

**Electronic supplementary information (ESI)**

For

**Reactivity of Copper(II)-Alkylperoxo Complexes**

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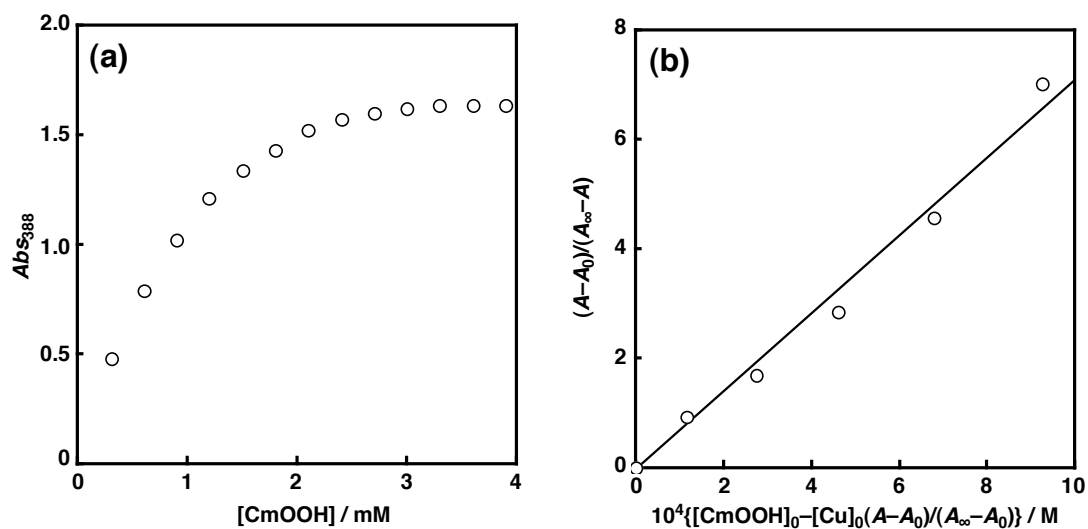
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Fig. S1



**Fig. S1.** (a) Spectrophotometric titration for the formation of cumylperoxo copper(II) complex from the reaction of  $1a^H$  (1.0 mM) and CmOOH in the presence of  $Et_3N$  (10 mM) in  $CH_3CN$  at  $-40^\circ C$ . (b) Plot of  $(A - A_0)/(A_\infty - A)$  against  $10^4\{[CmOOH]_0 - [Cu]_0(A - A_0)/(A_\infty - A_0)\} / M$ .

Fig. S2 and S3

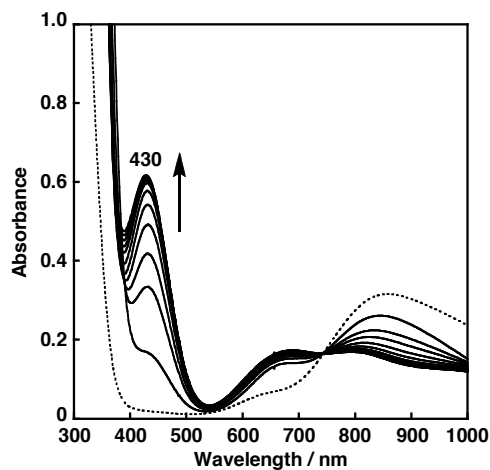


Fig. S2 Spectral change for the reaction of **1b** (1.0 mM) with CmOOH (2.5 mM) in the presence of Et<sub>3</sub>N (10 mM) in CH<sub>3</sub>CN at -40°C.

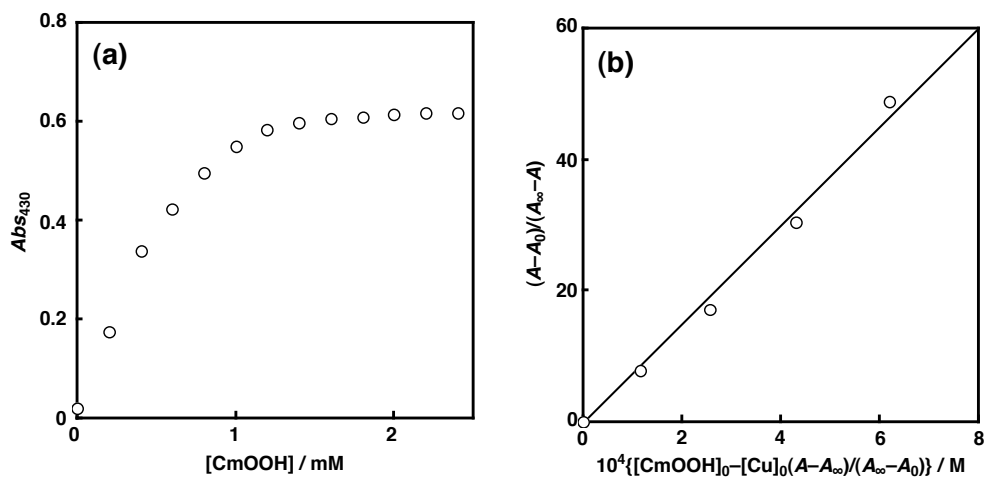
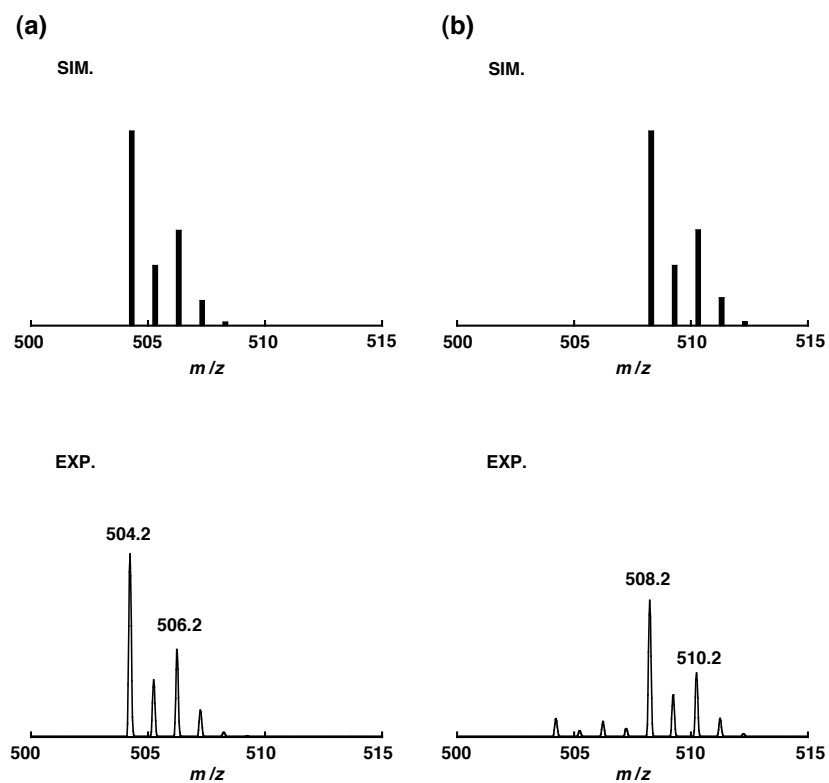


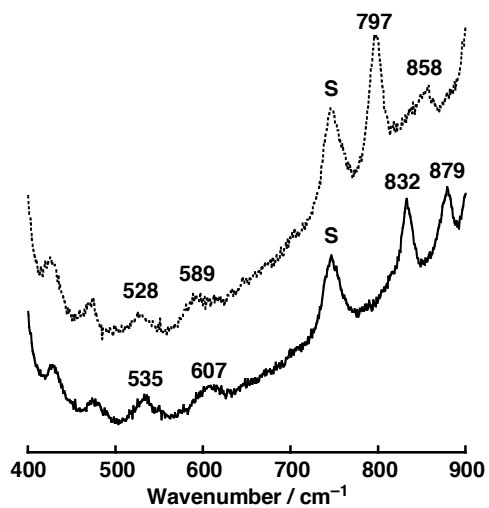
Fig. S3 (a) Spectrophotometric titration for the formation of cumylperoxo copper(II) complex from the reaction of **1b** (1.0 mM) and CmOOH in the presence of Et<sub>3</sub>N (10 mM) in CH<sub>3</sub>CN at -40°C. (b)  $(A - A_0)/(A_\infty - A)$  against  $\{[CmOOH]_0 - [Cu]_0(A - A_0)/(A_\infty - A_0)\}$ .

**Fig. S4**



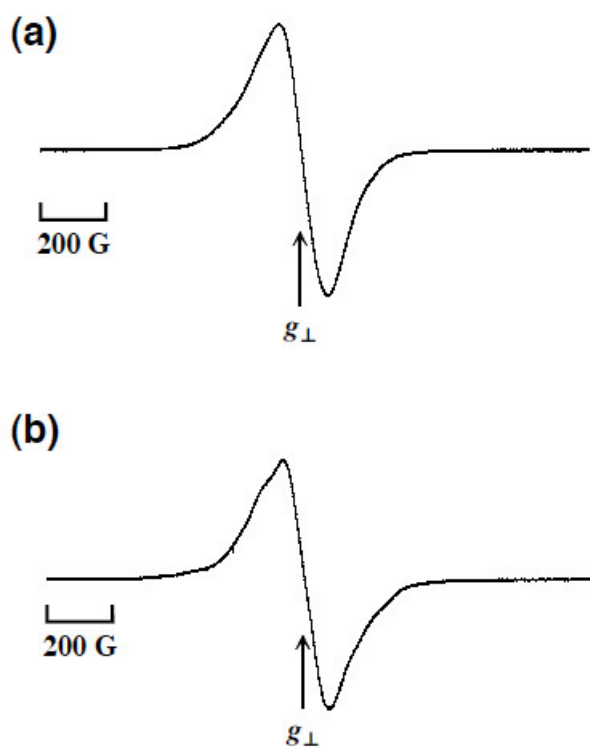
**Fig. S4** Experimental (bottom) and simulated (top) peak envelopes in the positive-ion ESI-MS spectra of the product derived from the reaction of **1b** (1.0 mM) with CmOOH (1.0 mM) in the presence of Et<sub>3</sub>N (1.0 mM) in CH<sub>3</sub>CN at -40°C; (a) with Cm<sup>16</sup>O<sub>2</sub>H and (b) with Cm<sup>18</sup>O<sub>2</sub>H.

**Fig. S5**



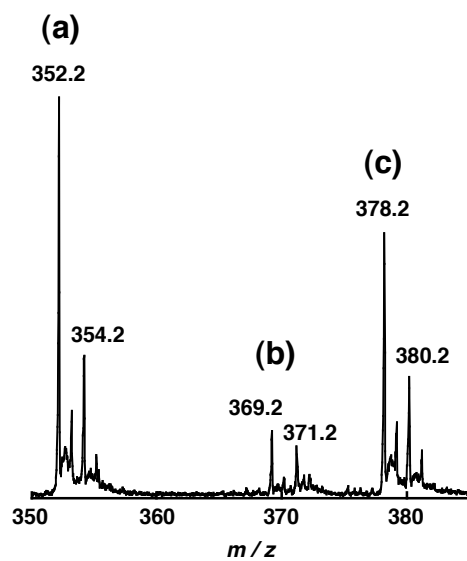
**Fig. S5** Resonance Raman spectra of the product derived from the reaction of **1b** (4.0 mM) with CmOOH (12 mM) in the presence of Et<sub>3</sub>N (40 mM) generated by using Cm<sup>16</sup>O<sub>2</sub>H (solid line, below) and Cm<sup>18</sup>O<sub>2</sub>H (dotted line, above) obtained with  $\lambda_{\text{ex}} = 441.6$  nm in CH<sub>3</sub>CN -40°C; s denotes the solvent band.

**Fig. S6**



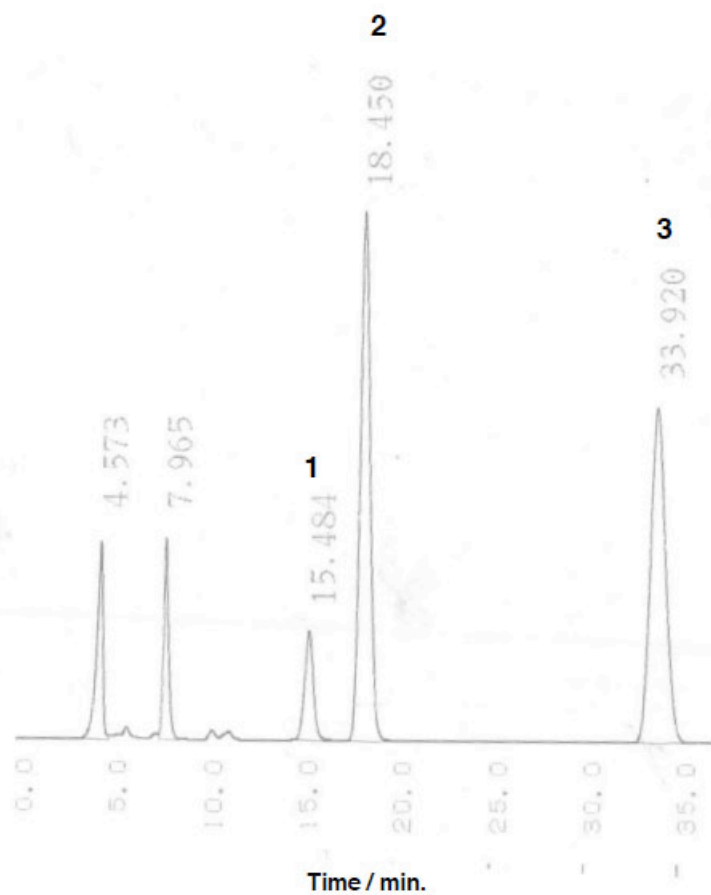
**Fig. S6** (a) ESR spectrum of **1b** (starting material) ( $2.0 \times 10^{-3}$  M) in  $\text{CH}_3\text{CN}$  at  $-196^\circ\text{C}$ . ESR parameter  $g_{\perp} = 2.112$ . (b) ESR spectrum of the **2b** generated in the reaction of **1b** ( $2.0 \times 10^{-3}$  M) and  $\text{CmOOH}$  ( $1.0 \times 10^{-2}$  M) in the presence of  $\text{Et}_3\text{N}$  ( $2.0 \times 10^{-3}$  M) in  $\text{CH}_3\text{CN}$  at  $-196^\circ\text{C}$ . ESR parameters  $g_{\perp} = 2.118$ . Low resolution of the spectrum prohibits precise assignment of the  $g_{\parallel}$  value.

**Fig. S7**



**Figure S7.** ESI-MS (pos.) spectrum after the self-decomposition of  $2\mathbf{a}^{\text{H}}$  in  $\text{CH}_3\text{CN}$ . (a)  $m/z = 352.2$  ( $[\text{Cu}^{\text{I}}(\text{bpa}^{\text{H}})]^+$ ), (b)  $m/z = 369.2$  ( $[\text{Cu}^{\text{II}}(\text{bpa}^{\text{H}})(\text{OH})]^+$ ), (c)  $m/z = 378.2$  ( $[\text{Cu}^{\text{II}}(\text{bpa}^{\text{H}})(\text{CN})]^+$ ).

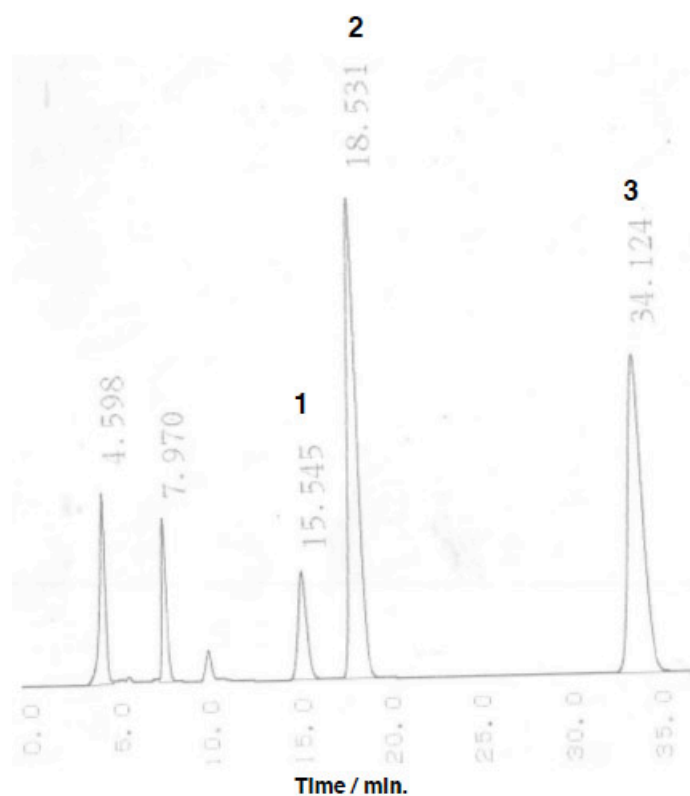
**Fig. S8**



**Fig. S8** HPLC diagram of the self-decomposition products of **2a**. Peak 1: cumyl alcohol (CmOH); peak 2: acetophenone (PhCOMe); peak 3: anisole (internal standard material).

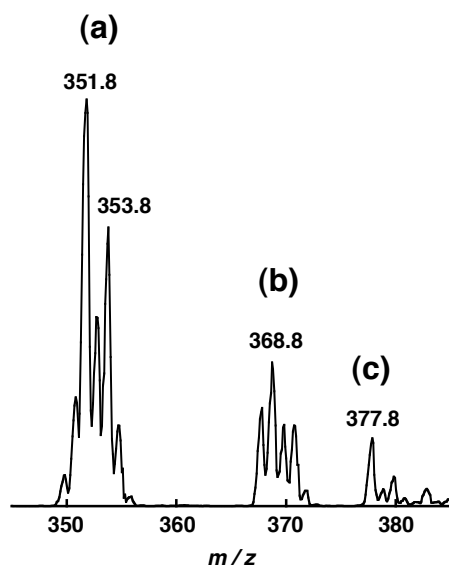


**Fig. S9**



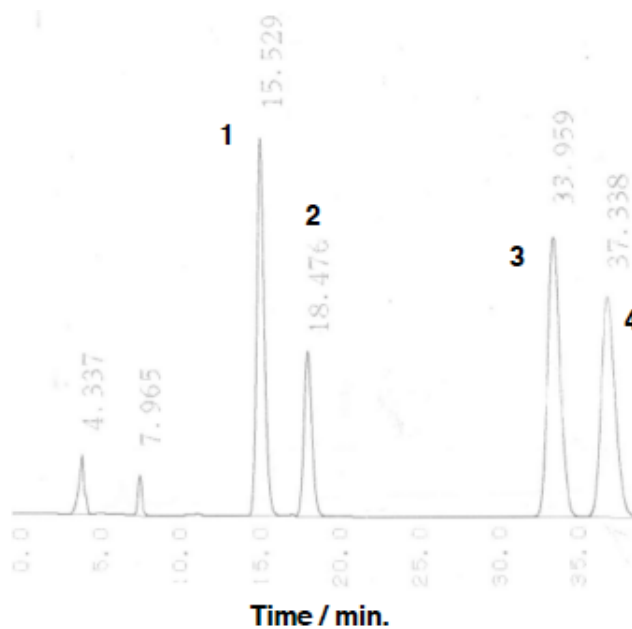
**Fig. S9** HPLC diagram of the self-decomposition products of **2b**. Peak 1: cumyl alcohol (CmOH); peak 2: acetophenone (PhCOME); peak 3: anisole (internal standard material).

**Fig. S10**



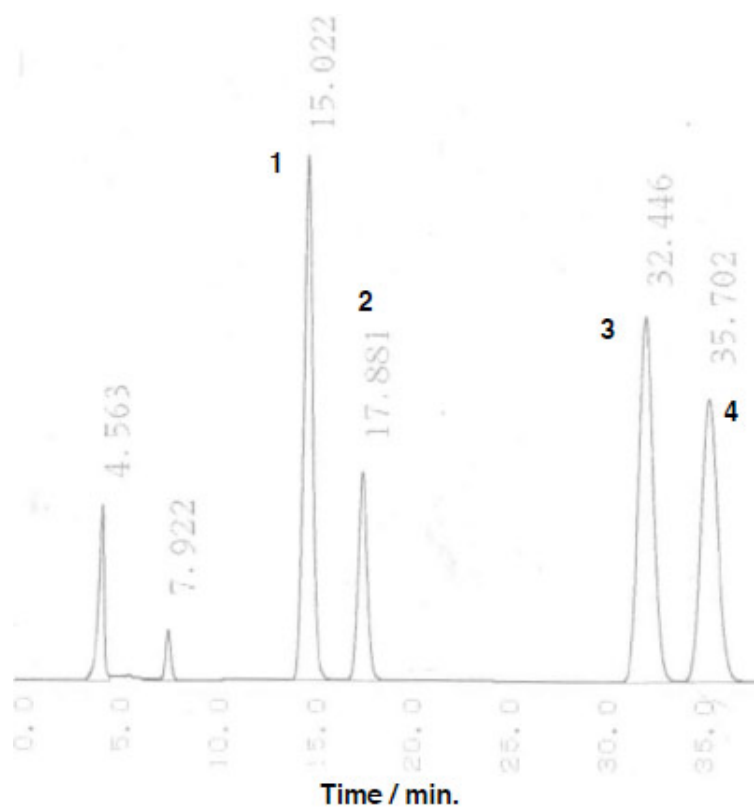
**Fig. S10** ESI-MS (pos.) spectrum of the final reaction mixture of **2a** and CHD. (a)  $m/z = 351.8$  ( $[\text{Cu}^{\text{I}}(\text{bpa})]^+$ ), (b)  $m/z = 368.8$  ( $[\text{Cu}^{\text{II}}(\text{bpa})(\text{OH})]^+$ ), (c)  $m/z = 377.8$  ( $[\text{Cu}^{\text{II}}(\text{bpa})(\text{CN})]^+$ ).

**Fig. 11**



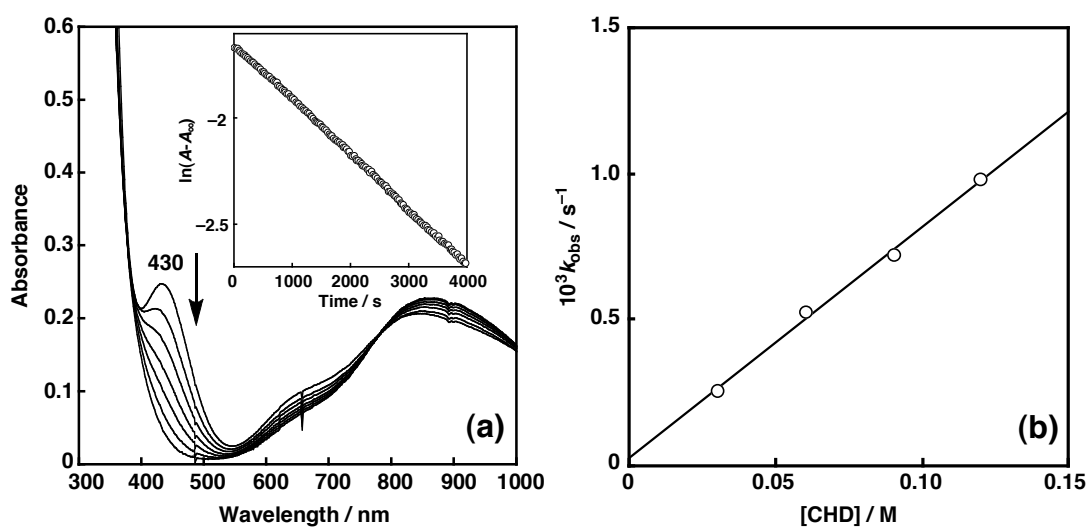
**Fig. S11** HPLC diagram of the products derived from the reaction of **2a** and CHD. Peak 1: cumyl alcohol (CmOH); peak 2: acetophenone (PhCOMe) ; peak 3: anisole (internal standard material); peak 4: benzene.

**Fig. S12**



**Fig. S12** HPLC diagram of the products of derived from the reaction of **2b** and CHD. Peak 1: cumyl alcohol (CmOH); peak 2: acetophenone (PhCOMe); peak 3: anisole (internal standard material); peak 4: benzene.

Fig. S13



**Fig. S13** (a) Spectral change for the reaction of **2b** (1.0 mM) and CHD (30 mM) in  $\text{CH}_3\text{CN}$  at 30 °C under anaerobic conditions; Inset: the pseudo-first-order plot based on the absorption change at 430 nm. (b) Plots of  $k_{\text{obs}}$  vs substrate concentration for the reaction of **2b** with CHD.

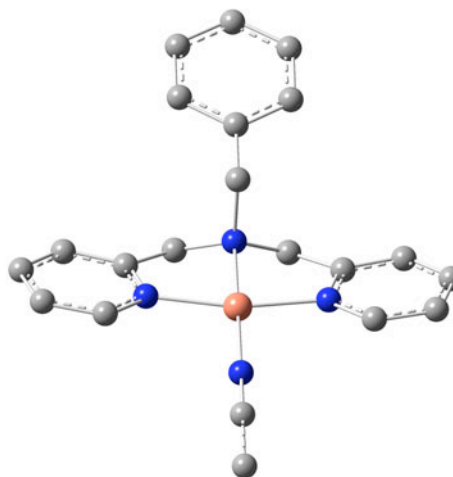
## DFT calculation results

### I – Cartesian Coordinates (ang) and Energies ( $E_h$ , doublet electronic states)

#### 1) – $[\text{Cu}^{\text{II}}(\text{bpa})(\text{CH}_3\text{CN})]^{2+}$

Energy: -1229.29162036 a.u.

C	-1.90034300	-2.91672300	-0.40538600
C	-1.59170000	-4.26747700	-0.36107500
C	-0.40265500	-4.66204100	0.24649700
C	0.43989600	-3.69295600	0.78585100
C	0.06858400	-2.35762000	0.71358200
N	-1.09166900	-1.98149700	0.12370600
H	-0.12953700	-5.71357900	0.29426500
H	-2.81073400	-2.55225200	-0.87499000
H	-2.27131500	-4.99213000	-0.80015800
H	1.37853200	-3.96789800	1.26247100
C	0.87213900	-1.23935700	1.30959800
H	0.54770700	-1.06208700	2.34422700
H	1.94450600	-1.47578500	1.34735200
N	0.63393900	-0.00040100	0.53733000
C	0.87280900	1.23811200	1.31010500
H	1.94531500	1.47388400	1.34805200
H	0.54817300	1.06063000	2.34463500
C	0.06999200	2.35709000	0.71443600
C	0.44209100	3.69217800	0.78726000
N	-1.09039500	1.98187900	0.12424800
C	-0.39978800	4.66196100	0.24811400
H	1.38081200	3.96638300	1.26413500
C	-1.89840300	2.91777600	-0.40466900
C	-1.58895200	4.26832800	-0.35983200
H	-0.12605100	5.71331900	0.29631300
H	-2.80889200	2.55398500	-0.87462300
H	-2.26802500	4.99355100	-0.79881100
C	1.36894100	-0.00033000	-0.79820300
H	1.00873500	0.88597000	-1.33590000
H	1.00851100	-0.88640500	-1.33612000
C	2.85992800	-0.00051800	-0.67821900
C	3.56836700	-1.20840500	-0.62993200
C	3.56862400	1.20720300	-0.62956500
C	4.95494000	-1.20899200	-0.52056300
H	3.03064500	-2.15485400	-0.71707800
C	4.95519500	1.20746700	-0.52019500
H	3.03110000	2.15379200	-0.71642200
C	5.64781700	-0.00084500	-0.45865300
H	5.49832700	-2.15071100	-0.50057500
H	5.49878100	2.14906400	-0.49992000
H	6.73242500	-0.00097200	-0.37991100
Cu	-1.35882000	0.00029300	0.06167500
C	-4.47374600	0.00129900	-0.47138200
N	-3.31836200	0.00092300	-0.34882800
C	-5.90467000	0.00155800	-0.62851100
H	-6.34141000	-0.86207000	-0.11530300
H	-6.33216900	0.91470300	-0.20031500

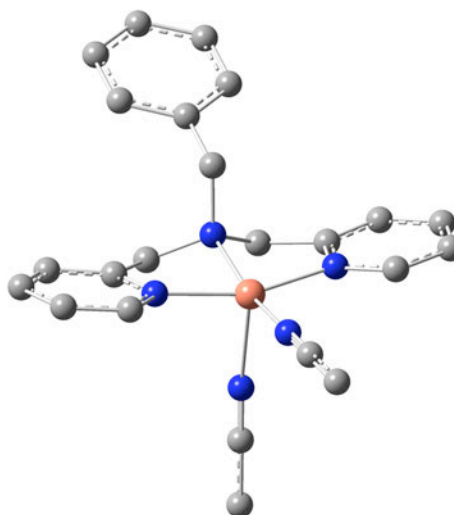


H -6.16863700 -0.04761200 -1.69063000

2) – [Cu<sup>II</sup>(bpa)(CH<sub>3</sub>CN)<sub>2</sub>]<sup>2+</sup>

Energy: -1362.07096036 a.u.

C	-1.52792500	-2.94647400	-0.90498000
C	-1.18817200	-4.29052200	-0.85294900
C	-0.06691300	-4.66756600	-0.11959300
C	0.67576800	-3.68832400	0.53477400
C	0.27366900	-2.36197800	0.44662200
N	-0.81735900	-2.00231200	-0.26853200
H	0.23157600	-5.71177200	-0.06376000
H	-2.38917600	-2.59655700	-1.46923200
H	-1.78991300	-5.02237600	-1.38419700
H	1.56218700	-3.94695500	1.11049900
C	0.97261400	-1.23575100	1.15019600
H	0.49927300	-1.06452000	2.12687700
H	2.03318700	-1.45904600	1.33316500
N	0.81515300	0.00004100	0.35866700
C	0.97284900	1.23580200	1.15021100
H	2.03346400	1.45891400	1.33315000
H	0.49949500	1.06467400	2.12690200
C	0.27407000	2.36214600	0.44666700
C	0.67652000	3.68840000	0.53465600
N	-0.81720600	2.00271500	-0.26823600
C	-0.06606800	4.66778600	-0.11960100
H	1.56312300	3.94684000	1.11017900
C	-1.52773100	2.94702300	-0.90453200
C	-1.18761900	4.29098900	-0.85263700
H	0.23270800	5.71192000	-0.06391500
H	-2.38924800	2.59733400	-1.46850700
H	-1.78933800	5.02296300	-1.38375000
C	1.67537000	-0.00003300	-0.89088100
H	1.37109300	0.88472100	-1.46376300
H	1.37086600	-0.88466200	-1.46383000
C	3.14915600	-0.00022000	-0.62538300
C	3.84942700	-1.20695300	-0.50456200
C	3.84970200	1.20634400	-0.50448400
C	5.21800900	-1.20800200	-0.25440400
H	3.32188600	-2.15305900	-0.64315900
C	5.21828400	1.20706800	-0.25432900
H	3.32237900	2.15257900	-0.64302300
C	5.90153200	-0.00054900	-0.12319700
H	5.75596800	-2.15006800	-0.17792900
H	5.75645900	2.14900600	-0.17779500
H	6.97269300	-0.00067700	0.06474300
Cu	-1.15835700	0.00023600	-0.23095700
C	-3.90340500	0.00012300	-1.83264800
N	-2.90084000	0.00034100	-1.24662100
C	-2.61457200	-0.00033600	2.87691700
N	-1.99571200	-0.00036500	1.89108200
C	-3.37866100	-0.00012000	4.10199700
H	-4.11557000	-0.80988100	4.09071600
H	-2.71848700	-0.14289600	4.96384300
H	-3.90609900	0.95193800	4.22141500
C	-5.14643600	-0.00006300	-2.56204200
H	-5.70610100	-0.91911100	-2.35782900



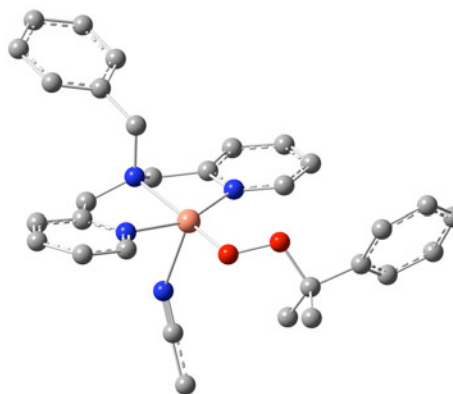
H	-5.76148600	0.85574900	-2.26394400
H	-4.95363800	0.06242500	-3.63850700

3) – [Cu<sup>II</sup>(bpa)(CH<sub>3</sub>CN)(O<sub>2</sub>Cm)]<sup>+</sup>

3a (structure *i* in Figure 8)

Energy: -1729.49998905 a.u.

C	-1.01104800	3.28802300	-1.24670200
C	-1.90923300	4.30272900	-1.55229900
C	-3.21226600	4.20607300	-1.07295100
C	-3.57473500	3.10311300	-0.30447300
C	-2.61912500	2.13216800	-0.02698700
N	-1.36138000	2.23429400	-0.49830700
H	-3.94414900	4.97745700	-1.30288000
H	0.02121300	3.27866100	-1.59603100
H	-1.59249600	5.14376800	-2.16296900
H	-4.58783800	2.99173500	0.07836700
C	-2.88753800	0.92675000	0.83412000
H	-2.59616300	1.15783100	1.86760400
H	-3.95880000	0.67232600	0.84318200
N	-2.05228500	-0.19582000	0.38968600
C	-1.79495800	-1.19727300	1.42823200
H	-2.64644900	-1.88073900	1.57260900
H	-1.64612900	-0.65526000	2.37162100
C	-0.54062700	-1.96115500	1.09955400
C	-0.35450900	-3.28322600	1.48707500
N	0.41279200	-1.28028800	0.42525400
C	0.84694900	-3.91920600	1.18742800
H	-1.14919000	-3.80332200	2.01939700
C	1.56217900	-1.90292300	0.11946600
C	1.82239200	-3.21611700	0.48961900
H	1.01089600	-4.95266200	1.48556300
H	2.27869800	-1.30733500	-0.44294400
H	2.77382900	-3.66730400	0.21937300
C	-2.54163800	-0.80338500	-0.89077400
H	-1.76961400	-1.51743200	-1.20596900
H	-2.54947400	0.00760500	-1.63099700
C	-3.88525500	-1.46690900	-0.80671300
C	-5.05563800	-0.74267500	-1.06079200
C	-3.99311200	-2.81913400	-0.46247000
C	-6.30393400	-1.34943600	-0.95735400
H	-4.98198500	0.30276900	-1.36751700
C	-5.23976500	-3.42890100	-0.35735000
H	-3.08538700	-3.40415700	-0.30041200
C	-6.39715100	-2.69257600	-0.60005400
H	-7.20520100	-0.77720200	-1.16781300
H	-5.30841300	-4.48352300	-0.09839300
H	-7.37199000	-3.16976500	-0.52515800
Cu	-0.13110700	0.65587200	-0.03812600
C	0.58630500	1.88013500	3.11528300
N	-0.10665300	1.32530900	2.36004200
C	1.45433200	2.56683100	4.04575500
H	1.78696100	3.51998100	3.62155200
H	0.93039400	2.76698400	4.98593700
H	2.33731400	1.95554300	4.26011100



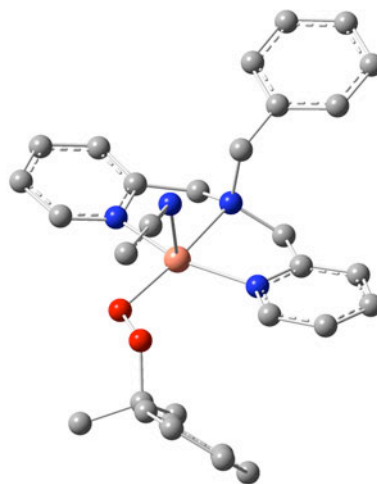


O	1.34149800	1.60085400	-0.74757800
O	2.41217100	0.73060300	-1.07971100
C	3.62805300	1.07842900	-0.32958300
C	3.30777700	1.21161100	1.14876700
H	2.84857300	0.29780300	1.54975500
H	4.21589000	1.42850200	1.72302600
H	2.60491300	2.03834300	1.28239200
C	4.16427500	2.39457400	-0.87786200
H	5.08690400	2.68461000	-0.36198700
H	4.38319700	2.31534800	-1.94742100
H	3.41844200	3.18464700	-0.73490900
C	4.53321600	-0.09410000	-0.66424600
C	5.14473600	-0.87922400	0.31737700
C	4.72836800	-0.43414200	-2.00972500
C	5.93886100	-1.96912800	-0.03505600
H	5.01018100	-0.64232100	1.37139700
C	5.50957700	-1.52904500	-2.36209700
H	4.24478600	0.15891700	-2.78422900
C	6.12042400	-2.29988400	-1.37461500
H	6.41849600	-2.55992000	0.74359300
H	5.64616900	-1.77919200	-3.41253400
H	6.74037800	-3.15108600	-1.64952800

### 3b

Energy: -1729.50013576 a.u.

C	0.94054800	3.53998900	0.14988500
C	1.81482300	4.61441500	0.25425200
C	3.13504400	4.44185400	-0.15017300
C	3.53807200	3.20618500	-0.65048600
C	2.60527100	2.18030000	-0.73884600
N	1.33095500	2.35641200	-0.33991700
H	3.84805100	5.25967400	-0.07189200
H	-0.10549400	3.58800700	0.45114300
H	1.46537100	5.56310700	0.65211800
H	4.56372500	3.03641400	-0.97339500
C	2.90520200	0.82712200	-1.32450000
H	2.60032000	0.82508800	-2.38071600
H	3.98400400	0.60977700	-1.30650400
N	2.11784800	-0.20501900	-0.63317700
C	1.84557100	-1.38793800	-1.46011600
H	2.70706100	-2.07177000	-1.51143500
H	1.65603000	-1.03826900	-2.48519400
C	0.61993000	-2.09471900	-0.94981000
C	0.47892100	-3.47693600	-0.98767100
N	-0.35948700	-1.29494800	-0.47714700
C	-0.70678800	-4.05133500	-0.53811400
H	1.29248000	-4.09078600	-1.37017900
C	-1.49277100	-1.85199100	-0.02456600
C	-1.71111400	-3.22353300	-0.04845500
H	-0.83874600	-5.13088100	-0.56370000
H	-2.24019000	-1.15141300	0.34680000
H	-2.65445000	-3.62238600	0.31568800
C	2.69254100	-0.55952100	0.70798600
H	1.95820100	-1.21691400	1.18913100
H	2.69691700	0.36989800	1.29089400
C	4.05298600	-1.19038700	0.66752100

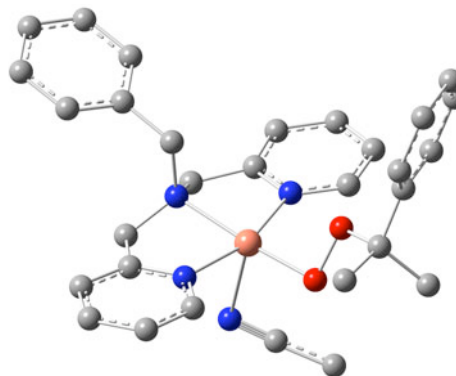


C	5.20788600	-0.40151600	0.72746200
C	4.19492200	-2.57942200	0.56741500
C	6.47130800	-0.98222600	0.66955100
H	5.11078200	0.67934100	0.84883800
C	5.45658300	-3.16411200	0.50900700
H	3.30251200	-3.20878100	0.56461600
C	6.59661900	-2.36479200	0.55426600
H	7.35994300	-0.35693800	0.72749500
H	5.55143400	-4.24601100	0.44140300
H	7.58352500	-2.82096500	0.51531400
Cu	0.17657600	0.68342000	-0.29641700
C	-1.00587300	0.65344600	2.63880700
N	0.01863200	0.44766800	2.12096000
C	-2.28586600	0.92084600	3.25287300
H	-2.21077100	0.88977000	4.34454600
H	-2.63797800	1.91027300	2.94258700
H	-3.02329500	0.18197800	2.91889600
O	-1.38403800	1.77560700	-0.27091000
O	-2.52120200	1.02895900	0.13420000
C	-3.53270200	0.99049000	-0.94014300
C	-2.90842300	0.50839700	-2.23723400
H	-2.46334200	-0.48823800	-2.13590700
H	-3.66099500	0.46732300	-3.03233800
H	-2.12570900	1.20642700	-2.54602800
C	-4.09004800	2.39678800	-1.11534200
H	-4.87023400	2.41156000	-1.88458200
H	-4.52486500	2.77367700	-0.18380700
H	-3.28502400	3.07405300	-1.41985300
C	-4.55046000	0.03291100	-0.34525600
C	-4.91744000	-1.16251100	-0.96973300
C	-5.11284600	0.32868000	0.90407700
C	-5.82202400	-2.03467700	-0.36598700
H	-4.50548200	-1.41926200	-1.94405900
C	-6.00661400	-0.54480300	1.51426900
H	-4.84350400	1.26049500	1.40044600
C	-6.36490600	-1.73271800	0.87909900
H	-6.10689100	-2.95269500	-0.87722200
H	-6.43552500	-0.29260100	2.48268800
H	-7.07241100	-2.41317300	1.34870900

3c

Energy: -1729.49282065 a.u.

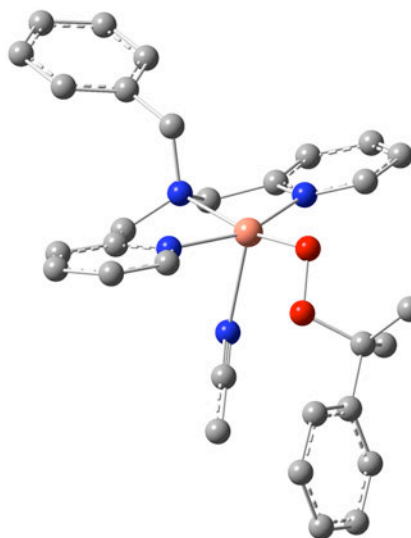
C	-0.05486100	3.27751000	-0.75459200
C	-0.63394100	4.35456700	-1.41169000
C	-2.02118700	4.40757300	-1.51024000
C	-2.78381900	3.38938100	-0.94477000
C	-2.13825000	2.34707100	-0.29044100
N	-0.79240000	2.29958000	-0.21156600
H	-2.50684500	5.23311600	-2.02592800
H	1.02081900	3.16107600	-0.63664800
H	-0.00608800	5.13053300	-1.84062700
H	-3.87066400	3.40133900	-1.00282500
C	-2.86533900	1.23994000	0.42287400
H	-2.99816600	1.53334700	1.47287800
H	-3.86439500	1.07021800	-0.00586200
N	-2.04483600	0.01863600	0.41558600



C	-2.35517000	-0.91209300	1.51097500
H	-3.24049800	-1.52734400	1.29063100
H	-2.58851800	-0.30489800	2.39608800
C	-1.15276600	-1.76266100	1.82204900
C	-1.24426100	-3.03532600	2.37454000
N	0.04160000	-1.18390300	1.58933200
C	-0.07376600	-3.70904200	2.71130300
H	-2.22127200	-3.48519100	2.54203800
C	1.17139500	-1.82577900	1.91977000
C	1.15429900	-3.09330400	2.48701800
H	-0.12122400	-4.70635000	3.14332100
H	2.08801700	-1.28397000	1.69338100
H	2.08841500	-3.58857900	2.73843600
C	-2.02375900	-0.65855700	-0.92647800
H	-1.27375100	-1.45709400	-0.85332800
H	-1.63400500	0.08278600	-1.63644800
C	-3.34613400	-1.19828300	-1.38547200
C	-4.22057000	-0.39961900	-2.13148500
C	-3.73114700	-2.50706200	-1.07253700
C	-5.45720800	-0.88972900	-2.54010000
H	-3.91434400	0.60937600	-2.41534100
C	-4.96722400	-3.00019000	-1.47971000
H	-3.04088900	-3.15286100	-0.52594100
C	-5.83366500	-2.18965700	-2.20968600
H	-6.12321000	-0.26156800	-3.12804200
H	-5.25002000	-4.02277200	-1.23851600
H	-6.79725100	-2.57656100	-2.53418600
Cu	-0.07861300	0.67638800	0.74062200
C	0.17402000	1.63538500	3.52087800
N	-0.87427400	1.56208600	3.01191000
C	1.50122400	1.68962200	4.08937300
H	1.76845500	2.71774100	4.35321600
H	1.56491000	1.06797300	4.98813000
H	2.20419500	1.32079100	3.33053900
O	1.74294900	1.16363200	0.95122900
O	2.32537600	0.20650000	-0.00415600
C	3.61163500	0.70222000	-0.46578800
C	3.44332000	2.04337800	-1.15921200
H	3.07848900	2.77672600	-0.43369200
H	4.39871300	2.40987400	-1.55035000
H	2.73064700	1.97489800	-1.99006700
C	4.54879000	0.84425500	0.73157500
H	4.62932700	-0.10051000	1.28188100
H	5.55479100	1.12895600	0.40373800
H	4.17451500	1.61516300	1.41432900
C	4.06812900	-0.41838500	-1.38674000
C	4.13260600	-1.72682400	-0.89035400
C	4.44113000	-0.19431300	-2.71387400
C	4.55777200	-2.77820000	-1.69360200
H	3.84198700	-1.92021800	0.14195300
C	4.87688500	-1.24481800	-3.51898500
H	4.40262900	0.80941000	-3.13193700
C	4.93503600	-2.53930500	-3.01352700
H	4.60147500	-3.78746000	-1.28771800
H	5.17170400	-1.04661700	-4.54779400
H	5.27552000	-3.35896800	-3.64319900

Energy: -1729.50175755 a.u.

C	-0.69042800	-2.45924800	-1.27012400
C	-0.64683600	-3.84761700	-1.29445900
C	0.31813100	-4.49798900	-0.53044600
C	1.20414800	-3.74379800	0.23417900
C	1.09432900	-2.35756700	0.22107800
N	0.15987400	-1.73817300	-0.52688400
H	0.38685900	-5.58375200	-0.53551000
H	-1.40921200	-1.87615900	-1.84407800
H	-1.34921200	-4.40380500	-1.90938700
H	1.97499800	-4.22161500	0.83661900
C	1.96423800	-1.45467200	1.06010900
H	1.46755300	-1.27876900	2.02333800
H	2.93582300	-1.92610500	1.27486500
N	2.11255600	-0.15241900	0.40018800
C	2.38688100	0.97127500	1.30519000
H	3.43923500	1.00631100	1.62698800
H	1.76822800	0.82382800	2.20082300
C	1.97911600	2.26130100	0.64087700
C	2.60984400	3.47667300	0.88076300
N	0.92816800	2.17567000	-0.20111700
C	2.13983900	4.62127500	0.24277100
H	3.45923900	3.52013100	1.56018700
C	0.48091400	3.27369900	-0.82632600
C	1.05955500	4.52005500	-0.62910800
H	2.61954900	5.58174400	0.41790700
H	-0.36326500	3.11335000	-1.49655800
H	0.67252400	5.38875100	-1.15435300
C	3.05861700	-0.20788500	-0.76160800
H	2.96687700	0.75533900	-1.28041400
H	2.66454600	-0.97611700	-1.44004400
C	4.48859800	-0.48854400	-0.40264800
C	4.96796300	-1.80241700	-0.35081100
C	5.36684600	0.55981300	-0.10512400
C	6.28759400	-2.06398700	0.00593000
H	4.30337600	-2.62620500	-0.61929800
C	6.68684900	0.30189500	0.25212100
H	5.01478300	1.59076800	-0.18078300
C	7.14706700	-1.01158600	0.31276100
H	6.64993500	-3.08961800	0.03221000
H	7.36151900	1.12698900	0.47108400
H	8.18062100	-1.21434800	0.58518500
Cu	0.18720700	0.31123100	-0.39813300
C	-1.65932500	-0.55278600	2.01413600
N	-0.66020900	0.03526300	1.87636000
C	-2.88506700	-1.29999200	2.17017500
H	-3.20307500	-1.69019200	1.19530500
H	-2.74336100	-2.12933800	2.87095900
H	-3.68938900	-0.65393000	2.54023700
O	-1.31528700	0.68832400	-1.48777700
O	-2.47587200	0.12340200	-0.86197500
C	-3.50208300	1.15626900	-0.70029000
C	-3.00583800	2.23433100	0.24923800
H	-2.05220400	2.62336100	-0.11988400
H	-3.71111400	3.07110800	0.30419900
H	-2.84564200	1.84973400	1.26307000
C	-3.83220400	1.74543700	-2.06727000
H	-4.12425900	0.95692200	-2.76901300
H	-4.66274500	2.45552800	-1.98575200



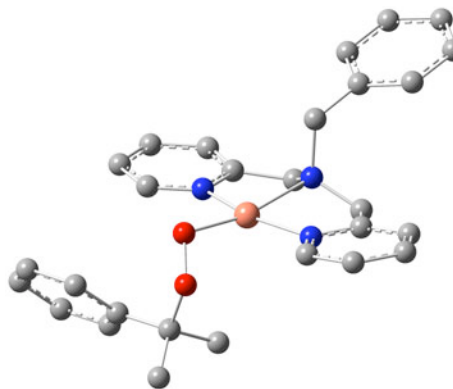
H	-2.96008900	2.26543000	-2.47708700
C	-4.67575500	0.35960500	-0.15868400
C	-5.00973700	-0.86293100	-0.75669500
C	-5.44258500	0.80449100	0.92168300
C	-6.06276300	-1.63089200	-0.26985000
H	-4.42429200	-1.21482100	-1.60496900
C	-6.50621800	0.04201600	1.40245400
H	-5.21599700	1.75744500	1.39717100
C	-6.81347100	-1.18204700	0.81543800
H	-6.30490700	-2.58019200	-0.74470900
H	-7.09697000	0.40950200	2.23968800
H	-7.64168200	-1.77823300	1.19330400

#### 4) – [Cu<sup>II</sup>(bpa)(O<sub>2</sub>Cm)]<sup>+</sup>

##### 4a (structure *ii* in Figure 8)

Energy: -1596.74023326 a.u.

C	-1.56188600	-2.19384600	-0.55155500
C	-1.68993800	-3.57365500	-0.44945800
C	-0.68892500	-4.29320600	0.19439100
C	0.40398400	-3.61402400	0.73014600
C	0.46236400	-2.23237500	0.60591700
N	-0.50461400	-1.54683200	-0.03863600
H	-0.75544700	-5.37552200	0.28210700
H	-2.30583300	-1.56007600	-1.03664400
H	-2.56265900	-4.06477900	-0.87112600
H	1.20041000	-4.14733200	1.24624500
C	1.54568700	-1.39146100	1.23524500
H	1.21505500	-1.08664600	2.23876200
H	2.47322700	-1.96826100	1.37189700
N	1.76213900	-0.16783100	0.45119800
C	2.26971300	0.97440900	1.22220000
H	3.35835100	0.92497900	1.37830400
H	1.80503400	0.93315700	2.21808200
C	1.87223700	2.26673100	0.55427800
C	2.64506800	3.41931600	0.61573800
N	0.67804300	2.25550000	-0.07603900
C	2.16751500	4.58607200	0.02386700
H	3.60691900	3.39939100	1.12507300
C	0.21536300	3.37733100	-0.64964400
C	0.93244600	4.56638100	-0.61631600
H	2.75737300	5.49932900	0.05936200
H	-0.75956500	3.28740300	-1.12604600
H	0.52746200	5.45556300	-1.09134500
C	2.55641400	-0.42087200	-0.79875500
H	2.51175900	0.50817000	-1.38308100
H	2.00146000	-1.18299600	-1.36219600
C	3.97752200	-0.84513100	-0.57327500
C	4.30858800	-2.19993600	-0.45453100
C	4.99691400	0.10874200	-0.47145000
C	5.62349200	-2.59148200	-0.22045000
H	3.52949900	-2.95530100	-0.57589600
C	6.31250700	-0.27976100	-0.23731200
H	4.75734400	1.16561200	-0.60620200
C	6.62572600	-1.63079700	-0.10596000

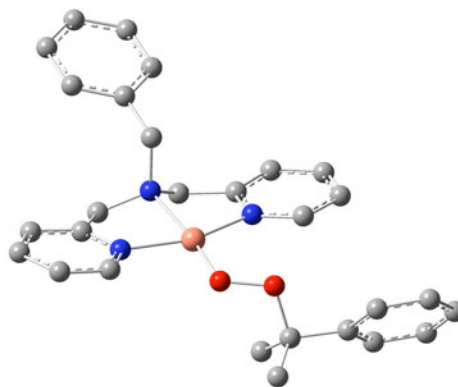


H	5.86919600	-3.64836700	-0.14103100
H	7.09704800	0.47113700	-0.17126900
H	7.65492100	-1.93628000	0.06969500
Cu	-0.16337600	0.43494300	-0.24296600
O	-1.77251200	0.73609600	-1.16321700
O	-2.51897200	1.86181800	-0.74303600
C	-3.33612900	1.52093700	0.42246400
C	-4.30916100	2.69077500	0.49604200
H	-4.92114100	2.74258600	-0.40988700
H	-4.97788200	2.57244000	1.35495100
H	-3.76925100	3.63886000	0.60673000
C	-2.43749200	1.49605100	1.65260200
H	-3.02052900	1.41641400	2.57675600
H	-1.74358200	0.64112400	1.63203300
H	-1.85608900	2.42399600	1.70494300
C	-4.06083200	0.21138500	0.16765700
C	-4.21143400	-0.76311300	1.15581400
C	-4.60246600	-0.03094900	-1.10065100
C	-4.88650300	-1.95442300	0.88614000
H	-3.80349300	-0.60352100	2.15292400
C	-5.26628100	-1.22075200	-1.37496400
H	-4.46932600	0.71454000	-1.88299200
C	-5.41162000	-2.18895200	-0.38020700
H	-5.00063100	-2.69835900	1.67293200
H	-5.67540000	-1.39355700	-2.36876900
H	-5.94067400	-3.11661700	-0.59178500

#### 4b

Energy: -1596.73797663 a.u.

C	-1.56188600	-2.19384600	-0.55155500
C	-1.68993800	-3.57365500	-0.44945800
C	-0.68892500	-4.29320600	0.19439100
C	0.40398400	-3.61402400	0.73014600
C	0.46236400	-2.23237500	0.60591700
N	-0.50461400	-1.54683200	-0.03863600
H	-0.75544700	-5.37552200	0.28210700
H	-2.30583300	-1.56007600	-1.03664400
H	-2.56265900	-4.06477900	-0.87112600
H	1.20041000	-4.14733200	1.24624500
C	1.54568700	-1.39146100	1.23524500
H	1.21505500	-1.08664600	2.23876200
H	2.47322700	-1.96826100	1.37189700
N	1.76213900	-0.16783100	0.45119800
C	2.26971300	0.97440900	1.22220000
H	3.35835100	0.92497900	1.37830400
H	1.80503400	0.93315700	2.21808200
C	1.87223700	2.26673100	0.55427800
C	2.64506800	3.41931600	0.61573800
N	0.67804300	2.25550000	-0.07603900
C	2.16751500	4.58607200	0.02386700
H	3.60691900	3.39939100	1.12507300
C	0.21536300	3.37733100	-0.64964400
C	0.93244600	4.56638100	-0.61631600
H	2.75737300	5.49932900	0.05936200
H	-0.75956500	3.28740300	-1.12604600
H	0.52746200	5.45556300	-1.09134500

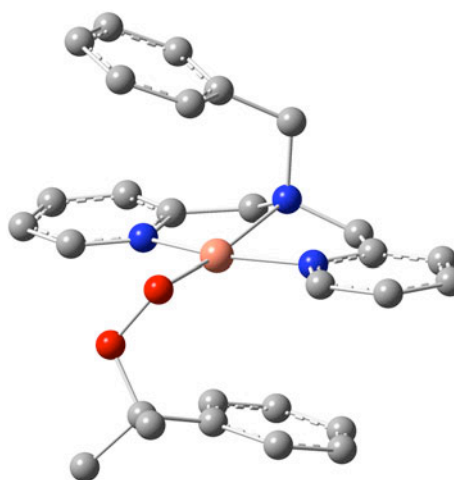


C	2.55641400	-0.42087200	-0.79875500
H	2.51175900	0.50817000	-1.38308100
H	2.00146000	-1.18299600	-1.36219600
C	3.97752200	-0.84513100	-0.57327500
C	4.30858800	-2.19993600	-0.45453100
C	4.99691400	0.10874200	-0.47145000
C	5.62349200	-2.59148200	-0.22045000
H	3.52949900	-2.95530100	-0.57589600
C	6.31250700	-0.27976100	-0.23731200
H	4.75734400	1.16561200	-0.60620200
C	6.62572600	-1.63079700	-0.10596000
H	5.86919600	-3.64836700	-0.14103100
H	7.09704800	0.47113700	-0.17126900
H	7.65492100	-1.93628000	0.06969500
Cu	-0.16337600	0.43494300	-0.24296600
O	-1.77251200	0.73609600	-1.16321700
O	-2.51897200	1.86181800	-0.74303600
C	-3.33612900	1.52093700	0.42246400
C	-4.30916100	2.69077500	0.49604200
H	-4.92114100	2.74258600	-0.40988700
H	-4.97788200	2.57244000	1.35495100
H	-3.76925100	3.63886000	0.60673000
C	-2.43749200	1.49605100	1.65260200
H	-3.02052900	1.41641400	2.57675600
H	-1.74358200	0.64112400	1.63203300
H	-1.85608900	2.42399600	1.70494300
C	-4.06083200	0.21138500	0.16765700
C	-4.21143400	-0.76311300	1.15581400
C	-4.60246600	-0.03094900	-1.10065100
C	-4.88650300	-1.95442300	0.88614000
H	-3.80349300	-0.60352100	2.15292400
C	-5.26628100	-1.22075200	-1.37496400
H	-4.46932600	0.71454000	-1.88299200
C	-5.41162000	-2.18895200	-0.38020700
H	-5.00063100	-2.69835900	1.67293200
H	-5.67540000	-1.39355700	-2.36876900
H	-5.94067400	-3.11661700	-0.59178500

4c

Energy: -1596.75394445 a.u.

C	-2.08450800	2.10558300	0.09453400
C	-3.19448000	2.71383500	0.66428000
C	-3.78596100	2.11973000	1.77524700
C	-3.25942600	0.93106300	2.26867500
C	-2.14896400	0.37414800	1.64398200
N	-1.56817100	0.96768900	0.58484000
H	-4.65638900	2.57077700	2.24675400
H	-1.56713100	2.51597600	-0.76993700
H	-3.58503500	3.63437100	0.23948700
H	-3.70807000	0.43009400	3.12487100
C	-1.50157100	-0.89570600	2.14449800
H	-0.78234800	-0.63340800	2.93383500
H	-2.25493300	-1.54978200	2.61457600
N	-0.76156900	-1.59933200	1.08579100
C	0.43685900	-2.31324800	1.55248400
H	0.19096200	-3.30386500	1.96845700
H	0.89057400	-1.72431900	2.36178100
C	1.44028300	-2.43533100	0.43214900



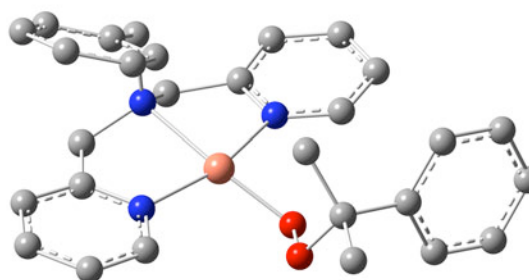


C	2.40667000	-3.43446100	0.38701200
N	1.37752900	-1.48206600	-0.51635000
C	3.32328700	-3.44001900	-0.66019700
H	2.43467100	-4.19837700	1.16173400
C	2.26169500	-1.48129500	-1.52381300
C	3.25085400	-2.44809300	-1.63462500
H	4.08400900	-4.21558600	-0.71676000
H	2.14335700	-0.66412200	-2.23553100
H	3.94573600	-2.42330300	-2.46960300
C	-1.62937300	-2.52468900	0.29075700
H	-2.16565400	-3.18828100	0.98981000
H	-0.94546900	-3.15104500	-0.29655900
C	-2.57530400	-1.80064200	-0.62011500
C	-3.88800500	-1.52629300	-0.23280800
C	-4.72422700	-0.77458900	-1.05509300
H	-4.25849700	-1.90463600	0.72171200
C	-2.94808200	-0.57111100	-2.67730500
C	-4.25240600	-0.29039800	-2.27358400
H	-5.74725400	-0.56979700	-0.74548300
H	-2.57709100	-0.20569500	-3.63241500
H	-4.90642100	0.29588300	-2.91586400
Cu	-0.03086800	-0.06165200	-0.23461100
O	0.51746900	1.05578900	-1.66862600
O	0.66564700	2.39722700	-1.21708500
C	2.06133900	2.65759600	-0.88918900
C	2.02922000	4.10816200	-0.42315900
H	3.03374300	4.43574100	-0.13597000
H	1.67071400	4.75721100	-1.22929800
H	1.36996500	4.23572700	0.44251300
C	2.47010500	1.72796200	0.24488800
C	3.62927500	0.95143500	0.21579300
C	1.64004700	1.63822100	1.37295100
C	3.95163600	0.10362900	1.27647100
H	4.29586100	1.00185100	-0.64365100
C	1.96112200	0.79836900	2.43664100
H	0.74127500	2.25414200	1.41677300
C	3.12027800	0.02195400	2.38938700
H	4.86474300	-0.48830500	1.23405700
H	1.32164900	0.77462900	3.32002600
H	3.38405300	-0.62481400	3.22520000
C	2.90343300	2.51460300	-2.14467200
H	2.49369500	3.15559400	-2.93108500
H	3.94081200	2.81805700	-1.96434900
H	2.89737200	1.48374700	-2.51200700
C	-2.11879900	-1.32923700	-1.85686900
H	-1.10313700	-1.56578700	-2.18355300

4d

Energy: -1596.74171808 a.u.

C	-1.67891100	-2.11462000	-1.40309900
C	-2.83474800	-2.85708400	-1.59736200
C	-4.05392600	-2.18987300	-1.66607900
C	-4.07588200	-0.80378500	-1.55214300
C	-2.88091700	-0.12092700	-1.36370100
N	-1.70517800	-0.77753000	-1.28317000
H	-4.98023600	-2.74245100	-1.80721900
H	-0.68812800	-2.56500400	-1.34002400
H	-2.77465700	-3.93790600	-1.68971600





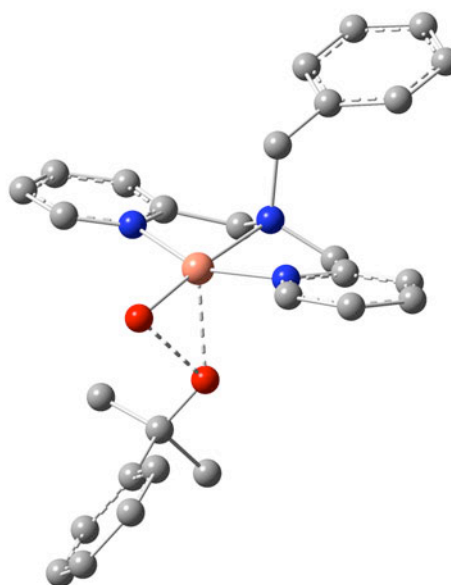
H	-5.01197200	-0.25047500	-1.59848700
C	-2.81136300	1.38644500	-1.31552500
H	-2.61979700	1.75562900	-2.33280800
H	-3.78108300	1.80646700	-1.00588400
N	-1.71079900	1.85174600	-0.45383500
C	-1.05030600	3.08544100	-0.91905700
H	-1.61532800	3.98638400	-0.62964300
H	-1.02447700	3.06274500	-2.01770500
C	0.36575500	3.14695100	-0.40412200
C	1.01219800	4.32771600	-0.06505000
N	1.00277000	1.96000300	-0.35127400
C	2.35007800	4.27516500	0.32232300
H	0.47649500	5.27386700	-0.10861400
C	2.29224700	1.90297400	0.01447000
C	3.00197600	3.04675400	0.35821300
H	2.87552100	5.18809300	0.59399500
H	2.73487000	0.90614800	0.00988000
H	4.04545300	2.96401900	0.65023200
C	-2.14483700	2.03636300	0.96448000
H	-2.81048900	2.91573000	1.00618000
H	-1.23847100	2.28601700	1.53352200
C	-2.83284700	0.83569000	1.53602200
C	-4.22579500	0.79180400	1.63527900
C	-4.86509200	-0.35034000	2.11115000
H	-4.81385500	1.66375900	1.34410200
C	-2.72300100	-1.42151500	2.40894600
C	-4.11484400	-1.46090300	2.49015300
H	-5.94993000	-0.37057500	2.19271100
H	-2.13178300	-2.27928200	2.72568000
H	-4.61281900	-2.35259300	2.86540400
Cu	-0.14703200	0.36349700	-0.78344100
O	1.41155900	-0.60281700	-1.23412800
O	1.43820500	-2.00527600	-1.07298500
C	2.03625600	-2.33309000	0.21880700
C	2.17887500	-3.84722800	0.14475700
H	2.64486600	-4.22610300	1.06031300
H	1.19961100	-4.32901900	0.03111600
H	2.80916700	-4.13429500	-0.70296900
C	3.38952700	-1.65039800	0.33659300
C	3.87087200	-1.17607800	1.55947900
C	4.18468300	-1.49203500	-0.80436100
C	5.11440000	-0.54956500	1.64166100
H	3.27736700	-1.28938200	2.46575600
C	5.42131200	-0.86199100	-0.72514600
H	3.80887400	-1.84201200	-1.76390200
C	5.89071800	-0.38575500	0.49876400
H	5.47453500	-0.19211400	2.60484700
H	6.02237900	-0.74058300	-1.62444400
H	6.86125500	0.10309100	0.56066300
C	1.06407600	-1.92431500	1.31612500
H	0.05993900	-2.29922800	1.07863900
H	1.34976400	-2.33423900	2.29106800
H	1.02358300	-0.83038900	1.41270300
C	-2.08928400	-0.27550800	1.94164500
H	-0.99967500	-0.23425600	1.88990400

## 5) – Self – Decomposition Structures (Bpa)

### 5a (structure *iii* in Figure 8)

Energy: -1596.69181842 a.u.

C	0.17641400	2.97542500	-1.61467200
C	-0.19753100	4.30801400	-1.50748800
C	-1.14596200	4.65953900	-0.55122400
C	-1.68696400	3.67197700	0.26799000
C	-1.25952100	2.35934200	0.11072000
N	-0.34795100	2.02721400	-0.82637100
H	-1.46337800	5.69428200	-0.44352000
H	0.92239300	2.63349400	-2.33017000
H	0.24738100	5.05120800	-2.16313200
H	-2.42820000	3.91416600	1.02744200
C	-1.71016800	1.22610200	0.99758000
H	-1.01696700	1.14260400	1.84835100
H	-2.71246100	1.41044700	1.41353200
N	-1.64015900	-0.03815000	0.25091400
C	-1.52779800	-1.24169100	1.09132000
H	-2.49401400	-1.53099100	1.53121300
H	-0.84941100	-0.99808400	1.92216700
C	-0.92001200	-2.36150200	0.28510200
C	-1.15688700	-3.70781400	0.53333100
N	-0.06299400	-1.96745900	-0.67521900
C	-0.46970200	-4.65876600	-0.21770000
H	-1.86078100	-4.00426900	1.30901800
C	0.60939100	-2.87575400	-1.39049400
C	0.43247000	-4.23942600	-1.19096900
H	-0.63655900	-5.71904200	-0.04108200
H	1.30638000	-2.46702400	-2.12118100
H	0.99051400	-4.95419600	-1.78936100
C	-2.73192600	-0.15679900	-0.77574800
H	-2.49015200	-1.04410400	-1.37407900
H	-2.62706700	0.71471200	-1.43431300
C	-4.11883600	-0.24543100	-0.21139100
C	-4.87121000	0.91209200	0.01931000
C	-4.68199100	-1.48843000	0.09990800
C	-6.14951400	0.83115500	0.56366600
H	-4.45826000	1.88449700	-0.25731300
C	-5.95993500	-1.57249200	0.64423800
H	-4.11941900	-2.39996900	-0.11221000
C	-6.69280100	-0.41166100	0.88127300
H	-6.72818300	1.73769400	0.72811000
H	-6.39024300	-2.54545600	0.87190900
H	-7.69464800	-0.47659000	1.30020700
Cu	0.19549600	0.07221000	-0.74237400
O	1.85903800	0.10246000	-1.47476700
O	1.76476000	-0.20343600	0.73369300
C	2.80765400	0.58411400	1.18673700
C	2.55645200	2.06653800	0.90908700
H	1.58317800	2.37055000	1.31743000
H	3.32684500	2.69981600	1.36107800
H	2.56000600	2.22810300	-0.17369900
C	2.74807300	0.32641400	2.72489300
H	2.88890100	-0.73600100	2.94225000
H	3.55365700	0.89434600	3.20256500
H	1.78662200	0.66046100	3.13066700
C	4.15972900	0.12042300	0.66591400
C	5.32461600	0.81398200	1.01258500
C	4.26592400	-1.01605100	-0.13847700
C	6.56593400	0.39681900	0.54484100
H	5.26720400	1.69222100	1.65689000

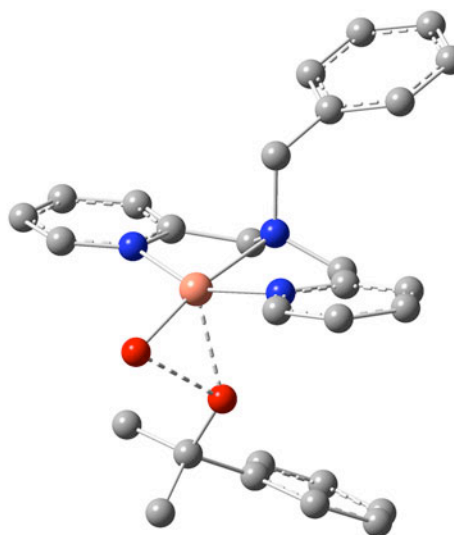


C	5.50747700	-1.43248200	-0.60976100
H	3.36212800	-1.55840200	-0.40456200
C	6.66064800	-0.72900900	-0.27077200
H	7.46152100	0.95077000	0.81942600
H	5.57576300	-2.31250100	-1.24706700
H	7.63103700	-1.05803400	-0.63719500

### 5b

Energy: -1596.69531235 a.u.

C	0.11300200	3.28784700	-1.87075700
C	-0.18058900	4.57587800	-1.44374800
C	-0.79441900	4.74407900	-0.20592600
C	-1.08861800	3.62349600	0.56655800
C	-0.75646400	2.36478800	0.08061000
N	-0.17491700	2.21091400	-1.12761500
H	-1.04223800	5.73931500	0.15632700
H	0.60505400	3.08764000	-2.82080900
H	0.06715900	5.42619600	-2.07285100
H	-1.56388100	3.72034000	1.54108100
C	-0.93415200	1.09510900	0.87310300
H	-0.00655300	0.89520700	1.43368900
H	-1.74824900	1.18631200	1.60841900
N	-1.13357500	-0.03362300	-0.04662100
C	-0.79310800	-1.34924900	0.52033000
H	-1.58557500	-1.73193600	1.18092900
H	0.11287700	-1.21717600	1.13122900
C	-0.47975600	-2.31126100	-0.59675800
C	-0.65437800	-3.68638600	-0.49948000
N	0.05458900	-1.74967900	-1.69757500
C	-0.24295500	-4.49144200	-1.55909100
H	-1.09758300	-4.11757100	0.39649200
C	0.46894400	-2.51959800	-2.70940300
C	0.33456500	-3.90224200	-2.67978900
H	-0.36933000	-5.57064600	-1.50692200
H	0.93018200	-1.98849400	-3.54020900
H	0.67617000	-4.50034800	-3.52002500
C	-2.48713400	-0.01868700	-0.69471900
H	-2.46443200	-0.80300700	-1.46169900
H	-2.56524100	0.94247800	-1.21880800
C	-3.63789100	-0.21457400	0.24767500
C	-4.24712400	0.88325800	0.86609900
C	-4.11697800	-1.49870400	0.53090900
C	-5.29953600	0.70217600	1.75853800
H	-3.90728200	1.89217500	0.62267800
C	-5.16930200	-1.68306600	1.42279400
H	-3.67459100	-2.35933600	0.02509300
C	-5.75834400	-0.58245300	2.04116500
H	-5.77164500	1.56481000	2.22412200
H	-5.53946100	-2.68577500	1.62603300
H	-6.58584200	-0.72490100	2.73285500
Cu	0.34757700	0.28055000	-1.48887000
O	1.83809200	0.43601100	-2.52506300
O	2.12648400	-0.22972100	-0.40714800
C	3.23442300	0.49933600	0.05769800
C	2.98500000	2.00002200	0.01080100
H	2.05835400	2.27750200	0.52830600
H	3.81450000	2.55736100	0.46156200
H	2.89050500	2.29487400	-1.03941000

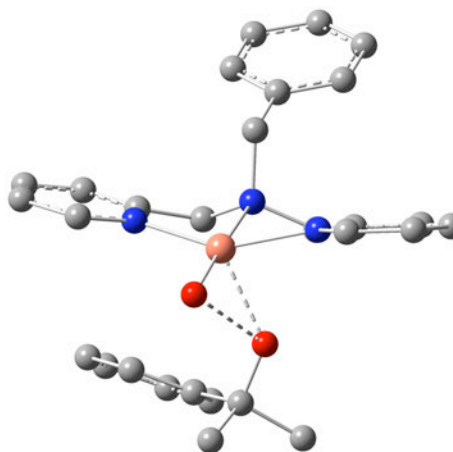


C	4.48799100	0.14775300	-0.73170300
H	5.36984900	0.65113200	-0.31916100
H	4.67474300	-0.93005400	-0.73364500
H	4.35044900	0.46732500	-1.77032900
C	3.22086200	-0.08574200	1.47837500
C	2.90415700	0.68476100	2.60578200
C	3.44382300	-1.46440800	1.64216300
C	2.87272800	0.10275100	3.86859000
H	2.73026400	1.75414800	2.50730100
C	3.39867900	-2.04507500	2.90335500
H	3.65325200	-2.07703100	0.76793000
C	3.11449500	-1.26273400	4.02160800
H	2.66840100	0.72028300	4.74119700
H	3.58865600	-3.11056300	3.01606400
H	3.08496500	-1.71360800	5.01149700

### 5c

Energy: -1596.69438272 a.u.

C	-1.25177800	-2.10463000	-2.47963200
C	-1.23977000	-3.48966600	-2.57873200
C	-0.56423700	-4.22211600	-1.60585200
C	0.06404400	-3.55101900	-0.56034600
C	-0.00011900	-2.16406900	-0.51690100
N	-0.63569800	-1.46289600	-1.47823200
H	-0.52824900	-5.30796600	-1.66005200
H	-1.76418500	-1.47243400	-3.20332600
H	-1.74524800	-3.97874400	-3.40676300
H	0.58954000	-4.09306300	0.22389700
C	0.56895200	-1.32605600	0.59572200
H	-0.23147000	-1.11198300	1.32274000
H	1.37500700	-1.84872500	1.13210500
N	1.01800000	-0.04375800	0.02683300
C	1.14761000	1.06010300	0.99043100
H	2.04371200	0.95696900	1.62093800
H	0.26691100	1.01628300	1.64946900
C	1.13714700	2.36811300	0.23845700
C	1.75071500	3.52409800	0.70462300
N	0.44256000	2.35689000	-0.91538000
C	1.61729700	4.69866200	-0.03250000
H	2.31777200	3.50406700	1.63383200
C	0.30071100	3.48525500	-1.61719200
C	0.87689700	4.68294800	-1.21006700
H	2.08661600	5.61735800	0.31242900
H	-0.30286300	3.40588900	-2.51960300
H	0.74568000	5.58079800	-1.80764700
C	2.24649000	-0.20651900	-0.82596100
H	2.40047200	0.75435000	-1.33006300
H	1.98703400	-0.93854200	-1.60066700
C	3.47362900	-0.62907700	-0.07376100
C	3.78098500	-1.98511000	0.08495400
C	4.32910600	0.32602800	0.48743700
C	4.90779600	-2.37908100	0.80035300
H	3.14128000	-2.73731600	-0.38157900
C	5.45641800	-0.06475200	1.20364500
H	4.11896000	1.38715100	0.33795800
C	5.74390400	-1.41838000	1.36478500
H	5.14152700	-3.43631900	0.90713900
H	6.11926500	0.68761900	1.62593600

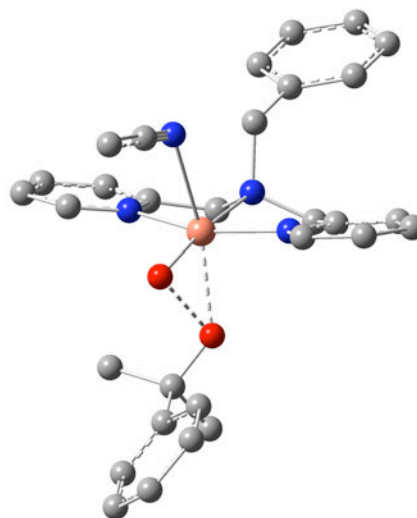


H	6.62875400	-1.72467000	1.91855100
Cu	-0.60480700	0.54098200	-1.13184500
O	-2.08513300	1.04845000	-2.02633200
O	-1.89906100	1.70511900	0.19926300
C	-3.02414100	1.32464400	0.93512200
C	-4.30324800	1.59434800	0.13970200
H	-5.18925500	1.32808200	0.72710600
H	-4.35695200	2.65537900	-0.12352200
H	-4.30185900	1.02432600	-0.79266100
C	-2.89977700	-0.13176200	1.37529900
C	-2.50434400	-0.50536200	2.66554600
C	-3.13628300	-1.14513000	0.43659500
C	-2.34664900	-1.84843000	3.00681700
H	-2.33086500	0.25234500	3.42746800
C	-2.98844200	-2.48604300	0.77769100
H	-3.43319500	-0.87389500	-0.57630400
C	-2.58571400	-2.84427400	2.06291000
H	-2.04950100	-2.11533400	4.01947700
H	-3.19004300	-3.25636300	0.03353400
H	-2.47644100	-3.89338100	2.33240500
C	-2.97461800	2.31587600	2.12304400
H	-3.79698700	2.08650900	2.81108300
H	-2.02707900	2.25464500	2.66801800
H	-3.09492600	3.33668400	1.75247600

**5d (structure *iv* in Figure 8)**

**Energy:** -1729.45013694 a.u.

C	-0.17785200	2.98304400	1.29248000
C	0.22532300	4.30986000	1.22153600
C	1.21524800	4.65559400	0.30576400
C	1.76603600	3.66896100	-0.50748300
C	1.30351800	2.36356200	-0.38523900
N	0.35003800	2.03820600	0.50725800
H	1.55794000	5.68490900	0.22628300
H	-0.95557800	2.64205700	1.97534500
H	-0.22734200	5.05356700	1.87153900
H	2.54196700	3.90560800	-1.23341800
C	1.76312500	1.23067900	-1.26459500
H	1.07961700	1.15195900	-2.12339100
H	2.77131400	1.41177200	-1.66759400
N	1.67975400	-0.03852400	-0.52483700
C	1.58841200	-1.22365700	-1.39550500
H	2.56617600	-1.50416400	-1.81519800
H	0.93485800	-0.95850000	-2.23939100
C	0.95476100	-2.36214900	-0.64004800
C	1.23013600	-3.70277900	-0.88326900
N	0.03650300	-1.99054100	0.26885100
C	0.51871800	-4.67086400	-0.17881000
H	1.98410800	-3.98085300	-1.61762600
C	-0.65272600	-2.91488100	0.94368500
C	-0.44293800	-4.27418300	0.74619400
H	0.71403300	-5.72688500	-0.35212400
H	-1.39306900	-2.52053200	1.64009800
H	-1.02000900	-5.00369800	1.30785300
C	2.76013600	-0.17072200	0.51389700
H	2.50691000	-1.06220500	1.10022200
H	2.63805400	0.68452800	1.18926100
C	4.15310600	-0.24869500	-0.03614300

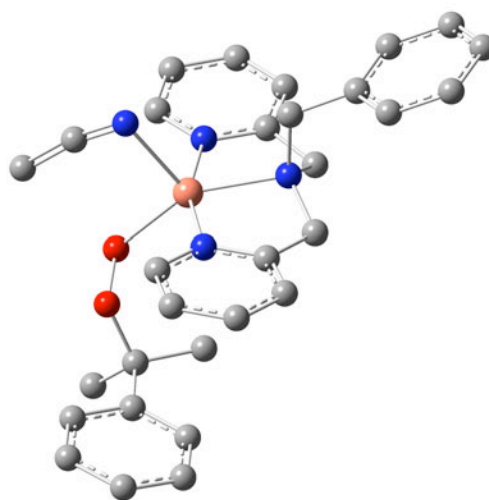


C	4.90596400	0.91284200	-0.24473400
C	4.72536600	-1.48577500	-0.35465200
C	6.19115500	0.84221500	-0.77421400
H	4.48596800	1.88052700	0.03769400
C	6.01022200	-1.56036800	-0.88410000
H	4.16263300	-2.40100800	-0.15944700
C	6.74257900	-0.39503900	-1.09935600
H	6.76878200	1.75248900	-0.92164800
H	6.44613700	-2.52958800	-1.11762600
H	7.74958800	-0.45219400	-1.50711600
Cu	-0.16479800	0.04910600	0.46614900
O	-1.88122900	0.10154300	1.10818200
O	-1.70947700	-0.06522500	-1.13345800
C	-2.77188100	0.71491300	-1.54979400
C	-2.56602000	2.18413500	-1.17988500
H	-1.60076100	2.53919900	-1.56377800
H	-3.35263400	2.82229300	-1.59587100
H	-2.57495600	2.27702000	-0.08913700
C	-2.69211000	0.55434000	-3.09923600
H	-2.80126100	-0.49627500	-3.38286600
H	-3.51008400	1.12777100	-3.54891700
H	-1.73720300	0.93884300	-3.47449100
C	-4.11395100	0.17450000	-1.07357400
C	-5.29644100	0.87274200	-1.33965400
C	-4.19074400	-1.04549100	-0.39878400
C	-6.52615300	0.37573100	-0.92003300
H	-5.26381200	1.81720600	-1.88392500
C	-5.42035900	-1.54338100	0.02241700
H	-3.27211700	-1.59065400	-0.19633900
C	-6.59169400	-0.83536700	-0.23480600
H	-7.43582600	0.93441500	-1.13222000
H	-5.46529000	-2.49269200	0.55418600
H	-7.55298600	-1.22738900	0.09182200
C	-0.22933000	-0.12747800	3.76278800
N	0.54995300	-0.12756800	2.89526500
C	-1.22750400	-0.13863800	4.80899600
H	-1.10661500	-1.01834300	5.44918000
H	-1.14485300	0.75671400	5.43332900
H	-2.22723900	-0.16344000	4.36035700

**5e (structure *v* in Figure 8)**

**Energy:** -1729.44511464 a.u.

C	1.49248100	3.53083300	0.27680900
C	2.46521600	4.44286400	-0.10675700
C	3.48236600	4.01419700	-0.95441900
C	3.48850000	2.69421900	-1.39569600
C	2.47332000	1.83913300	-0.98398500
N	1.49737200	2.26204400	-0.15372500
H	4.26698200	4.69982500	-1.26621100
H	0.67781800	3.80166900	0.94806300
H	2.42641500	5.46403400	0.26141200
H	4.27029400	2.32548100	-2.05702400
C	2.34497200	0.41799200	-1.46190000
H	1.70939500	0.40220300	-2.35939700
H	3.32153500	0.00306700	-1.75561900
N	1.68535800	-0.39931500	-0.43508700
C	0.98029000	-1.57643000	-0.95823200
H	1.66328900	-2.42294000	-1.12858800
H	0.56398700	-1.30648400	-1.93974100
C	-0.14447700	-1.95789100	-0.03327000
C	-0.64203700	-3.25269600	0.05236400
N	-0.68787700	-0.94777100	0.67765700
C	-1.73138500	-3.50463500	0.88111600
H	-0.17989400	-4.04799500	-0.52959100
C	-1.72528700	-1.19341400	1.49158300
C	-2.27952800	-2.45933100	1.61650500
H	-2.14253600	-4.50895100	0.95685300
H	-2.11037800	-0.33850800	2.04075600
H	-3.12890900	-2.61314100	2.27594400
C	2.59556700	-0.73225700	0.71953000
H	1.95787300	-1.18757700	1.48731100
H	2.92975000	0.22852800	1.13082200
C	3.75378500	-1.61525800	0.36356800
C	4.97101000	-1.06282100	-0.05231300
C	3.63804900	-3.00851000	0.43777100
C	6.04054400	-1.88143100	-0.40276200
H	5.08789600	0.02272800	-0.07122300
C	4.70567300	-3.82984700	0.08784500
H	2.70865100	-3.45045300	0.80274100
C	5.90635200	-3.26652600	-0.33844600
H	6.98474100	-1.43867300	-0.71299900
H	4.60597900	-4.91080100	0.16131000
H	6.74390800	-3.90748400	-0.60522700
Cu	0.21621400	0.83767700	0.45336100
C	-0.35468800	2.01828300	2.74784200
N	0.47617000	1.18102000	2.56680300
C	-1.36358100	2.95993700	2.66223400
H	-1.07454500	3.98784300	2.88686100
H	-1.53638000	2.63843300	1.07973600
H	-2.30872200	2.67429200	3.12768300
O	-1.43691600	2.16909700	0.08164100
O	-2.56715600	1.23015800	0.15251600
C	-3.10912900	1.03472900	-1.18627200
C	-1.98931000	0.71493300	-2.16602200
H	-1.40580400	-0.15222400	-1.82995100
H	-2.39535000	0.48952800	-3.15828100
H	-1.31992600	1.57550100	-2.26494500
C	-3.85589000	2.28785700	-1.62134300
H	-4.30899400	2.14571400	-2.60892200
H	-4.65358400	2.53742900	-0.91487400
H	-3.16570700	3.13682900	-1.67595300
C	-4.03815700	-0.13940900	-0.91483600





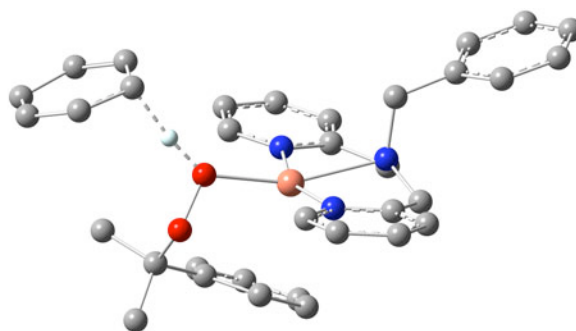
C	-3.92454800	-1.36040000	-1.58449600
C	-5.01595000	-0.00996500	0.08102000
C	-4.77454800	-2.42107900	-1.27766600
H	-3.17834400	-1.49196600	-2.36612400
C	-5.85627400	-1.07180500	0.39693900
H	-5.10830500	0.93186200	0.61978400
C	-5.73929800	-2.28233300	-0.28421500
H	-4.68333200	-3.35889800	-1.82332800
H	-6.61132400	-0.95108800	1.17152000
H	-6.40549600	-3.10994400	-0.04804300

## 6) – Cyclohexadiene (CHD) Oxidation (Bpa)

### 6a (structure *vi* in Figure 8)

Energy: -1830.10369032 a.u.

C	-1.03632500	-2.35038000	0.16175800
C	-1.01386100	-3.71705900	0.40122200
C	0.15060400	-4.28150500	0.91333700
C	1.24551500	-3.45886900	1.16030600
C	1.14982600	-2.09644500	0.89484200
N	0.01883100	-1.55631400	0.39674100
H	0.20940800	-5.34960700	1.11174700
H	-1.92017300	-1.84957800	-0.23671100
H	-1.89214200	-4.32067800	0.18556600
H	2.17543200	-3.86522800	1.55525000
C	2.28127100	-1.14116300	1.19797500
H	2.13426800	-0.75072100	2.21613600
H	3.24530300	-1.67775000	1.20080600
N	2.25926200	-0.00705800	0.28557000
C	2.80038400	1.24202700	0.80277100
H	3.89596900	1.31763600	0.69580100
H	2.59114400	1.27063900	1.88250800
C	2.12645800	2.42744300	0.14977500
C	2.79799000	3.62250300	-0.08365700
N	0.81938000	2.28377600	-0.15713200
C	2.10601300	4.69802600	-0.63263400
H	3.85461700	3.70318600	0.16713600
C	0.15255800	3.32135800	-0.68891100
C	0.75744500	4.54583000	-0.93930900
H	2.61528700	5.64032400	-0.82260500
H	-0.89934300	3.13760100	-0.90361800
H	0.17970700	5.35868200	-1.37095800
C	2.73730200	-0.33641200	-1.08314900
H	2.50121900	0.53289700	-1.71301700
H	2.11184500	-1.16670300	-1.43995600
C	4.19485800	-0.68657200	-1.17496300
C	4.62022200	-2.01092300	-1.01962300
C	5.15756200	0.30637100	-1.38991300
C	5.97339600	-2.33376300	-1.06181700
H	3.87629900	-2.79986300	-0.89003400
C	6.51178800	-0.01261400	-1.43237300
H	4.83604100	1.33714900	-1.55332300
C	6.92150400	-1.33319000	-1.26312200
H	6.28863200	-3.36929300	-0.95004800
H	7.24846500	0.76820800	-1.61073200
H	7.97923200	-1.58476100	-1.30285800
Cu	0.02585300	0.44174300	0.11321200



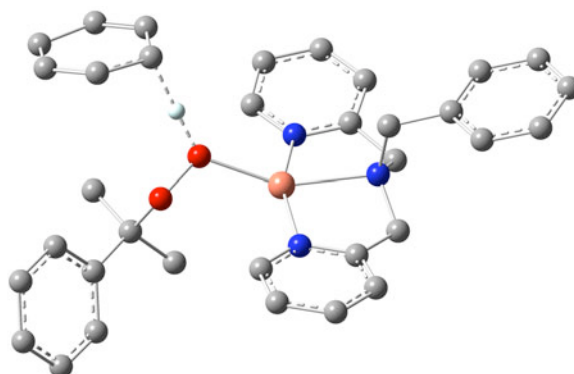


O	-1.85687000	0.67356700	-0.71305400
O	-2.65654500	1.67663400	-0.02979200
C	-3.32829600	1.05687400	1.10338700
C	-4.33190300	0.03227700	0.60605600
H	-3.83786300	-0.79836800	0.08514300
H	-4.92382700	-0.37881700	1.43148000
H	-5.01795200	0.51018600	-0.10054900
C	-4.04055400	2.24786300	1.73645000
H	-4.59527900	1.92209500	2.62252900
H	-3.32750200	3.01918200	2.04619600
H	-4.74808000	2.69125900	1.02760900
C	-2.27713000	0.49100800	2.04853200
C	-2.37821700	-0.77320300	2.63147500
C	-1.15580200	1.27754000	2.35737900
C	-1.38718400	-1.24750900	3.49169600
H	-3.23522600	-1.40772800	2.41146600
C	-0.16466300	0.80744400	3.21872400
H	-1.08107200	2.27940800	1.93409700
C	-0.27711500	-0.46199500	3.78706700
H	-1.48823100	-2.23724400	3.93448100
H	0.68112100	1.44902300	3.46780100
H	0.48714000	-0.82765600	4.47146500
C	-4.34623900	0.50019600	-2.96849900
C	-5.49694200	-0.15707400	-2.69303200
C	-4.18751100	-2.26174500	-2.38443600
C	-3.05971800	-1.57884100	-2.68890400
H	-4.38253100	1.54995200	-3.25867500
H	-6.45263600	0.36049500	-2.76604900
H	-4.15071300	-3.34073500	-2.23363300
H	-2.11346900	-2.11553500	-2.77800200
C	-5.52428500	-1.59900000	-2.30500800
H	-5.94578500	-1.70820800	-1.28497600
H	-6.25451000	-2.14745800	-2.92756000
C	-3.05343200	-0.14211100	-2.87749200
H	-2.25968100	0.26527100	-3.51232500
H	-2.46297600	0.34943000	-1.66366800

## 6b

Energy: -1830.09259931 a.u.

C	0.23792100	2.77218300	-1.29844000
C	0.72030600	4.04813200	-1.55530100
C	2.07916100	4.20861300	-1.80560100
C	2.90094300	3.08486100	-1.79354400
C	2.34709200	1.83575700	-1.53785400
N	1.02711800	1.68503200	-1.28802500
H	2.49605300	5.19388200	-2.00205200
H	-0.81398900	2.59027800	-1.07706200
H	0.03750900	4.89444700	-1.55142800
H	3.96964300	3.16899600	-1.98433200
C	3.16414300	0.56794300	-1.58864900
H	3.02492500	0.10960300	-2.57819900
H	4.23915400	0.79484900	-1.49975500
N	2.70046200	-0.39222700	-0.58963300
C	2.85723400	-1.79615000	-0.96294100
H	3.86023000	-2.19244800	-0.73425900
H	2.73807900	-1.86155000	-2.05404500
C	1.79294900	-2.64878400	-0.31753200
C	2.05134500	-3.94855300	0.09986800

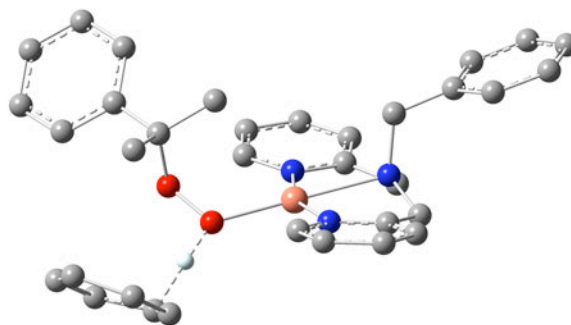


N	0.55761800	-2.10402000	-0.21974500
C	1.01553600	-4.71963200	0.61944600
H	3.05999800	-4.34891500	0.01039200
C	-0.44033400	-2.84991500	0.28993800
C	-0.25315900	-4.15922200	0.71337900
H	1.20019300	-5.73923700	0.95059500
H	-1.40683900	-2.35166300	0.35827900
H	-1.09319600	-4.71965500	1.11454500
C	3.18067300	-0.08821200	0.78813500
H	2.62354400	-0.75389700	1.46258100
H	2.85430800	0.93843200	1.00804400
C	4.66048300	-0.23447000	0.99669900
C	5.52378800	0.84573900	0.78041800
C	5.20633600	-1.46122400	1.39207600
C	6.89910200	0.69997700	0.93682200
H	5.10685800	1.81910400	0.51327900
C	6.58099700	-1.61072600	1.54969200
H	4.53947700	-2.29947100	1.60443100
C	7.42958200	-0.53086900	1.31647900
H	7.55752600	1.55109800	0.77518200
H	6.99054700	-2.56749500	1.86739700
H	8.50383800	-0.64450100	1.44552400
Cu	0.46830700	-0.12008500	-0.54591100
O	-1.24430200	0.61808000	0.26666700
O	-2.33429900	-0.33542100	0.33355400
C	-3.17590900	-0.21662800	-0.86465200
C	-2.33460400	-0.49140200	-2.10039100
H	-1.81983300	-1.45834300	-2.03310400
H	-2.95249100	-0.49477600	-3.00529100
H	-1.58128700	0.29678500	-2.22457900
C	-3.79296500	1.17294500	-0.93183700
H	-4.41156100	1.27059300	-1.83101300
H	-4.42226900	1.36399300	-0.05758100
H	-3.01133600	1.94320000	-0.96583900
C	-4.22098300	-1.28005800	-0.57282100
C	-4.46560900	-2.35360900	-1.43259500
C	-4.96064300	-1.18697800	0.61395700
C	-5.44018400	-3.30069300	-1.12398400
H	-3.90619900	-2.45329000	-2.36087100
C	-5.92453100	-2.13741300	0.92745100
H	-4.76520200	-0.36218900	1.29942100
C	-6.17046400	-3.19664000	0.05564700
H	-5.62775800	-4.12294700	-1.81194700
H	-6.48919100	-2.05064700	1.85388200
H	-6.93080400	-3.93742700	0.29515500
C	-3.12816400	1.93763800	2.57969400
C	-4.26649900	2.60463300	2.27420100
C	-2.90216100	4.34371900	1.11008700
C	-1.78361400	3.66268200	1.44640200
H	-3.17746600	1.03730600	3.19203800
H	-5.22618500	2.24588800	2.64569400
H	-2.82723700	5.30747100	0.60707400
H	-0.80502600	4.08494000	1.21316300
C	-4.26926200	3.85326900	1.45565000
H	-4.86433600	3.70205200	0.53280800
H	-4.83344800	4.64800400	1.97712400
C	-1.83294700	2.36839000	2.09817400
H	-0.96990000	2.09924800	2.71711500
H	-1.52816500	1.42616900	1.09067200

6c

Energy: -1830.09266567 a.u.

C	0.18392300	2.55821900	1.41913600
C	-0.13369700	3.87516000	1.72469400
C	-1.45357100	4.19289200	2.02474900
C	-2.40776500	3.17967900	2.00929000
C	-2.02041100	1.88094800	1.70094300
N	-0.73683200	1.57699900	1.40409200
H	-1.74015600	5.21524600	2.26180800
H	1.19759900	2.24936200	1.16599200
H	0.64633600	4.63177400	1.71834900
H	-3.45243900	3.38761600	2.23548400
C	-3.00127500	0.73221300	1.72438600
H	-2.92780600	0.22684200	2.69831900
H	-4.03469200	1.10994300	1.64576700
N	-2.66962400	-0.24445400	0.69478500
C	-3.06794400	-1.61875200	0.97045700
H	-4.11466600	-1.82986400	0.69373400
H	-2.99596900	-1.77580400	2.05649400
C	-2.13731400	-2.58855700	0.28004400
C	-2.57391100	-3.81937800	-0.19771100
N	-0.84369400	-2.21407300	0.18350900
C	-1.65708800	-4.69304900	-0.77525400
H	-3.62619400	-4.08583700	-0.11187100
C	0.03604800	-3.05340500	-0.38635900
C	-0.32493700	-4.30299600	-0.87058800
H	-1.98104100	-5.66076200	-1.15198500
H	1.06339100	-2.69102000	-0.44126200
H	0.42757100	-4.94780600	-1.31807700
C	-3.01189400	0.20618600	-0.68116000
H	-2.54152200	-0.51055800	-1.36999000
H	-2.50225900	1.16943000	-0.82836800
C	-4.48257800	0.32972600	-0.95717200
C	-5.15863200	1.52796300	-0.69980300
C	-5.21095400	-0.76018700	-1.44740800
C	-6.53060000	1.63009300	-0.91032500
H	-4.59448900	2.39693800	-0.35455900
C	-6.58302700	-0.66165800	-1.65933000
H	-4.68788500	-1.68787600	-1.68921800
C	-7.24536800	0.53283900	-1.38543700
H	-7.04175200	2.57071500	-0.71512600
H	-7.13498500	-1.51406800	-2.05032500
H	-8.31681900	0.61316200	-1.55614500
Cu	-0.39973100	-0.32232800	0.79391600
O	1.62919800	-0.62601900	0.72442000
O	2.36002900	0.57080900	0.34669700
C	2.44681100	0.67772900	-1.11481100
C	1.04888900	0.69040600	-1.71510400
H	0.41571200	1.46057800	-1.25471100
H	1.08743800	0.88089000	-2.79362300
H	0.57091100	-0.28877800	-1.57821400
C	3.25264400	-0.48476000	-1.67530700
H	3.28562500	-0.43402700	-2.76958100
H	4.27917400	-0.47103900	-1.29830200
H	2.79664500	-1.44195300	-1.38797800
C	3.18606700	1.99911100	-1.24302100
C	2.65154000	3.10104700	-1.91545800

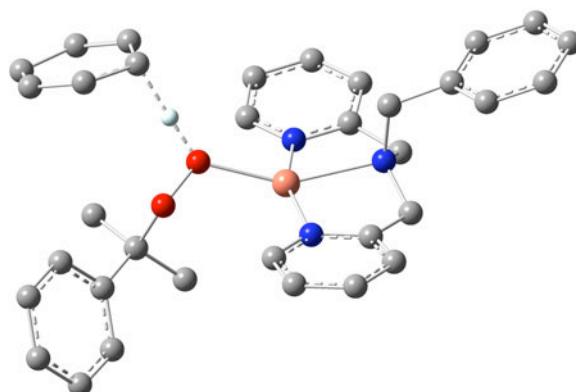


C	4.44233900	2.12730900	-0.63540200
C	3.36452200	4.29534900	-1.99875100
H	1.67662200	3.03397400	-2.39474900
C	5.14907400	3.32162800	-0.70907700
H	4.85900400	1.28079400	-0.08952800
C	4.61321900	4.40953600	-1.39589600
H	2.93985700	5.13892800	-2.53978500
H	6.12324500	3.40410200	-0.23085900
H	5.16913500	5.34273100	-1.46144800
C	4.67821900	-1.51937600	1.49534600
C	5.58150900	-1.85717100	0.54431300
C	4.17386000	-3.83351500	-0.04944100
C	3.30219500	-3.47839700	0.92277100
H	4.87216800	-0.66609900	2.14519100
H	6.50108300	-1.28248700	0.43554100
H	4.03116200	-4.76245700	-0.60103600
H	2.45797200	-4.13068500	1.15226400
C	5.38816200	-3.02430100	-0.36700900
H	5.35490200	-2.68367200	-1.42154300
H	6.28480300	-3.67075000	-0.35206200
C	3.44004100	-2.24578100	1.67098700
H	2.99775100	-2.22542500	2.67241200
H	2.45540200	-1.35265200	1.12604900

6d

Energy: -1830.09259928 a.u.

C	0.23789700	2.77229400	-1.29829200
C	0.72025000	4.04826400	-1.55510900
C	2.07910000	4.20878600	-1.80541500
C	2.90090600	3.08505200	-1.79340800
C	2.34708700	1.83592600	-1.53775700
N	1.02711900	1.68516000	-1.28791900
H	2.49596800	5.19407200	-2.00183100
H	-0.81400600	2.59036100	-1.07691500
H	0.03743100	4.89456200	-1.55119700
H	3.96960300	3.16921900	-1.98419900
C	3.16417700	0.56813800	-1.58861300
H	3.02501700	0.10985600	-2.57819800
H	4.23917700	0.79507300	-1.49966200
N	2.70050100	-0.39210800	-0.58966500
C	2.85725700	-1.79600600	-0.96308300
H	3.86029000	-2.19230200	-0.73456000
H	2.73794900	-1.86133400	-2.05417400
C	1.79306600	-2.64868100	-0.31758200
C	2.05152700	-3.94844700	0.09978500
N	0.55773500	-2.10394200	-0.21967800
C	1.01577900	-4.71954800	0.61945300
H	3.06017800	-4.34879200	0.01020900
C	-0.44015700	-2.84985600	0.29009100
C	-0.25291800	-4.15916300	0.71350700
H	1.20048400	-5.73915200	0.95057700
H	-1.40666500	-2.35162200	0.35851500
H	-1.09290700	-4.71961800	1.11474400
C	3.18076100	-0.08819800	0.78811300
H	2.62363000	-0.75390700	1.46253400
H	2.85443300	0.93844300	1.00809200
C	4.66057100	-0.23450700	0.99663600
C	5.52389300	0.84571200	0.78046900

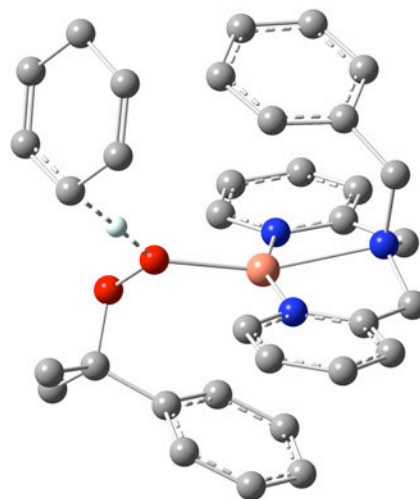


C	5.20640600	-1.46131200	1.39187800
C	6.89920400	0.69991100	0.93685400
H	5.10697800	1.81911200	0.51343700
C	6.58106400	-1.61085400	1.54947500
H	4.53953200	-2.29957000	1.60414700
C	7.42966600	-0.53098400	1.31637800
H	7.55764200	1.55104000	0.77530700
H	6.99060000	-2.56766200	1.86707700
H	8.50392000	-0.64464600	1.44541100
Cu	0.46837700	-0.11998300	-0.54578600
O	-1.24438200	0.61798000	0.26658100
O	-2.33435400	-0.33556900	0.33342800
C	-3.17592600	-0.21677500	-0.86480000
C	-2.33461100	-0.49167300	-2.10050300
H	-1.81976700	-1.45856500	-2.03307200
H	-2.95250300	-0.49523500	-3.00540000
H	-1.58135000	0.29654800	-2.22481100
C	-3.79288100	1.17283800	-0.93209000
H	-4.41151700	1.27043100	-1.83124400
H	-4.42211900	1.36403100	-0.05781900
H	-3.01120000	1.94303000	-0.96622500
C	-4.22108500	-1.28010600	-0.57291500
C	-4.46562300	-2.35383000	-1.43249700
C	-4.96088200	-1.18677300	0.61375800
C	-5.44026600	-3.30082300	-1.12381600
H	-3.90609900	-2.45371500	-2.36068200
C	-5.92483900	-2.13711300	0.92732200
H	-4.76548600	-0.36186200	1.29908900
C	-6.17069600	-3.19650600	0.05569900
H	-5.62777600	-4.12321200	-1.81163500
H	-6.48961000	-2.05014600	1.85366700
H	-6.93108900	-3.93722300	0.29525900
C	-3.12844800	1.93737600	2.57956200
C	-4.26671700	2.60444600	2.27398600
C	-2.90215300	4.34359300	1.11022700
C	-1.78367700	3.66248100	1.44663100
H	-3.17786600	1.03699200	3.19182200
H	-5.22646500	2.24571100	2.64532800
H	-2.82712400	5.30739700	0.60732900
H	-0.80504000	4.08472500	1.21356700
C	-4.26932100	3.85316100	1.45555500
H	-4.86427900	3.70206100	0.53261900
H	-4.83354400	4.64786600	1.97703400
C	-1.83315200	2.36811700	2.09824700
H	-0.97020000	2.09886500	2.71727300
H	-1.52827500	1.42596700	1.09064700

6e

Energy: -1830.10634117 a.u.

C	-1.46420400	-1.13221900	2.33856000
C	-2.33748800	-1.88316400	3.11088900
C	-2.59769700	-3.19791400	2.73331200
C	-1.98334000	-3.70393400	1.59478000
C	-1.11945300	-2.89104600	0.86539100
N	-0.85831300	-1.62643400	1.24389200
H	-3.27813100	-3.81811200	3.31290600
H	-1.21485600	-0.09881200	2.58096600
H	-2.80454200	-1.44201300	3.98727400
H	-2.17454200	-4.72258500	1.26010800
C	-0.39035700	-3.42747600	-0.35012600
H	0.51914400	-3.93834900	-0.00187400
H	-1.00812600	-4.20576100	-0.83242100
N	0.01082000	-2.39023000	-1.29684900
C	1.33155400	-2.55997900	-1.89465900
H	1.32456400	-3.23637400	-2.76782700
H	1.98551800	-3.02239300	-1.14037500
C	1.92908800	-1.22650000	-2.28161000
C	2.81172300	-1.09907400	-3.34927800
N	1.59715700	-0.17052200	-1.51232200
C	3.36492400	0.14584700	-3.63194400
H	3.05567400	-1.97078900	-3.95404300
C	2.12965500	1.02902800	-1.78995000
C	3.01397600	1.23452600	-2.83951300
H	4.05358200	0.26504500	-4.46561100
H	1.82219400	1.83404100	-1.12186400
H	3.41520200	2.22672500	-3.02913500
C	-1.02572200	-2.09391900	-2.31590900
H	-1.30730400	-3.02345300	-2.84284300
H	-0.55746900	-1.42738800	-3.05297000
C	-2.21938000	-1.43267900	-1.69114200
C	-3.34774300	-2.16702800	-1.32567300
C	-4.37284500	-1.57167800	-0.59187600
H	-3.41755000	-3.22004600	-1.60485400
C	-3.15281000	0.51075700	-0.58091500
C	-4.26623500	-0.23848500	-0.20198900
H	-5.24886300	-2.15435200	-0.31306700
H	-3.04959800	1.54967100	-0.26973500
H	-5.05539300	0.21995700	0.39149500
Cu	0.31848200	-0.53299500	0.02129100
O	0.14478900	1.44195400	0.65136400
O	0.34118300	1.58740400	2.08375200
C	1.75539200	1.81175900	2.36042100
C	-2.27363100	3.59097100	-2.13009700
C	-3.08958700	4.20582300	0.14816000
C	-1.81660600	4.13849100	0.60452900
C	-1.01274100	3.53410600	-1.64203000
H	-2.45851600	3.40620400	-3.18773400
H	-3.89537800	4.49070100	0.82355600
H	-1.60725000	4.36606900	1.65045700
H	-0.18868800	3.31002600	-2.32252000
C	-0.71085300	3.74733800	-0.24210300
H	-0.29570400	2.45585900	0.28381200
H	0.26118600	4.19963000	-0.01590800
C	-3.44481700	3.96264800	-1.28225300
H	-3.94249900	4.85745500	-1.70301100
H	-4.23511000	3.19115300	-1.36143100
C	1.77324400	1.81853900	3.88536100
H	2.79507700	1.97411400	4.24626400
H	1.14187200	2.62539100	4.27296700

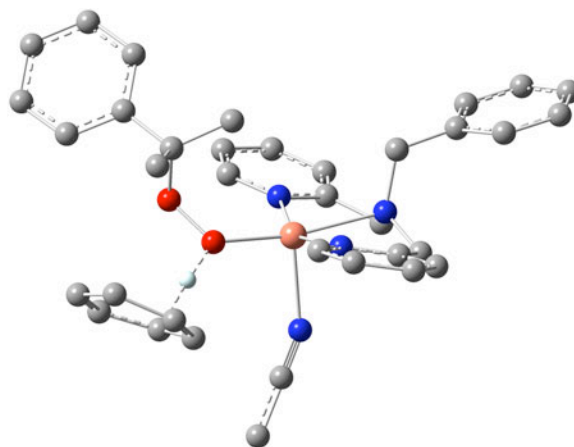


H	1.41026300	0.86840400	4.29152400
C	2.56227600	0.64711700	1.80337000
C	3.70062800	0.81679600	1.01316600
C	2.13959300	-0.66034300	2.08308400
C	4.39004100	-0.28404400	0.50329700
H	4.06135600	1.81784400	0.78183100
C	2.82250300	-1.76288200	1.57337200
H	1.26838700	-0.81030400	2.72015900
C	3.95142400	-1.57644600	0.77522200
H	5.27562100	-0.12641700	-0.11045000
H	2.48030700	-2.76857300	1.81957600
H	4.49695800	-2.43426500	0.38449100
C	2.17419700	3.16585900	1.81521100
H	1.49139200	3.93828400	2.18539200
H	3.18715000	3.42851400	2.13977600
H	2.15489300	3.18246100	0.71939200
C	-2.14832400	-0.07978600	-1.33992500
H	-1.29051500	0.51866700	-1.65848000

6f

Energy: -1962.85346300 a.u.

C	0.05282200	2.52030200	1.57255400
C	-0.33197900	3.73770100	2.12069200
C	-1.65318400	3.90306900	2.52187800
C	-2.54178300	2.84455100	2.35748900
C	-2.08616000	1.65157600	1.80768600
N	-0.80215100	1.49549200	1.41692800
H	-1.99128700	4.84466700	2.94941900
H	1.07095000	2.33208200	1.23173100
H	0.39585700	4.53855900	2.22058800
H	-3.58662200	2.93596900	2.65084100
C	-2.98852500	0.45302800	1.63488900
H	-2.83942300	-0.23044500	2.48410100
H	-4.04722900	0.76428600	1.65296900
N	-2.62169000	-0.27444700	0.42712400
C	-2.98597500	-1.68327200	0.39349300
H	-4.03439300	-1.85495500	0.09462200
H	-2.87732400	-2.07485700	1.41565200
C	-2.04794700	-2.44232600	-0.51599300
C	-2.45429700	-3.56176900	-1.23536200
N	-0.77618100	-1.99481000	-0.56738900
C	-1.52429600	-4.24941100	-2.00973000
H	-3.49218800	-3.88753800	-1.18294300
C	0.11492100	-2.65441000	-1.32066800
C	-0.21175600	-3.78904700	-2.05156600
H	-1.82291400	-5.12847400	-2.57694500
H	1.12721000	-2.24686100	-1.31277100
H	0.54887100	-4.29019000	-2.64528500
C	-2.95238100	0.44999500	-0.82698800
H	-2.45900400	-0.09647600	-1.64305400
H	-2.46111700	1.43062500	-0.76028400
C	-4.42279000	0.60311600	-1.09192400
C	-5.12549500	1.70490800	-0.59106100
C	-5.12479500	-0.36835000	-1.81416800
C	-6.49693700	1.82694500	-0.79415500
H	-4.58151600	2.48644500	-0.05620200
C	-6.49640800	-0.24983900	-2.01961400
H	-4.58112000	-1.21422200	-2.24038300





C	-7.18509500	0.84638600	-1.50528100
H	-7.02859200	2.69419300	-0.40734300
H	-7.02752800	-1.00776500	-2.59215100
H	-8.25612600	0.94354500	-1.67033800
Cu	-0.37755800	-0.37425100	0.67158000
O	1.64934900	-0.44844700	0.41035300
O	2.33020600	0.81627200	0.18814900
C	2.40843200	1.10095900	-1.24796600
C	1.00699500	1.14795000	-1.83680200
H	0.36102900	1.84356600	-1.28591400
H	1.03368800	1.45954600	-2.88720000
H	0.55034300	0.15132700	-1.80068800
C	3.24444500	0.03644400	-1.94491000
H	3.27497000	0.22172600	-3.02471500
H	4.27115100	0.02639500	-1.56710000
H	2.81294000	-0.95963300	-1.77698800
C	3.11565100	2.44603400	-1.22437200
C	2.55682600	3.60012600	-1.77872500
C	4.36930600	2.53843900	-0.60493100
C	3.24223600	4.81246500	-1.73448200
H	1.58343600	3.56090000	-2.26376300
C	5.04866600	3.74951300	-0.55066100
H	4.80679000	1.64891300	-0.15204400
C	4.48808000	4.89127800	-1.12038300
H	2.79785100	5.69849100	-2.18417300
H	6.02120700	3.80300500	-0.06483200
H	5.02255900	5.83865800	-1.08641800
C	4.73268600	-1.54394100	0.97417400
C	5.53312300	-1.84933400	-0.07344000
C	3.91126400	-3.62268600	-0.75649700
C	3.14814200	-3.30708900	0.31470100
H	5.04995800	-0.78776900	1.69243300
H	6.49115700	-1.34458600	-0.19458300
H	3.64114500	-4.46630900	-1.39180800
H	2.25403200	-3.89763800	0.52976100
C	5.16547500	-2.88035400	-1.09100900
H	5.07470200	-2.40935600	-2.09103800
H	5.99988700	-3.59134700	-1.23299700
C	3.44475800	-2.17321600	1.16566800
H	3.07164300	-2.21099900	2.19480500
H	2.48189900	-1.18261200	0.73851200
C	0.14465800	-2.29598600	3.28930500
N	-0.42017800	-1.62583400	2.52127700
C	0.84936400	-3.12657600	4.24030100
H	0.14688300	-3.58635400	4.94302900
H	1.39460000	-3.92263800	3.72160800
H	1.56748400	-2.52709000	4.80959800

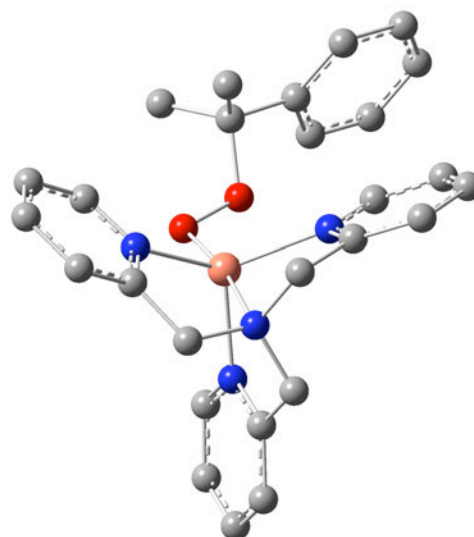
7) – [Cu<sup>II</sup>(tpa)(O<sub>2</sub>Cm)]<sup>+</sup>

7a

Energy: -1612.79766701 a.u.



C	-1.66522600	3.00459100	-0.54824000
C	-2.47745400	4.11950200	-0.38993900
C	-3.70547400	3.96366000	0.24583100
C	-4.08658200	2.69747000	0.68026400
C	-3.22725700	1.62483300	0.46851000
N	-2.02699800	1.78626900	-0.12039200
H	-4.36215200	4.81705900	0.39943100
H	-0.69280400	3.04846500	-1.03836400
H	-2.14791700	5.08882500	-0.75387500
H	-5.04492700	2.53795400	1.17105800
C	-3.61097200	0.20489600	0.79496600
H	-4.35882900	0.17110100	1.60489100
H	-4.09166700	-0.23398100	-0.09216000
N	-2.43862200	-0.62255300	1.09943300
C	-1.92470100	-0.40951900	2.45722500
H	-2.55477800	-0.89644200	3.22092600
H	-1.97025900	0.67305400	2.65097900
C	-0.49750800	-0.88068100	2.55701300
C	0.01918400	-1.44811300	3.71599500
N	0.25334600	-0.70462500	1.44985000
C	1.35564700	-1.83840200	3.74040000
H	-0.62010800	-1.58047600	4.58694900
C	1.53497300	-1.10254900	1.47139000
C	2.12617700	-1.66544600	2.59631900
H	1.78233600	-2.28094900	4.63791500
H	2.08853900	-0.94520500	0.54662700
H	3.17094100	-1.96354600	2.56151700
C	-2.64917300	-2.04101100	0.77526700
H	-3.62028000	-2.40586800	1.14868800
H	-1.87434000	-2.61334500	1.30560400
C	-2.50514500	-2.28875300	-0.70594400
C	-3.20111400	-3.29083500	-1.37308800
C	-2.94613800	-3.49734600	-2.72657300
H	-3.92729100	-3.90207900	-0.83991700
C	-1.36810700	-1.70337200	-2.63824100
C	-2.01102400	-2.69397200	-3.37158900
H	-3.47636000	-4.27567900	-3.27104600
H	-0.63247700	-1.02790300	-3.07488400
H	-1.78622300	-2.82517600	-4.42669500
Cu	-0.81537200	0.10921100	-0.19031000
N	-1.61104100	-1.50713300	-1.33671500
O	0.36154400	0.83729400	-1.48929200
O	1.66511800	0.34099700	-1.24995000
C	2.58134200	1.43058300	-0.86763900
C	2.70731300	2.38092800	-2.05133200
H	3.05990200	1.85218700	-2.94274100
H	1.73200500	2.82581800	-2.27888900
H	3.41793900	3.18426200	-1.82712900
C	2.04913300	2.16303800	0.35255200
H	1.97877000	1.50914000	1.22922600
H	2.69506700	3.00986300	0.60934500
H	1.05095200	2.55669600	0.13741700
C	3.87108600	0.67110900	-0.61341300
C	4.60769600	0.81320700	0.56616600
C	4.33687200	-0.21941600	-1.58993000
C	5.78304800	0.09017900	0.76199700
H	4.27385200	1.50043600	1.34181000
C	5.50304100	-0.94948700	-1.39053000
H	3.76663200	-0.34680100	-2.50854300
C	6.23217000	-0.79537900	-0.21290100

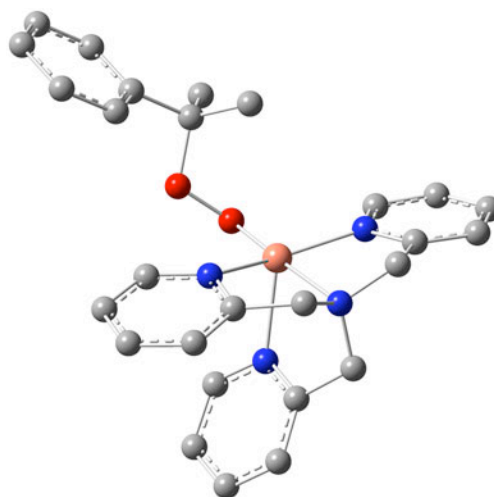


H	6.35067600	0.22473100	1.68120800
H	5.84745900	-1.63830700	-2.15969300
H	7.15021700	-1.35927400	-0.05918800

7b

Energy: -1612.79060311 a.u.

C	0.90822900	-2.25278000	-0.05084500
C	0.98981300	-3.62397500	-0.26393200
C	0.08891900	-4.22131700	-1.13816800
C	-0.85764100	-3.42348200	-1.77489300
C	-0.86994500	-2.05711800	-1.52214200
N	0.00364100	-1.47852600	-0.67219800
H	0.11632300	-5.29361900	-1.31952900
H	1.57735800	-1.72811200	0.62929000
H	1.74462100	-4.20631700	0.25769200
H	-1.58260500	-3.85346300	-2.46380500
C	-1.81952300	-1.12416100	-2.22756700
H	-1.28433800	-0.65650000	-3.06575600
H	-2.66170800	-1.68455600	-2.66559000
N	-2.28752900	-0.04396800	-1.34522600
C	-2.53213800	1.23032600	-2.04027700
H	-3.51305800	1.25080500	-2.54264800
H	-1.77093900	1.32742400	-2.82688100
C	-2.39046900	2.38893500	-1.08697200
C	-3.13569500	3.55687800	-1.19691200
N	-1.44660000	2.24169300	-0.13736600
C	-2.88837500	4.60085700	-0.30927700
H	-3.89650100	3.64602300	-1.97014200
C	-1.20999400	3.24420100	0.72031600
C	-1.90784500	4.44396400	0.66546300
H	-3.45943400	5.52416100	-0.37630000
H	-0.43103000	3.04334200	1.45637300
H	-1.68761700	5.23404700	1.37813400
C	-3.45804700	-0.44221200	-0.53343200
H	-4.21351000	-0.94291200	-1.16139400
H	-3.91468200	0.48547800	-0.15930500
C	-3.07917000	-1.29373100	0.64895200
C	-3.78237600	-2.43490500	1.01735300
C	-3.38312900	-3.12563100	2.15983600
H	-4.62804500	-2.77619800	0.42252500
C	-1.64059500	-1.51248700	2.44223800
C	-2.29517000	-2.65700200	2.88841000
H	-3.91398300	-4.02234400	2.47235700
H	-0.76653200	-1.10664400	2.95234500
H	-1.95173100	-3.17012200	3.78291300
Cu	-0.64791200	0.36586700	0.07303400
N	-2.02736200	-0.84209500	1.35242000
O	0.62936000	0.87518400	1.38819000
O	1.91231200	0.36333600	1.09162900
C	2.77376300	1.39591800	0.49559800
C	2.10017600	1.98295100	-0.74005900
H	1.77843600	1.19165500	-1.43054300
H	1.22357300	2.57670100	-0.45844200
H	2.79803200	2.63374800	-1.27853300
C	3.01325600	2.47171100	1.53913500
H	3.47738100	2.05612600	2.43916800
H	3.65353300	3.27043400	1.14786200
H	2.05302600	2.91136200	1.82623900

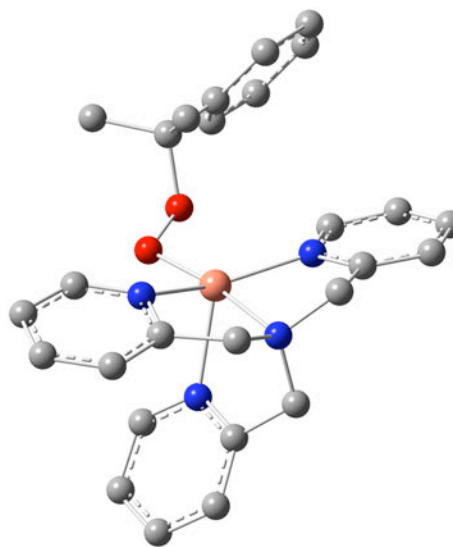


C	4.00862400	0.59800500	0.11569800
C	5.27580000	0.88789200	0.62500100
C	3.87964000	-0.47044700	-0.78099500
C	6.38457200	0.13379500	0.24556400
H	5.40994300	1.71251700	1.32180600
C	4.98150800	-1.23060600	-1.15404500
H	2.89749000	-0.70671600	-1.19125800
C	6.24157700	-0.92858500	-0.64079600
H	7.36485100	0.37924300	0.64949800
H	4.85934100	-2.05771100	-1.85172300
H	7.10825100	-1.51788600	-0.93382800

7c

Energy: -1612.79286012 a.u.

C	-2.08887200	-2.45578300	-0.93292000
C	-3.26149400	-3.16270400	-1.16369600
C	-4.39511400	-2.45959000	-1.56001000
C	-4.31160000	-1.08025000	-1.72504300
C	-3.09666000	-0.44473300	-1.49178000
N	-2.00671500	-1.12710800	-1.09645900
H	-5.33592600	-2.97713200	-1.73439800
H	-1.17269100	-2.93219400	-0.58360200
H	-3.28427700	-4.23990400	-1.02254800
H	-5.17904300	-0.49916500	-2.03351800
C	-2.90664300	1.03144700	-1.73892400
H	-2.59349800	1.16361500	-2.78387900
H	-3.86544700	1.56425800	-1.63824100
N	-1.87374200	1.63072200	-0.87467400
C	-0.97088000	2.55316100	-1.57680700
H	-1.42960600	3.54230800	-1.74296600
H	-0.77416400	2.12427700	-2.56941400
C	0.33713800	2.69250600	-0.84325400
C	1.07400400	3.86998600	-0.87782100
N	0.77994400	1.59164000	-0.19754300
C	2.31615300	3.91344500	-0.25010500
H	0.67816800	4.73940300	-1.39955800
C	1.97074800	1.64372100	0.42247300
C	2.77281100	2.77823300	0.40866800
H	2.91185100	4.82339600	-0.27268300
H	2.27370900	0.72782700	0.92575100
H	3.73507600	2.75783500	0.91394200
C	-2.45280500	2.25307700	0.33343400
H	-3.26629500	2.94764500	0.06510000
H	-1.65571700	2.84945900	0.80038400
C	-2.92118700	1.21081700	1.31121000
C	-4.15847000	1.25445300	1.94311200
C	-4.48252900	0.24281000	2.84530300
H	-4.85522400	2.06451100	1.73397600
C	-2.34915200	-0.74360400	2.40070900
C	-3.56404000	-0.77491300	3.07969700
H	-5.44408400	0.24860800	3.35417500
H	-1.59073900	-1.51664300	2.52707600
H	-3.78239800	-1.58261800	3.77347700
Cu	-0.56281500	0.01661600	-0.12895500
N	-2.03350800	0.22825100	1.54004200
O	0.30590500	-1.55164700	0.51332700
O	1.67116200	-1.31267400	0.74136400
C	2.51124900	-1.87331800	-0.33819400

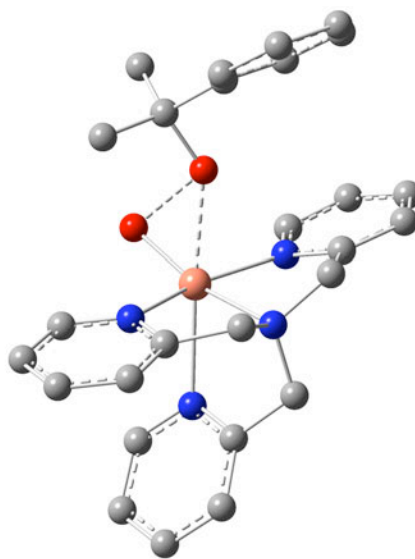


C	2.49093900	-3.38960500	-0.20490100
H	2.85725000	-3.70385000	0.77762100
H	1.46608300	-3.75954300	-0.32642500
H	3.12270200	-3.85490100	-0.96995800
C	1.97945200	-1.44594100	-1.69478000
H	1.94678200	-0.35320700	-1.79251200
H	2.61175500	-1.84201600	-2.49683600
H	0.96889100	-1.84006700	-1.84123900
C	3.86594700	-1.28068700	0.00603900
C	4.63411300	-0.56964100	-0.91992100
C	4.34769500	-1.41070700	1.31574000
C	5.85459800	-0.00785400	-0.54996000
H	4.28792900	-0.45232700	-1.94510000
C	5.55819900	-0.83759200	1.68980400
H	3.75408100	-1.95209600	2.05077300
C	6.31789700	-0.13494500	0.75604800
H	6.44475000	0.53108500	-1.28911300
H	5.91356000	-0.94582500	2.71291300
H	7.27077600	0.30467300	1.04466700

**8) – Self – Decomposition Structures (Tpa) (structure *vii* in Figure 8)**

Energy: --1612.74308465 a.u.

C	-2.13245200	-2.22350000	1.12975900
C	-2.92626700	-3.29377800	0.73732500
C	-3.09372100	-3.53120900	-0.62425100
C	-2.45544500	-2.70420700	-1.54453400
C	-1.66855300	-1.65872200	-1.07267900
N	-1.52403300	-1.42880600	0.24287600
H	-3.71584000	-4.35461900	-0.96834400
H	-1.95229400	-1.97252000	2.17531200
H	-3.40444700	-3.92229600	1.48369700
H	-2.56167000	-2.86920300	-2.61522600
C	-0.84725200	-0.77440100	-1.97707800
H	0.15362700	-1.22267100	-2.06408000
H	-1.27242800	-0.74107800	-2.99325600
N	-0.66849400	0.58131100	-1.42251100
C	0.62262400	1.19542900	-1.79105600
H	0.60863600	1.58653000	-2.82124000
H	1.38586800	0.40472300	-1.75090200
C	1.01392200	2.26364800	-0.80177500
C	1.92268100	3.27125000	-1.10824800
N	0.50603000	2.12651400	0.43347900
C	2.33008500	4.13476600	-0.09570400
H	2.31305300	3.36702100	-2.11993500
C	0.90742500	2.94339800	1.41255900
C	1.82137700	3.96568600	1.18914800
H	3.04265000	4.92905400	-0.30757700
H	0.48659000	2.73367900	2.39438100
H	2.12581200	4.61327600	2.00690300
C	-1.79780800	1.48129000	-1.75217800
H	-2.03957400	1.41347800	-2.82527900
H	-1.45142300	2.50537800	-1.55824600
C	-3.00835800	1.21518900	-0.89976700
C	-4.27790700	1.02777800	-1.43557100
C	-5.34713000	0.81729200	-0.56709900
H	-4.42759400	1.04786100	-2.51402700
C	-3.80244000	0.99007300	1.24900800
C	-5.10770400	0.80035700	0.80218100



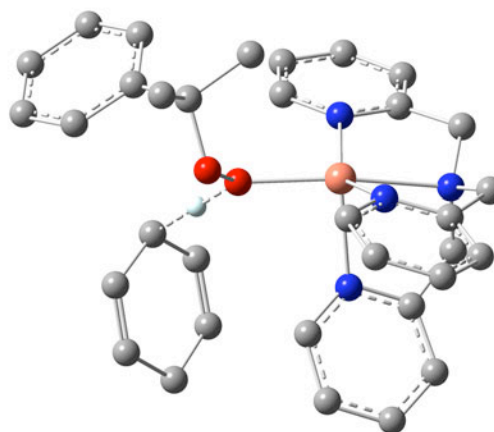
H	-6.35150800	0.66695000	-0.95708500
H	-3.56048100	0.97280100	2.31211700
H	-5.91317700	0.64162600	1.51469000
Cu	-0.56587000	0.35568500	0.69522100
N	-2.77209600	1.19516400	0.42374200
O	-0.06228400	0.00463300	2.41406200
O	1.53059100	-0.36515200	0.85253500
C	2.29886500	-1.42096600	1.35113200
C	2.87470200	-1.09034900	2.72232500
H	3.42967500	-0.14694400	2.70516700
H	2.04887500	-0.98175100	3.43391200
H	3.54670200	-1.88203600	3.07340200
C	1.50209300	-2.71681800	1.39863300
H	1.03235500	-2.93683000	0.43212100
H	2.12712100	-3.56908500	1.69070800
H	0.70764400	-2.59524200	2.14302400
C	3.34579300	-1.36938700	0.22651700
C	3.52438700	-2.41316500	-0.68964600
C	4.07769600	-0.18073000	0.05332500
C	4.45885500	-2.29453600	-1.71367700
H	2.96457500	-3.33933300	-0.57955600
C	4.99588200	-0.05871600	-0.98155000
H	3.90807300	0.65080000	0.73579600
C	5.19242700	-1.11807000	-1.86682000
H	4.61974700	-3.12843300	-2.39438200
H	5.56352500	0.86283300	-1.09727700
H	5.91716900	-1.02959900	-2.67379300

## 9) – Cyclohexadiene (CHD) Oxidation (Tpa)

### 9a (structure *viii* in Figure 8)

Energy: -1846.15236083 a.u.

C	1.72951600	-1.33066500	2.49124600
C	2.70090400	-2.15976300	3.03667700
C	4.03844800	-1.80664800	2.89194900
C	4.35006600	-0.63071200	2.21621000
C	3.32329500	0.15800300	1.70926300
N	2.02563900	-0.19184200	1.84010700
H	4.82835100	-2.43805800	3.29285300
H	0.66740000	-1.57313600	2.54019700
H	2.40826100	-3.06952000	3.55434400
H	5.38508300	-0.32018300	2.08132900
C	3.61061100	1.48745400	1.04833700
H	3.50061900	2.27227200	1.80983500
H	4.66394500	1.52148800	0.72013900
N	2.69064900	1.79819800	-0.04737400
C	2.24004300	3.18813800	-0.11862400
H	2.92789900	3.83093200	-0.69487400
H	2.23150000	3.58312200	0.90688700
C	0.83878500	3.29890200	-0.67369300
C	0.43500200	4.39287600	-1.43155900
N	-0.02154700	2.31440800	-0.33712200
C	-0.89338000	4.49163700	-1.83625500
H	1.15858000	5.16272100	-1.69467300
C	-1.30294300	2.41330700	-0.73011000
C	-1.78176100	3.48449800	-1.47157200
H	-1.22670300	5.34111700	-2.42825800

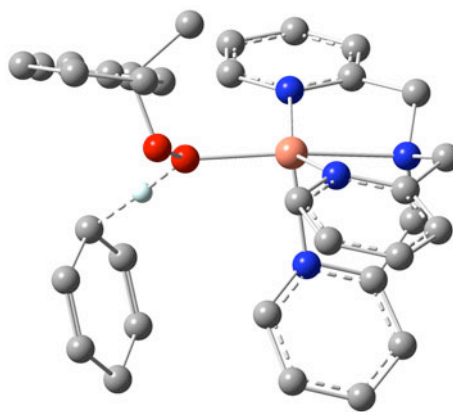


H	-1.94909900	1.58933300	-0.42239100
H	-2.82977700	3.51728800	-1.75993200
C	3.14077700	1.28256700	-1.34550500
H	4.18387800	1.57827300	-1.55606600
H	2.51095500	1.75412100	-2.11443700
C	2.97836800	-0.21225600	-1.44763200
C	3.97703600	-1.04821900	-1.93505800
C	3.72757400	-2.41652300	-2.01649700
H	4.93566100	-0.63338900	-2.24268500
C	1.54159300	-1.99416800	-1.14120100
C	2.48681100	-2.89991900	-1.61396500
H	4.49459300	-3.09454200	-2.38485400
H	0.55046500	-2.31438800	-0.81027300
H	2.25252100	-3.96127800	-1.65519100
Cu	0.78787300	0.60205900	0.40647000
N	1.78020100	-0.68133400	-1.05586600
O	-0.94208700	-0.49879300	0.40936600
O	-1.36627600	-1.24292200	1.57838800
C	-2.29363700	-0.42413700	2.35903500
C	-1.59759600	0.85377500	2.79750800
H	-0.67257200	0.60588100	3.33141400
H	-1.33638400	1.49189200	1.94552200
H	-2.23322600	1.43314200	3.47712700
C	-0.73331100	-1.40482800	-3.59863100
C	-1.64998400	-3.42896700	-2.46090900
C	-2.38638000	-2.62417500	-1.66039500
C	-1.47632600	-0.62921400	-2.77722300
H	-0.12723500	-0.94781700	-4.38073700
H	-1.74403300	-4.51129700	-2.37937700
H	-3.06557500	-3.06595700	-0.93073900
H	-1.46020300	0.45463700	-2.90758900
C	-2.28612900	-1.17947900	-1.70691600
H	-1.58709600	-0.86793200	-0.52472500
H	-3.18452000	-0.61568200	-1.42826400
C	-0.74197500	-2.89541800	-3.51970800
H	-1.01651000	-3.32413200	-4.50223500
H	0.28939000	-3.27462100	-3.37379000
C	-3.55119200	-0.20194400	1.53399200
C	-4.25370700	-1.31560800	1.05724300
C	-4.02450200	1.06995900	1.20204500
C	-5.38656600	-1.16613200	0.26606200
H	-3.89122500	-2.31541400	1.29556000
C	-5.15859100	1.22555700	0.40444500
H	-3.51170800	1.95743500	1.57070300
C	-5.84170200	0.10917300	-0.06778000
H	-5.91520100	-2.04676700	-0.09515800
H	-5.51363900	2.22602700	0.16169400
H	-6.72831500	0.22972200	-0.68700600
C	-2.56107900	-1.31550700	3.56662500
H	-3.28740900	-0.83433000	4.22973900
H	-2.96534000	-2.28826400	3.27050300
H	-1.63774000	-1.48410300	4.13311200

9b

Energy: -1846.14680416 a.u.

C	-0.79657300	2.48219400	-0.15649800
C	-0.88029500	3.81628500	0.22101600
C	0.17286100	4.66774700	-0.09450700
C	1.26446500	4.15089400	-0.78583100
C	1.27163900	2.80779600	-1.14569600
N	0.25184100	1.97956900	-0.83305100
H	0.15086200	5.71548100	0.19752400
H	-1.57453000	1.76182400	0.09482000
H	-1.75351000	4.16949900	0.76360700
H	2.11241700	4.78241200	-1.04676700
C	2.40122400	2.21960300	-1.95911400
H	2.09157100	2.20858300	-3.01356900
H	3.28646400	2.87678300	-1.90243100
N	2.71871400	0.84246200	-1.57682200
C	3.05516700	-0.05337600	-2.68290900
H	4.11976500	0.00062200	-2.96957800
H	2.47799200	0.27518800	-3.55855000
C	2.67242400	-1.47996900	-2.37106400
C	3.42917800	-2.55773200	-2.81705500
N	1.52485000	-1.65444100	-1.68089700
C	2.98972200	-3.85347700	-2.56207400
H	4.35387500	-2.37728500	-3.36266700
C	1.10645100	-2.90726700	-1.43694100
C	1.80167300	-4.03150000	-1.86033700
H	3.56841300	-4.70908800	-2.90270400
H	0.17455900	-2.98067700	-0.87482800
H	1.41798300	-5.02390000	-1.63857000
C	3.67731000	0.75293900	-0.46754500
H	4.57642000	1.36358400	-0.66332800
H	4.00438700	-0.29548700	-0.40962900
C	3.04591200	1.13606500	0.84552200
C	3.62248500	2.04932700	1.72095800
C	2.95765600	2.35583000	2.90642600
H	4.57195000	2.52081200	1.47199200
C	1.24348200	0.82020100	2.25224700
C	1.74416600	1.73263400	3.17697300
H	3.37889200	3.07754100	3.60316700
H	0.29133100	0.30706800	2.41166600
H	1.18435600	1.95237500	4.08353400
Cu	0.77157900	-0.01475500	-0.72521300
N	1.87543800	0.52719600	1.11110900
O	-0.76338500	-0.98212100	0.22910600
O	-2.08704000	-0.38046000	0.17470500
C	-2.89496200	-1.04316100	-0.85531100
C	-2.19541800	-0.93856800	-2.20558800
H	-1.93251500	0.09888000	-2.44224200
H	-1.27297500	-1.53162200	-2.21024700
H	-2.84687400	-1.31362700	-3.00298900
C	-3.09614800	-2.49919500	-0.47372600
H	-3.52020300	-2.59669800	0.53184400
H	-3.76071700	-3.00469700	-1.18313100
H	-2.13286400	-3.02078500	-0.49134200
C	-4.16663700	-0.20997100	-0.81244900
C	-5.39326600	-0.74073000	-0.40487200
C	-4.11717100	1.14123000	-1.17945400
C	-6.53836100	0.05189200	-0.37495100
H	-5.46983100	-1.78656500	-0.11607600
C	-5.25611800	1.93680800	-1.14218800
H	-3.17299000	1.57644100	-1.50508800
C	-6.47396500	1.39256800	-0.74010100



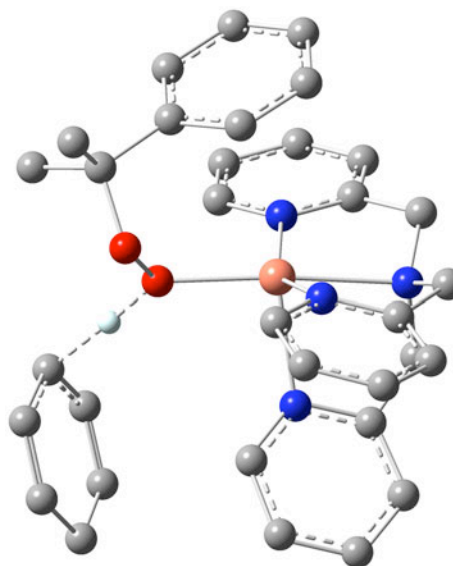


H	-7.48543600	-0.38433400	-0.06341000
H	-5.19526600	2.98335900	-1.43569300
H	-7.36929000	2.01059600	-0.71577100
C	1.22462500	-2.33127900	3.67364600
C	-0.89048700	-1.21086500	4.38817600
C	-1.51629100	-1.74212800	3.31193700
C	0.57129200	-2.84359900	2.60614700
H	2.27112900	-2.58154100	3.84450600
H	-1.45273500	-0.60993100	5.10223600
H	-2.57901900	-1.55243300	3.15960500
H	1.10403100	-3.50745400	1.92330100
C	-0.81367600	-2.52824300	2.31815200
H	-0.77876900	-1.66035000	1.19830100
H	-1.39607800	-3.30269300	1.80611200
C	0.55043300	-1.46739000	4.68747900
H	0.65148500	-1.91817100	5.69324700
H	1.10066200	-0.51205100	4.79864800

9c

Energy: -1846.15636108 a.u.

C	-1.26146300	-0.69252400	2.63393600
C	-2.25303400	-1.22612600	3.44701100
C	-2.66561000	-2.53565600	3.22211900
C	-2.05760700	-3.26449900	2.20424300
C	-1.06293500	-2.66572000	1.43833200
N	-0.67653700	-1.39038800	1.64548900
H	-3.45011100	-2.98420800	3.82775700
H	-0.90877600	0.33357900	2.74740100
H	-2.69602300	-0.62004000	4.23306000
H	-2.35099800	-4.29322700	1.99979900
C	-0.31143600	-3.43694700	0.37588900
H	0.61860700	-3.81309900	0.82541300
H	-0.89120000	-4.32727500	0.07606200
N	0.05475100	-2.61211700	-0.77632000
C	1.38868900	-2.85578900	-1.32393400
H	1.41747200	-3.71655900	-2.01513600
H	2.04825800	-3.10367600	-0.47944100
C	1.94161000	-1.62557300	-2.00284900
C	2.81537800	-1.71466100	-3.08139300
N	1.58482900	-0.43741600	-1.47635200
C	3.34029900	-0.54857500	-3.63037700
H	3.07757800	-2.69130900	-3.48494100
C	2.08885900	0.68360500	-2.01198900
C	2.96768700	0.67645700	-3.08657800
H	4.02312500	-0.59702300	-4.47582400
H	1.76510800	1.60832800	-1.53356300
H	3.34843500	1.61292900	-3.48615900
C	-0.98584500	-2.57294600	-1.81263700
H	-1.28841400	-3.59071100	-2.11679700
H	-0.54398200	-2.08746000	-2.69473500
C	-2.18012400	-1.77313300	-1.36108300
C	-3.48178000	-2.25705700	-1.43323300
C	-4.52282700	-1.45936300	-0.96273300
H	-3.67464900	-3.24802300	-1.84140700
C	-2.89533100	0.20794500	-0.41940100
C	-4.22475600	-0.20573200	-0.43999700
H	-5.54946200	-1.81815500	-0.99512800
H	-2.60651700	1.18170500	-0.01519100



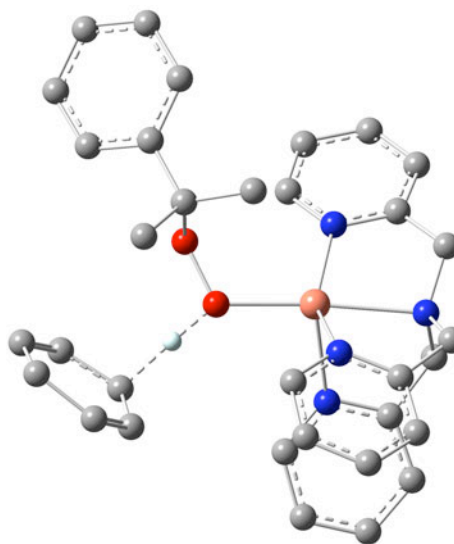


H	-5.00392900	0.44270500	-0.04501900
Cu	0.16152300	-0.46379900	-0.01368700
N	-1.89297200	-0.55413100	-0.86823800
O	0.16345800	1.54808500	0.41331900
O	0.45464600	1.91930500	1.78929000
C	1.86861200	2.25111000	1.91423700
C	-2.59708700	3.01062300	-2.39757900
C	-3.32010000	3.82008900	-0.14767100
C	-2.01984100	3.99569800	0.18726700
C	-1.30822600	3.19435600	-2.02862700
H	-2.83256400	2.66147500	-3.40234600
H	-4.10514700	4.08904100	0.55842200
H	-1.76675300	4.39712300	1.16937500
H	-0.51403300	2.99115600	-2.74882000
C	-0.93654000	3.63640400	-0.70172000
H	-0.35684800	2.47332400	-0.05796700
H	-0.01528500	4.22247000	-0.61786000
C	-3.74274300	3.33111100	-1.49505100
H	-4.40291000	4.07857900	-1.97589100
H	-4.41022100	2.45193500	-1.40017300
C	1.98652500	2.52645500	3.40985800
H	3.02054700	2.78488400	3.66040500
H	1.33949800	3.36126100	3.70099500
H	1.70571300	1.64582000	3.99765300
C	2.70666200	1.04589300	1.51226800
C	3.80420100	1.13456300	0.65399800
C	2.36951600	-0.21094600	2.02915100
C	4.53590100	-0.00186200	0.30821400
H	4.09880100	2.09766900	0.23949100
C	3.09407300	-1.34782200	1.68584400
H	1.52261600	-0.29366300	2.70901600
C	4.18058000	-1.24737700	0.81666100
H	5.38786200	0.09074200	-0.36365300
H	2.81709700	-2.31243200	2.11274600
H	4.75805000	-2.13226800	0.55206400
C	2.16807100	3.50700100	1.11419000
H	1.46753600	4.29957500	1.39948100
H	3.18307000	3.86966300	1.31027000
H	2.07268900	3.33056900	0.03645700

9d

Energy: -1846.14697952 a.u.

C	-1.47205000	1.86059000	1.59716600
C	-2.37876700	2.81632300	2.03581100
C	-3.67255600	2.41041300	2.34773400
C	-3.99902400	1.06262100	2.22587900
C	-3.03108500	0.16361400	1.79070000
N	-1.78391700	0.56136600	1.46647200
H	-4.41774200	3.13000300	2.67987200
H	-0.45338700	2.12778600	1.31064900
H	-2.07190300	3.85634100	2.12129900
H	-4.99969200	0.70541100	2.46499900
C	-3.30285300	-1.32236200	1.72253200
H	-2.93594500	-1.77508000	2.65430900
H	-4.39044300	-1.50684300	1.69889600
N	-2.61723000	-1.97674700	0.60564000
C	-1.99445200	-3.26128100	0.91754900
H	-2.70995800	-4.10212200	0.89506500
H	-1.61674300	-3.19720900	1.94821100
C	-0.82866800	-3.54852100	0.00309200
C	-0.51984800	-4.84548900	-0.39029800
N	-0.06566000	-2.49237500	-0.35630400
C	0.61913300	-5.07359700	-1.15670700
H	-1.16735600	-5.66742600	-0.08950000
C	1.03573800	-2.71811400	-1.09535500
C	1.41446700	-3.98894600	-1.50864200
H	0.87832800	-6.08164000	-1.47286300
H	1.62530700	-1.83414700	-1.33169800
H	2.31755600	-4.11567800	-2.09965200
C	-3.42794700	-2.02510900	-0.61519800
H	-4.41181300	-2.49229700	-0.43083200
H	-2.89406100	-2.66464000	-1.33354000
C	-3.59308300	-0.65215500	-1.20811200
C	-4.83137900	-0.13947600	-1.57907600
C	-4.89906400	1.14644200	-2.10948300
H	-5.72999900	-0.74042600	-1.44881500
C	-2.52693000	1.28199700	-1.86206100
C	-3.72324900	1.87469600	-2.25230300
H	-5.85625500	1.57308700	-2.40139800
H	-1.57767400	1.81048800	-1.95302200
H	-3.72680300	2.88288300	-2.65900800
Cu	-0.84264400	-0.64240200	0.03132300
N	-2.45199000	0.04928600	-1.34899000
O	0.64046600	0.73608600	-0.35899100
O	1.97177700	0.16381500	-0.40158500
C	2.61026900	0.23494300	0.91981900
C	2.78121500	1.68729300	1.34151600
H	3.43379600	2.22808700	0.65047200
H	1.80870800	2.19786800	1.36402900
H	3.21938700	1.74125800	2.34458900
C	1.77216200	-0.51419400	1.94212000
H	1.58349800	-1.54854700	1.63178000
H	2.27471500	-0.53096700	2.91604400
H	0.80663000	-0.01263100	2.07667500
C	3.94465800	-0.42339100	0.60996500
C	4.38764000	-1.57072100	1.27227400
C	4.75489100	0.12778300	-0.39172500
C	5.61820600	-2.14260700	0.95591300
H	3.78031500	-2.02247600	2.05410600
C	5.97735000	-0.44846400	-0.71589000
H	4.41173200	1.01331200	-0.92664000
C	6.41518200	-1.58535200	-0.03893900

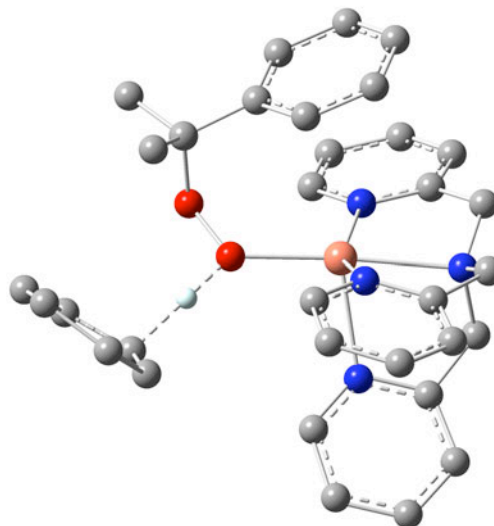


H	5.95369400	-3.02845400	1.49211700
H	6.59314600	-0.00734100	-1.49754900
H	7.37592300	-2.03305400	-0.28571700
C	3.02579100	4.09060000	-1.14100700
C	2.27872700	3.21070500	-1.84750500
C	0.24153200	3.97709000	-0.69612400
C	0.96198300	4.84721700	0.04626000
H	4.08891600	4.19961300	-1.35415100
H	2.74472000	2.61142400	-2.62961600
H	-0.84726800	3.96541200	-0.60510900
H	0.46016600	5.53367800	0.72798400
C	0.86655300	3.02333800	-1.59271400
H	0.27174600	2.69313300	-2.45271700
H	0.76874900	1.77178400	-0.90526100
C	2.44831100	4.95150800	-0.06566600
H	2.92129000	4.70943800	0.90746200
H	2.74189500	6.00534600	-0.22210800

9e

Energy: -1846.15326491 a.u.

C	1.64164500	1.30850500	1.58710900
C	2.34429500	2.33392200	2.20558200
C	1.64334400	3.46312500	2.61725500
C	0.26796200	3.51097100	2.40787900
C	-0.36533900	2.43942400	1.78650200
N	0.31834500	1.35484100	1.36969700
H	2.15748500	4.29547000	3.09297700
H	2.14726300	0.41201900	1.22341600
H	3.41861300	2.24452000	2.34933400
H	-0.31587600	4.37546600	2.72083900
C	-1.86671100	2.39940000	1.60835800
H	-2.29085400	1.83050300	2.44794100
H	-2.28257700	3.41922600	1.68478800
N	-2.27451000	1.73518400	0.37056600
C	-3.44339400	0.86514900	0.48049400
H	-4.39660300	1.42018100	0.42560000
H	-3.40579400	0.38920600	1.47102400
C	-3.41840300	-0.22578800	-0.56213200
C	-4.59425000	-0.75615200	-1.08245100
N	-2.20647100	-0.69382300	-0.92482600
C	-4.52446100	-1.80275800	-1.99624100
H	-5.55375100	-0.34693200	-0.77049800
C	-2.14261500	-1.70239200	-1.80975800
C	-3.27366600	-2.28398700	-2.36745500
H	-5.43284300	-2.22909700	-2.41647100
H	-1.13731300	-2.04751100	-2.04738900
H	-3.16863400	-3.09625800	-3.08211200
C	-2.36358900	2.65372200	-0.77026900
H	-3.01355500	3.51731000	-0.54181200
H	-2.83570700	2.10036900	-1.59473800
C	-0.99978400	3.11463200	-1.20879200
C	-0.68243500	4.45808200	-1.37988100
C	0.60907200	4.80244900	-1.77171700
H	-1.43701200	5.22285000	-1.20190700
C	1.12898300	2.47128300	-1.79961600
C	1.53684300	3.78882500	-1.98349700
H	0.88555500	5.84621600	-1.90458200
H	1.81749500	1.64018600	-1.95532200

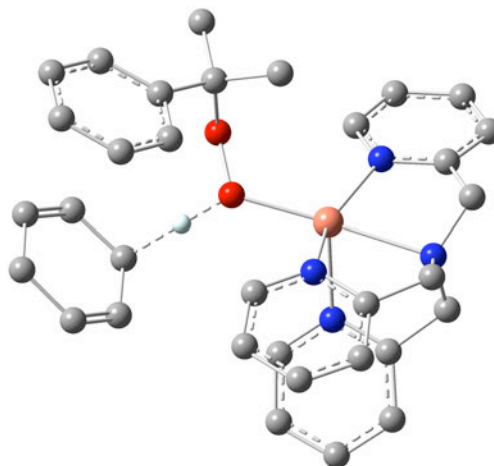


H	2.55708500	4.00850600	-2.28891900
Cu	-0.58416800	0.28001400	-0.17541700
N	-0.10557300	2.13040200	-1.41729200
O	1.07472100	-0.88929300	-0.60188100
O	0.87026700	-2.28078900	-0.94864700
C	0.85408500	-3.12566300	0.25347000
C	2.12156500	-2.92259700	1.06760400
H	2.99385800	-3.23455600	0.48507600
H	2.26752000	-1.87284200	1.34275700
H	2.08125500	-3.51427300	1.98905800
C	4.96867300	-2.32760700	-0.96000700
C	4.01381400	-1.80840700	-1.76697900
C	4.16452100	0.35158500	-0.59912800
C	5.10011000	-0.14323000	0.24290200
H	5.34652400	-3.33384400	-1.13828200
H	3.62050500	-2.40330100	-2.59089800
H	3.89520000	1.40919300	-0.53943500
H	5.58491100	0.50888000	0.96933500
C	3.47542900	-0.48097800	-1.56435100
H	3.09022100	0.01697300	-2.46177300
H	2.15565900	-0.70280900	-1.00010100
C	5.55362100	-1.56574200	0.18392300
H	5.32261700	-2.08041200	1.13890300
H	6.65727400	-1.60898700	0.14747800
C	0.86099500	-4.50898200	-0.38299400
H	0.73507800	-5.28302200	0.38159500
H	0.06081100	-4.62124400	-1.12229900
H	1.81346000	-4.67587400	-0.89604500
C	-0.41357200	-2.82787500	1.04478100
C	-0.42980400	-1.80602400	2.00170200
C	-1.60944500	-3.51449800	0.80299700
C	-1.59693500	-1.47798800	2.68948000
H	0.48539500	-1.26274500	2.22725300
C	-2.77876100	-3.19188400	1.48634300
H	-1.63696000	-4.32201700	0.07381100
C	-2.77801900	-2.17059800	2.43397600
H	-1.57143000	-0.69170200	3.44475400
H	-3.69152200	-3.75101400	1.28615500
H	-3.68756300	-1.93216600	2.98427200

9f

Energy: -1846.14536742 a.u.

C	-0.43539900	-1.99008000	1.18532700
C	-0.53320900	-3.31404400	1.59286500
C	0.55955900	-3.90015600	2.22234800
C	1.70439600	-3.13325600	2.42144100
C	1.72513100	-1.81252900	1.98758500
N	0.66613500	-1.24415700	1.37186200
H	0.52640100	-4.93736600	2.54876600
H	-1.26324900	-1.49550600	0.67758800
H	-1.45160200	-3.86646400	1.40817400
H	2.58247300	-3.55370600	2.90925800
C	2.91385400	-0.91479800	2.23021100
H	2.68298200	-0.26720900	3.08773200
H	3.79202000	-1.51812300	2.51980300
N	3.19566700	-0.04774600	1.08711400
C	3.66395100	1.29625500	1.42283200
H	4.74735000	1.33654000	1.63112000



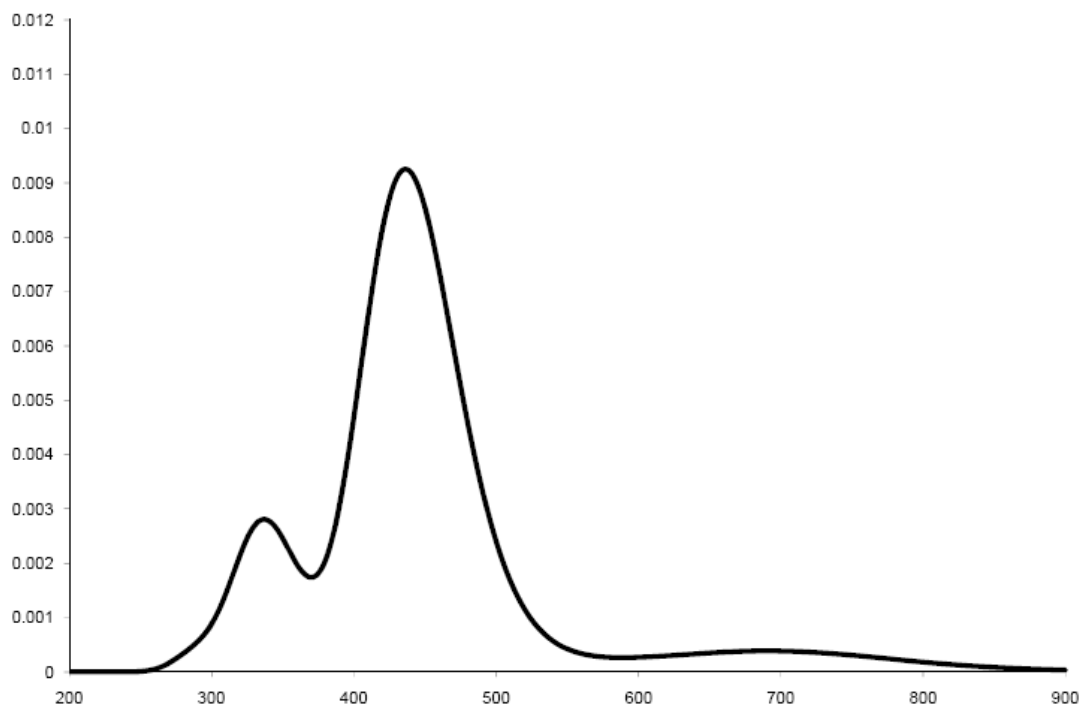
H	3.15328700	1.59684300	2.34890800
C	3.30548500	2.28024300	0.33684200
C	4.16051100	3.31389100	-0.02772700
N	2.08826900	2.12837600	-0.22904600
C	3.75147900	4.22991600	-0.99266200
H	5.13689100	3.39756100	0.44665900
C	1.69795600	3.01392400	-1.16200100
C	2.49468000	4.07718800	-1.56799200
H	4.40617900	5.04545500	-1.29175400
H	0.70110200	2.84669100	-1.56866600
H	2.13184000	4.76623500	-2.32620800
C	4.01208600	-0.69497700	0.05561300
H	4.87614600	-1.22229900	0.49720800
H	4.42008100	0.10302700	-0.58211700
C	3.21403600	-1.62883500	-0.81922700
C	3.68582100	-2.88403600	-1.18980500
C	2.92043600	-3.66831700	-2.04921400
H	4.64198200	-3.24025700	-0.80959400
C	1.31236200	-1.90389800	-2.09248300
C	1.70961200	-3.16786300	-2.51548300
H	3.26633700	-4.65519500	-2.34913000
H	0.37134300	-1.46307400	-2.42411900
H	1.08115200	-3.74147500	-3.19254600
Cu	1.14014600	0.35038100	0.10940200
N	2.03709500	-1.14781000	-1.26069900
O	-0.79676600	0.55364200	-0.57499300
O	-1.25426900	1.89030400	-0.88357500
C	-1.89031200	2.52300700	0.28191600
C	-4.74335000	-0.78623200	-1.58183100
C	-3.63205200	-0.21358800	-2.09801400
C	-2.34597500	-2.26682500	-1.66343500
C	-3.43559500	-2.86028000	-1.12602300
H	-5.68505400	-0.23980500	-1.57857800
H	-3.68488400	0.79474200	-2.50889000
H	-1.42099500	-2.84119600	-1.75652000
H	-3.38702800	-3.90033900	-0.80256200
C	-2.34858400	-0.88319600	-2.10030400
H	-1.68571800	-0.63625300	-2.94012700
H	-1.54448600	-0.13200000	-1.20077800
C	-4.75086400	-2.16602700	-1.01638000
H	-5.08232700	-2.13328800	0.03976400
H	-5.53754100	-2.77406400	-1.50126000
C	-2.22593000	3.88643500	-0.30577000
H	-2.75337100	4.50085800	0.43134100
H	-1.30589300	4.40938700	-0.58828400
H	-2.85244900	3.79723800	-1.19920400
C	-0.87198200	2.67908000	1.40472700
H	-1.33950800	3.14259200	2.28113100
H	-0.45883400	1.71210800	1.71793100
H	-0.03883400	3.31334000	1.08085900
C	-3.10941900	1.73769400	0.73863700
C	-4.41243800	2.15076900	0.44395700
C	-2.94685100	0.57250600	1.49962000
C	-5.51428500	1.42837400	0.89517900
H	-4.58295200	3.05730800	-0.13293300
C	-4.04329300	-0.16445500	1.93332500
H	-1.94569800	0.24926100	1.77479700
C	-5.33530000	0.26413900	1.63613300
H	-6.51861400	1.78193100	0.66794600
H	-3.88658100	-1.06819600	2.52281400

H            -6.19716200   -0.29873200   1.99149200

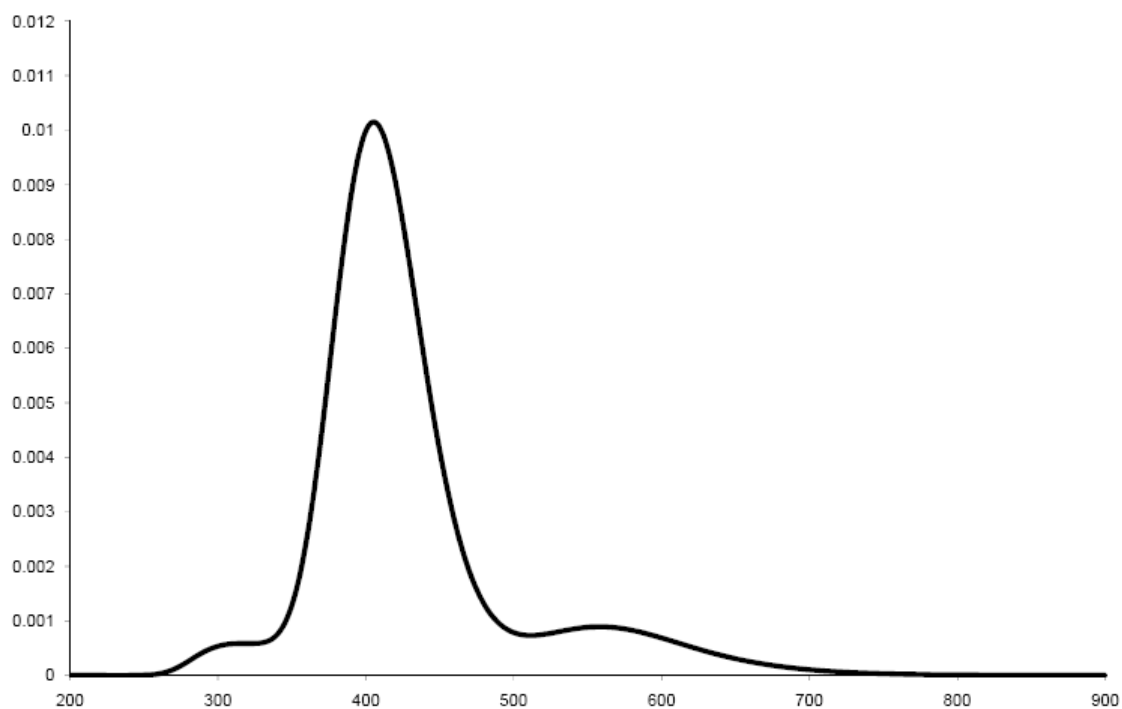
## II – Calculated UV-Vis Spectra

TD-DFT spectra (see Computational Methods section for details) generated by applying Gaussian broadening to computed peak positions and scaling arbitrary absorption intensities to predicted oscillator strengths.

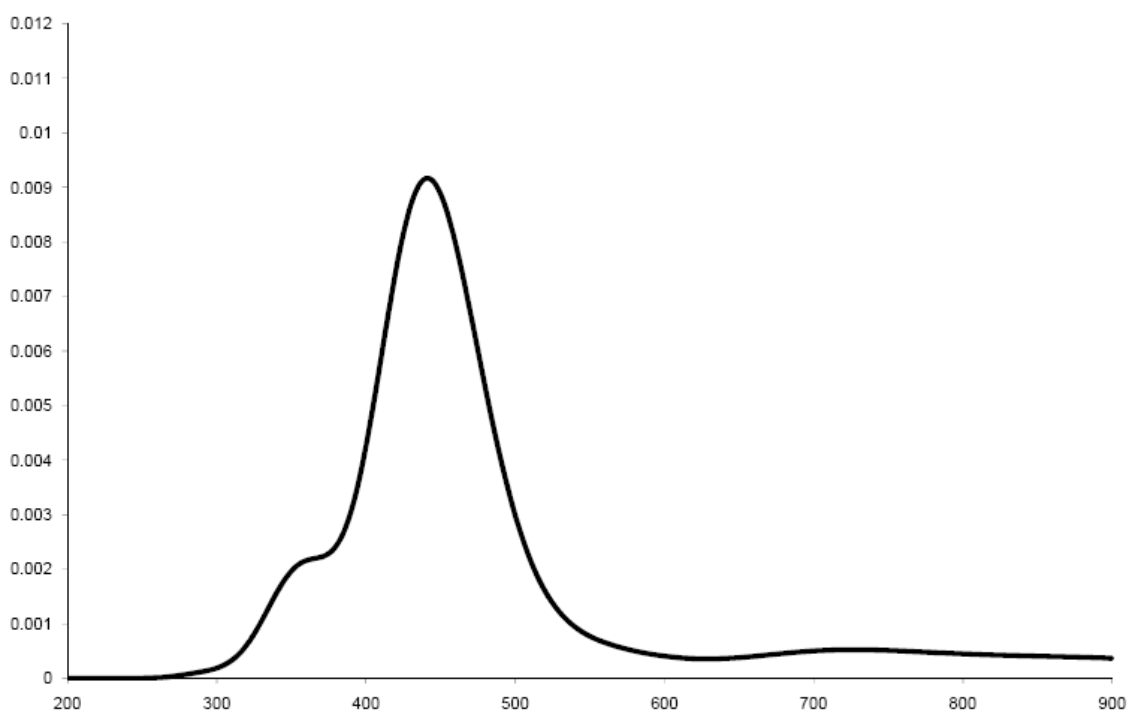
### a) $[\text{Cu}^{\text{II}}(\text{bpa})(\text{CH}_3\text{CN})(\text{O}_2\text{Cm})]^+$



### b) $[\text{Cu}^{\text{II}}(\text{bpa})(\text{O}_2\text{Cm})]^+$



c)  $[\text{Cu}^{\text{II}}(\text{tpa})(\text{O}_2\text{Cm})]^+$



III - Selected M06-L vibrational frequencies ( $\text{cm}^{-1}$ ) with mode assignment and  $^{18}\text{O}_2$  isotope shift

**a) Computed for structure *i***

896.5 ( $\Delta\nu = 32.7$ ) — mixed O–O stretching mode

812.4 ( $\Delta\nu = 15.4$ ) — mixed O–O stretching mode

619.4 ( $\Delta\nu = 7.4$ ) — C–C–O deformation mode

499 ( $\Delta\nu = 16$ ) — Cu–O stretching mode

**b) Computed for structure *ii***

903.4 ( $\Delta\nu = 41.6$ ) — mixed O–O stretching mode

833.4 ( $\Delta\nu = 17.2$ ) — mixed O–O stretching mode

604.8 ( $\Delta\nu = 7.9$ ) — C–C–O deformation mode

515.7 ( $\Delta\nu = 15.7$ ) — Cu–O stretching mode