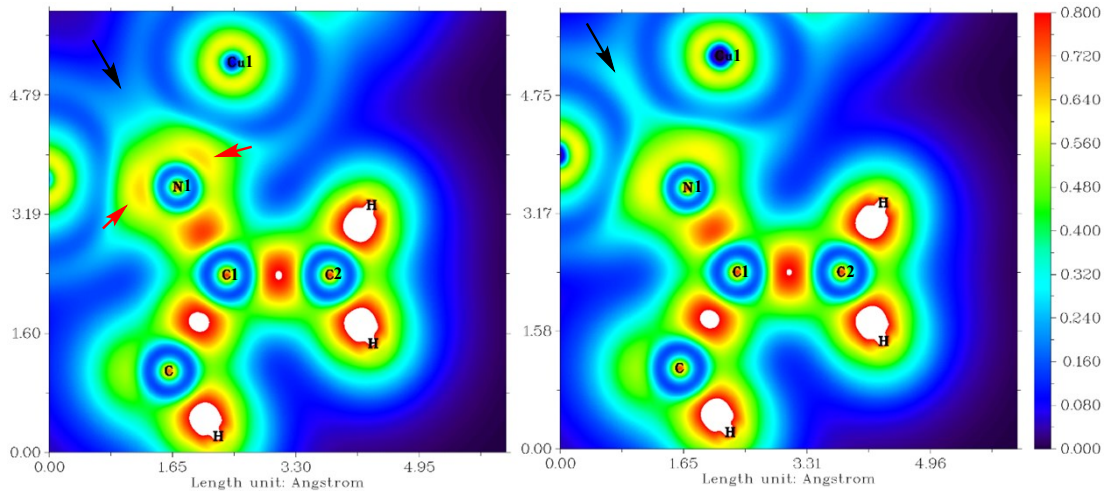


Figure S4. Color-filled map of localized orbital locator (LOL) for (a) P2-4s and (b) P2-4t on the C1-C2-N1 plane. The region where electron density higher than the upper limit of color scale is depicted as white.

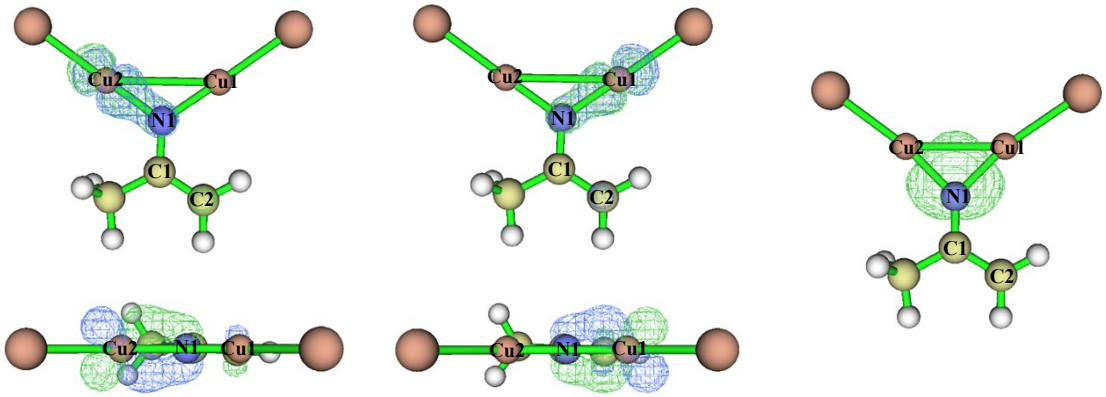


Figure S5. Map of localized molecular orbital (LMO) of P2-4s and P2-4t

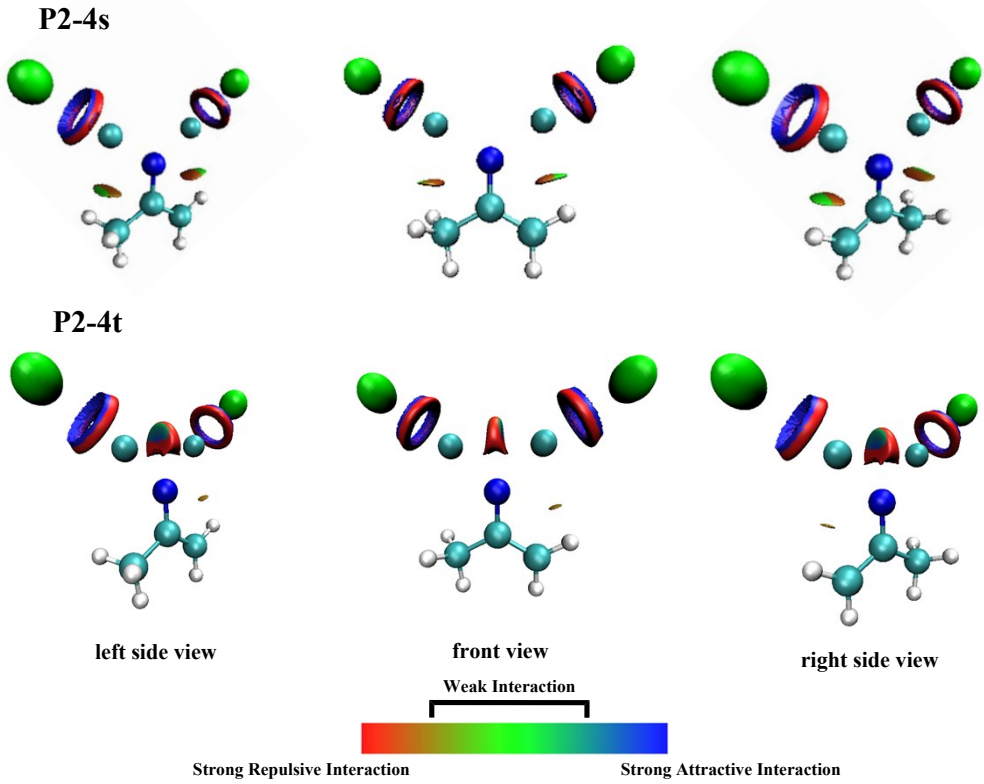


Figure S6. Gradient Isosurfaces (s = 0.5 a.u.) of P2-4s and P2-4t. The surfaces are colored on a blue-green-red scale according to values of sign(λ_2)ρ, ranging from -0.04 to +0.02 a.u.. Blue indicates strong attractive interactions, and red indicates strong non-bonded overlap.

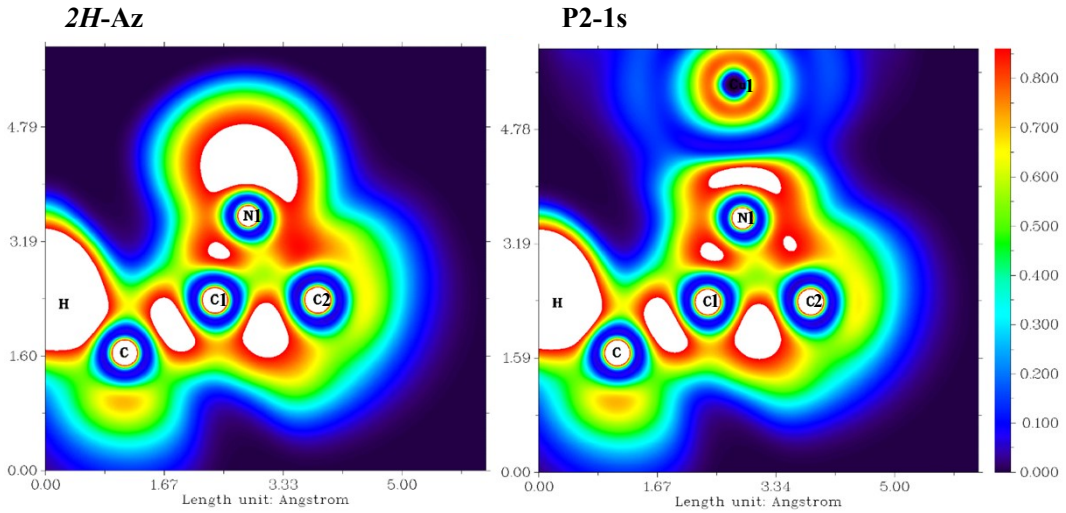


Figure S7. Color-filled map of electron localization function (ELF) for (a) *2H*-Az and (b) P2-1s on the C1-C2-N1 plane. The region where electron density higher than the upper limit of color scale is depicted as white.

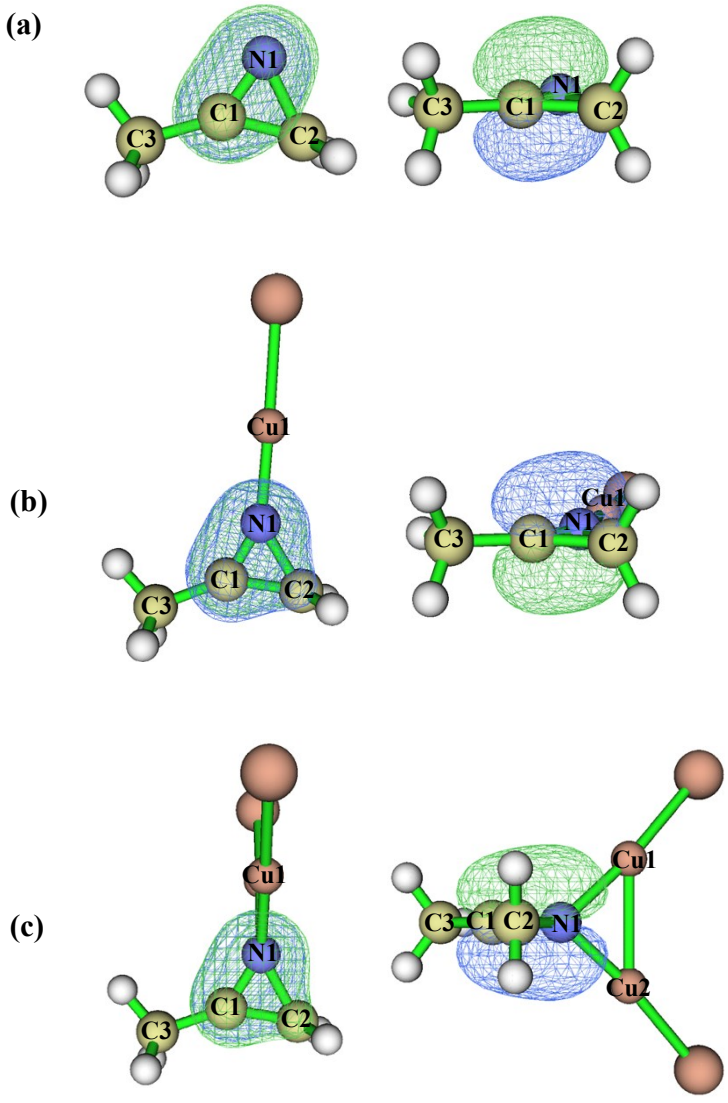


Figure S8. Ring π bond plotted by AdNDP (a) 2H-Az (b) P2-1s and (c)P2-2s.

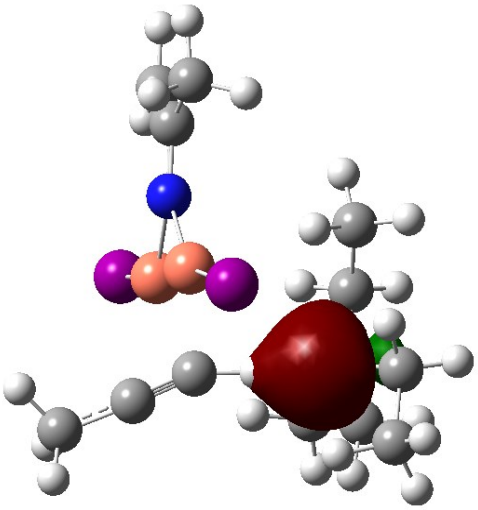


Figure S9. Highest occupied molecular orbital (HOMO) of P2-6t.

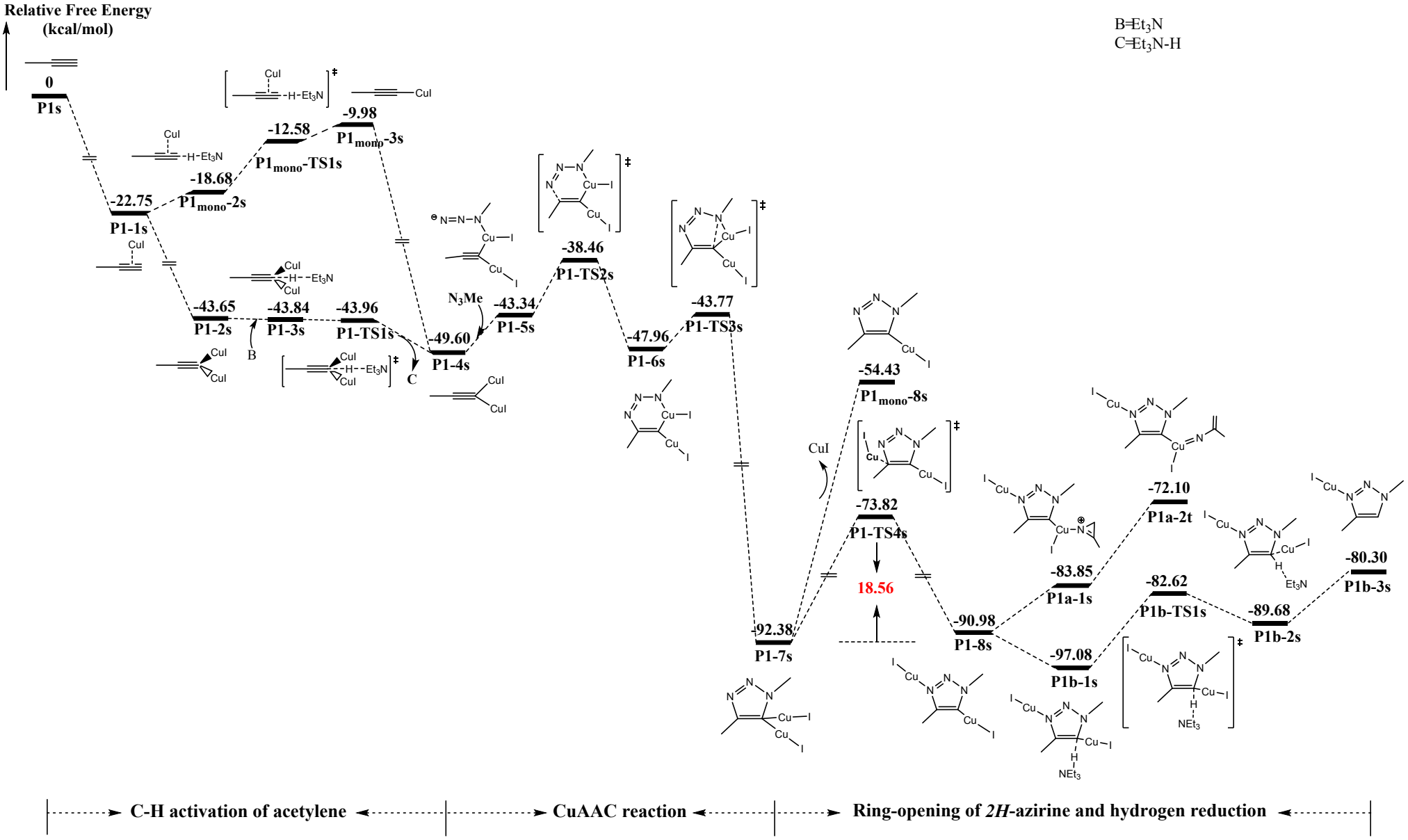


Figure S10. The potential energy surface profiles for the 5-"Interrupted" click reaction (named as Path 1).

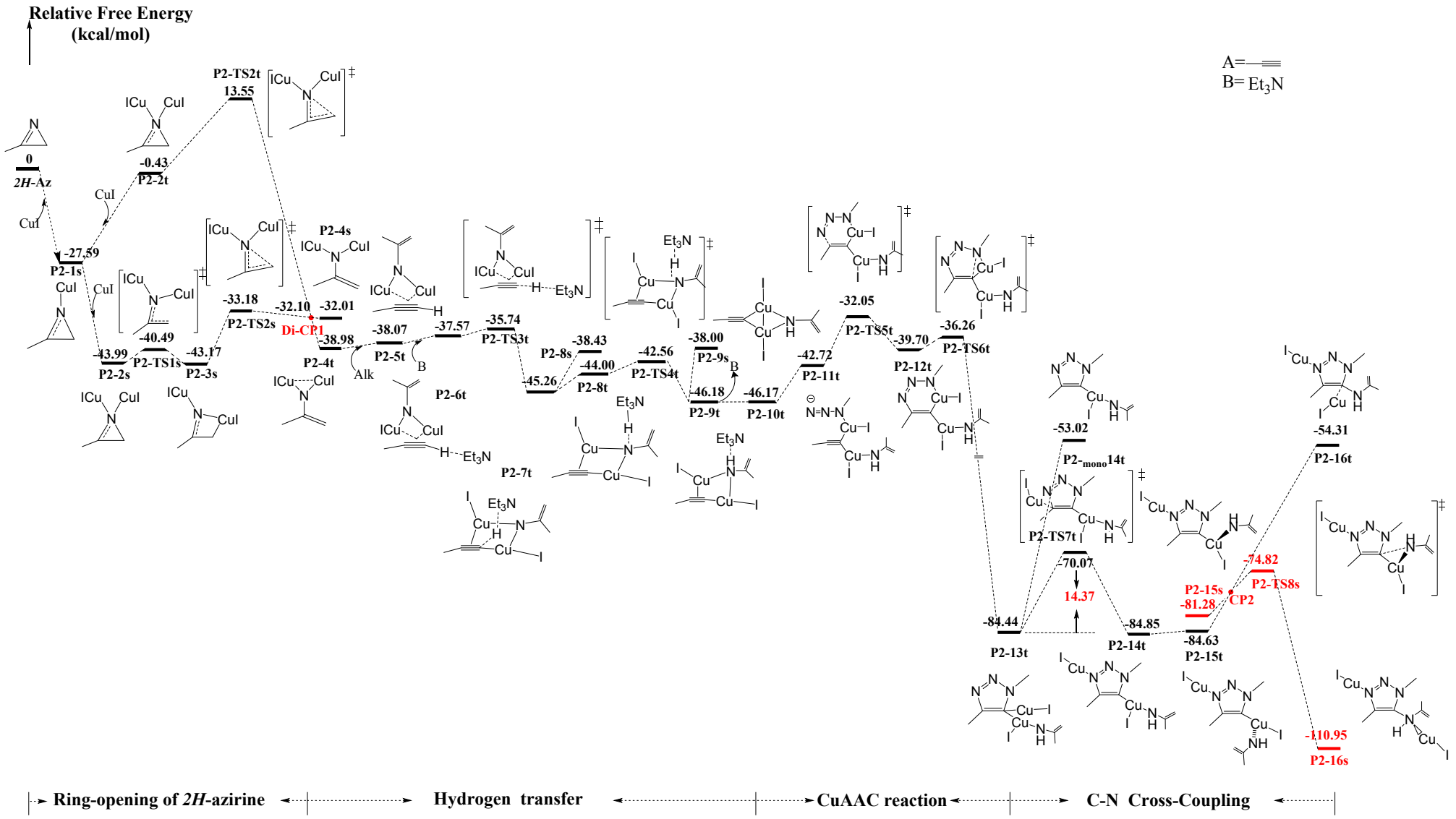


Figure S11. Total potential energy surface profiles discussed in the text (named as Path 2).

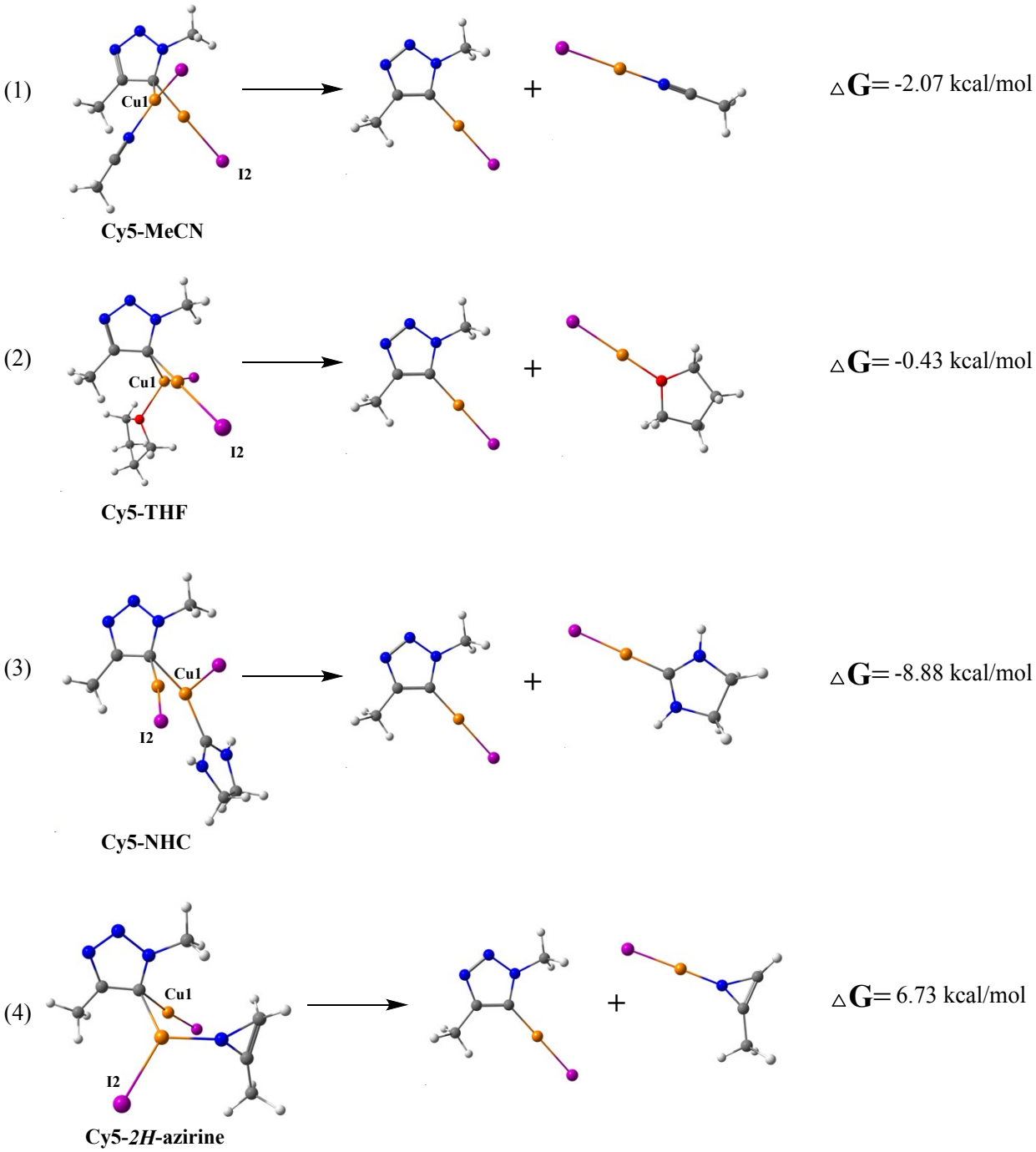
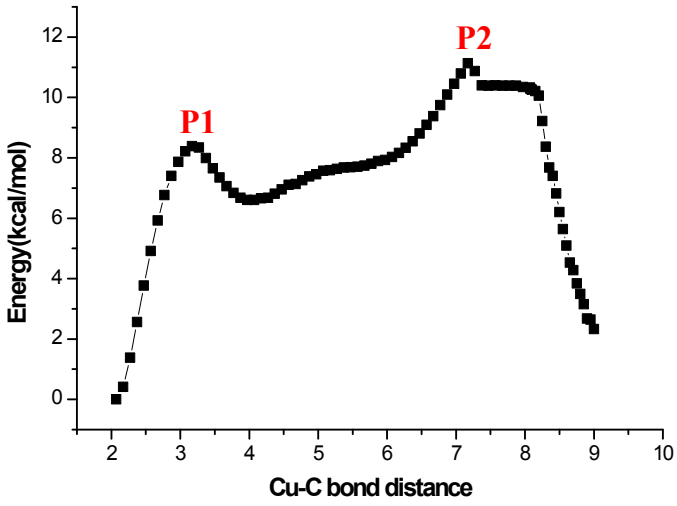
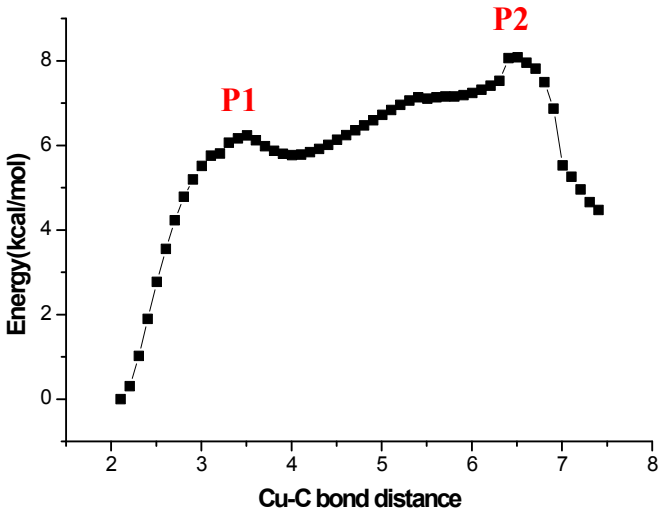


Figure S12. Calculated free Gibbs energies (kcal/mol) for (1) Cy5-MeCN, (2) Cy5-THF, (3) Cy5-NHC and (4) Cy5-*2H*-azirine chemical reactions from dicopper to monocopper 1,2,3-triazole.

(a)



(b)



(c)

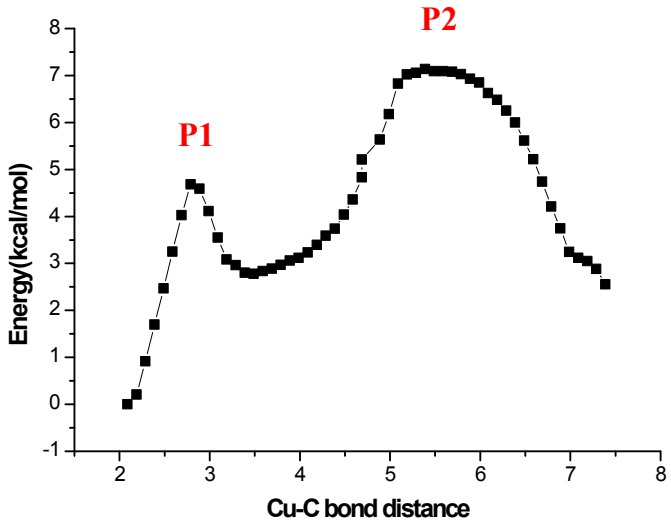


Figure S13. Potential energy scan along the Cu-C bond distances (Å) with the step size 0.1 Å for (a)Cy5-MeCN, (b)Cy5-THF and (b)Cy5-NHC.

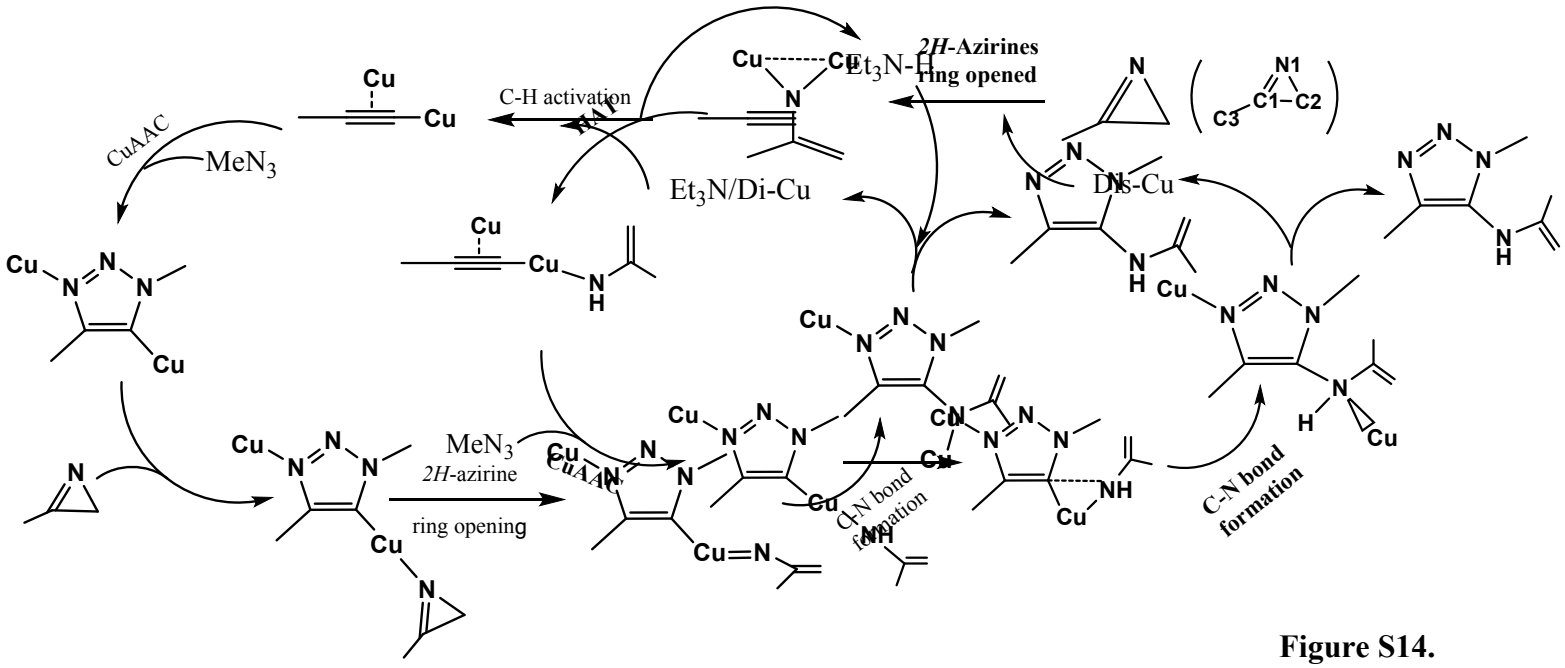


Figure S14.

Detailed reaction processes by dicopper(I) catalyst.

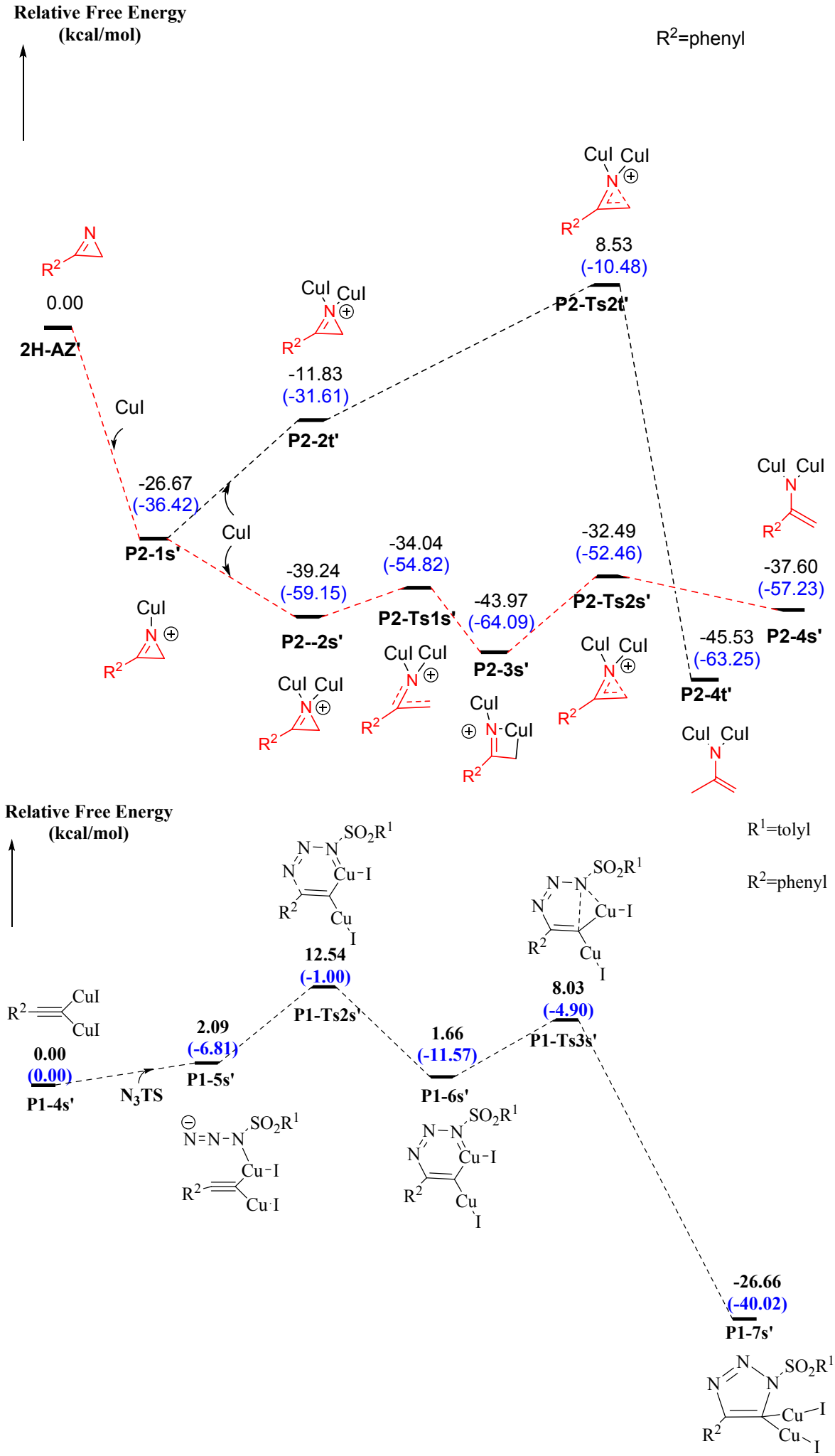


Figure S15. Calculated energy profiles of binuclear 3-phenyl-2H-azirine ring-opening and [3+2] cycloaddition in the

phenylacetylene and TsN_3 reaction. The relative Gibbs and total energies calculated at the (U)M06-L-D3BJ-IEFPCM/6-31+G(d,p)/Lanl2TZ+ level in dichloromethane are given in kcal/mol.

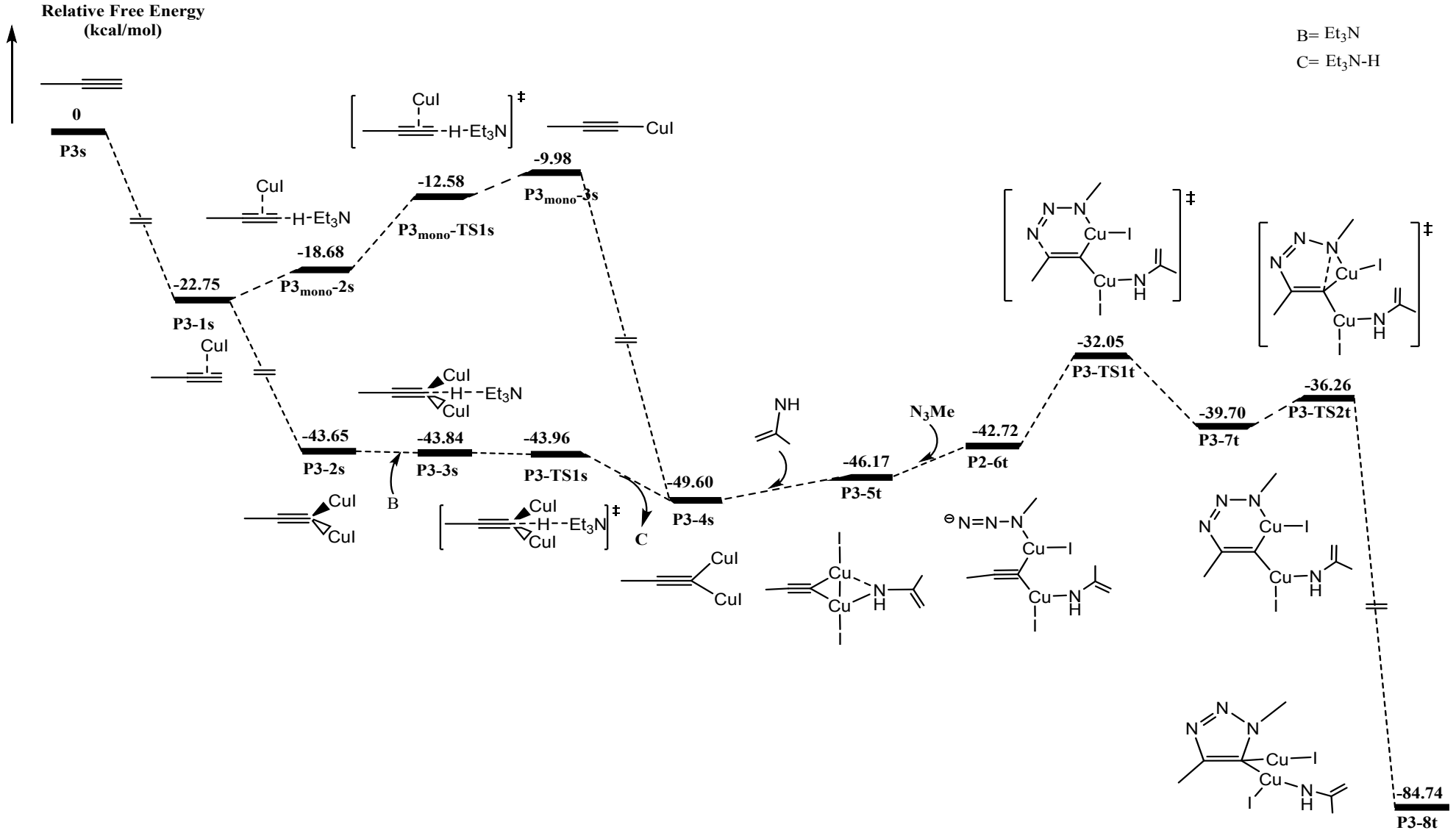


Figure S16. Calculated energy profiles of the formation of dinuclear Cu(I)-acetylide from alkyne and copper iodide followed by the ring-opening of 2H-Azirines to form P2-10t and finally [3+2] cycloaddition. The relative Gibbs and total energies calculated at the (U)M06-L-D3BJ-IEFPCM/6-31+G(d,p)/Lanl2TZ+ level in dichloromethane are given in kcal/mol. (named as Path 3).

Table S1. Atom contributions of π orbital of P2-1s and P2-2s with AdNDP by B3LYP method (unit:%)

	N1	**C1**	**C2**	**Cu***
P2-1s	53.92	33.15	7.92	3.84
P2-2s	50.96	28.22	7.02	12.86

*Total contributions from two copper.

Table S2. RFC of *2H*-Az, P2-1s and P2-2s on N1-C2 and C1-C2 bond (unit: mdyn/Å).

	***2H*-Az**	**P2-1s**	**P2-2s**
N1-C2	3.175	3.300	3.165
C1-C2	5.848	5.650	5.618

Table S3. Optimized Cartesian coordinates and corresponding energies at M06-L/6-31G*/LANL2TZ+ level for all reactants, intermediates, transition states and products in Path1.

P1-1s

E= -324.3033204 a.u.

ZPE_G= 0.022975 a.u.

G= -324.280345 au

C	2.572436000	-1.230237000	0.020743000
H	2.645172000	-2.303704000	0.034361000
C	2.838553000	-0.020807000	0.010230000
C	3.370142000	1.332042000	0.002666000
H	3.040726000	1.896865000	0.880490000
H	4.465465000	1.288933000	0.013923000
H	3.058244000	1.880652000	-0.891694000
Cu	0.798879000	-0.345315000	-0.015030000
I	-1.590666000	0.151093000	-0.055400000

$P1_{mono}$-2s

E= -616.6781317 a.u.

ZPE_G= -0.214664 a.u.

G= -616.463468 au

N	2.708140000	-0.708370000	0.017878000
C	4.034559000	-0.617742000	-0.607109000
C	1.849913000	-1.662713000	-0.699745000
C	2.834259000	-1.110357000	1.427405000
C	4.791924000	0.634710000	-0.213022000
C	1.389087000	-1.176630000	-2.059943000
C	1.599224000	-0.823006000	2.259318000
H	3.893834000	-0.617833000	-1.693661000
H	4.627915000	-1.524168000	-0.370812000
H	0.965157000	-1.843698000	-0.075623000
H	2.366243000	-2.640110000	-0.792302000
H	3.683517000	-0.564314000	1.854673000
H	3.097578000	-2.186058000	1.485776000
H	5.765679000	0.663073000	-0.714503000
H	4.980990000	0.691634000	0.865154000
H	4.236904000	1.534964000	-0.503271000
H	0.693172000	-1.901289000	-2.497049000
H	2.213543000	-1.045310000	-2.769950000

H	0.858431000	-0.218117000	-1.981277000
H	1.754717000	-1.161903000	3.289675000
H	0.704742000	-1.334812000	1.883233000
H	1.380826000	0.251318000	2.291710000
C	0.939813000	1.765485000	-0.043497000
H	1.732900000	0.993442000	-0.038484000
C	0.138310000	2.709884000	-0.040952000
C	-0.587742000	3.971345000	-0.046974000
H	-1.227071000	4.070207000	0.836155000
H	0.124097000	4.804657000	-0.048649000
H	-1.222449000	4.062406000	-0.934468000
Cu	-0.856940000	0.882554000	-0.011310000
I	-2.578727000	-0.845574000	0.004974000

P1mono-TS1s

E= -616.6675294 au

ZPE_G= 0.213779 au

G= -616.453750 a.u.

N	-1.588958000	1.266651000	-3.250532000
C	-2.281758000	-0.023042000	-3.012572000
C	-2.334515000	2.422100000	-2.688426000
C	-0.182124000	1.235808000	-2.769900000
C	-1.561805000	-1.213359000	-3.609770000
C	-3.782877000	2.484855000	-3.122726000
C	0.552023000	2.549325000	-2.942870000
H	-3.272473000	0.067651000	-3.468805000
H	-2.428900000	-0.147844000	-1.928187000
H	-1.816066000	3.321676000	-3.045715000
H	-2.241995000	2.403479000	-1.591516000
H	0.325098000	0.456175000	-3.347559000
H	-0.181590000	0.917187000	-1.715555000
H	-2.220103000	-2.086769000	-3.570269000
H	-0.645430000	-1.471317000	-3.069813000
H	-1.305528000	-1.038053000	-4.661279000
H	-4.195806000	3.457982000	-2.838214000
H	-4.402784000	1.714403000	-2.653508000
H	-3.877573000	2.392667000	-4.211885000
H	1.619220000	2.387434000	-2.761283000

H	0.212723000	3.320461000	-2.244008000
H	0.444693000	2.941996000	-3.962540000
C	-1.484480000	1.887594000	-5.859485000
H	-1.546434000	1.492142000	-4.503716000
C	-1.358757000	2.157446000	-7.076568000
C	-1.199106000	2.211286000	-8.525862000
H	-0.306898000	2.778076000	-8.814679000
H	-1.096887000	1.197565000	-8.931318000
H	-2.061541000	2.680683000	-9.012313000
Cu	-1.590526000	3.852935000	-5.816453000
I	-1.781445000	6.159559000	-4.995994000

$P1_{mono}$-3s

E= -323.8389623 a.u.

ZPE_G= 0.014117 a.u.

G= -323.824845 a.u.

C	-2.427582000	0.000349000	-0.000498000
C	-3.663803000	0.000080000	-0.000170000
C	-5.119381000	-0.000459000	0.000718000
H	-5.531458000	-0.729354000	0.712611000
H	-5.532413000	0.980008000	0.276208000
H	-5.532794000	-0.252652000	-0.985818000
Cu	-0.577890000	0.000304000	-0.000457000
I	1.898492000	-0.000125000	0.000188000

P1-2s

E= -531.9675486 a.u.

ZPE_G= 0.015080 a.u.

G= -531.952469 a.u.

C	-1.031819000	1.510037000	0.252751000
H	0.048694000	1.465258000	0.302718000
C	-2.168188000	1.285325000	-0.277615000
C	-3.220848000	0.838800000	-1.184933000
H	-4.219688000	1.106139000	-0.830792000
H	-3.066367000	1.296019000	-2.168547000
H	-3.168285000	-0.250616000	-1.288952000
Cu	-2.077407000	3.197862000	0.519235000
I	-2.756694000	5.456298000	1.098049000

Cu	-2.226651000	0.995895000	1.775770000
I	-3.097591000	0.421754000	3.968680000

P1-3s

E= -824.3506578 a.u.

ZPE_G= 0.208517 a.u.

G= -824.1721408 a.u.

Cu	-0.554077000	-1.135960000	-0.663628000
C	0.153494000	0.075289000	0.765800000
H	-0.667554000	0.522751000	1.439380000
C	1.183203000	-0.579724000	0.399613000
Cu	0.790687000	1.064470000	-0.846718000
I	-2.226604000	-2.271037000	-2.019218000
I	1.030201000	2.750250000	-2.583381000
C	2.439623000	-1.323720000	0.385129000
H	3.222984000	-0.730449000	0.869562000
H	2.318191000	-2.261751000	0.938450000
H	2.766441000	-1.563531000	-0.630427000
N	-2.096180000	1.056868000	2.191932000
C	-2.492810000	2.254641000	1.428376000
C	-1.919029000	1.369033000	3.616765000
C	-3.020681000	-0.066304000	1.974094000
C	-2.787951000	1.998669000	-0.037587000
C	-0.876433000	2.438454000	3.875868000
C	-2.639149000	-1.328891000	2.721015000
H	-1.665579000	2.971491000	1.504374000
H	-3.368938000	2.728710000	1.911711000
H	-1.611293000	0.444325000	4.116307000
H	-2.890941000	1.663421000	4.058623000
H	-3.011045000	-0.283451000	0.897184000
H	-4.055933000	0.234854000	2.223883000
H	-2.876677000	2.955861000	-0.561789000
H	-3.720601000	1.446723000	-0.194172000
H	-1.982436000	1.436998000	-0.531809000
H	-0.647312000	2.477780000	4.945775000
H	-1.209246000	3.438150000	3.578509000
H	0.057067000	2.218076000	3.342535000
H	-3.215128000	-2.172429000	2.325989000

H	-2.840599000	-1.268050000	3.795492000
H	-1.574847000	-1.564833000	2.588309000

P1-TS1s

E= -824.3487568 a.u.

ZPE_G= 0.206431 a.u.

G= -824.142326 a.u.

Cu	-0.926865000	-0.779186000	0.724299000
C	-0.240436000	1.053818000	1.118202000
H	-0.755295000	1.916752000	0.371661000
C	0.019151000	0.428434000	2.201385000
Cu	1.475937000	0.172999000	0.665500000
I	-2.145682000	-2.523863000	-0.465648000
I	3.502599000	-0.485806000	-0.516278000
C	0.206117000	0.062560000	3.602180000
H	0.904314000	0.759683000	4.078680000
H	-0.752902000	0.115992000	4.129893000
H	0.602001000	-0.950670000	3.715298000
N	-1.420874000	2.769526000	-0.590623000
C	-0.501713000	2.806625000	-1.752357000
C	-1.650111000	4.116201000	-0.031507000
C	-2.678468000	2.053380000	-0.890280000
C	-0.304850000	1.467137000	-2.434845000
C	-0.374599000	4.821499000	0.381399000
C	-3.628630000	1.971148000	0.286471000
H	0.465240000	3.162574000	-1.376439000
H	-0.864386000	3.559312000	-2.473234000
H	-2.293373000	3.991928000	0.845516000
H	-2.213088000	4.719921000	-0.764419000
H	-2.395407000	1.034190000	-1.184608000
H	-3.168141000	2.514767000	-1.764530000
H	0.526295000	1.545413000	-3.142823000
H	-1.187604000	1.140742000	-2.993706000
H	-0.045115000	0.673759000	-1.720617000
H	-0.625745000	5.718367000	0.956060000
H	0.229714000	5.141091000	-0.473338000
H	0.246766000	4.181297000	1.019648000
H	-4.414022000	1.242333000	0.061584000

H	-4.117618000	2.924522000	0.510015000
H	-3.113985000	1.628402000	1.193719000

P1-4s

E= -531.5328455 a.u.

ZPE_G= 0.006292 a.u.

G= -531.526554 a.u.

C	2.076452000	-0.001123000	0.009112000
C	3.315473000	0.016943000	0.014464000
C	4.762952000	0.034982000	0.020026000
H	5.157737000	0.673553000	0.820520000
H	5.168556000	-0.972042000	0.181649000
H	5.172050000	0.401563000	-0.929993000
Cu	0.599507000	-1.215022000	0.010218000
I	-1.002822000	-3.087553000	0.013603000
Cu	0.595654000	1.210365000	-0.010146000
I	-1.008699000	3.081444000	-0.035508000

P1-5s (Cy6-1s)

E= -735.6325235 a.u.

ZPE_G= 0.049601 a.u.

G= -735.582923 a.u.

Cu	-0.622877000	0.622508000	-0.042568000
Cu	1.751533000	1.017550000	-0.124814000
C	0.792691000	-0.678161000	0.062822000
C	0.911979000	-1.907568000	0.186497000
C	0.978257000	-3.349367000	0.334088000
H	-0.027960000	-3.783047000	0.405289000
H	1.479209000	-3.825428000	-0.518316000
H	1.524941000	-3.643379000	1.239047000
N	3.882316000	-1.970039000	0.075995000
N	3.982058000	-0.827602000	-0.019484000
N	3.790627000	0.394818000	-0.123150000
C	4.987115000	1.247902000	-0.168824000
H	5.616741000	0.997245000	-1.028701000
H	4.615817000	2.269918000	-0.272370000
H	5.567167000	1.161030000	0.755847000
I	1.857917000	3.533716000	-0.365338000

I	-2.770111000	1.847355000	-0.127806000

P1-TS2s

E= -735.6238102 a.u.

ZPE_G= 0.051225 a.u.

G= -735.572585 a.u.

Cu	-1.036487000	0.829725000	0.000172000
Cu	1.248175000	0.030852000	0.000443000
C	0.594930000	1.817649000	0.000424000
C	1.107787000	2.977544000	0.000255000
C	1.004900000	4.439532000	0.001032000
H	-0.045483000	4.749549000	0.000314000
H	1.491828000	4.872357000	0.882934000
H	1.493527000	4.873563000	-0.879312000
N	3.074353000	2.823339000	-0.000967000
N	3.547796000	1.729462000	-0.000834000
N	3.182762000	0.503063000	0.001570000
C	4.272527000	-0.473762000	-0.002703000
H	4.881783000	-0.393680000	-0.910818000
H	4.916856000	-0.361986000	0.877200000
H	3.804923000	-1.460787000	0.023498000
I	0.884353000	-2.478251000	0.000360000
I	-3.397516000	0.116127000	-0.000437000

P1-6s

E= -735.6413846 a.u.

ZPE_G= 0.053663 a.u.

G= -735.587722 a.u.

Cu	-0.745555000	-0.672595000	0.119753000
Cu	1.410095000	0.486381000	-0.052711000
C	1.017941000	-1.313899000	0.128426000
C	1.825263000	-2.361189000	0.203092000
C	1.383476000	-3.785118000	0.350559000
H	0.293954000	-3.871034000	0.390535000
H	1.751519000	-4.384777000	-0.490915000
H	1.802831000	-4.218539000	1.266749000
N	3.262735000	-2.273180000	0.152216000
N	3.854502000	-1.162675000	0.029933000

N	3.285301000	-0.001864000	-0.062049000
C	4.219814000	1.117536000	-0.196506000
H	4.027715000	1.654151000	-1.132247000
H	4.079862000	1.822177000	0.630774000
H	5.249338000	0.747394000	-0.191679000
I	0.739270000	2.916161000	-0.264649000
I	-3.195540000	-0.420701000	0.171952000

P1-TS3s

E= -735.6359834 a.u.

ZPE_G= 0.054949 a.u.

G= -735.5810344 a.u.

Cu	-1.212222000	0.717688000	-0.050489000
Cu	1.225639000	0.093421000	-0.106380000
C	0.331021000	1.737781000	-0.299350000
C	0.877571000	2.914675000	-0.632323000
C	0.213357000	3.878663000	-1.568542000
H	-0.756443000	3.512617000	-1.915883000
H	0.066328000	4.845185000	-1.071618000
H	0.851885000	4.054060000	-2.442214000
N	2.107975000	3.386007000	-0.131266000
N	2.699576000	2.626316000	0.714128000
N	2.187936000	1.478131000	1.035367000
C	2.903656000	0.769704000	2.099909000
H	2.182713000	0.186554000	2.680284000
H	3.649649000	0.080515000	1.683149000
H	3.399540000	1.487997000	2.760216000
I	1.774997000	-2.333165000	-0.356281000
I	-3.373201000	-0.420179000	0.241743000

P1-7s (Cy5-1s)

E= -735.7146687 a.u.

ZPE_G= 0.056164 a.u.

G= -735.6585047 a.u.

Cu	-0.548312000	-0.271821000	0.083493000
Cu	1.650674000	0.676573000	-0.156049000
C	1.180477000	-1.217788000	0.115154000
C	1.483145000	-2.191471000	-0.853254000

C	1.276494000	-2.121290000	-2.322982000
H	0.901237000	-1.135107000	-2.616874000
H	2.209548000	-2.306578000	-2.868147000
H	0.551815000	-2.871533000	-2.662729000
N	2.018686000	-3.287883000	-0.259108000
N	2.079978000	-3.079281000	1.042205000
N	1.584676000	-1.854985000	1.273808000
C	1.526738000	-1.351346000	2.629504000
H	2.119554000	-0.435991000	2.719446000
H	0.491287000	-1.134670000	2.909265000
H	1.932712000	-2.117349000	3.292625000
I	-2.913333000	0.400664000	0.105408000
I	2.744824000	2.849989000	-0.509558000

P1-TS4s (Cy5-TS1s)

E= -735.687365 a.u.

ZPE_G= 0.058435 a.u.

G= -735.628930 a.u.

Cu	-2.052592000	0.407374000	0.368013000
C	0.396100000	1.463741000	0.064942000
C	-0.568449000	1.672841000	1.080172000
Cu	1.943011000	0.381088000	0.017443000
C	-0.459408000	1.346614000	2.535956000
H	-1.437491000	1.371842000	3.028269000
H	-0.020650000	0.355156000	2.689201000
H	0.185668000	2.072725000	3.048994000
N	-1.540505000	2.566028000	0.617413000
N	-1.232332000	2.922456000	-0.609614000
N	-0.076646000	2.271831000	-0.924730000
C	0.461345000	2.430414000	-2.259406000
H	1.537232000	2.613639000	-2.204124000
H	0.281117000	1.526231000	-2.849522000
H	-0.036402000	3.279117000	-2.732528000
I	3.971676000	-1.018197000	-0.009510000
I	-3.525690000	-1.432520000	-0.259735000

$P1_{mono}$-8s

E= -528.0237943 a.u.

ZPE_G= 0.064324 a.u.

G= -527.959471 a.u.

Cu	-0.124009000	0.019003000	-0.002586000
C	1.782815000	0.031836000	-0.001143000
C	2.721531000	1.072554000	0.001004000
N	2.599902000	-1.067686000	-0.001401000
C	2.485883000	2.554738000	0.000745000
N	3.988639000	0.561248000	0.002060000
N	3.917201000	-0.750760000	0.000865000
C	2.215191000	-2.471094000	0.001452000
H	1.412451000	2.769065000	0.011717000
H	2.934961000	3.036955000	0.878950000
H	2.916210000	3.034272000	-0.888416000
H	1.648762000	-2.709509000	0.906573000
H	1.599674000	-2.696943000	-0.873932000
H	3.126459000	-3.071752000	-0.027337000
I	-2.619150000	0.014321000	0.000838000

P1-8s

E= -735.7145488 a.u.

ZPE_G= 0.058283 a.u.

G= -735.656266 a.u.

Cu	0.055841000	0.168158000	0.939261000
C	1.802230000	0.381898000	1.634634000
C	2.594660000	1.488379000	1.944193000
N	2.638575000	-0.649478000	1.974056000
C	2.287495000	2.935362000	1.813417000
N	3.797663000	1.058309000	2.426331000
N	3.834612000	-0.265725000	2.448729000
C	2.361472000	-2.066448000	1.871831000
H	1.279103000	3.073359000	1.410393000
H	2.336710000	3.453307000	2.780135000
H	2.990573000	3.443971000	1.140934000
H	1.493160000	-2.322422000	2.485478000
H	2.152303000	-2.332013000	0.831747000
H	3.236884000	-2.615140000	2.223936000
I	-2.212571000	-0.199272000	0.036378000
Cu	5.291296000	2.064633000	3.016137000

I	7.208070000	3.366387000	3.773142000

P1a-1s

E= -907.7228999 a.u.

ZPE_G= 0.126363 a.u.

G= -907.596537 a.u.

Cu	2.417986000	0.487120000	0.348438000
C	0.598599000	-0.095767000	0.484072000
C	-0.611744000	0.455033000	0.055684000
N	0.168368000	-1.269018000	1.046321000
C	-0.862822000	1.727780000	-0.667360000
N	-1.633766000	-0.388321000	0.380638000
N	-1.162276000	-1.460477000	1.001485000
C	0.984218000	-2.259624000	1.714473000
H	0.016701000	2.378043000	-0.607891000
H	-1.078085000	1.561978000	-1.731626000
H	-1.719375000	2.270856000	-0.247412000
H	1.937712000	-2.340695000	1.182495000
H	1.174934000	-1.962499000	2.751430000
H	0.460380000	-3.217747000	1.702336000
I	4.201006000	-1.471596000	-0.739460000
Cu	-3.491266000	-0.162250000	0.088447000
I	-5.873344000	0.220477000	-0.265112000
C	4.523322000	2.797687000	0.296278000
C	5.153060000	1.944247000	1.277845000
H	5.914698000	1.221037000	0.975960000
H	5.133111000	2.202497000	2.338297000
N	3.804290000	1.800991000	0.603637000
C	4.545386000	3.961627000	-0.588133000
H	5.380469000	3.879554000	-1.294127000
H	3.609927000	4.049048000	-1.148297000
H	4.712159000	4.877872000	-0.010235000

P1a-2t

E= -907.696937 a.u.

ZPE_G= 0.119122 a.u.

G= -907.577815 a.u.

Cu	-3.466215000	-0.124575000	0.122872000

C	0.624909000	-0.156652000	0.494552000
C	-0.569019000	0.415807000	0.054662000
Cu	2.457550000	0.464135000	0.249259000
C	-0.783717000	1.662246000	-0.723671000
H	0.138963000	2.251666000	-0.759314000
H	-1.083284000	1.453988000	-1.759343000
H	-1.569341000	2.287842000	-0.280914000
N	-1.614007000	-0.373752000	0.438432000
N	-1.167884000	-1.425374000	1.108772000
N	0.168461000	-1.280087000	1.126195000
C	0.954250000	-2.270550000	1.830659000
H	0.312619000	-3.124123000	2.056669000
H	1.792992000	-2.580970000	1.200455000
H	1.346367000	-1.850207000	2.762406000
C	4.525718000	2.743595000	0.246578000
N	3.493445000	1.946351000	0.314910000
C	4.405287000	4.091607000	0.610327000
C	5.855444000	2.203631000	-0.234074000
H	6.143514000	1.320591000	0.345430000
H	5.782118000	1.887904000	-1.280616000
H	6.645350000	2.956985000	-0.151658000
H	3.449939000	4.485580000	0.949127000
H	5.257611000	4.766372000	0.566036000
I	4.039240000	-1.542658000	-0.621799000
I	-5.835522000	0.261320000	-0.303341000

P1b-1s

E= -1028.5592507 a.u.

ZPE_G= 0.268492 a.u.

G= -1028.290759 a.u.

Cu	-2.439200000	-0.930367000	0.214016000
C	-0.608384000	-0.706813000	0.674607000
C	0.563494000	-0.760262000	-0.083560000
C	0.740854000	-0.963316000	-1.543702000
H	-0.230608000	-1.040604000	-2.042668000
H	1.302360000	-0.141676000	-2.008765000
H	1.295822000	-1.885589000	-1.756281000
N	1.638240000	-0.615434000	0.745712000

N	1.232889000	-0.471610000	1.997719000
N	-0.105714000	-0.526968000	1.939839000
C	-0.853338000	-0.384119000	3.172717000
H	-1.572271000	-1.201820000	3.264626000
H	-0.149610000	-0.412073000	4.006036000
H	-1.390700000	0.569888000	3.182626000
H	-1.548105000	1.300355000	0.133188000
I	-4.798481000	-1.119726000	-0.456216000
Cu	3.468913000	-0.469167000	0.267781000
I	5.777725000	-0.202060000	-0.447666000
N	-1.659388000	2.273119000	-0.225691000
C	-0.882712000	3.190063000	0.684181000
C	-3.137277000	2.570626000	-0.197359000
C	-1.094399000	2.260461000	-1.624202000
C	0.594048000	2.884890000	0.734762000
C	-3.729099000	2.454752000	1.185599000
C	-1.892342000	1.410451000	-2.583185000
H	-1.330202000	3.080767000	1.674626000
H	-1.086475000	4.207295000	0.331484000
H	-3.602177000	1.832430000	-0.857428000
H	-3.264213000	3.565971000	-0.637329000
H	-0.076279000	1.873730000	-1.522558000
H	-1.030385000	3.306223000	-1.945321000
H	1.045725000	3.494255000	1.522920000
H	1.114245000	3.120363000	-0.198291000
H	0.784482000	1.835648000	0.986885000
H	-4.819265000	2.474547000	1.098538000
H	-3.432741000	3.265343000	1.857265000
H	-3.465777000	1.491626000	1.643923000
H	-1.294262000	1.243001000	-3.483868000
H	-2.831930000	1.879939000	-2.887993000
H	-2.126540000	0.427347000	-2.150204000

P1b-TS1s

E= -1028.5298993 a.u.

ZPE_G= 0.262181 a.u.

G= -1028.267718 a.u.

Cu	-2.258291000	-0.728901000	0.203615000

C	-0.622049000	0.347474000	0.470315000
C	0.555686000	0.068896000	-0.242151000
C	0.751745000	-0.237262000	-1.677414000
H	-0.204352000	-0.322589000	-2.200996000
H	1.348314000	0.540855000	-2.170267000
H	1.289540000	-1.183976000	-1.805336000
N	1.603868000	0.119655000	0.620420000
N	1.176654000	0.428743000	1.841129000
N	-0.134553000	0.567352000	1.749396000
C	-0.888854000	0.905736000	2.940976000
H	-1.630572000	0.128959000	3.143811000
H	-0.189165000	0.978792000	3.773652000
H	-1.393253000	1.866502000	2.802300000
H	-1.443031000	1.244493000	0.037354000
I	-4.264731000	-2.068255000	-0.116521000
Cu	3.447177000	-0.198401000	0.267274000
I	5.777258000	-0.620311000	-0.265081000
N	-2.128970000	2.453084000	-0.518932000
C	-1.599852000	3.658754000	0.156205000
C	-3.586540000	2.303389000	-0.307466000
C	-1.775655000	2.449427000	-1.958894000
C	-0.108427000	3.862682000	-0.011268000
C	-3.991993000	2.208616000	1.147384000
C	-2.418036000	1.327686000	-2.748942000
H	-1.838051000	3.562463000	1.220685000
H	-2.152868000	4.539263000	-0.213481000
H	-3.891030000	1.379274000	-0.813578000
H	-4.108444000	3.134456000	-0.811483000
H	-0.683593000	2.358181000	-2.014441000
H	-2.035883000	3.429038000	-2.393907000
H	0.217496000	4.674261000	0.646529000
H	0.167990000	4.141045000	-1.032881000
H	0.464286000	2.968677000	0.264551000
H	-5.057016000	1.962376000	1.205993000
H	-3.838202000	3.137775000	1.705214000
H	-3.451082000	1.400780000	1.659049000
H	-1.909412000	1.224468000	-3.712713000
H	-3.479111000	1.504013000	-2.950259000

H	-2.339300000	0.362417000	-2.227242000

P1b-2s

E= -1028.5388558 a.u.

ZPE_G= -1028.5388558 a.u.

G= -1028.278960 a.u.

Cu	1.123538000	0.811449000	0.086756000
C	0.886163000	-1.230301000	0.427627000
C	-0.269419000	-0.876921000	-0.288089000
C	-0.542585000	-0.825259000	-1.748852000
H	0.384119000	-0.836743000	-2.328794000
H	-1.137062000	-1.697605000	-2.046637000
H	-1.110032000	0.070971000	-2.020759000
N	-1.294836000	-0.818590000	0.636555000
N	-0.851789000	-1.121949000	1.837935000
N	0.446296000	-1.378161000	1.720557000
C	1.234897000	-1.696641000	2.896685000
H	1.743299000	-0.798301000	3.258682000
H	0.559816000	-2.074137000	3.664775000
H	1.971620000	-2.458436000	2.634028000
H	1.895373000	-1.552983000	0.102156000
I	2.246338000	2.961815000	0.060357000
Cu	-3.125298000	-0.443454000	0.282387000
I	-5.429142000	0.013858000	-0.328009000
N	3.777631000	-1.855368000	-0.582717000
C	4.176585000	-3.191055000	-0.121761000
C	4.708231000	-0.836898000	-0.078869000
C	3.672810000	-1.834973000	-2.047627000
C	3.143888000	-4.271052000	-0.382799000
C	4.548240000	-0.565117000	1.403887000
C	3.271880000	-0.490695000	-2.624893000
H	4.356653000	-3.127035000	0.957790000
H	5.146031000	-3.474271000	-0.581650000
H	4.503976000	0.096423000	-0.614500000
H	5.755433000	-1.115424000	-0.315345000
H	2.913585000	-2.578679000	-2.321327000
H	4.622414000	-2.175692000	-2.510014000
H	3.447367000	-5.201740000	0.108661000

H	3.021772000	-4.494579000	-1.448192000
H	2.160371000	-3.990336000	0.016725000
H	5.212695000	0.249878000	1.711102000
H	4.779299000	-1.432225000	2.033367000
H	3.519668000	-0.247056000	1.625003000
H	2.914094000	-0.613552000	-3.652876000
H	4.094114000	0.231933000	-2.649137000
H	2.459834000	-0.030957000	-2.040757000

P1b-2s

E= -528.513437 a.u.

ZPE_G= 0.075997 a.u.

G= -528.437440 a.u.

C	3.674296000	0.755183000	-0.006602000
C	2.359554000	1.163211000	-0.001736000
C	1.761966000	2.518374000	0.000166000
H	2.532366000	3.284501000	-0.118491000
H	1.038968000	2.631166000	-0.815630000
H	1.228560000	2.715753000	0.937385000
N	1.603107000	0.025946000	0.006182000
N	2.375048000	-1.049215000	0.007054000
N	3.630126000	-0.597531000	-0.000934000
C	4.735231000	-1.536697000	-0.006263000
H	5.353070000	-1.386280000	0.881888000
H	4.315093000	-2.542380000	0.000186000
H	5.339414000	-1.392349000	-0.904810000
H	4.605391000	1.304021000	-0.016101000
Cu	-0.293273000	-0.104581000	0.006543000
I	-2.723626000	-0.144083000	-0.002900000

Figure S15. Optimized Cartesian coordinates and corresponding energy at M06-L/6-31G*/LANL2TZ+ level for all reactants, intermediates, transition states and products in Path2.

2H-azirine

E= -171.9991647 a.u.

ZPE_G= 0.047528 a.u.

G= -171.951637 a.u.

C	-0.116172000	0.029022000	0.000004000
C	1.198785000	-0.559809000	-0.000001000
H	1.641345000	-0.940665000	0.923161000
H	1.641286000	-0.940703000	-0.923175000
N	0.788279000	0.912757000	-0.000004000
C	-1.572695000	-0.127165000	-0.000018000
H	-1.889916000	-0.700074000	0.878993000
H	-2.080445000	0.842117000	-0.001212000
H	-1.889733000	-0.702261000	-0.877650000

P2-1s

E= -379.6742906 a.u.

ZPE_G= 0.040119 a.u.

G= -379.634171 a.u.

C	-3.386255000	0.101988000	-0.000166000
C	-3.310781000	-1.343315000	-0.000434000
H	-3.452202000	-1.903146000	0.924917000
H	-3.451321000	-1.902742000	-0.926165000
N	-2.193795000	-0.322000000	0.000348000
C	-4.167047000	1.334676000	-0.000169000
H	-4.823479000	1.358400000	0.877204000
H	-3.521587000	2.216634000	0.000976000
H	-4.821670000	1.359485000	-0.878874000
Cu	-0.336679000	-0.148406000	0.000371000
I	2.082548000	0.091869000	-0.000125000

P2-2s

E= -587.3295907 a.u.

ZPE_G= 0.030721 a.u.

G= -587.298870 a.u.

C	0.557092000	3.083806000	0.000000000
C	-0.874221000	3.271376000	0.000000000

N	-0.086166000	1.968434000	0.000000000
C	1.910266000	3.608628000	0.000000000
H	-1.391660000	3.516143000	0.926942000
H	2.054198000	4.253038000	0.875955000
H	2.652987000	2.807323000	0.000000000
Cu	-0.078864000	0.465945000	1.236968000
I	-0.078864000	-1.122004000	3.075170000

P2-TS1s

E= -587.3254678 a.u.

ZPE_G= 0.032179 a.u.

G= -587.293289 a.u.

C	0.375435000	-0.344601000	-3.082377000
C	-0.673097000	-1.300756000	-2.856950000
H	-1.704342000	-1.042212000	-3.093844000
H	-0.428133000	-2.356183000	-2.743071000
N	0.074088000	-0.314880000	-1.845701000
C	1.257495000	0.331176000	-4.022197000
H	0.664721000	0.772727000	-4.831298000
H	1.848729000	1.105356000	-3.527284000
H	1.924001000	-0.402274000	-4.490805000
Cu	-0.835108000	-1.226814000	-0.355437000
I	-1.925165000	-2.346197000	1.493572000
Cu	0.358601000	0.952717000	-0.396627000
I	0.760344000	2.669541000	1.267618000

P2-3s

E= -587.3282703 a.u.

ZPE_G= 0.030708 a.u.

G= -587.297562 a.u.

C	-0.362585000	2.849972000	0.000053000
C	-1.811032000	2.600599000	0.000420000
H	-2.356934000	2.747906000	0.934645000
H	-2.357476000	2.748119000	-0.933455000
N	0.032886000	1.629048000	-0.000480000
C	0.432509000	4.086370000	0.000274000
H	0.182103000	4.692381000	0.879438000
H	1.504366000	3.869723000	0.000720000

H	0.182868000	4.692161000	-0.879269000
Cu	-1.539309000	0.605850000	-0.000184000
I	-3.113694000	-1.270847000	0.000066000
Cu	1.423789000	0.432736000	-0.000229000
I	3.423347000	-0.946026000	0.000100000

P2-TS2s

E= -587.3095711 a.u.

ZPE_G= 0.027928 a.u.

G= -587.281643 a.u.

C	-0.018658000	2.711251000	-0.061451000
C	-1.345386000	3.154551000	0.126560000
H	-1.596330000	3.897973000	0.884287000
H	-2.168579000	2.684244000	-0.409570000
N	0.030513000	1.403619000	-0.205433000
C	1.171856000	3.589869000	0.076299000
H	1.165217000	4.104127000	1.044631000
H	2.095971000	3.007745000	-0.005881000
H	1.169431000	4.364953000	-0.698575000
Cu	1.492629000	0.326929000	0.039885000
I	3.526124000	-0.996667000	0.008177000
Cu	-1.519233000	0.407095000	-0.155519000
I	-3.506401000	-1.001542000	0.050844000

P2-4s

E= -587.311492 a.u.

ZPE_G= 0.031724 a.u.

G= -587.279768 a.u.

C	-0.075732000	2.758748000	0.008720000
C	1.081474000	3.503872000	-0.079634000
H	1.061864000	4.590271000	-0.140581000
H	2.054058000	3.014708000	-0.117493000
N	0.004522000	1.408868000	0.002692000
C	-1.418507000	3.425578000	0.076338000
H	-2.026492000	3.147616000	-0.792983000
H	-1.960574000	3.093383000	0.969545000
H	-1.341303000	4.516017000	0.107080000
Cu	-1.482826000	0.347568000	-0.019504000

I	-3.455660000	-1.062142000	-0.000903000
Cu	1.523781000	0.400318000	0.015446000
I	3.521125000	-0.976386000	0.001671000

P2-1t

E= -379.575125 a.u.

ZPE_G= 0.035232 a.u.

G= -379.539893 a.u.

C	-3.421539000	0.110957000	-0.450128000
C	-3.294361000	-1.211807000	0.142641000
H	-3.687898000	-1.360247000	1.156288000
H	-3.261290000	-2.136832000	-0.441183000
N	-2.137235000	-0.357402000	-0.018888000
C	-4.075558000	1.313878000	0.107945000
H	-3.945233000	1.365040000	1.202233000
H	-3.642142000	2.228495000	-0.312850000
H	-5.150446000	1.309620000	-0.101352000
Cu	-0.343103000	-0.196973000	-0.031543000
I	2.063140000	0.104336000	0.013983000

P2-2t

E= -587.2601038 a.u.

ZPE_G= 0.030650 a.u.

G= -587.229454 a.u.

C	-0.218477000	3.162018000	0.315172000
C	-0.135030000	3.083684000	-1.131925000
H	-1.042743000	3.194425000	-1.732617000
H	0.784390000	3.348252000	-1.657326000
N	-0.057466000	1.875285000	-0.281237000
C	-1.318205000	3.541442000	1.221702000
H	-2.288613000	3.196998000	0.822216000
H	-1.191953000	3.087623000	2.211394000
H	-1.375023000	4.627820000	1.343203000
Cu	-1.217127000	0.400543000	-0.198056000
I	-2.936040000	-1.299278000	0.035699000
Cu	1.318952000	0.610302000	-0.108570000
I	3.173654000	-0.938826000	0.104758000

P2-TS2t

E= -587.2332526 a.u.

ZPE_G= 0.026079 a.u.

G= -587.207174 a.u.

C	0.172542000	3.065975000	-0.081367000
C	0.122909000	3.006723000	1.315771000
H	0.983627000	3.263802000	1.947920000
H	-0.778991000	2.695330000	1.837187000
N	0.034626000	1.674902000	-0.018542000
C	1.094828000	3.780940000	-0.986850000
H	2.143482000	3.482658000	-0.817791000
H	0.859026000	3.561052000	-2.033565000
H	1.025016000	4.861504000	-0.830133000
Cu	1.305954000	0.356786000	0.120093000
I	3.148294000	-1.222108000	-0.021794000
Cu	-1.371890000	0.489911000	-0.072124000
I	-3.354031000	-0.914962000	-0.031984000

P2-4t

E= -587.3184457 a.u.

ZPE_G= 0.027565 a.u.

G= -587.290881 a.u.

C	0.045130000	2.947227000	-0.000073000
C	-1.138297000	3.690539000	0.000067000
H	-1.116057000	4.777166000	0.000018000
H	-2.107140000	3.194821000	0.000280000
N	0.007127000	1.628480000	0.000022000
C	1.384509000	3.633537000	-0.000392000
H	1.965694000	3.342289000	0.881700000
H	1.964778000	3.343123000	-0.883372000
H	1.274531000	4.721011000	0.000165000
Cu	1.273263000	0.307316000	0.000610000
I	3.255572000	-1.092766000	-0.000148000
Cu	-1.303975000	0.353975000	-0.000197000
I	-3.310083000	-1.012573000	-0.000013000

P2-TS$_{mono}$s

E= -379.6124096 a.u.

ZPE_G= 0.038662 a.u.

G= -379.573747 a.u.

C	3.131218000	0.063462000	0.000003000
C	4.394714000	-0.514622000	0.000006000
H	5.316098000	0.069939000	0.000002000
H	4.476500000	-1.599332000	0.000010000
N	2.114636000	-0.800454000	0.000002000
C	2.963180000	1.560207000	-0.000002000
H	2.389242000	1.870229000	-0.880863000
H	2.389287000	1.870239000	0.880886000
H	3.915366000	2.101044000	-0.000028000
Cu	0.375474000	-0.355807000	-0.000006000
I	-2.020988000	0.093494000	0.000002000

P2-TS$_{mono}$t

E= -379.5457124 a.u.

ZPE_G= 0.032937 a.u.

G= -379.512776 a.u.

C	3.383762000	-0.074773000	-0.111846000
C	2.997402000	-1.095017000	0.755709000
H	2.830474000	-2.109963000	0.400237000
H	2.833879000	-0.928303000	1.829306000
N	2.133412000	-0.303807000	-0.713681000
C	3.867342000	1.285371000	0.229702000
H	3.153008000	1.825369000	0.873645000
H	4.821537000	1.223872000	0.762422000
H	4.009557000	1.885271000	-0.675144000
Cu	0.382998000	-0.227343000	-0.332832000
I	-1.984534000	0.115658000	0.117284000

P2-Nit

E= -379.6396173 a.u.

ZPE_G= 0.032728 a.u.

G= -379.606889 a.u.

C	3.353939000	-0.075151000	-0.000110000
N	2.058178000	-0.046842000	-0.000013000
C	4.042843000	-1.301049000	-0.000001000
C	4.115648000	1.229590000	-0.000010000

H	4.761260000	1.286313000	-0.882592000
H	3.437340000	2.085482000	-0.004145000
H	4.754448000	1.289890000	0.887310000
Cu	0.287747000	-0.016780000	-0.000001000
H	3.499913000	-2.242018000	0.000326000
H	5.129736000	-1.321654000	-0.000105000
I	-2.139796000	0.011248000	0.000001000

Di-CP1

E= -587.3128348 a.u.

ZPE_G= 0.032916 a.u.

G= -587.2799188 a.u.

C	-0.083715000	2.769290000	0.040779000
C	1.081918000	3.512746000	-0.164683000
H	1.038132000	4.570008000	-0.419103000
H	2.051344000	3.017784000	-0.200148000
N	-0.008824000	1.444005000	0.038151000
C	-1.416483000	3.450221000	0.154044000
H	-1.979946000	3.348370000	-0.781481000
H	-2.014464000	2.988701000	0.947236000
H	-1.307224000	4.516199000	0.373974000
Cu	-1.414603000	0.289460000	-0.144799000
I	-3.392790000	-1.116305000	-0.062860000
Cu	1.451859000	0.355099000	0.170133000
I	3.480525000	-0.977159000	0.079152000

Mono-CP1

E= -379.627978 a.u.

ZPE_G= 0.040610 a.u.

G= -379.587368 a.u.

C	3.349822000	0.092096000	0.061820000
N	2.083462000	0.174653000	-0.043600000
C	3.870190000	-1.254748000	0.039775000
C	4.255947000	1.283532000	0.064374000
H	4.947465000	1.232682000	-0.784489000
H	3.687707000	2.214960000	0.007987000
H	4.862063000	1.284579000	0.977625000
Cu	0.328665000	-0.086159000	-0.048296000

H	3.233543000	-2.079321000	0.348616000
H	4.750315000	-1.480732000	-0.563074000
I	-2.067923000	-0.482511000	-0.060078000

Alkyne C-H active

P2-5t

E= -703.9738381 a.u.

ZPE_G= 0.079042 a.u.

G= -703.8947961 a.u.

C	10.930960000	7.784824000	1.690435000
N	11.764599000	7.163545000	0.878880000
C	9.665331000	8.361091000	1.107761000
Cu	11.772009000	6.844040000	-0.935017000
I	11.445867000	6.738460000	-3.349138000
C	13.786765000	4.715054000	-0.583533000
H	12.971408000	4.023998000	-0.698900000
C	14.881566000	5.266266000	-0.649097000
C	16.154271000	5.942251000	-0.744172000
H	16.682256000	5.922832000	0.215874000
H	16.780080000	5.444097000	-1.493533000
H	16.028064000	6.987190000	-1.049116000
Cu	13.387450000	6.200562000	0.974167000
C	11.205939000	7.912687000	3.054044000
H	9.903465000	9.136700000	0.370867000
H	9.091372000	7.585092000	0.589183000
I	14.861923000	6.369331000	3.025865000
H	9.033417000	8.802570000	1.883014000
H	12.124784000	7.501565000	3.468262000
H	10.511630000	8.424395000	3.715876000

P2-6t

E= -996.3555136 a.u.

ZPE_G= 0.271734 a.u.

G= -996.0837796 a.u.

C	0.307067000	-2.601969000	-1.572315000
N	0.203635000	-1.712405000	-0.605778000
C	-0.946878000	-3.271453000	-2.072580000
Cu	-1.199938000	-0.878288000	0.333085000

I	-3.659348000	-0.773317000	0.527460000
C	-0.087949000	0.891322000	1.301682000
H	-0.408157000	1.618541000	0.497179000
C	0.411855000	0.561004000	2.385048000
C	0.955032000	0.105892000	3.642450000
H	1.997207000	0.426608000	3.755011000
H	0.375138000	0.509757000	4.479884000
H	0.930417000	-0.988045000	3.712397000
Cu	1.338522000	-0.490290000	0.305588000
C	1.552670000	-2.910621000	-2.126776000
H	-1.494920000	-3.729625000	-1.241976000
H	-1.615084000	-2.532352000	-2.531224000
I	3.822456000	-0.295179000	0.201382000
H	-0.721348000	-4.042279000	-2.814659000
H	2.451221000	-2.413617000	-1.763421000
H	1.644828000	-3.645202000	-2.923092000
N	-0.528772000	2.734497000	-0.910455000
C	0.286750000	3.899984000	-0.535243000
C	-1.907928000	3.131871000	-1.224518000
C	0.116107000	1.972631000	-1.990127000
C	1.730805000	3.568354000	-0.212730000
C	-2.612376000	3.811172000	-0.066244000
C	-0.757115000	0.920301000	-2.642050000
H	-0.180387000	4.353999000	0.346101000
H	0.244126000	4.656740000	-1.344618000
H	-2.460518000	2.222414000	-1.483971000
H	-1.924133000	3.785375000	-2.120025000
H	1.003629000	1.482830000	-1.551107000
H	0.504227000	2.661780000	-2.765278000
H	2.224072000	4.452486000	0.204855000
H	2.302155000	3.261986000	-1.095888000
H	1.806026000	2.764653000	0.531176000
H	-3.685490000	3.876331000	-0.274852000
H	-2.252974000	4.829851000	0.114585000
H	-2.487777000	3.236540000	0.860674000
H	-0.135226000	0.265542000	-3.262686000
H	-1.530037000	1.355015000	-3.284427000
H	-1.262947000	0.284169000	-1.900719000

P2-TS3t

E= -996.3540974 a.u.

ZPE_G= 0.273213 a.u.

G= -996.0808844 a.u.

C	0.062195000	-2.829315000	-1.122926000
N	0.071786000	-1.811621000	-0.288088000
C	-1.258317000	-3.463196000	-1.476229000
Cu	-1.205385000	-0.643908000	0.531976000
I	-3.698674000	-0.652557000	0.498153000
C	-0.067040000	1.023268000	1.153365000
H	-0.345767000	1.711056000	0.177607000
C	0.708546000	1.102915000	2.130295000
C	1.542908000	1.241109000	3.300915000
H	2.498437000	1.712350000	3.036608000
H	1.050756000	1.855113000	4.063565000
H	1.774103000	0.265676000	3.745506000
Cu	1.296072000	-0.513285000	0.409682000
C	1.256099000	-3.305479000	-1.674647000
H	-1.768706000	-3.812560000	-0.571822000
H	-1.917891000	-2.725126000	-1.948275000
I	3.779972000	-0.473462000	0.082757000
H	-1.130157000	-4.308266000	-2.158439000
H	2.202482000	-2.831535000	-1.417082000
H	1.260113000	-4.145330000	-2.365551000
N	-0.417553000	2.564198000	-1.060787000
C	0.435651000	3.741521000	-0.795605000
C	-1.824759000	2.945829000	-1.289451000
C	0.148067000	1.711161000	-2.127845000
C	1.906125000	3.413690000	-0.628554000
C	-2.425388000	3.729621000	-0.140670000
C	-0.781792000	0.628869000	-2.634441000
H	0.060891000	4.205577000	0.123794000
H	0.292794000	4.474581000	-1.609147000
H	-2.392294000	2.018345000	-1.420059000
H	-1.901443000	3.512791000	-2.234232000
H	1.055128000	1.246982000	-1.706174000
H	0.483270000	2.346626000	-2.964880000

H	2.433670000	4.301185000	-0.264272000
H	2.381970000	3.112117000	-1.567651000
H	2.065897000	2.608615000	0.100106000
H	-3.509981000	3.793058000	-0.274884000
H	-2.041997000	4.753007000	-0.075588000
H	-2.241480000	3.231393000	0.819529000
H	-0.210234000	-0.081532000	-3.241683000
H	-1.592824000	1.026077000	-3.253354000
H	-1.238834000	0.059364000	-1.813063000

P2-7t

E= -996.3777201 a.u.

ZPE_G= 0.281690 a.u.

G= -996.0960301 a.u.

C	-1.681299000	1.806181000	1.319580000
N	-0.651380000	1.402754000	0.602006000
C	-2.935575000	2.250495000	0.610085000
Cu	-0.241632000	0.780869000	-1.213103000
I	-2.001229000	0.980176000	-3.020243000
C	1.469187000	-0.176923000	-1.086873000
H	0.074912000	-1.729844000	-0.676641000
C	2.545097000	-0.588705000	-0.601769000
C	3.838569000	-1.124523000	-0.210315000
H	3.829939000	-1.457317000	0.836149000
H	4.122741000	-1.977486000	-0.839558000
H	4.624014000	-0.364489000	-0.300732000
Cu	1.071604000	0.541147000	0.857871000
C	-1.619395000	1.824930000	2.716600000
H	-2.713835000	3.071825000	-0.080248000
H	-3.341954000	1.433877000	0.000254000
I	2.126728000	0.265724000	3.141597000
H	-3.702929000	2.580474000	1.316762000
H	-0.712797000	1.503361000	3.227584000
H	-2.467299000	2.158033000	3.311480000
N	-0.372908000	-2.665569000	-0.598324000
C	0.758526000	-3.636490000	-0.364633000
C	-1.058035000	-2.912018000	-1.918546000
C	-1.339134000	-2.623896000	0.557391000

C	1.379046000	-3.520916000	1.007127000
C	-0.102515000	-2.885555000	-3.086304000
C	-2.519533000	-1.712684000	0.320028000
H	1.494872000	-3.418008000	-1.143517000
H	0.349629000	-4.636292000	-0.550354000
H	-1.798641000	-2.113892000	-2.025744000
H	-1.586901000	-3.866843000	-1.820511000
H	-0.759357000	-2.282356000	1.420387000
H	-1.644412000	-3.659809000	0.742867000
H	2.316241000	-4.085842000	1.013811000
H	0.740814000	-3.929801000	1.795843000
H	1.619561000	-2.480367000	1.263884000
H	-0.686908000	-2.874532000	-4.010944000
H	0.558672000	-3.756448000	-3.120752000
H	0.508275000	-1.974150000	-3.074309000
H	-3.027674000	-1.543310000	1.274494000
H	-3.249090000	-2.132514000	-0.378612000
H	-2.201937000	-0.732180000	-0.060625000

P2-8t

E= -996.3767469 a.u.

ZPE_G= 0.282728 a.u.

G= -996.0940189 a.u.

C	-0.761255000	0.835624000	1.227276000
N	-0.153709000	0.117274000	0.271511000
C	-2.026960000	1.572958000	0.869710000
Cu	0.146282000	0.640448000	-1.616742000
I	-1.859655000	0.894743000	-3.118355000
C	2.077978000	0.690000000	-1.797248000
H	-0.866031000	-1.584593000	-0.067423000
C	3.300980000	0.554672000	-1.599770000
C	4.748678000	0.453722000	-1.531384000
H	5.063615000	-0.550552000	-1.223693000
H	5.200325000	0.664192000	-2.508135000
H	5.167558000	1.164177000	-0.808586000
Cu	1.775694000	-0.133703000	0.087024000
C	-0.272074000	0.877626000	2.523502000
H	-1.810294000	2.381535000	0.160677000

H	-2.742167000	0.906613000	0.373583000
I	3.116524000	-1.337329000	1.858249000
H	-2.502939000	2.005487000	1.754838000
H	0.654276000	0.364172000	2.780353000
H	-0.802188000	1.416868000	3.305694000
N	-1.140555000	-2.589359000	-0.149925000
C	-0.231033000	-3.347566000	0.783093000
C	-0.932093000	-2.983621000	-1.588028000
C	-2.585308000	-2.695394000	0.265233000
C	-0.434493000	-2.991544000	2.234943000
C	0.510301000	-2.895189000	-2.025353000
C	-3.541223000	-2.031233000	-0.695387000
H	0.790522000	-3.095071000	0.479596000
H	-0.400014000	-4.412256000	0.583368000
H	-1.549755000	-2.299237000	-2.177631000
H	-1.338759000	-3.995657000	-1.698437000
H	-2.647039000	-2.229341000	1.252273000
H	-2.794088000	-3.764955000	0.383340000
H	0.371383000	-3.448361000	2.817042000
H	-1.385126000	-3.355350000	2.636261000
H	-0.368517000	-1.906884000	2.392939000
H	0.551000000	-2.982603000	-3.115241000
H	1.138526000	-3.683678000	-1.600712000
H	0.954688000	-1.922077000	-1.768119000
H	-4.523380000	-1.963479000	-0.218402000
H	-3.664135000	-2.591691000	-1.626787000
H	-3.223482000	-1.012303000	-0.952001000

P2-TS4t

E= -996.3675626 a.u.

ZPE_G= 0.275837 a.u.

G= -996.091726 a.u.

C	0.227610000	0.498261000	2.136576000
N	0.118861000	0.448428000	0.785364000
C	0.766051000	1.756889000	2.757392000
Cu	1.135449000	-1.205973000	0.036856000
I	3.593991000	-0.882468000	-0.069383000
C	-0.313188000	-2.429913000	-0.299187000

H	0.362359000	1.515976000	0.051576000
C	-1.085744000	-3.366108000	-0.535823000
C	-1.974509000	-4.470366000	-0.825419000
H	-3.020715000	-4.139565000	-0.814775000
H	-1.774642000	-4.898666000	-1.814741000
H	-1.874514000	-5.271832000	-0.083983000
Cu	-1.330295000	-0.713576000	0.085094000
C	-0.128643000	-0.574205000	2.929381000
H	1.780763000	1.963884000	2.394678000
H	0.142205000	2.621188000	2.498942000
I	-3.684481000	0.102670000	-0.004821000
H	0.803362000	1.680477000	3.847287000
H	-0.498697000	-1.498681000	2.484145000
H	-0.045611000	-0.529813000	4.012323000
N	0.481277000	2.494698000	-0.781715000
C	-0.905577000	2.971456000	-1.038727000
C	1.104302000	1.935366000	-2.014196000
C	1.320729000	3.579390000	-0.203805000
C	-1.601472000	3.504451000	0.192697000
C	0.298089000	0.840127000	-2.677201000
C	2.771957000	3.198650000	-0.009641000
H	-1.468587000	2.113072000	-1.419940000
H	-0.865466000	3.725273000	-1.839979000
H	2.079036000	1.536891000	-1.713004000
H	1.287066000	2.765935000	-2.713492000
H	0.873432000	3.843024000	0.759320000
H	1.227359000	4.462245000	-0.854781000
H	-2.654989000	3.682367000	-0.043805000
H	-1.180211000	4.447943000	0.554468000
H	-1.578273000	2.769386000	1.007626000
H	0.912250000	0.366419000	-3.449684000
H	-0.617365000	1.202145000	-3.155251000
H	0.018470000	0.048901000	-1.964802000
H	3.253532000	3.938665000	0.637340000
H	3.330931000	3.168850000	-0.950073000
H	2.876213000	2.216269000	0.469047000

P2-9t

E= -996.3763513 a.u.

ZPE_G= 0.278851 a.u.

G= -996.0975003 a.u.

C	-0.539335000	0.792785000	1.053675000
N	-0.020310000	-0.142353000	0.210089000
C	-1.926051000	0.578880000	1.574665000
Cu	0.476920000	0.660012000	-1.687688000
I	-1.579161000	0.983050000	-3.014895000
C	2.382132000	0.728283000	-1.498633000
H	-0.621302000	-0.996673000	0.073959000
C	3.613572000	0.778574000	-1.379343000
C	5.055783000	0.852148000	-1.280130000
H	5.528485000	-0.080230000	-1.610648000
H	5.449197000	1.665719000	-1.900604000
H	5.371023000	1.039737000	-0.246834000
Cu	1.930989000	-0.448770000	0.112389000
C	0.200494000	1.906178000	1.377789000
H	-2.650419000	0.591191000	0.749648000
H	-2.015579000	-0.397264000	2.066839000
I	3.048686000	-1.867056000	1.821567000
H	-2.209687000	1.354671000	2.290137000
H	1.199684000	2.049962000	0.965043000
H	-0.188448000	2.666595000	2.048309000
N	-1.379189000	-2.678508000	-0.167043000
C	-0.653307000	-3.539063000	0.780738000
C	-1.089922000	-3.056308000	-1.559964000
C	-2.824593000	-2.710265000	0.103106000
C	-0.748571000	-3.091246000	2.224341000
C	0.367187000	-2.922624000	-1.956939000
C	-3.651530000	-1.841280000	-0.822306000
H	0.402622000	-3.533448000	0.488250000
H	-1.007888000	-4.583809000	0.677157000
H	-1.686816000	-2.399777000	-2.202302000
H	-1.438177000	-4.091646000	-1.747066000
H	-2.967648000	-2.374604000	1.136579000
H	-3.184420000	-3.758244000	0.064153000
H	-0.090641000	-3.712072000	2.841698000
H	-1.759128000	-3.173369000	2.639160000

H	-0.407318000	-2.053251000	2.337562000
H	0.464984000	-3.048913000	-3.040472000
H	1.021597000	-3.659686000	-1.479380000
H	0.759933000	-1.921402000	-1.716190000
H	-4.653033000	-1.700638000	-0.402076000
H	-3.773366000	-2.277501000	-1.819337000
H	-3.195398000	-0.850701000	-0.951868000

P2-10t

E= -703.833344 a.u.

ZPE_G= 0.077045 a.u.

G= -703.910389 a.u.

C	0.056376000	-1.964407000	1.208834000
N	0.027254000	-1.220698000	0.061920000
C	0.135469000	-3.449836000	1.074715000
Cu	-1.258641000	0.335135000	-0.037272000
I	-3.606122000	-0.292380000	-0.487259000
C	-0.016457000	1.825979000	0.353533000
H	0.051173000	-1.793564000	-0.782675000
C	-0.127110000	3.007256000	0.697035000
C	-0.253522000	4.391565000	1.089509000
H	0.619805000	4.970512000	0.766045000
H	-1.137359000	4.850831000	0.630938000
H	-0.343539000	4.498803000	2.176635000
Cu	1.269691000	0.391316000	-0.031412000
C	0.016775000	-1.326393000	2.424508000
H	-0.726824000	-3.834071000	0.516250000
H	1.036699000	-3.738367000	0.519971000
I	3.624226000	-0.204140000	-0.479686000
H	0.160070000	-3.938885000	2.051036000
H	-0.038130000	-0.238992000	2.486365000
H	0.038180000	-1.887915000	3.353118000

P2-11t (Cy6)

E= -908.0928169 a.u.

ZPE_G= 0.127410 a.u.

G= -907.965407 a.u.

Cu	-1.427943000	0.529671000	-0.040586000

C	0.102968000	1.719730000	-0.034813000
C	0.496052000	2.899012000	-0.009335000
Cu	0.955354000	-0.026986000	-0.152347000
C	0.990303000	4.252025000	0.009936000
H	0.511753000	4.868390000	-0.760489000
H	0.838373000	4.732044000	0.983715000
H	2.069570000	4.251064000	-0.196409000
N	-2.449746000	4.070348000	0.595386000
N	-2.838866000	3.000380000	0.471075000
N	-3.095600000	1.796483000	0.311681000
C	-4.523984000	1.431690000	0.395063000
H	-5.104488000	1.968988000	-0.360569000
H	-4.570347000	0.358857000	0.200626000
H	-4.917542000	1.642368000	1.393886000
C	1.436279000	-2.829223000	0.683544000
N	1.037788000	-1.950511000	-0.227103000
C	2.005136000	-2.364698000	1.874836000
C	1.243239000	-4.294838000	0.440173000
H	1.854273000	-4.901560000	1.113087000
H	0.192013000	-4.563555000	0.605250000
H	1.489666000	-4.562721000	-0.592364000
H	2.114398000	-1.296634000	2.053863000
H	2.352966000	-3.055162000	2.637777000
I	3.535759000	0.526198000	-0.208427000
I	-2.456757000	-1.751308000	-0.332175000
H	0.612348000	-2.388208000	-1.045087000

P2-TS5t (Cy6-TS1t)

E= -908.0738819 a.u.

ZPE_G= 0.1254836 a.u.

G= -907.948398 a.u.

Cu	1.645140000	0.330319000	-0.139921000
C	0.260004000	1.550210000	0.412823000
C	0.225539000	2.773039000	0.739601000
Cu	-0.781944000	-0.096825000	0.300269000
C	-0.502241000	4.004324000	1.043390000
H	-0.230611000	4.804910000	0.346226000
H	-0.273587000	4.362172000	2.053550000

H	-1.580150000	3.823854000	0.963533000
N	2.059715000	3.420834000	0.990218000
N	2.954884000	2.679562000	0.738107000
N	3.154543000	1.492762000	0.316513000
C	4.548339000	1.051077000	0.230654000
H	5.137418000	1.717480000	-0.408032000
H	4.540663000	0.054792000	-0.215737000
H	5.009026000	0.990292000	1.222705000
C	-1.257759000	-2.591246000	1.808941000
N	-1.673274000	-1.716444000	0.912979000
C	-0.001067000	-2.395432000	2.418722000
C	-2.082645000	-3.782003000	2.185114000
H	-2.304760000	-3.775101000	3.257815000
H	-1.529122000	-4.705423000	1.980134000
H	-3.026819000	-3.817650000	1.635734000
H	0.607310000	-1.527528000	2.168109000
H	0.384064000	-3.099502000	3.150958000
I	-2.924655000	1.070087000	-0.698947000
I	1.343844000	-1.967629000	-1.055466000
H	-2.599479000	-1.919895000	0.536921000

P2-12t

E= -908.0924101 a.u.

ZPE_G= 0.131818 a.u.

G=-907.960592 a.u.

Cu	-1.471894000	0.665596000	-0.091515000
C	0.101381000	1.495364000	0.552898000
C	0.300071000	2.793270000	0.798393000
Cu	0.781313000	-0.258554000	0.490628000
C	1.635819000	3.431869000	1.019540000
H	2.004174000	3.862497000	0.080486000
H	1.533421000	4.243842000	1.746864000
H	2.377548000	2.709084000	1.367417000
N	-0.752362000	3.740246000	0.927018000
N	-1.976037000	3.425962000	0.760473000
N	-2.406007000	2.272837000	0.383411000
C	-3.861440000	2.111299000	0.413061000
H	-4.339336000	3.083141000	0.560310000

H	-4.195177000	1.670144000	-0.530771000
H	-4.143826000	1.440288000	1.232350000
C	0.425990000	-2.843550000	1.887999000
N	1.146703000	-2.074337000	1.094773000
C	-0.782971000	-2.338432000	2.412844000
C	0.851746000	-4.235215000	2.234823000
H	0.899787000	-4.366293000	3.321168000
H	0.118762000	-4.958535000	1.859403000
H	1.827998000	-4.483581000	1.810619000
H	-1.103250000	-1.322241000	2.185303000
H	-1.414709000	-2.946111000	3.054420000
I	2.943055000	0.353609000	-0.812570000
I	-1.804430000	-1.528253000	-1.208360000
H	2.004728000	-2.520896000	0.770384000

P2-TS6t

E= -908.0874317 a.u.

ZPE_G= 0.132329 a.u.

G= -907.955103 a.u.

Cu	-9.080721000	-6.397088000	0.038348000
C	-10.899411000	-5.767956000	-0.167897000
C	-11.774609000	-6.374470000	-0.992832000
Cu	-10.496069000	-4.732206000	1.347841000
C	-13.174820000	-6.747101000	-0.619400000
H	-13.735989000	-6.981773000	-1.529022000
H	-13.182521000	-7.627741000	0.032680000
H	-13.673699000	-5.939394000	-0.076362000
N	-11.450551000	-6.673335000	-2.326941000
N	-10.283263000	-6.301430000	-2.703874000
N	-9.432556000	-5.856574000	-1.837900000
C	-8.310113000	-5.077501000	-2.366382000
H	-8.484353000	-4.010976000	-2.187001000
H	-7.379470000	-5.377364000	-1.874565000
H	-8.229848000	-5.249574000	-3.443060000
C	-8.404735000	-2.975289000	2.504450000
N	-9.629922000	-3.464399000	2.531553000
C	-7.595555000	-3.212325000	1.373333000
C	-7.850867000	-2.188666000	3.649893000

H	-8.613251000	-1.963705000	4.400226000
H	-7.049704000	-2.757406000	4.137243000
H	-7.409026000	-1.248499000	3.304286000
H	-7.997720000	-3.737276000	0.508842000
H	-6.567645000	-2.863737000	1.330100000
I	-12.478517000	-5.447572000	2.886552000
I	-7.454229000	-6.897024000	1.814145000
H	-10.136952000	-3.224580000	3.383806000

P2-13t (Cy5-1t)

E= -908.167058 au

ZPE_G= 0.134686 au

G= -908.032372 au

Cu	-1.237334000	-0.936576000	0.004517000
C	0.648704000	-1.499705000	0.115236000
C	1.220948000	-2.344701000	-0.870851000
Cu	0.715769000	0.480884000	-0.118713000
C	1.091322000	-2.248265000	-2.342579000
H	0.891788000	-3.228764000	-2.787259000
H	0.288580000	-1.561765000	-2.629666000
H	2.024638000	-1.878383000	-2.785731000
N	1.983216000	-3.289130000	-0.280107000
N	1.943657000	-3.102092000	1.030878000
N	1.159388000	-2.057383000	1.275597000
C	0.970554000	-1.601873000	2.638270000
H	1.415268000	-0.609092000	2.764170000
H	-0.096885000	-1.556002000	2.871560000
H	1.464400000	-2.311320000	3.303189000
C	-0.994474000	2.815803000	0.338340000
N	-0.026318000	2.253537000	-0.357100000
C	-1.450376000	2.180452000	1.514560000
C	-1.619676000	4.105494000	-0.088246000
H	-1.195557000	4.479158000	-1.023737000
H	-2.699307000	3.972461000	-0.224657000
H	-1.488890000	4.871418000	0.684163000
H	-0.965806000	1.276972000	1.882623000
H	-2.274118000	2.589513000	2.092600000
I	3.258141000	1.009275000	-0.165137000

I	-3.581094000	-0.267718000	-0.196605000
H	0.256147000	2.790564000	-1.176513000

P2-TS7t (Cy5-TS1t)

E= -908.144483 au

ZPE_G= 0.135022 au

G= -908.009461 au

Cu	-8.831667000	-7.250432000	-0.720684000
C	-10.512039000	-5.242977000	-0.855387000
C	-10.812167000	-6.616060000	-0.695491000
Cu	-10.277283000	-3.907794000	0.469859000
C	-11.426318000	-7.307572000	0.476200000
H	-11.319594000	-8.393356000	0.394492000
H	-10.978292000	-6.984701000	1.422201000
H	-12.499099000	-7.080634000	0.528201000
N	-10.705246000	-7.237952000	-1.938263000
N	-10.408983000	-6.323029000	-2.843234000
N	-10.325396000	-5.136043000	-2.196779000
C	-9.984731000	-3.944554000	-2.948326000
H	-10.731583000	-3.169011000	-2.758781000
H	-8.996816000	-3.582939000	-2.649028000
H	-9.977347000	-4.204045000	-4.007390000
C	-8.596300000	-3.331484000	2.782589000
N	-9.471123000	-2.892313000	1.894220000
C	-8.188132000	-4.680930000	2.725168000
C	-8.046231000	-2.438327000	3.848315000
H	-8.394585000	-2.768516000	4.833840000
H	-6.952506000	-2.485511000	3.866293000
H	-8.349322000	-1.397516000	3.708309000
H	-8.581749000	-5.357197000	1.964807000
H	-7.468786000	-5.082777000	3.432843000
I	-12.677619000	-2.844209000	0.307415000
I	-6.544144000	-7.523914000	0.055438000
H	-9.719055000	-1.911171000	2.021226000

P2-14t (Cy5-2t)

E= -908.1658604 au

ZPE_G= 0.132827 au

G= -908.033033 au

Cu	-3.255636000	-0.003606000	0.195840000
C	0.816473000	-0.016638000	0.608318000
C	-0.346671000	0.380695000	-0.048980000
Cu	2.629434000	0.444627000	0.271608000
C	-0.515408000	1.265409000	-1.226821000
H	-1.101406000	2.159853000	-0.980828000
H	0.457688000	1.593798000	-1.605476000
H	-1.037054000	0.752108000	-2.043535000
N	-1.410144000	-0.183507000	0.589812000
N	-0.994177000	-0.931374000	1.602944000
N	0.338834000	-0.830630000	1.594264000
C	1.101563000	-1.545982000	2.597220000
H	0.406833000	-2.134752000	3.197136000
H	1.822850000	-2.205017000	2.105010000
H	1.634620000	-0.836870000	3.236492000
C	4.483295000	2.722515000	0.056319000
N	4.292498000	1.416243000	0.095274000
C	3.365074000	3.578207000	0.151584000
C	5.849544000	3.311816000	-0.095627000
H	6.630528000	2.547303000	-0.088143000
H	5.919660000	3.868095000	-1.037220000
H	6.052207000	4.025735000	0.709675000
H	2.357704000	3.175223000	0.253387000
H	3.481844000	4.657635000	0.125669000
I	3.393175000	-1.874617000	-0.728824000
I	-5.614568000	0.256798000	-0.344071000
H	5.155932000	0.880433000	0.007132000

P2-mono14t

E= -700.4817542 au

ZPE_G= 0.138008 au

G= -700.343746 au

C	1.366296000	-0.914453000	0.120657000
C	1.993920000	-1.711025000	-0.848252000
Cu	-0.433948000	-0.344147000	0.229864000
C	1.408257000	-2.309853000	-2.074911000
H	1.240103000	-3.389008000	-1.961839000

H	0.442180000	-1.850728000	-2.313957000
H	2.070922000	-2.178449000	-2.937483000
N	3.288606000	-1.918893000	-0.491788000
N	3.530420000	-1.278659000	0.634391000
N	2.380878000	-0.666204000	0.994199000
C	2.339764000	0.120045000	2.207487000
H	3.343531000	0.134875000	2.635510000
H	2.019680000	1.141477000	1.978199000
H	1.641725000	-0.322768000	2.924641000
C	-3.179851000	-1.391105000	0.281058000
N	-2.362893000	-0.360687000	0.409202000
C	-2.630583000	-2.660645000	0.005146000
C	-4.662530000	-1.242637000	0.413208000
H	-4.951559000	-0.222774000	0.679491000
H	-5.156124000	-1.506520000	-0.528920000
H	-5.051004000	-1.925638000	1.176218000
H	-1.552668000	-2.792660000	-0.089921000
H	-3.265426000	-3.534109000	-0.111940000
I	-0.056982000	2.191305000	-0.380444000
H	-2.847548000	0.516516000	0.599079000

P2-15t

E= -908.166404 au

ZPE_G= 0.133722 au

G= -908.032682 au

Cu	-3.135186000	-0.444655000	0.051098000
C	0.943239000	-0.246641000	0.150649000
C	-0.290768000	0.192167000	-0.315711000
Cu	2.746733000	0.423530000	-0.191720000
C	-0.636798000	1.287842000	-1.254854000
H	0.245924000	1.624944000	-1.805521000
H	-1.387498000	0.962862000	-1.984833000
H	-1.054389000	2.156059000	-0.726913000
N	-1.256382000	-0.579591000	0.263119000
N	-0.711793000	-1.474261000	1.073338000
N	0.609280000	-1.261152000	0.996667000
C	1.494909000	-2.099076000	1.780108000
H	0.880821000	-2.740513000	2.413178000

H	2.114323000	-2.710392000	1.118030000
H	2.142843000	-1.473547000	2.400337000
C	1.796484000	3.154139000	0.548782000
N	2.427795000	2.354588000	-0.289730000
C	1.291467000	2.632319000	1.758128000
C	1.586743000	4.602126000	0.232155000
H	1.893436000	5.236176000	1.070027000
H	2.134494000	4.912228000	-0.661441000
H	0.519826000	4.792104000	0.062177000
H	1.453868000	1.591046000	2.026835000
H	0.743815000	3.266522000	2.449526000
I	4.677235000	-1.115793000	-0.392906000
I	-5.541203000	-0.209837000	-0.227170000
H	2.773966000	2.839181000	-1.118571000

P2-15s

E= -908.411308 au

ZPE_G= 0.137878 au

G= -908.027343 au

C	-2.714601000	-3.058862000	-0.278294000
N	-2.517507000	-2.029375000	-1.167533000
C	-3.912747000	-3.115189000	0.375651000
C	-1.622350000	-4.057844000	-0.067693000
H	-1.938861000	-4.883611000	0.574461000
H	-1.285465000	-4.475893000	-1.023649000
H	-0.750044000	-3.576756000	0.395701000
H	-4.696522000	-2.389705000	0.164670000
H	-4.120080000	-3.887936000	1.110194000
H	-1.635745000	-2.153988000	-1.671657000
Cu	3.082476000	0.142524000	0.214938000
C	-0.970662000	-0.187035000	0.102283000
C	0.250960000	-0.034469000	-0.531509000
C	0.582919000	0.083312000	-1.971397000
H	1.312051000	0.882256000	-2.147674000
H	1.019282000	-0.845254000	-2.361118000
H	-0.309967000	0.309554000	-2.562079000
N	1.205251000	-0.011498000	0.445229000
N	0.656491000	-0.155686000	1.642666000

N	-0.659853000	-0.272606000	1.421021000
C	-1.560428000	-0.442659000	2.543651000
H	-0.966799000	-0.416295000	3.457717000
H	-2.296196000	0.366822000	2.550313000
H	-2.076373000	-1.405114000	2.467266000
I	5.484062000	0.290536000	-0.130682000
Cu	-2.771691000	-0.292770000	-0.565018000
I	-4.019481000	1.765948000	-0.024556000

P2-TS8s

E= -908.156751 au

ZPE_G= 0.139703 au

G= -908.017048 au

Cu	-2.909557000	0.171946000	0.265505000
C	1.149578000	0.388467000	0.011007000
C	-0.098653000	0.266131000	-0.589023000
Cu	2.984407000	-0.089646000	-0.547834000
C	-0.468191000	0.191468000	-2.020348000
H	0.310697000	-0.305096000	-2.607616000
H	-1.401020000	-0.367417000	-2.151393000
H	-0.630008000	1.190339000	-2.448646000
N	-1.015234000	0.241426000	0.416097000
N	-0.423373000	0.366280000	1.597277000
N	0.884396000	0.490978000	1.343000000
C	1.823979000	0.528433000	2.447210000
H	1.258407000	0.714410000	3.360402000
H	2.348677000	-0.429393000	2.518648000
H	2.546691000	1.333794000	2.286485000
C	2.478868000	2.818785000	-0.120931000
N	2.439573000	1.670122000	-0.924312000
C	3.564942000	3.030025000	0.650403000
C	1.303882000	3.739082000	-0.190633000
H	1.454871000	4.631301000	0.422163000
H	1.115594000	4.063865000	-1.221850000
H	0.390863000	3.235166000	0.156784000
H	4.399523000	2.331325000	0.654729000
H	3.639069000	3.911673000	1.280454000
I	4.138323000	-2.211507000	-0.203290000

I	-5.323560000	0.144361000	0.001621000
H	1.752365000	1.770654000	-1.671077000

P2-16t

E= -908.1203583 au

ZPE_G= 0.136001 au

G= -907.984357 au

N	4.121284000	7.715303000	2.984378000
N	3.356409000	6.606892000	2.892938000
N	5.971427000	8.306774000	4.453310000
C	4.569042000	7.961006000	4.343660000
C	7.038427000	7.473094000	4.648902000
C	4.092788000	6.733730000	4.986961000
N	3.370857000	6.036885000	4.112152000
C	6.963228000	6.117361000	4.461939000
H	6.070968000	5.618290000	4.097275000
H	7.839367000	5.505196000	4.651440000
H	6.188600000	9.297293000	4.422935000
C	4.243787000	6.358948000	6.410043000
H	4.191608000	5.272271000	6.538453000
H	5.203119000	6.706236000	6.810060000
H	3.452856000	6.804681000	7.030372000
C	4.035787000	8.718438000	1.956316000
H	3.327812000	9.510203000	2.244408000
H	5.020541000	9.165229000	1.789657000
H	3.696188000	8.243541000	1.034312000
C	8.303484000	8.150447000	5.063362000
H	9.138300000	7.447233000	5.078168000
H	8.558082000	8.968243000	4.378576000
H	8.201228000	8.586578000	6.064166000
Cu	3.562415000	9.423582000	5.248003000
I	1.925585000	11.023124000	6.136377000
Cu	2.386308000	4.430744000	4.370560000
I	1.248521000	2.320491000	4.749915000

P2-16s

E= -908.121775 au HF=-908.3175027 au

ZPE_G= 0.133766 au

G= -907.988009 au

Cu	-3.02814500	0.05040700	0.23985400
C	0.72424800	1.58182200	0.37992000
C	-0.24859700	0.84852800	-0.27016300
C	-0.20562800	0.15731500	-1.57752100
H	0.74503500	-0.37642600	-1.70914100
H	-1.01932500	-0.57256600	-1.64775500
H	-0.30510000	0.85906100	-2.41473200
N	-1.33238400	0.85377100	0.55266200
N	-1.08743900	1.52866900	1.66340500
N	0.16815100	1.98454400	1.54808000
C	0.76346500	2.74739000	2.62786500
H	0.00324300	2.86052400	3.40025300
H	1.62293800	2.21226200	3.04118000
H	1.06629400	3.73626900	2.27293000
C	2.11184900	2.58463900	-1.33278400
N	2.05394600	1.87381500	-0.03050500
C	2.82204500	2.04338300	-2.31885800
C	1.35230600	3.86322000	-1.39087900
H	0.28303500	3.70636700	-1.19456200
H	1.71225000	4.57908700	-0.63958400
H	1.44952600	4.32600800	-2.37566600
H	3.34637100	1.09492900	-2.20115100
H	2.89855700	2.54219000	-3.28126100
I	-5.17721000	-0.97762700	-0.23793700
H	2.50343700	2.46692900	0.67291600
Cu	3.02345000	0.13227500	0.04306800
I	4.10732000	-2.02946300	0.14418000

Other Complex

CuI

E= -207.6138135 au

ZPE_G= -0.024748 au

G= -207.638562 au

Cu	0.000000000	0.000000000	-1.556267000
I	0.000000000	0.000000000	0.851542000

Et_3N

E= -292.3619923 au

ZPE_G= 0.172210 au

G= -292.189782 au

N	-0.000523000	0.000561000	-0.068290000
C	0.077113000	-1.387144000	0.395509000
C	-1.241227000	0.626012000	0.396543000
C	1.161073000	0.761658000	0.398873000
C	1.078368000	-2.224801000	-0.375621000
C	-2.467155000	0.180681000	-0.376522000
C	1.392087000	2.043358000	-0.377167000
H	-0.917383000	-1.834403000	0.280529000
H	0.302983000	-1.419039000	1.483411000
H	-1.130877000	1.711281000	0.285228000
H	-1.382210000	0.442722000	1.483816000
H	2.045336000	0.122142000	0.292164000
H	1.069499000	0.978175000	1.485216000
H	1.072622000	-3.258344000	-0.010570000
H	2.104591000	-1.852126000	-0.275739000
H	0.830687000	-2.238626000	-1.443366000
H	-3.359650000	0.699848000	-0.008481000
H	-2.656519000	-0.895050000	-0.282236000
H	-2.355929000	0.407702000	-1.443227000
H	2.286682000	2.557495000	-0.007207000
H	0.555143000	2.746005000	-0.288644000
H	1.537142000	1.829702000	-1.442552000

Et_3NH

E= -292.8135098

ZPE_G= 0.188747 au

G= -292.624763 au

N	-0.000729000	-0.000508000	-0.013907000
C	0.382032000	-1.392493000	0.438063000
C	-1.397581000	0.364961000	0.438556000
C	1.013055000	1.026526000	0.441088000
C	1.497742000	-1.979407000	-0.388834000
C	-2.465721000	-0.303735000	-0.389199000
C	0.970897000	2.283857000	-0.389891000

H	-0.521847000	-2.002567000	0.368043000
H	0.644336000	-1.295910000	1.496180000
H	-1.471799000	1.453263000	0.371003000
H	-1.446623000	0.087136000	1.496387000
H	1.993298000	0.547347000	0.379530000
H	0.793189000	1.210707000	1.497552000
H	1.722097000	-2.981997000	-0.014600000
H	2.422844000	-1.397590000	-0.331077000
H	1.211684000	-2.077485000	-1.441533000
H	-3.444876000	0.007375000	-0.015026000
H	-2.429427000	-1.395981000	-0.332596000
H	-2.406537000	-0.005687000	-1.441696000
H	1.727700000	2.978108000	-0.014748000
H	0.005589000	2.797182000	-0.338082000
H	1.203027000	2.081644000	-1.441227000
H	-0.000099000	-0.000241000	-1.039462000

N_3Me

E= -204.0877889 au

ZPE_G= 0.024116 au

G= -204.063673 au

N	-1.807096000	0.264453000	0.000004000
N	-0.713263000	-0.091197000	0.000008000
N	0.394244000	-0.624762000	-0.000015000
C	1.552901000	0.281125000	-0.000010000
H	1.564797000	0.911786000	0.895827000
H	2.438497000	-0.353664000	-0.002633000
H	1.562108000	0.915661000	-0.893112000

Acetylene

E= -116.6367348 au

ZPE_G= 0.031374 au

G= -116.605361 au

C	-1.425482000	0.000032000	-0.000052000
H	-2.495193000	0.000057000	-0.000338000
C	-0.212963000	-0.000107000	0.000272000
C	1.236778000	0.000010000	-0.000036000
H	1.635457000	-0.851440000	0.563290000

H	1.634707000	-0.062211000	-1.019408000
H	1.635032000	0.913984000	0.455358000

B1s

E= -380.052369 au

ZPE_G= 0.052287 au

G= -380.000082 au

C	3.181982000	0.173878000	0.000020000
C	2.969201000	1.553257000	0.000061000
H	3.804054000	2.248889000	-0.000045000
H	1.963328000	1.969639000	-0.000478000
N	2.096420000	-0.609076000	-0.000154000
C	4.550255000	-0.418424000	0.000086000
H	4.691704000	-1.052703000	0.881853000
H	4.692239000	-1.051508000	-0.882470000
H	5.324344000	0.350311000	0.000801000
Cu	0.292785000	-0.298453000	-0.000005000
I	-2.079336000	0.079300000	0.000011000
H	2.354772000	-1.601133000	-0.000029000

Et_3N-CuI

E= -500.044833 au

ZPE_G= 0.166586 au

G= -499.878247 au

N	-2.040261000	-0.000240000	-0.000158000
C	-2.547540000	1.099863000	-0.873237000
C	-2.547471000	0.205075000	1.389259000
C	-2.547069000	-1.306267000	-0.517134000
C	-1.806809000	1.212880000	-2.186784000
C	-1.810538000	1.289439000	2.142860000
C	-1.809577000	-2.501142000	0.044254000
H	-2.441914000	2.034714000	-0.313439000
H	-3.626547000	0.940494000	-1.034627000
H	-2.437385000	-0.746359000	1.919516000
H	-3.627420000	0.420166000	1.332555000
H	-2.438011000	-1.289208000	-1.606315000
H	-3.626867000	-1.365139000	-0.301920000
H	-2.221549000	2.036568000	-2.777506000

H	-1.878865000	0.305037000	-2.795750000
H	-0.741447000	1.423525000	-2.019364000
H	-2.223532000	1.386355000	3.152525000
H	-1.888660000	2.270718000	1.662076000
H	-0.743708000	1.044370000	2.238978000
H	-2.221925000	-3.423834000	-0.377681000
H	-1.888203000	-2.576511000	1.134342000
H	-0.742679000	-2.461112000	-0.215634000
Cu	-0.044641000	0.000512000	-0.000485000
I	2.391305000	-0.000227000	0.000417000