Supporting Information

Mechanistically Guided Predictive Models for Ligand and Initiator Effects in Copper-Catalyzed Atom Transfer Radical Polymerization (Cu-ATRP)

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Selection of experimental ATRP activation rate constants (k_{act})

The experimental Gibbs free energy barriers ($\Delta G_{exp}^{\ddagger}$) of the Cu-ATRP activation were calculated using the Eyring equation and experimentally measured k_{act} values.

1. Experimental k_{act} values used in the training set to develop the computational model for initiator effects (eq. 3)

The experimental k_{act} values for Cu-ATRP with different initiators (Figure 6a) were taken from an experimental study reported by Fantin *et al.* in 2016.[1] These k_{act} values were measured with chronoamperometry in MeCN. The $Cu(OTf)_2$ pre-catalyst and TPMA ligand were used. Because these rate-constant values were measured under the same experimental conditions, they offer a reliable data set to develop eq. 3 for the prediction of relative reactivity of different initiators.

2. Experimental k_{act} values used in the training set to develop the computational model for ligand effects (eq. 4)

The k_{act} values of different Cu-ATRP catalysts have been measured using different experimental techniques (chronoamperometry, gas chromatography, and UV-Vis analysis) and with different Cu pre-catalysts (*e.g.* CuBr or $Cu(OTf)_2$).[2] To reliably describe the reactivity trend of a larger number of Cu catalysts, the experimental rate constant values used in the training set should all be determined under the same or similar experimental conditions. Although some more recent measurements were performed using $Cu(OTf)_2$ and chronoamperometry or cyclic voltammetry,[1] only three ligands have been measured using this method. In contrast, a majority of the experimental k_{act} values were measured with CuBr pre-catalyst using either GC or UV-Vis. Because the experimental k_{act} values measured using the two different pre-catalysts could differ by up to two orders of magnitude for the same ligand, we only included k_{act} values measured with the CuBr pre-catalyst in the training set. Specifically,

- The k_{act} values of most of the ligands in Figure 8 (i.e. N[2,3,2], N[3,2,3], TMEDA, Et_6TREN, bpy, N[2,2,2], Me_4Cyclam, PMDTA, BPED, TPMA, Me_6TREN, Cyclam-B) were taken from *Macromolecules*, **2006**, *39*, 4953-4959 (ref. 2(a)). These experimental measurements were performed in acetonitrile at 35 °C.
- The k_{act} values of $TPMA^{*3}$ (8400 M^{-1} s^{-1}) and BPMPA (0.1 M^{-1} s^{-1}) is taken from ref. 2(b) (*ACS Macro Lett.* **2012**, 1, 1037−1040), and ref. 2(c) (*J. Am. Chem. Soc. 2*0**08,** 1*30*, 10702-10713), respectively, which were both measured using the same method as in ref. 2(a) at a slightly lower temperature (22 °C). It has been shown experimentally the temperature has a relatively small impact on the activation rate constants ($k_{35°C}/k_{25°C} \approx 2$),[3c] and thus, the activation free energies derived from the k_{act} values are not expected to be significantly impacted by the temperature difference.
- The k_{act} values of $TPMA^{NMe2}$ and $TPMA^{Ph}$ (3.1×10^5 M^{-1} s^{-1} and 0.038 M^{-1} s^{-1}) are calculated based on the relative rate constants of these ligands as compared with TPMA: k_L/k_{TPMA} = 3.5 and 17.6 for $TPMA^{NMe2}$ and $TPMA^{Ph}$, respectively. These relative rate constants were reported in ref. 2(d) (*J. Am. Chem. Soc.,* **2018**, 140, 1525–1534), and ref. 2(e) (*Polymer*, **2017**, 128, 169-176).
- The k_{act} values of $TPMA^{*2}$ (1017.2 M^{-1} s^{-1}) and $TPMA^{*1}$ (536.3 M^{-1} s^{-1}) are calculated from the k_{act} of $TPMA^{*3}$ and using the well-known correlation of k_{act} with $E_{1/2}$ of the catalysts.[3]

Therefore, all of the experimental rate constants in Figure 8 correspond to values measured with CuBr using GC or UV-Vis.

Marcus theory calculations for the free energy of activation of single electron transfer

We used the modified Marcus theory to estimate the barriers for the stepwise outer-sphere single electron transfer (OSET-SW) and the concerted dissociative electron transfer (DET) processes in the reduction of MMA-Br by $[Cu^{I}$-$TPMA]^{+}$. The DFT calculations were performed at the ω-B97XD/def2-TZVP//ω-B97XD/SDD-6-31G(d) level of theory in acetonitrile at 25°C (see Computational Methods in the manuscript for details).

The OSET-SW pathway is shown as:

$[Cu^{I}\text{-TPMA}]^{+}$ + MMA-Br $\rightleftharpoons$ $[Cu^{II}\text{-TPMA}]^{2+}$ + $[MMA\text{-Br}]^{\bullet -}$ (s1)

$[MMA\text{-Br}]^{\bullet -}$ $\rightleftharpoons$ MMA• + Br^{-} (s2)

The DET pathway is shown as:

$[Cu^{I}\text{-TPMA}]^{+}$ + MMA-Br $\rightleftharpoons$ $[Cu^{II}\text{-TPMA}]^{2+}$ + MMA• + Br^{-} (s3)

The following equation was used to calculate the activation free energy of activation ($\Delta G^{\ddagger}_{OSET-SW}$) in the OSET-SW pathway:

$$\Delta G^{\ddagger}_{OSET-SW} = \Delta G^{\ddagger}_{0}(1 + \frac{\Delta_r G^{\ominus}}{4\Delta G^{\ddagger}_{0}})^2$$

Here, $\Delta_r G^{\ominus}$ = 36.1 kcal/mol is the reaction energy of eq. s1 obtained from DFT calculations. The intrinsic barrier is determined using $\Delta G^{\ddagger}_{0} = \lambda_0/4$, where λ_0 is the solvent reorgamization energy that can be calculated as follows:

$$\lambda_0 = A\times[(2r_D)^{-1} + (2r_A)^{-1} - (r_D + r_A)^{-1}]$$

where r_D and r_A are the hard sphere radii of electron donor and acceptor, respectively. A is an empirical constant. Here we use A = 99 kcal mol^{-1} Å as suggested in the Coote and Matyjaszewski's study.[4] Thus,

$$\begin{aligned}\lambda_0 &= 99\times[(2r_{[CuI\text{-}TPMA]^{+}})^{-1} + (2r_{MMA\text{-}Br})^{-1} - (r_{[CuI\text{-}TPMA]^{+}} + r_{MMA\text{-}Br})^{-1}] \\ &= 99\times [1/(4.29\times2) + 1/(3.58\times2) - 1/(4.29+3.58)] \\ &= 12.8 \text{ kcal/mol}\end{aligned}$$

leading to

$$\Delta G^{\ddagger}_{0} = \lambda_0/4 = 3.2 \text{ kcal/mol}$$

Thus,

$$\Delta G^{\ddagger}_{OSET-SW} = 3.2 \times (1 + \frac{36.1}{4 \times 3.2})^2 = 46.7 \text{ kcal/mol}$$

The dissociation of the radical anion $[MMA\text{-Br}]^{\bullet -}$ is highly exothermic (Figure 3) and is expected to be very fast. Therefore, the rate-determining step in the OSET-SW pathway is the outer-sphere single electron transfer (eq. s1).

In the DET pathway (eq. s3), the electron transfer occurs with simultaneous alkyl halide bond dissociation to form the MMA• radical and the Br^{-} anion in a polar solvent (MeCN) cage. Thus, the "sticky" model[5] is used to estimate the free energy of activation of the DET pathway:

$$\Delta G^{\ddagger}_{DET} = \Delta G^{\ddagger}_{0}(1 + \frac{\Delta_r G^{\ominus} - D_p}{4\Delta G^{\ddagger}_{0}})^2$$

$$\Delta G^{\ddagger}_{0} = \frac{\left(\sqrt{D_{MMA-Br}} - \sqrt{D_p}\right)^2 + \lambda_0}{4}$$

where $\Delta G^{\ddagger}_{0}$ is the the intrinsic barrier; $\Delta_r G^{\ominus}$= 26.0 kcal/mol is the DFT-calculated reaction energy for eq. s3; D_p is the interaction energy between MMA• and Br^{-} in the solvent cage, and the experimental data of D_p = 0.24 kcal/mol is used in our calculation;[6] $D_{MMA\text{-}Br}$ is the MMA–Br bond dissociation enthalpy calculated using DFT ($D_{MMA\text{-}Br}$ = 56.7 kcal/mol); λ_0 is the solvent reorgamization energy that is the same as that in the OSET-SW pathway (λ_0 = 12.8 kcal/mol).

Thus,

$$\Delta G_0^{\ddagger} = \frac{\left(\sqrt{D_{MMA-Br}} - \sqrt{D_p}\right)^2 + \lambda_0}{4} = \frac{\left(\sqrt{56.7} - \sqrt{0.24}\right)^2 + 12.8}{4} = 15.59\ kcal/mol$$

$$\Delta G_{DET}^{\ddagger} = \Delta G_0^{\ddagger}(1 + \frac{\Delta_r G^{\circ} - D_p}{4\Delta G_0^{\ddagger}})^2 = 15.59 \times (1 + \frac{26.0 - 0.24}{4 \times 15.59})^2 = 31.1\ kcal/mol$$

Distortion/interaction energy analysis of initiator effects on reactivity

To investigate the origin of initiator effect on Cu-ATRP reactivity, distortion/interaction model (eq s4) was used to decompose the total activation energies of 8 initiators (the structures are shown in Figure 6) with the $[Cu^{I}\text{-TPMA}]^{+}$ catalyst into distortion energies (ΔE_{dist}) and interaction energies (ΔE_{int}) using the eq s4. The results are shown in Table S1, and the correlation of distortion energies and interaction energies with the experimental reactivities are plotted in Figure S1 and Figure S2, respectively.

$$\begin{aligned} \Delta E^{\ddagger} &= \Delta E_{dist} + \Delta E_{int} \\ &= \Delta E_{dist(R\text{-}X)} + \Delta E_{dist(CuL)} + \Delta E_{int} \end{aligned} \qquad \text{(eq s4)}$$

Table S1. Distortion and interaction energies for transition states of 8 initiators with $[Cu^{I}\text{-TPMA}]^{+}$.

	$\Delta E_{dist(R\text{-}X)}$	$\Delta E_{dist(CuL)}$	ΔE_{dist}	ΔE_{int}	$\Delta E^{\ddagger}$	$\Delta G^{\ddagger}_{exp}$
MAc-Br	27.1	2.3	29.4	-18.1	11.3	17.1
MA-Br	24.1	2.2	26.3	-17.2	9.1	14.3
MMA-Br	20.9	2.1	22.9	-16.9	6.0	12.5
MeCN-Br	23.4	1.7	25.1	-15.8	9.3	12.8
MeCN-Cl	25.9	1.5	27.5	-14.7	12.7	15.3
AN-Cl	24.0	1.4	25.4	-14.0	11.3	14.7
MAc-Cl	30.2	2.1	32.3	-17.0	15.3	19.2
MA-Cl	26.6	2.0	28.7	-16.7	12.0	17.3

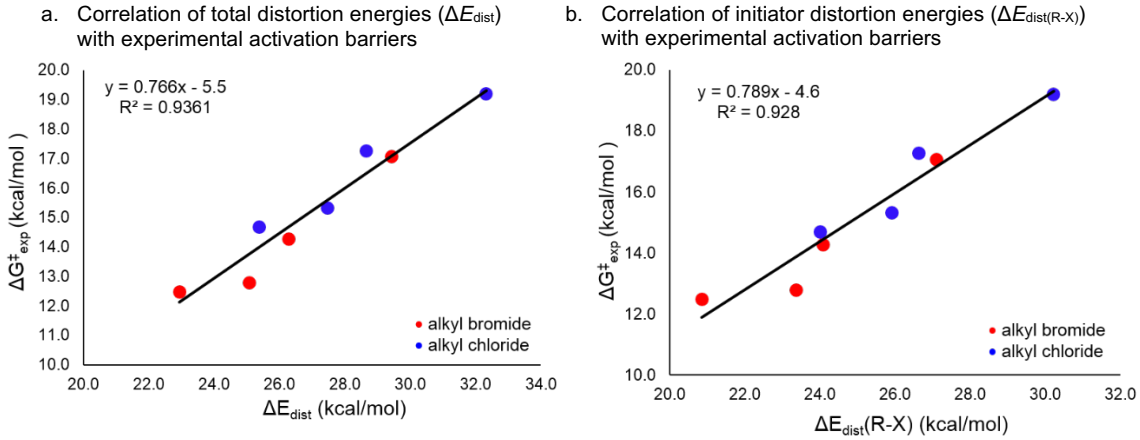


Figure S1. Correlation of distortion energies with experimental reactivities of alkyl halide initiators.

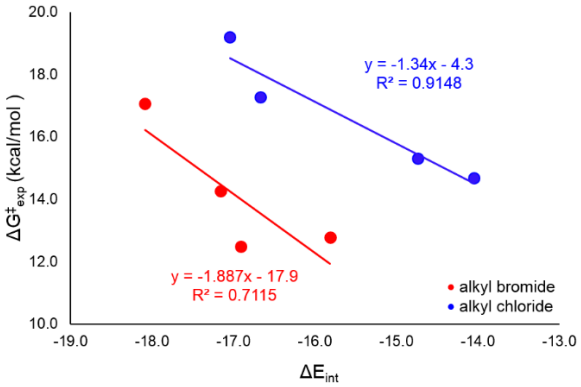


Figure S2. Correlation of interaction energies (ΔE_{int}) with experimental reactivities of alkyl halide initiators.

From the above correlation plots, we observed that distortion and interaction energies both contribute to the overall activation energies. The total distortion energies and the distortion energies of the initiators (R-X) both have a good overall correlation with the experimental activation barriers. Although the interaction energies do not have a good overall correlation with the reactivities, they correlate well within each type of halides. In addition, the computed interaction energy plot (Figure S2) indicates the alkyl bromides in general have stronger interaction with the catalyst than the alkyl chlorides.

Correlation between the HOMO energy of the TPMA family ligands (E_{HOMO}) and their reactivities

We calculated the HOMO energies (E_{HOMO}) for five $[Cu^{I}L]^{+}$ catalysts with TPMA family ligands. We observed a good correlation between the activation free energies and E_{HOMO} (Figure S3). These results suggest E_{HOMO} is an appropriate descriptor to describe the electronic effects of the ancillary ligand.

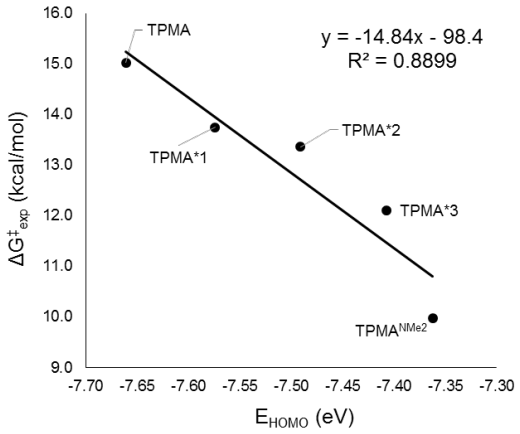


Figure S3. Correlation of experimental reactivities and the HOMO energies of five $[Cu^{I}L]^{+}$ catalysts with TPMA family ligands.

Effects of catalyst distortion of flexible ligands L7, L8

As discussed in the main manuscript, the reactivities of tetradentate Cyclam family ligands are significantly affected by the ligand backbone flexibility. Except for the most rigid ligand, **L9**, the other three more flexible ligands (**L6-L8**) undergo a conformational change from the $[Cu^{I}L]^{+}$ catalyst to achieve the geometries in their ISET transition states. Thus, reactions with catalysts supported with these ligands have lower reactivities due to the relatively large

distortion energy of the CuL catalyst in the ISET transition state. For instance, in reactions using **L7** and **L8**, the CuL catalyst is distorted from the tetrahedral geometry in the Cu^{I} ground state to a square pyramidal geometry in the ISET transition state (Figure S4).

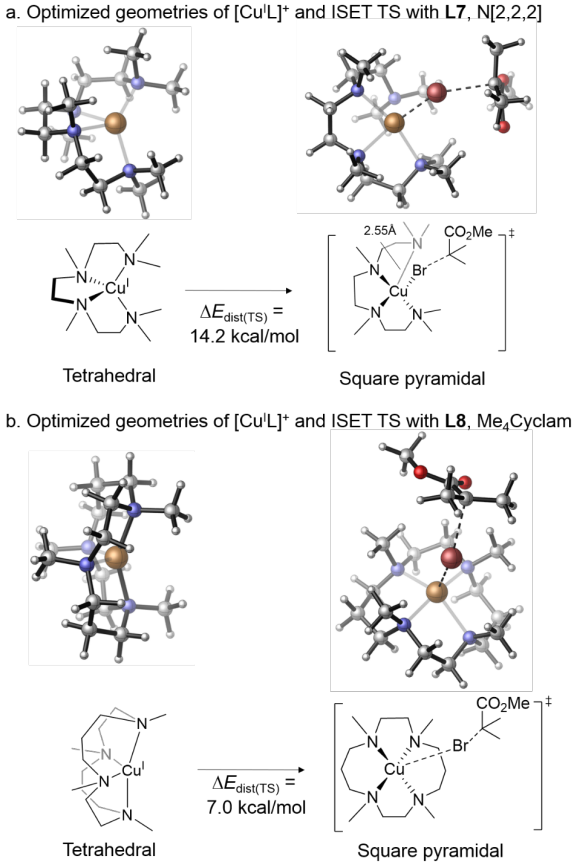


Figure S4. Optimized geometries of $[Cu^{I}L]^{+}$ catalysts and ISET transition states with Cyclam family ligands (**L7** and **L8**).

Correlation between $\Delta E_{dist}(BrCu^{II}L)$ and $\Delta E_{dist}(TS)$

As discussed in the manuscript, the ligand backbone flexibility has a significant role on reactivity. We found that both the computed distortion energy of CuL in the ISET transition state ($\Delta E_{dist(TS)}$) and in the $[Br\text{-}Cu^{II}L]^{+}$ product ($\Delta E_{dist(BrCuIIL)}$) can be used as appropriate parameters to quantitatively describe the ligand flexibility effect. Table S2 summarizes the computed $\Delta E_{dist(TS)}$ and $\Delta E_{dist(BrCu^{II}L)}$ for all 9 ligands in the training set. Importantly, an excellent linear correlation between the distortion of the ISET transition and that of the Cu^{II} intermediate is observed (Figure S5). Thus, $\Delta E_{dist(BrCuIIL)}$ was chosen as the parameter to describe the ligand flexibility effect in our predictive model of ligand effect, since it is more feasible to compute.

Table S2. The computed distortion energies (in kcal/mol) for 9 ligands in the training set.

ligand	$\Delta E_{dist(TS)}$	$\Delta E_{dist(BrCu^{II}L)}$
TPMA	2.1	4.0
TPMA[*3]	2.0	3.6
PMA^{NMe2}	1.8	3.7
Me_6TREN	2.2	4.0
Et_6TREN	3.5	5.1
Cyclam-B	4.0	5.2
Me_4Cyclam	7.0	9.0
N_4[2,2,2]	14.2	17.0
N_4[2,3,2]	11.9	14.4

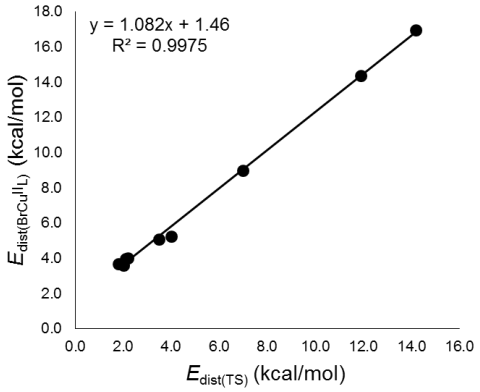


Figure S5. Correlation of $\Delta E_{dist(TS)}$ and $\Delta E_{dist(BrCu^{II}L)}$ for 9 ligands in the training set

Standardized multivariate linear equation for ligand effect prediction

In the manuscript, a multivariate linear equation (eq.4) was established using three DFT-calculated parameters:

$$\Delta G^{\ddagger}_{predicted} = -4.50 \times E_{HOMO} + 0.45 \times V_{bur}\% + 0.48 \times \Delta E_{dist} - 41.0.$$

However, since three parameters have different ranges and distributions of values, it is difficult to infer the significance of these three parameters from their weights in the linear equation. Hence, a data standardization strategy was used to transform the raw computed parameters to the normalized values with zero mean and unit variance (eq s5).

$$\text{Parameter}_{new} = \frac{\text{Parameter}_{raw} - \mu}{\sigma} \qquad \text{(eq. s5)}$$

where μ and σ are the mean and the standard deviation of individual parameters for 9 ligands in the training set, respectively.

Table S3 shows the standardized values for these three parameters. The standardized multivariate linear equation is therefore derived as follows:

$$\Delta G^{\ddagger}_{predicted} = -1.17 \times E_{HOMO}' + 2.56 \times V_{bur}'\% + 2.42 \times \Delta E_{dist}' + 15.7 \quad \text{(eq. s6)}$$

We can see that the relatively large coefficients of all three parameters in the standardized multivariate linear equation (eq. s6) indicate that electronic effects (E_{HOMO}'), steric effects (V_{bur}'%), and backbone flexibility effects (ΔE_{dist}') all have substantial contribution to the reactivity.

Table S3. Standardized electronic, steric, and backbone flexibility parameters for all 18 ligands.

ligand	$\Delta G^{\ddagger}_{exp}$	$\Delta G^{\ddagger}_{predicted}$	E_{HOMO} '	V_{bur}'%	ΔE_{dist}'
$TPMA^{NMe2}$	10.0	11.5	-0.45	-1.19	-0.72
$TPMA^{*3}$	12.1	12.2	-0.62	-0.96	-0.74
$TPMA^{*2}$	13.4	12.6	-0.94	-1.01	-0.69
Cyclam-B	13.6	13.6	1.69	0.32	-0.41
$TPMA^{*1}$	13.7	12.9	-1.26	-1.08	-0.65
Me_6TREN	13.8	14.5	-0.37	-0.01	-0.66
TPMA	15.0	13.0	-1.60	-1.15	-0.66
BPED	16.6	18.5	-0.88	-0.70	1.45
PMDTA	16.9	18.2	-0.84	-0.86	1.50
Me_4Cyclam	17.7	16.8	1.24	0.67	0.33
N[2,2,2]	18.6	20.3	-0.04	-0.03	1.91
BPMPA	18.8	17.7	-2.20	-1.45	1.30
bpy	19.1	16.3	-2.04	-1.26	0.57
Et_6TREN	19.3	19.9	-0.33	1.89	-0.44
$TPMA^{Ph}$	19.4	18.1	-1.45	0.34	-0.07
TMEDA	20.0	20.5	-0.56	0.29	1.40
N[3,2,3]	20.6	21.0	0.14	0.94	1.25
N[2,3,2]	21.5	19.7	0.48	0.46	1.39

Choosing the radius of the coordination sphere around the metal center in the percent buried volume (V_{bur}%) calculations

The percent buried volume offers a powerful and straightforward description of the size of the ligand based on the percentage of space occupied by the ligand in the first coordination sphere around the metal center. A radius (R) of 3.5 Å was recommended by Cavallo to define the first coordination sphere, as this sphere would account for the van der Waals volume occupied by the atoms directly coordinated to the metal.[7] It was also recognized a larger radius (*e.g.* R = 5.0 Å) would be necessary to accurately describe steric properties of substituents further away from the metal center, where the bulkiness of the ligand is not governed by the groups directly bound to the metal.[7] Considering the alkyl halide chain end is relatively far away from the Cu center in the bent ISET transition state, we surmised a larger radius may be necessary in the V_{bur}% calculations to provide a complete picture of the steric properties of the *N*-donor ligands.

To determine the optimum radius (*R*) for the percent buried volume parameters for the ligands used in this study, we calculated the V_{bur}% values using different radius (*i.e.* R = 3.5 Å, 4.0 Å, 4.5 Å, 5.0 Å, and 5.5 Å), and correlated the experimental activation energies with the three-variable linear equations using these V_{bur}% values in combination with computed electronic parameters (E_{HOMO}) and flexibility parameters (ΔE_{dist})[8] for the nine ligands in the training set (Table S4). As shown in Table S4, when using the default radius value of 3.5 Å, the difference in V_{bur}% between Me_6TREN and Et_6TREN is relatively small (6.6%), while the difference between TPMA and Me_6TREN is much larger (16.7%). These results indicate the V_{bur}% calculated using the radius of 3.5 Å is relatively insensitive to the steric

effects of *N*-Me and *N*-Et substituents as the Et groups are mainly located outside of the sphere. On the other hand, we suspected these V_{bur}% values overestimated the difference between the steric properties of sp^2 and sp^3 N atoms.

In contrast, when the radius value of 5.0 Å was used, the calculated V_{bur}% values are capable of capturing the steric difference between Me_6TREN and Et_6TREN (10.8%), as well as providing a reasonable difference between the V_{bur}% values of TPMA and Me_6TREN (6.5%). Furthermore, a better agreement between the experimental activation energies ($\Delta G^{\ddagger}_{exp}$) and the predicted activation energies ($\Delta G^{\ddagger}_{predicted}$) was achieved when using V_{bur}% values calculated with a radius of 5.0 Å. The overall predicted R^2 for all ligands in the training set is the largest (0.8793) using the radius of 5.0 Å, and is much greater than that with the default radius value of 3.5 Å (0.8359). With these considerations, we chose the radius of 5.0 Å in the V_{bur}% calculations in this study.

Table S4. Computed percent buried volumes (V_{bur}%) using different radii for the first-coordination sphere.

ligand	V_{bur}%				
	radius (*R*)				
	3.5 Å	4.0 Å	4.5 Å	5.0 Å	5.5 Å
TPMA	56.6	52.3	45.8	**39.2**	33.3
TPMA[*3]	56.6	52.3	45.9	40.3	36.0
$TPMA^{NMe2}$	56.1	51.9	45.5	39.0	33.2
Me_6TREN	73.3	70.1	59.2	**45.7**	34.4
Et_6TREN	78.9	76.5	67.8	**56.5**	45.3
Cyclam-B	73.5	70.5	60.7	47.6	35.9
Me_4Cyclam	78.8	75.5	64.1	49.6	37.4
N[2,2,2]	73.3	70.0	59.0	45.6	34.4
N[2,3,2]	76.7	73.4	62.4	48.4	36.6
R^2 [a]	0.8359	0.8335	0.8599	**0.8793**	0.8303

[a] The coefficient of determination of the linear regression for the relationship between $\Delta G^{\ddagger}_{exp}$ and a three-variable equation using V_{bur}%, E_{HOMO}, and ΔE_{dist} (see Table 4 in the main manuscript for computed E_{HOMO}, and ΔE_{dist} parameters).

The effect of initiator on the bent geometry of ISET transition state

As shown in the Figure 5 of the manuscript, the ISET transition state with the $[Cu^{I}$-TPMA$]^+$ catalyst and MMA-Br initiator has a bent geometry. Distortion/interaction model and energy decomposition analysis indicated the bent geometry is due to the attractive electrostatic interaction and dispersion interaction between the catalyst and the ester group on the initiator.

The optimized geometries of ISET transition states with 15 initiators and $[Cu^{I}$-TPMA$]^+$ catalyst are shown in Figure S6. All of the ISET transition states have a bent geometry. However, the Cu–X–C bond angle is affected by the initiator. Transition states with bromide initiators are typically more bent than transition states with chloride initiators. Because Cu–Br and C–Br bonds are both longer than corresponding Cu–Cl and C–Cl bonds, the smaller Cu–Br–C angle leads to a shorter distance between the catalyst and the alkyl group on the substrate, which allows more effective catalyst-substrate non-covalent interactions. Initiators with an ester group lead to more bent transition state structures than those with cyano groups, which is attributed to the stronger attractive electrostatic interactions with the more electronegative oxygen atoms in the ester. In addition, initiators with phenyl substituents also have bent ISET transition states which are stabilized by favorable π/π interactions.[9] Finally, the computed transition state with Me-Br as initiator has a completely linear geometry. Here, the favorable catalyst-substrate electrostatic and dispersion interactions between $[Cu^{I}$-TPMA$]^+$ and the Me group in the initiator are absent. Therefore, the Br transfer transition state prefers the linear geometry rather than bent.

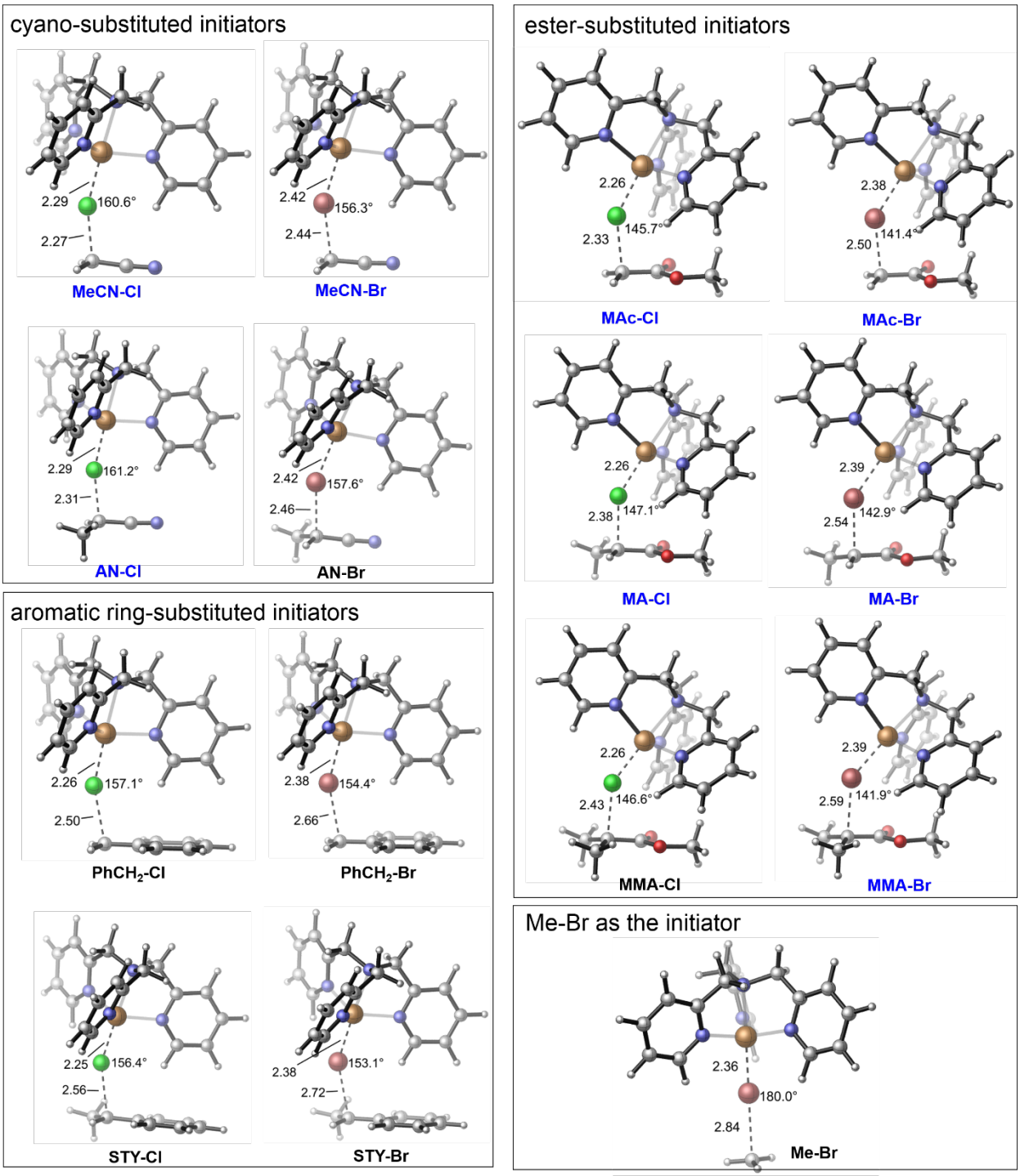


Figure S6. Optimized geometries of ISET TS of 15 initiators with $[Cu^{I}(TPMA)]^{+}$ catalyst. The initiators highlighted in blue are reported in the main manuscript.

Geometry of ISET transition state structures (TS1) optimized in gas phase and in acetonitrile

To investigate the solvation effect on the bent geometry of the ISET transition state, we have optimized the transition state (**TS1**) for the reaction between MMA-Br and $[Cu^{I}TPMA]^{+}$ both in gas phase and in acetonitrile using the CPCM solvation model (Figure S7). The calculations indicate the TS is bent in both cases and the Cu-Br-C angles are similar.

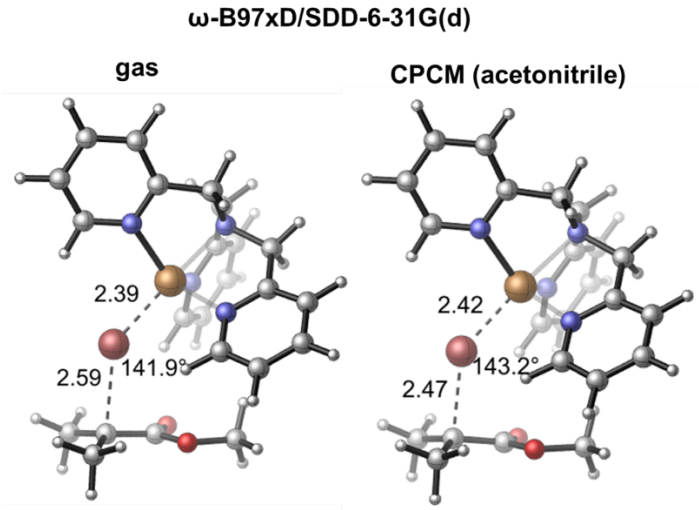


Figure S7. Geometry of **TS1** optimized in gas phase and in acetonitrile.

Benchmark of computational methods in the calculations of activation free energies for Cu-ATRP

We performed benchmark calculations to identify an appropriate DFT method and solvation model for the Cu-ATRP activation energy calculations. We evaluated the performance of different functionals, basis sets, and solvation models in activation energy calculations for 8 representative initiators (shown in Figure 6) in reactions with the $[Cu^{I}TPMA]^{+}$ catalyst. The computationally predicted activation energies were compared with experimental values (Figure S8). These benchmark calculations indicated the CPCM solvation model gives better correlation than the SMD solvation model. The def2-TZVP basis set performed better than the SDD-6-311++G(d,p) basis set. Finally, the use of the ω-B97XD yielded better correlation with experimental data in terms of both R^2 and the slope of the correlation. Because the ω-B97XD/def2-TZVP/CPCM//ω-B97XD/SDD-6-31G(d) method provides the best agreement with the experimentally determined k_{act} values, we chose this method in the present computational study.

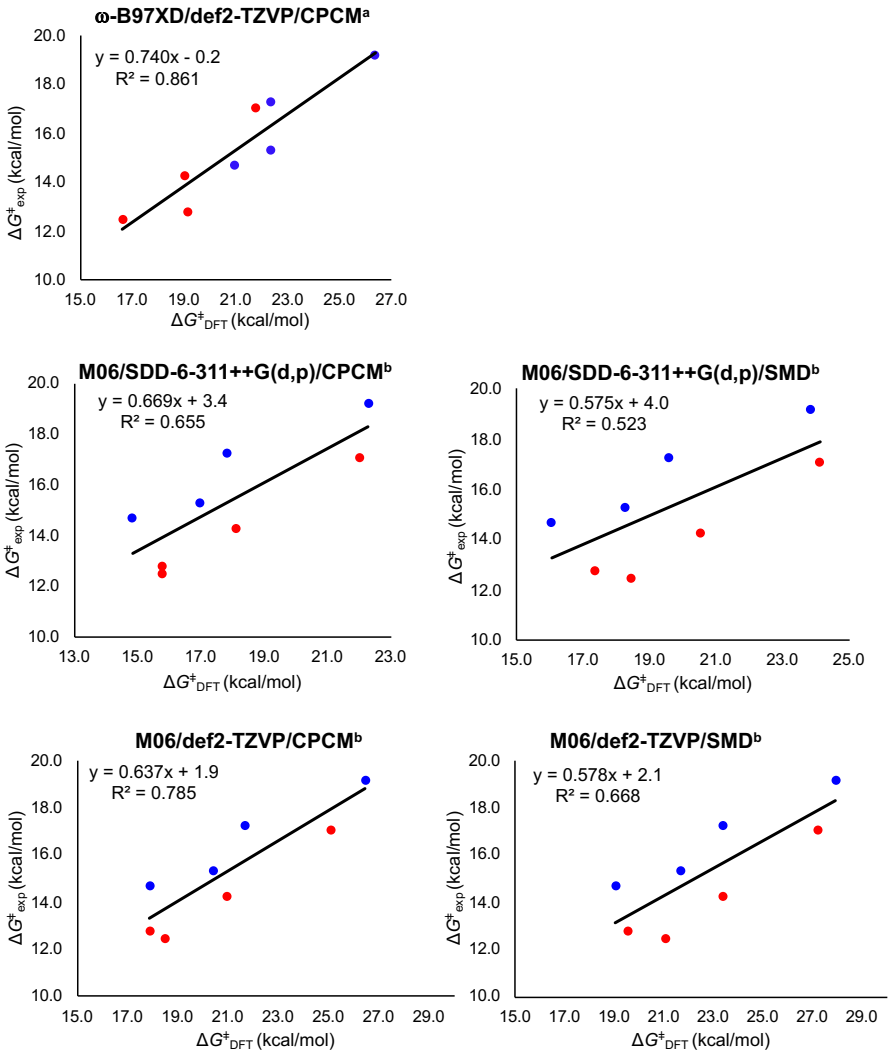


Figure S8. Benchmark of computational methods in the calculation of activation energies of different initiators with the $[Cu^{I}TPMA]^{+}$ catalysts. Blue dots stand for chloride initiators, and the red dots represent bromide initiators.

[a] Geometries were optimized with ω-B97XD/SDD-6-31G(d) in gas phase; [b] Geometries were optimized with M06/SDD-6-31G(d) in gas phase.

Possible partial dissociation of the TPMA ligand

In addition to the tetradentate-coordinated Cu-TPMA complexes reported in the manuscript, we considered the partial dissociation of the TPMA ligand (Figure S9). We calculated the possible partial dissociation of TPMA ligand for $[Cu^{I}L]^{+}$, $[Br\text{-}Cu^{II}L]^{+}$, and the ISET transition state, in which one of the pyridine arms dissociates (*e.g.* **9**, **12** and **TS3**) or is replaced with one or two acetonitrile ligands (*e.g.* **10**, **11**, **13**, and **TS4**). Although these partially dissociated complexes are energetically accessible, they are all less stable than the tetradentate-coordinated isomers reported in the main manuscript (*i.e.* **1**, **8**, and **TS1**).

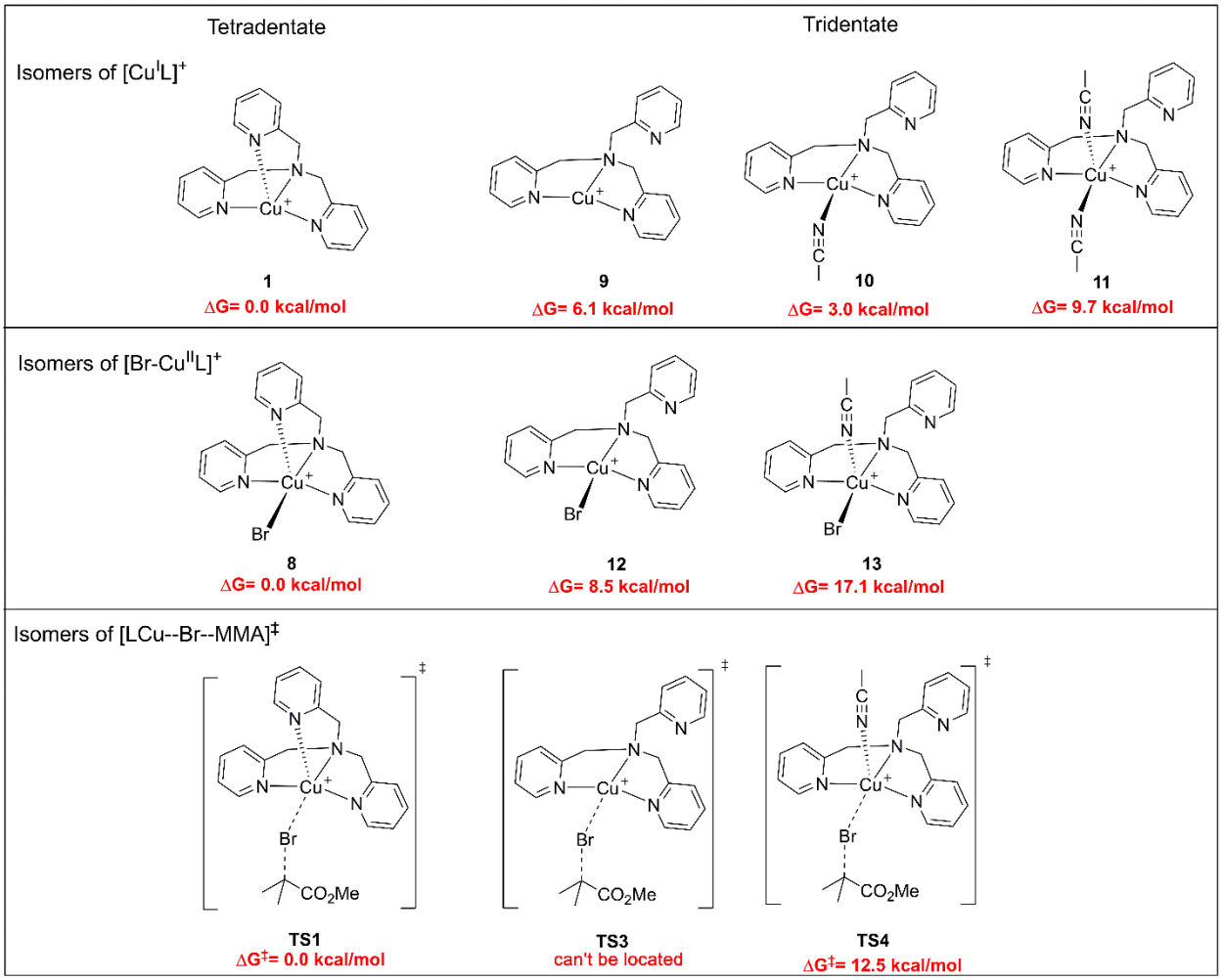


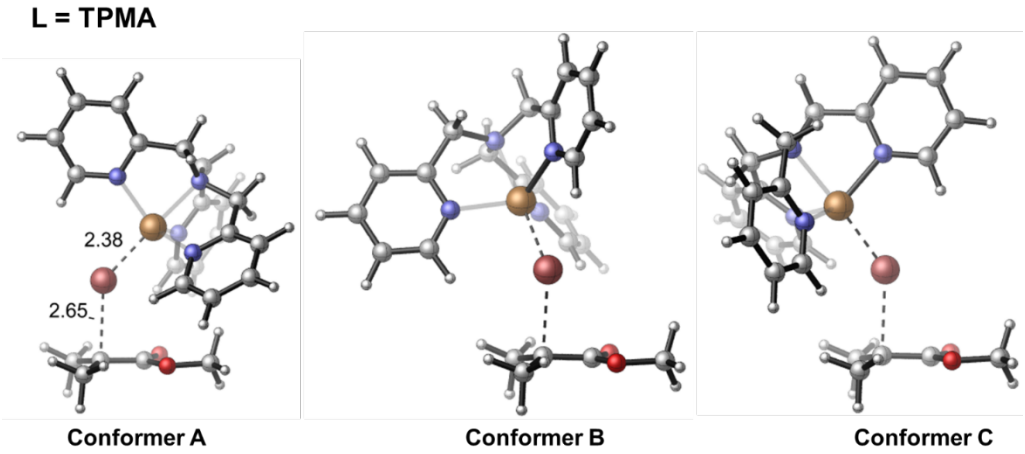
Figure S9. Partial dissociation of the TPMA ligand*.

*All Gibbs free energy values of the isomers of $[Cu^{I}L]^{+}$ are with respect to **1** and separated MeCN molecule(s); All Gibbs free energy values of the isomers of $[Br\text{-}Cu^{II}L]^{+}$ are with respect to **8** and a separated MeCN; All Gibbs free energy values of the [LCu--Br--MMA]‡ transition states are with respect to **TS1** and a separated MeCN. The geometry optimization of **TS3** was unsuccessful after multiple attempts. Constrained geometry optimization of **TS3** by fixing the forming/cleaving C-Br and Cu-Br bond distances suggested TS3, if it exists, should be higher in energy than **TS1**.

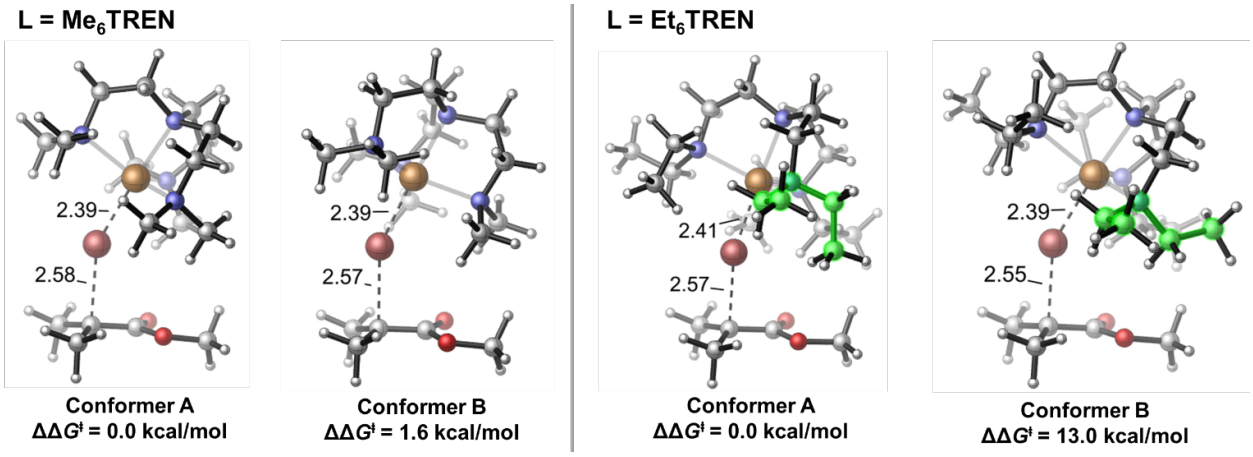
Conformational analysis of the ISET transition states

Multiple possible conformers of the ISET transition states have been considered in the geometry optimizations. The ISET transition state structures reported in the main manuscript are the lowest-energy conformers obtained from the DFT calculations.

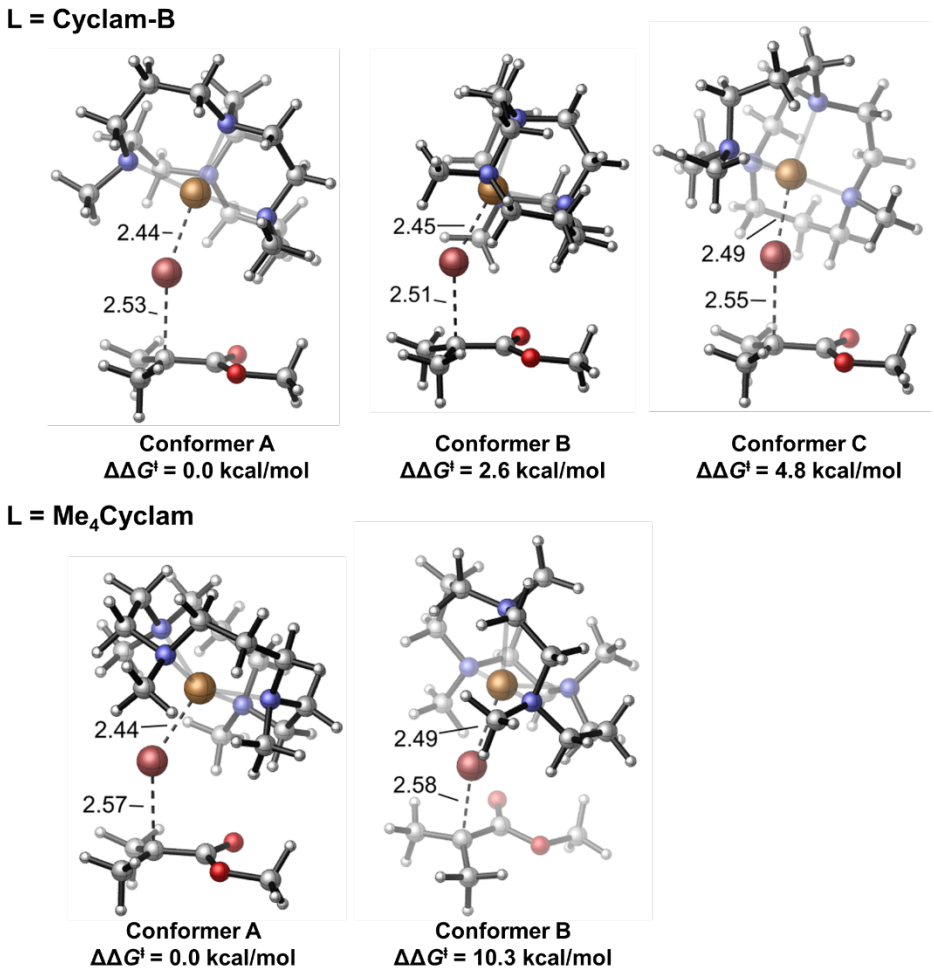
In the geometry optimizations of the ISET TS with TPMA family ligands, we have considered three different orientations through which the Cu(TPMA) catalyst approaches the MMA-Br. Only Conformer A can be successfully optimized to **TS1** in the main text, while the other two TS conformers cannot be located, which indicates these conformations are not stationary points on the potential energy surface, possibly due to weaker stabilizing through-space interactions between the catalyst and the MMA-Br. In addition, we have considered the partial dissociation of pyridine arms of TPMA ligand in the ISET TS (Figure S9). Taken together these calculations indicate the most stable TS conformer with the TPMA ligand is Conformer A.



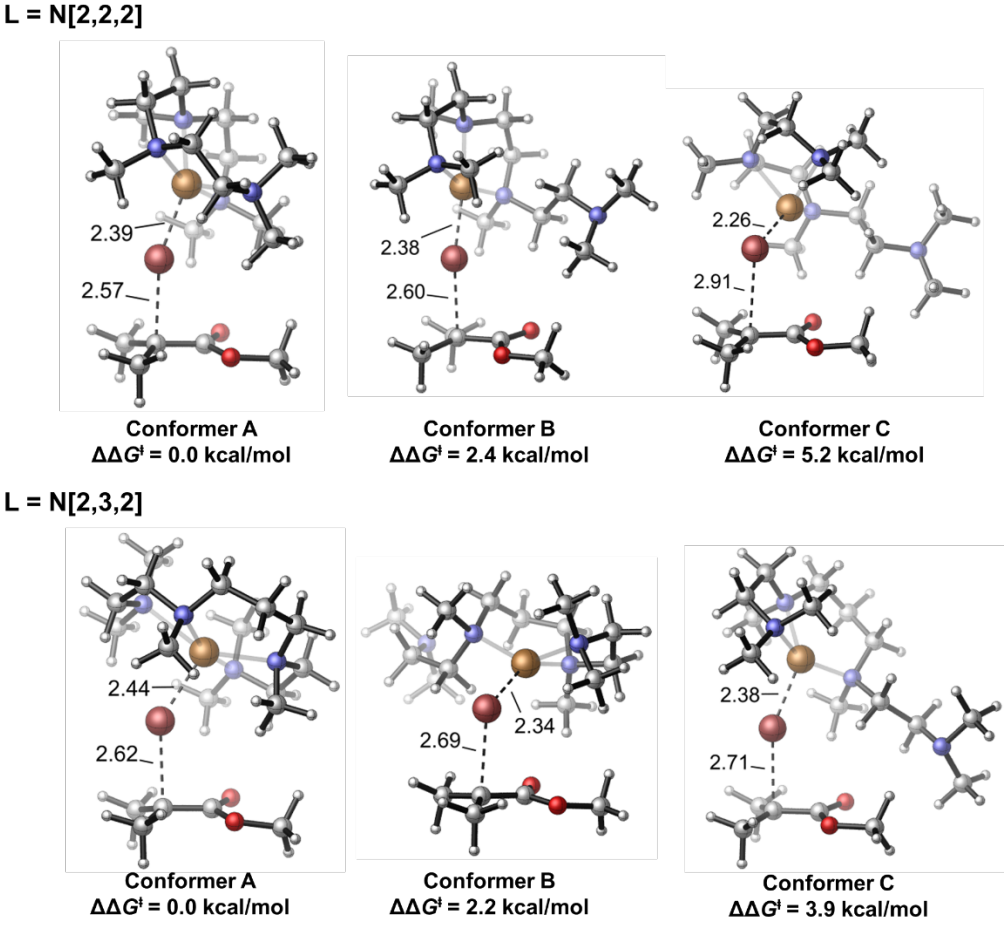
In the geometry optimizations of the ISET TS with the Me_6TREN ligand, two conformers have been located. Conformer A, in which the ester group of MMA-Br points towards the open region between the NMe_2 groups on the ligand, has a lower activation energy than Conformer B, in which the ester group points towards one of the NMe_2 arms. This is consistent with our hypothesis that minimizing the ligand-initiator steric repulsions stabilizes the transition state. For the transition state with the Et_6TREN ligand, two conformers have been located involving different conformations of the *N*-ethyl groups on the ligands (see the highlighted atoms in the TS structures shown below). In Conformer A, one of the *N*-ethyl groups is synclinal with respect to the ethylene group on the ligand backbone (defined as "equatorial") and the other *N*-ethyl is *anti*-periplanar (defined as "axial"). In Conformer B, both *N*-ethyl groups are synclinal ("equatorial"). Conformer A of the ISET TS with Et_6TREN has a much lower free energy than Conformer B. Here, conformer B is destabilized due to significant repulsions between the equatorial *N*-ethyl groups. We attempted to locate another TS conformer in which both N-ethyl groups are "axial". However, such TS structure cannot be located due to steric repulsions with the initiator.



In the geometry optimizations of the ISET TS with the more rigid Cyclam-B ligand, different orientations through which the Cu catalyst approaches the initiator were considered. The most favored conformer (Conformer A) was presented in the main text. Regarding more flexible Me4Cyclam ligand, two types of catalyst coordination geometries were calculated. The square planar conformer (Conformer A), which has a much lower activation energy than the see-saw conformer (Conformer B), was thereby reported in the main manuscript.



In the ISET TS calculations with acyclic Cyclam family ligands (*i.e*. N[2,2,2] and N[2,3,2]), we have located the tetradentate TS (Conformer A) as well as transition states involving ligand partial dissociation (Conformer B and C). With both ligands, the tetradentate transition state was favored, and thereby reported in the main manuscript.



Additional statistical tests of the training set and test set data

In the main manuscript, we have shown that the $\Delta G^{\ddagger}_{predicted}$ values calculated from equation 4 are typically within ± 2 kcal/mol of the experimentally derived activation free energies. In order to further validate equation 4, we performed additional statistical tests (Figure S10).

First, the training set data ($\Delta G^{\ddagger}_{predicted}$) are shown to have a good linear relationship with the experimentally derived $\Delta G^{\ddagger}_{exp}$ values, with the regression slope equals to 1, and the R^2 equals to 0.897. The $\Delta G^{\ddagger}_{predicted}$ values also demonstrated a satisfactory external predictivity on the test set with the regression slope of 0.78 and the R^2 equals to 0.756.

In addition, we have calculated the leave-one-out cross-validation Q^2 (Q^2_{LOOCV}) for the training set (Figure S10a). The Q^2_{LOOCV} (0.367) for the training set is relatively low, which is likely due to the small number of training set data points (only 9 compounds were included). Because of the relatively small number of available experimental k_{act} values, having a larger training set would require us to reduce the data points in the test set, which would make the validation of test set less meaningful. In Figure S11, we included all 18 ligands in the training set to generate the predictive equation (eq. 6). In this case, the Q^2_{LOOCV} is significantly improved due to the large training set while the R^2 value remained the same as the R^2 derived from the smaller training set as shown in Figure S10a. However, to validate the performance of eq. 6, an additional external test set would be required.

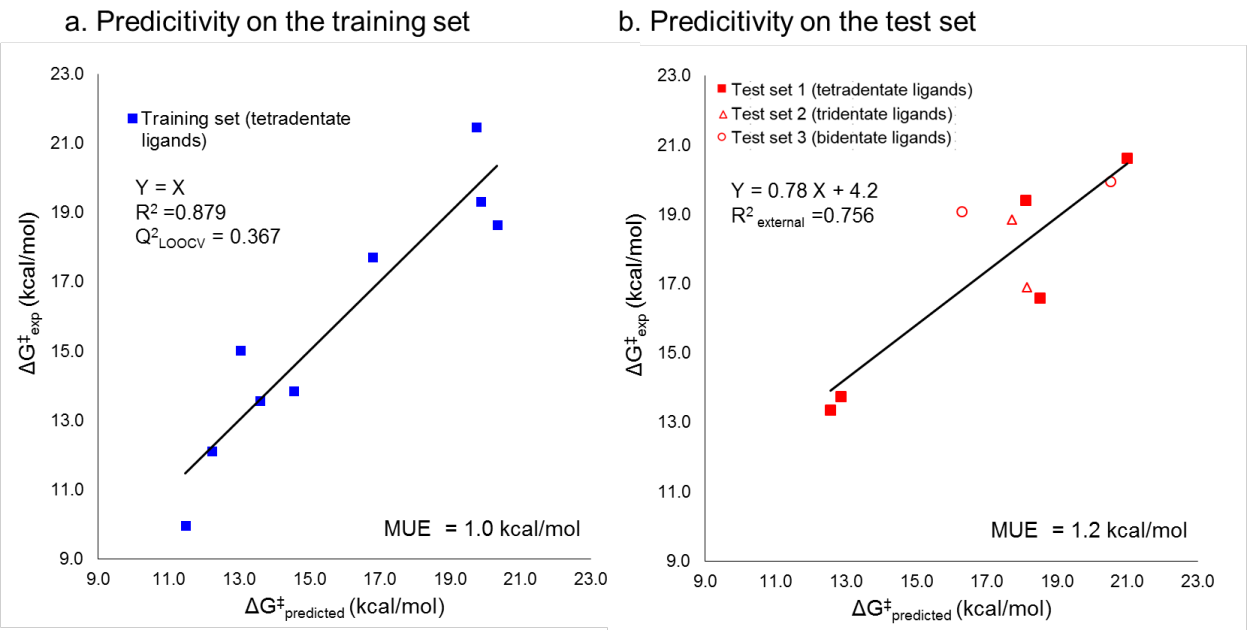


Figure S10. Statistical tests of the training set and test set data.

$$\Delta G^{\ddagger}_{predicted} = -6.28 \times HOMO + 0.47 \times V_{bur}\% + 0.42 \times E_{dist} - 54.2 \quad \text{(eq. 6)}$$

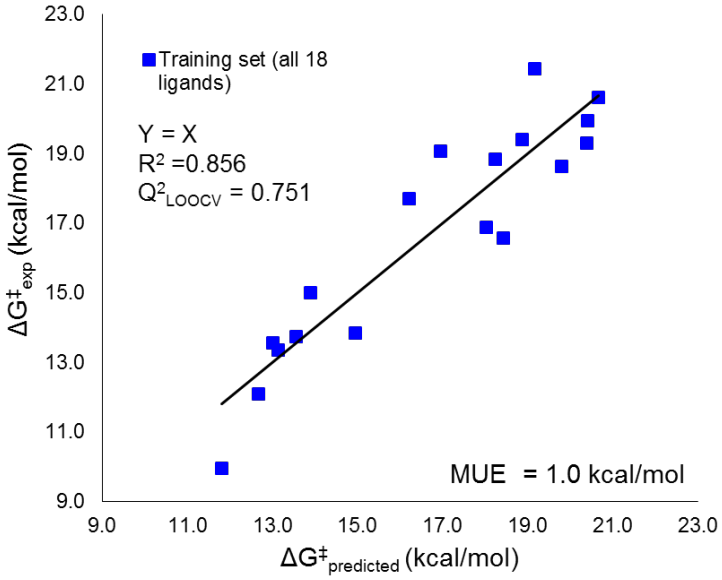


Figure S11. Predictive equation for ligand effect derived using all 18 ligands in the training set.

Calculated parameters used in the initiator-effect predictive model

Table S5. Calculated bond dissociation energy (*BDE*) and halogenophilicity (*E*(Cu, X•)) parameters for all 8 initiators[a]

Initiators	$\Delta G^{\ddagger}_{exp}$	$\Delta G^{\ddagger}_{predicted}$	**BDE(R-X)**	***E*(Cu, X•)**
MAc-Br	17.1	16.5	53.3	-46.2
MA-Br	14.3	13.9	48.7	-46.2
MMA-Br	12.5	12.3	45.8	-46.2
MeCN-Br	12.8	13.9	48.8	-46.2
MeCN-Cl	15.3	16.0	60.3	-57.4
AN-Cl	14.7	14.5	57.6	-57.4
MAc-Cl	19.2	19.5	66.6	-57.4
MA-Cl	17.3	16.3	60.9	-57.4

[a] All parameters, as well as experimental and predicted free energies are in kcal/mol

Cartesian coordinates (Å) and energies of optimized structures

1

ω-B97XD SCF energy: -1112.68419249 a.u.
ω-B97XD enthalpy: -1112.326379 a.u.
ω-B97XD free energy: -1112.394664 a.u.
ω-B97XD SCF energy in solution: -2556.28428343 a.u.
ω-B97XD enthalpy in solution: -2555.926470 a.u.
ω-B97XD free energy in solution: -2555.994755 a.u.

Cartesian coordinates

ATOM	X	Y	Z
Cu	-0.002239	-0.000565	-0.892664
N	1.129606	-1.690213	-0.580295
N	0.904061	1.820955	-0.579485
N	-2.031612	-0.125967	-0.581124
N	-0.002224	-0.000200	1.358364
C	2.372504	-4.048520	0.210490
C	1.468705	-1.881104	0.709180
C	-3.005135	0.119278	-1.468755
H	-2.686183	0.280497	-2.493170
C	2.081925	-3.052958	1.137286
C	2.032880	-3.843950	-1.121267
C	-3.688647	-0.279524	1.134762
C	1.408144	-2.654072	-1.468605
H	1.115218	-2.456028	-2.494327
C	-2.366847	-0.330420	0.707325
C	-4.348263	0.170885	-1.121981
C	-1.248446	-0.679604	1.677296
H	-1.580509	-0.489715	2.709607
H	-1.065202	-1.757990	1.596488
C	1.208295	-0.740002	1.680998
H	1.205233	-1.125917	2.712059
H	2.050306	-0.040943	1.607040
C	0.895816	2.212324	0.709240
C	1.604419	3.328884	1.137194
C	0.032317	1.418705	1.678151
H	0.361825	1.610781	2.710895
H	-0.992807	1.800326	1.597008
C	1.605601	2.539805	-1.466405
H	1.584144	2.183201	-2.490969
C	2.327020	4.074769	0.211777
C	2.325920	3.674412	-1.118944
C	-4.695603	-0.029961	0.208424
H	2.852283	-4.969289	0.525614
H	2.236941	-4.590714	-1.879823
H	2.328612	-3.181451	2.186338
H	-5.096752	0.371242	-1.879792
H	-5.733318	0.012032	0.522871
H	-3.923030	-0.437502	2.182602
H	2.875431	4.220876	-1.876721
H	2.883941	4.951041	0.527015
H	1.586339	3.610228	2.185288

2

ω-B97XD SCF energy: -2917.73423843 a.u.
ω-B97XD enthalpy: -2917.584355 a.u.
ω-B97XD free energy: -2917.630456 a.u.
ω-B97XD SCF energy in solution: -2920.66507167 a.u.
ω-B97XD enthalpy in solution: -2920.515188 a.u.
ω-B97XD free energy in solution: -2920.561289 a.u.

Cartesian coordinates

ATOM	X	Y	Z
H	3.332094	-1.655252	0.887712
C	3.006567	-0.944185	0.129506
O	1.721402	-0.491854	0.554735
C	1.122955	0.377984	-0.263318
C	-0.272206	0.767701	0.231997
C	-0.308438	1.004991	1.737556
H	0.032569	0.128525	2.289867
H	-1.326204	1.252101	2.051213
H	0.345177	1.850666	1.984119
C	-0.802904	1.952541	-0.559517
H	-1.833785	2.167349	-0.266632
H	-0.184920	2.832187	-0.347080
H	-0.763572	1.761247	-1.632675
Br	-1.414833	-0.809973	-0.175256
O	1.628959	0.816193	-1.267826
H	2.933459	-1.429720	-0.846518
H	3.705590	-0.106958	0.061348

3

ω-B97XD SCF energy: -4030.44790246 a.u.
ω-B97XD enthalpy: -4029.937794 a.u.
ω-B97XD free energy: -4030.034174 a.u.
ω-B97XD SCF energy in solution: -5476.96468633 a.u.
ω-B97XD enthalpy in solution: -5476.454578 a.u.
ω-B97XD free energy in solution: -5476.550958 a.u.

Cartesian coordinates

ATOM	X	Y	Z
Cu	-0.536652	0.067737	-0.218304
N	-0.089763	-1.872365	0.449901
N	-0.488905	1.716992	1.062044
N	-2.194461	0.107800	-1.511347
N	-2.306197	-0.406955	1.241687
C	0.313103	-4.435363	1.449831
C	-0.749326	-2.285785	1.545004
C	-2.220938	0.674001	-2.724596
H	-1.269867	1.036006	-3.103373
C	-0.571630	-3.560644	2.071774
C	0.980375	-4.011865	0.305819
C	-4.553923	-0.242237	-1.674154
C	0.743891	-2.724818	-0.157797
H	1.238743	-2.343180	-1.044311
C	-3.347406	-0.349798	-0.991043
C	-3.381212	0.808742	-3.475089

C	-3.279813	-1.032452	0.364775
H	-4.287207	-1.072708	0.808970
H	-2.965438	-2.070243	0.201731
C	-1.682339	-1.288456	2.208785
H	-2.413509	-1.827188	2.833606
H	-1.086919	-0.662670	2.885991
C	-1.500339	1.820047	1.943534
C	-1.503213	2.780108	2.948550
C	-2.689248	0.892765	1.758338
H	-3.255984	0.823526	2.700632
H	-3.357426	1.358093	1.023475
C	0.521615	2.591890	1.144868
H	1.312804	2.476848	0.413977
C	-0.445119	3.679378	3.035627
C	0.585874	3.587853	2.109900
C	-4.573528	0.341028	-2.936409
C	3.473046	0.374463	-1.167252
C	4.188575	1.655247	-1.558040
H	5.202040	1.629004	-1.142488
H	4.260746	1.735755	-2.645173
H	3.684994	2.536802	-1.159823
C	3.242550	0.317206	0.345431
O	3.308235	1.283288	1.067109
O	2.956157	-0.912870	0.766151
C	2.616673	-1.028468	2.151419
H	3.454834	-0.713898	2.776371
H	1.742961	-0.409136	2.370871
H	2.390974	-2.082859	2.307397
H	-5.505550	0.434329	-3.484241
H	-5.466693	-0.613297	-1.218961
H	-3.343869	1.276554	-4.452114
H	-1.124486	-3.862613	2.955719
H	0.467174	-5.434089	1.845526
H	1.665723	-4.662714	-0.224964
H	-2.328985	2.822704	3.651820
H	-0.429097	4.435904	3.813345
H	1.434051	4.262029	2.132509
Br	1.605615	0.473215	-1.927936
C	4.136715	-0.871987	-1.731694
H	4.231180	-0.790630	-2.817306
H	5.142901	-0.956099	-1.304817
H	3.586142	-1.779897	-1.483362

4

ω-B97XD SCF energy: -1112.33138298 a.u.
ω-B97XD enthalpy: -1111.972205 a.u.
ω-B97XD free energy: -1112.039393 a.u.
ω-B97XD SCF energy in solution: -2556.09258788 a.u.
ω-B97XD enthalpy in solution: -2555.733410 a.u.
ω-B97XD free energy in solution: -2555.800598 a.u.

Cartesian coordinates

ATOM	X	Y	Z
Cu	-0.002760	-0.000981	-0.733844

N	-2.028289	-0.141237	-0.574687
N	1.135152	-1.682555	-0.571726
N	0.894843	1.820800	-0.573253
N	-0.003441	0.000822	1.242862
C	-4.695437	-0.250064	0.156411
C	-2.372489	-0.427276	0.698958
C	1.586214	2.531645	-1.478195
H	1.633616	2.125262	-2.482948
C	-3.697018	-0.480801	1.101599
C	-4.337267	0.039475	-1.156118
C	1.425266	3.441835	1.099905
C	-2.990037	0.092827	-1.481695
H	-2.662791	0.327035	-2.489173
C	0.811623	2.266474	0.698309
C	2.213639	3.725080	-1.153114
C	-0.038651	1.432887	1.633053
H	0.280769	1.545446	2.675320
H	-1.079577	1.768216	1.567188
C	-1.226134	-0.744429	1.634783
H	-1.482055	-0.521980	2.676925
H	-0.995431	-1.813418	1.570026
C	1.557454	-1.834077	0.701460
C	2.270827	-2.951324	1.104741
C	1.252930	-0.684711	1.638412
H	1.182632	-1.022008	2.678705
H	2.062121	0.051622	1.581684
C	1.413932	-2.633577	-1.477353
H	1.043338	-2.471377	-2.483952
C	2.570717	-3.932593	0.160926
C	2.137441	-3.770878	-1.150767
C	2.131790	4.186606	0.156530
H	-3.947447	-0.703807	2.133407
H	2.616369	5.113403	0.445221
H	1.349423	3.776286	2.129268
H	2.757592	4.273594	-1.913192
H	-5.740439	-0.291399	0.445424
H	-5.084763	0.228443	-1.917591
H	3.131327	-4.815093	0.450846
H	2.347093	-4.514101	-1.911110
H	2.591616	-3.055074	2.135996

5

ω-B97XD SCF energy: -2917.76332737 a.u.
ω-B97XD enthalpy: -2917.615688 a.u.
ω-B97XD free energy: -2917.665583 a.u.
ω-B97XD SCF energy in solution: -2920.79565183 a.u.
ω-B97XD enthalpy in solution: -2920.648012 a.u.
ω-B97XD free energy in solution: -2920.697907 a.u.

Cartesian coordinates

ATOM	X	Y	Z
H	0.857485	-3.109825	1.140972
C	0.906885	-2.474705	0.253216
O	1.349528	-1.205881	0.707857

C	1.499131	-0.283623	-0.277025
C	1.359589	1.076697	0.207960
C	0.974162	1.349966	1.621739
H	1.489690	0.690494	2.326112
H	-0.107691	1.154120	1.706761
H	1.169639	2.395602	1.889271
C	1.236908	2.153180	-0.813327
H	0.164309	2.289846	-1.022893
H	1.642388	3.106865	-0.450578
H	1.727153	1.867202	-1.747107
Br	-1.974057	0.009278	-0.095196
O	1.747880	-0.593136	-1.433007
H	-0.090733	-2.356651	-0.185099
H	1.600437	-2.899334	-0.479754

6

ω-B97XD SCF energy: -4030.39715777 a.u.
ω-B97XD enthalpy: -4029.886635 a.u.
ω-B97XD free energy: -4029.977690 a.u.
ω-B97XD SCF energy in solution: -5476.91495763 a.u.
ω-B97XD enthalpy in solution: -5476.404435 a.u.
ω-B97XD free energy in solution: -5476.495490 a.u.

Cartesian coordinates

ATOM	X	Y	Z
Cu	-0.027099	-0.238821	-0.470573
N	-1.713671	1.097712	-0.316948
N	1.562730	-1.097940	0.751635
N	1.528641	1.333613	-0.686290
N	0.052371	1.037055	1.757172
C	-3.881454	2.824104	-0.297431
C	-2.114128	1.658005	0.833668
C	2.399977	1.300905	-1.703398
H	2.131480	0.654688	-2.530287
C	-3.198187	2.528294	0.877101
C	-3.444130	2.259013	-1.490144
C	2.988147	2.862853	0.436791
C	-2.352358	1.403444	-1.452669
H	-1.957551	0.939278	-2.353187
C	1.814847	2.120577	0.364499
C	3.582792	2.028310	-1.716659
C	0.767770	2.266249	1.438368
H	1.219154	2.708152	2.340459
H	0.039478	2.996155	1.065821
C	-1.331825	1.314188	2.089152
H	-1.441081	2.136383	2.814881
H	-1.753523	0.424431	2.561095
C	1.825688	-0.657944	1.988231
C	3.015147	-0.976977	2.636325
C	0.762859	0.170023	2.682366
H	0.045470	-0.526488	3.123570
H	1.225292	0.736059	3.506415
C	2.475877	-1.844182	0.117494
H	2.221335	-2.138409	-0.897469

C	3.953420	-1.769921	1.987317
C	3.681234	-2.211036	0.696655
C	3.891718	2.817470	-0.618233
C	-1.391962	-1.986869	-0.349235
C	-0.506621	-3.202562	-0.278057
H	-1.177308	-4.062689	-0.124854
H	0.025316	-3.360201	-1.216159
H	0.180989	-3.172297	0.564286
C	-1.971670	-1.663385	1.022080
O	-1.396699	-1.879239	2.066727
O	-3.226347	-1.223336	0.936866
C	-3.981758	-1.108916	2.147828
H	-3.649887	-1.847543	2.878474
H	-3.870051	-0.101891	2.557938
H	-5.020689	-1.274480	1.866570
H	4.814442	3.387481	-0.580772
H	3.184371	3.473403	1.312253
H	4.244699	1.959523	-2.572318
H	-3.491765	2.977233	1.821017
H	-4.729428	3.501239	-0.283726
H	-3.929092	2.477806	-2.434391
H	3.199292	-0.601757	3.637990
H	4.886973	-2.028441	2.476532
H	4.386863	-2.818634	0.141945
Br	0.223357	-0.959272	-2.724847
C	-2.433553	-2.042539	-1.438105
H	-2.014815	-2.414227	-2.369841
H	-3.207314	-2.742699	-1.091716
H	-2.931357	-1.088864	-1.609686

7

ω-B97XD SCF energy: -346.25376766 a.u.
ω-B97XD enthalpy: -346.108971 a.u.
ω-B97XD free energy: -346.153223 a.u.
ω-B97XD SCF energy in solution: -346.39915864 a.u.
ω-B97XD enthalpy in solution: -346.254362 a.u.
ω-B97XD free energy in solution: -346.298614 a.u.

Cartesian coordinates

ATOM	X	Y	Z
C	-1.086184	0.118456	0.002126
C	-2.175071	-0.898676	0.001285
H	-1.769824	-1.906590	-0.101450
H	-2.753038	-0.846135	0.935587
H	-2.886044	-0.708056	-0.814253
C	-1.444345	1.566524	-0.000449
H	-2.168542	1.784498	0.796265
H	-0.572897	2.209281	0.126949
H	-1.937311	1.836127	-0.946250
C	0.291077	-0.349508	-0.001081
O	1.194707	0.658425	0.000896
C	2.555328	0.245656	0.002213
H	2.781568	-0.351371	-0.885590
H	3.141726	1.164863	0.001947

H	2.780202	-0.349821	0.891475
O	0.622709	-1.524363	-0.004552

8

ω-B97XD SCF energy: -3684.15505854 a.u.
ω-B97XD enthalpy: -3683.793078 a.u.
ω-B97XD free energy: -3683.865894 a.u.
ω-B97XD SCF energy in solution: -5130.54723540 a.u.
ω-B97XD enthalpy in solution: -5130.185255 a.u.
ω-B97XD free energy in solution: -5130.258071 a.u.

Cartesian coordinates

ATOM	X	Y	Z
Br	-0.005606	0.004518	2.753525
Cu	-0.002430	0.001335	0.411449
N	-2.063885	0.216745	0.026755
N	1.221248	1.673718	0.026373
N	0.845848	-1.890680	0.032042
N	-0.002166	-0.002078	-1.705766
C	-4.700343	0.390285	-0.785311
C	-2.359066	0.509936	-1.249018
C	1.520482	-2.641115	0.909904
H	1.561801	-2.251676	1.922542
C	-3.668624	0.597118	-1.698371
C	-4.389157	0.098794	0.537698
C	1.312295	-3.476321	-1.689446
C	-3.051985	0.016223	0.905545
H	-2.737283	-0.207398	1.920190
C	0.733754	-2.297777	-1.241647
C	2.119926	-3.839374	0.542701
C	-0.111383	-1.410724	-2.127094
H	0.156535	-1.529775	-3.185320
H	-1.160787	-1.707134	-2.018456
C	-1.166565	0.794688	-2.133071
H	-1.399949	0.616734	-3.191220
H	-0.900306	1.852518	-2.027808
C	1.624743	1.780165	-1.249135
C	2.358785	2.868131	-1.698251
C	1.270537	0.606491	-2.133782
H	1.232421	0.899270	-3.191549
H	2.051884	-0.155237	-2.032007
C	1.543647	2.629495	0.904709
H	1.189826	2.471303	1.918794
C	2.697304	3.865186	-0.785981
C	2.287337	3.743682	0.536618
C	2.015780	-4.260787	-0.777996
H	-3.877687	0.825845	-2.738269
H	2.478205	-5.188294	-1.099338
H	1.211618	-3.776824	-2.727235
H	2.658804	-4.422275	1.280447
H	-5.734603	0.455826	-1.107153
H	-5.163816	-0.066809	1.277227
H	3.272469	4.727094	-1.108181
H	2.532221	4.497680	1.275410

H 2.663201 2.933775 -2.737722

Br^-

ω-B97XD SCF energy: -2571.49038592 a.u.
ω-B97XD enthalpy: -2571.488025 a.u.
ω-B97XD free energy: -2571.506561 a.u.
ω-B97XD SCF energy in solution: -2574.39923339 a.u.
ω-B97XD enthalpy in solution: -2574.396872 a.u.
ω-B97XD free energy in solution: -2574.415408 a.u.

Cartesian coordinates

ATOM	X	Y	Z
Br	0.000000	0.000000	0.000000

$Br^•$

ω-B97XD SCF energy: -2571.38275084 a.u.
ω-B97XD enthalpy: -2571.380390 a.u.
ω-B97XD free energy: -2571.399581 a.u.
ω-B97XD SCF energy in solution: -2574.17283507 a.u.
ω-B97XD enthalpy in solution: -2574.170474 a.u.
ω-B97XD free energy in solution: -2574.189665 a.u.

Cartesian coordinates

ATOM	X	Y	Z
Br	0.000000	0.000000	0.000000

$Cl^•$

ω-B97XD SCF energy: -460.11348646 a.u.
ω-B97XD enthalpy: -460.111126 a.u.
ω-B97XD free energy: -460.129164 a.u.
ω-B97XD SCF energy in solution: -460.14754002 a.u.
ω-B97XD enthalpy in solution: -460.145180 a.u.
ω-B97XD free energy in solution: -460.163218 a.u.

Cartesian coordinates

ATOM	X	Y	Z
Cl	0.000000	0.000000	0.000000

TS1

ω-B97XD SCF energy: -4030.41632720 a.u.
ω-B97XD enthalpy: -4029.908392 a.u.
ω-B97XD free energy: -4030.003189 a.u.
ω-B97XD SCF energy in solution: -5476.93974467 a.u.
ω-B97XD enthalpy in solution: -5476.431809 a.u.
ω-B97XD free energy in solution: -5476.526606 a.u.
Imaginary frequency: -588.8508 cm-1

Cartesian coordinates

ATOM	X	Y	Z
Cu	-0.692884	0.214679	-0.037061
N	-0.114340	-1.242821	-1.510094
N	-0.426064	-0.601505	1.913723
N	-2.278428	1.473079	-0.419814
N	-2.356279	-1.230140	0.081428
C	0.300449	-3.164206	-3.461800
C	-0.863084	-2.354834	-1.531905
C	-2.249272	2.810129	-0.346744
H	-1.275189	3.252464	-0.167246
C	-0.690849	-3.336516	-2.500364
C	1.084234	-2.016290	-3.425933
C	-4.635386	1.558044	-0.789168
C	0.839429	-1.076897	-2.432571
H	1.420157	-0.163823	-2.344680
C	-3.449242	0.851194	-0.643530
C	-3.391113	3.585979	-0.493632
C	-3.391385	-0.656183	-0.779628
H	-4.379366	-1.099388	-0.586562
H	-3.127472	-0.893870	-1.817180
C	-1.858488	-2.519808	-0.400540
H	-2.679013	-3.187003	-0.701844
H	-1.340381	-3.006812	0.433683
C	-1.483902	-1.290429	2.372169
C	-1.447419	-1.974951	3.578603
C	-2.723349	-1.250795	1.501071
H	-3.392949	-2.090090	1.739169
H	-3.272811	-0.326260	1.714226
C	0.699268	-0.571427	2.634331
H	1.531628	-0.018983	2.208413
C	-0.277777	-1.937663	4.335470
C	0.814714	-1.227550	3.854761
C	-4.605384	2.947782	-0.715881
C	3.777150	1.669936	-0.037783
C	4.020275	2.610599	1.096711
H	5.104036	2.708077	1.260188
H	3.631789	3.607104	0.869803
H	3.576612	2.242510	2.022862
C	3.745779	0.230408	0.302383
O	3.687925	-0.204225	1.437955
O	3.747317	-0.562933	-0.782480
C	3.605706	-1.955789	-0.513294
H	4.397329	-2.304709	0.153186
H	2.633649	-2.153035	-0.050706
H	3.672524	-2.451105	-1.481606
H	-5.520201	3.520620	-0.827197
H	-5.567335	1.028600	-0.958347
H	-3.321820	4.665437	-0.426571
H	-1.318985	-4.221764	-2.498663
H	0.455101	-3.916324	-4.228773
H	1.866521	-1.842263	-4.155916
H	-2.316633	-2.528286	3.919497
H	-0.222346	-2.464659	5.282551
H	1.750328	-1.182442	4.399806
Br	1.192002	1.670478	-0.165243
C	4.147885	2.103616	-1.419986

H	3.818905	3.130021	-1.603818
H	5.243095	2.084513	-1.524937
H	3.731746	1.446729	-2.184829

TS2

ω-B97XD SCF energy: -4030.39443125 a.u.
ω-B97XD enthalpy: -4029.885757 a.u.
ω-B97XD free energy: -4029.976686 a.u.
ω-B97XD SCF energy in solution: -5476.90954087 a.u.
ω-B97XD enthalpy in solution: -5476.400867 a.u.
ω-B97XD free energy in solution: -5476.491796 a.u.
Imaginary frequency: -67.3445 cm-1

Cartesian coordinates

ATOM	X	Y	Z
Cu	0.061035	-0.286758	0.321839
N	1.748168	1.104087	0.432445
N	-1.664772	-0.907722	-1.005156
N	-1.536588	1.028613	1.138034
N	-0.274266	1.512219	-1.387603
C	3.688283	3.049019	0.815835
C	1.923763	2.068350	-0.482100
C	-2.285352	0.637674	2.174014
H	-1.878391	-0.176730	2.765112
C	2.882934	3.063368	-0.318289
C	3.500844	2.047028	1.761472
C	-3.217252	2.634543	0.584567
C	2.513615	1.098678	1.529506
H	2.308436	0.304285	2.242510
C	-1.987723	2.024487	0.362186
C	-3.513466	1.209673	2.480777
C	-1.060161	2.541692	-0.712038
H	-1.629174	3.146369	-1.435504
H	-0.362842	3.226298	-0.214785
C	1.053215	2.003155	-1.722418
H	1.031159	2.990874	-2.209432
H	1.504414	1.302163	-2.430186
C	-2.026974	-0.097419	-2.007923
C	-3.286177	-0.169858	-2.593921
C	-0.979345	0.880024	-2.495929
H	-0.248198	0.314804	-3.080160
H	-1.445677	1.620891	-3.165085
C	-2.547312	-1.801879	-0.548324
H	-2.210220	-2.413752	0.284777
C	-4.196641	-1.112144	-2.127518
C	-3.821903	-1.946120	-1.080432
C	-3.994847	2.221837	1.660697
C	1.571848	-2.271015	-0.241888
C	0.594745	-3.242733	-0.815558
H	1.187457	-3.945529	-1.423966
H	0.093858	-3.812525	-0.032686
H	-0.124763	-2.764376	-1.477081
C	2.121288	-1.301624	-1.272489
O	1.533571	-0.998386	-2.289767

O	3.373658	-0.956338	-0.993289
C	4.084967	-0.196039	-1.976031
H	3.842806	-0.546886	-2.980485
H	3.832880	0.861736	-1.874579
H	5.140034	-0.347540	-1.754630
H	-4.957626	2.684275	1.853053
H	-3.555398	3.426369	-0.076218
H	-4.076308	0.855296	3.336748
H	2.991296	3.838868	-1.070337
H	4.442246	3.815638	0.963343
H	4.095026	2.003634	2.667076
H	-3.547937	0.506588	-3.401416
H	-5.184428	-1.188317	-2.570584
H	-4.500815	-2.688818	-0.676991
Br	0.114573	-1.784465	2.103692
C	2.594822	-2.817606	0.706079
H	2.165881	-3.553700	1.383076
H	3.356363	-3.309341	0.081050
H	3.105193	-2.039450	1.273601

TS1'

ω-B97XD SCF energy: -4030.41217158 a.u.
ω-B97XD enthalpy: -4029.905243 a.u.
ω-B97XD free energy: -4029.999593 a.u.
ω-B97XD SCF energy in solution: -5476.96468633 a.u.
ω-B97XD enthalpy in solution: -5476.457758 a.u.
ω-B97XD free energy in solution: -5476.552108 a.u.
Imaginary frequency: -470.0835 cm-1

Cartesian coordinates

ATOM	X	Y	Z
Cu	-0.741694	0.035064	-0.034113
N	-0.864436	-1.427057	-1.538298
N	-0.777574	-0.650792	1.955071
N	-1.691484	1.873145	-0.392278
N	-2.848621	-0.556815	0.146843
C	-1.359259	-3.271692	-3.544478
C	-1.997424	-2.147617	-1.528790
C	-1.114384	3.077978	-0.330199
H	-0.038739	3.074044	-0.181691
C	-2.283860	-3.074607	-2.522807
C	-0.182748	-2.531638	-3.542844
C	-3.816330	2.919054	-0.690826
C	0.023589	-1.614226	-2.520867
H	0.920815	-1.005354	-2.463658
C	-3.019272	1.787675	-0.574556
C	-1.840241	4.256186	-0.448107
C	-3.586140	0.387638	-0.695749
H	-4.662762	0.384360	-0.471315
H	-3.471083	0.061072	-1.736080
C	-2.913840	-1.936374	-0.340298
H	-3.943280	-2.235219	-0.586101
H	-2.573087	-2.590088	0.471264
C	-2.008433	-0.882017	2.440113

C	-2.208138	-1.450023	3.691393
C	-3.166210	-0.431237	1.571794
H	-4.084255	-0.975962	1.835922
H	-3.350988	0.630051	1.775613
C	0.290059	-0.959334	2.700696
H	1.256980	-0.740457	2.257121
C	-1.098387	-1.771801	4.468225
C	0.172619	-1.519346	3.966526
C	-3.215840	4.173429	-0.629493
C	4.050506	1.318151	-0.381908
C	4.050899	2.570967	0.430759
H	5.055603	3.018893	0.399936
H	3.352297	3.305932	0.020246
H	3.809307	2.366682	1.474729
C	4.495700	0.089102	0.322724
O	4.597323	-0.006190	1.528781
O	4.767792	-0.915794	-0.525088
C	5.182748	-2.132679	0.092235
H	6.108780	-1.982170	0.652248
H	4.410592	-2.498382	0.774128
H	5.340643	-2.838432	-0.722541
H	-3.816446	5.072913	-0.717637
H	-4.887950	2.818368	-0.828958
H	-1.334324	5.212922	-0.390700
H	-3.213141	-3.634488	-2.494346
H	-1.558466	-3.992805	-4.330536
H	0.563612	-2.654008	-4.319222
H	-3.214885	-1.632719	4.053221
H	-1.227991	-2.216308	5.449653
H	1.064214	-1.752419	4.537094
Br	1.560569	0.640234	-0.182209
C	4.203014	1.424983	-1.864757
H	3.570248	2.224124	-2.261250
H	5.247150	1.678314	-2.102398
H	3.968458	0.487150	-2.369754

AN•

ω-B97XD SCF energy: -171.347368271 a.u.
ω-B97XD enthalpy: -171.280649 a.u.
ω-B97XD free energy: -171.314276 a.u.
ω-B97XD SCF energy in solution: -171.422249303 a.u.
ω-B97XD enthalpy in solution: -171.35553 a.u.
ω-B97XD free energy in solution: -171.389157 a.u.

Cartesian coordinates

ATOM	X	Y	Z
C	-0.12463	1.0425	1.1824
N	-0.602	1.42154	2.18213
C	0.45228	0.5858	-0.00011
H	0.01653	0.93089	-0.93174
C	1.66028	-0.36936	-0.00007
H	2.25264	-0.19521	0.87382
H	1.31436	-1.3819	-0.00051
H	2.25317	-0.19462	-0.87348

AN-Cl

ω-B97XD SCF energy: -631.57218586 a.u.
ω-B97XD enthalpy: -631.499457 a.u.
ω-B97XD free energy: -631.535076 a.u.
ω-B97XD SCF energy in solution: -631.68125724 a.u.
ω-B97XD enthalpy in solution: -631.608528 a.u.
ω-B97XD free energy in solution: -631.644147 a.u.

Cartesian coordinates

ATOM	X	Y	Z
C	-1.290077	-0.287572	0.093909
N	-2.312996	-0.756143	-0.175188
C	-0.015935	0.348498	0.439912
H	0.055356	0.403571	1.528588
C	0.109664	1.737470	-0.179792
H	-0.708216	2.370973	0.177058
H	1.061439	2.185682	0.113895
H	0.062215	1.677960	-1.269431
Cl	1.346957	-0.713856	-0.085174

[AN--Cl—Cu(TPMA)]‡

ω-B97XD SCF energy: -1744.24041337 a.u.
ω-B97XD enthalpy: -1743.809826 a.u.
ω-B97XD free energy: -1743.895539 a.u.
ω-B97XD SCF energy in solution: -3187.94746346 a.u.
ω-B97XD enthalpy in solution: -3187.516876 a.u.
ω-B97XD free energy in solution: -3187.602589 a.u.
Imaginary frequency: -708.0729 cm-1

Cartesian coordinates

ATOM	X	Y	Z
Cu	-0.108666	0.142647	-0.129749
N	-1.239922	-1.047423	-1.437089
N	0.731498	-0.861648	1.530093
N	-0.715371	2.113497	0.158965
N	-1.892105	-0.190910	1.089858
C	-3.009553	-2.513113	-2.986245
C	-2.322391	-1.611463	-0.876652
C	0.033765	3.207047	-0.023248
H	1.010994	3.040273	-0.464392
C	-3.235516	-2.344908	-1.623630
C	-1.882491	-1.935961	-3.560131
C	-2.445130	3.470354	1.090598
C	-1.025012	-1.205891	-2.748156
H	-0.131393	-0.729693	-3.138926
C	-1.938942	2.237378	0.701662
C	-0.407081	4.476569	0.327143
C	-2.751311	0.963404	0.815430
H	-3.541771	1.075064	1.571734
H	-3.246164	0.787178	-0.146948
C	-2.459688	-1.458157	0.624729

H	-3.509733	-1.573187	0.930185
H	-1.895212	-2.268153	1.101481
C	-0.103330	-0.992910	2.574884
C	0.239952	-1.729672	3.699717
C	-1.417058	-0.244487	2.475370
H	-2.167391	-0.683939	3.148342
H	-1.251095	0.787263	2.806930
C	1.933145	-1.445752	1.577725
H	2.571968	-1.309904	0.711046
C	1.494272	-2.334136	3.751141
C	2.357986	-2.187848	2.673173
C	-1.667904	4.608904	0.896698
C	3.916995	0.138182	-2.221055
H	-2.042624	5.583695	1.191429
H	-3.431847	3.538181	1.537022
H	0.231527	5.336318	0.160885
H	-4.105836	-2.781317	-1.144261
H	-3.705491	-3.085993	-3.590340
H	-1.670205	-2.042519	-4.617585
H	-0.461096	-1.825785	4.522702
H	1.786847	-2.913003	4.621259
H	3.343603	-2.638426	2.661572
C	4.432063	-0.729864	-1.220012
N	4.781854	-1.451490	-0.376899
Cl	1.787626	0.435230	-1.378124
H	4.220541	1.176293	-2.123347
C	3.703556	-0.402993	-3.603150
H	3.109755	0.296345	-4.196145
H	4.672182	-0.537883	-4.102643
H	3.199666	-1.372368	-3.573799

MA•

ω-B97XD SCF energy: -306.943751866 a.u.
ω-B97XD enthalpy: -306.829076 a.u.
ω-B97XD free energy: -306.870943 a.u.
ω-B97XD SCF energy in solution: -307.076086882 a.u.
ω-B97XD enthalpy in solution: -306.961411 a.u.
ω-B97XD free energy in solution: -307.003278 a.u.

Cartesian coordinates

ATOM	X	Y	Z
C	1.20836	-0.67039	-0.00001
C	-0.02873	0.08555	0.0002
O	-1.11146	-0.72409	-0.00016
O	-0.10722	1.30225	0.00023
H	1.14377	-1.7538	-0.00014
C	-2.37111	-0.0472	-0.00018
H	-2.44646	0.56606	-0.87375
H	-3.1628	-0.76701	-0.00035
H	-2.44661	0.56582	0.87355
C	2.57544	0.03861	0.
H	3.35651	-0.69271	0.00196
H	2.66062	0.64909	-0.87462
H	2.65905	0.65208	0.87268

MA-Br

ω-B97XD SCF energy: -2878.42810527 a.u.
ω-B97XD enthalpy: -2878.307656 a.u.
ω-B97XD free energy: -2878.351521 a.u.
ω-B97XD SCF energy in solution: -2881.34710710 a.u.
ω-B97XD enthalpy in solution: -2881.226658 a.u.
ω-B97XD free energy in solution: -2881.270523 a.u.

Cartesian coordinates

ATOM	X	Y	Z
C	0.254875	0.706679	-0.583168
C	-1.104511	0.440732	0.044243
O	-1.750244	-0.530693	-0.606781
C	-3.019689	-0.893450	-0.062409
H	-3.694779	-0.034199	-0.057416
H	-3.402297	-1.678776	-0.713044
H	-2.902758	-1.263986	0.958834
O	-1.546490	1.037448	0.994924
H	0.207864	0.504784	-1.653109
Br	1.488544	-0.658011	0.120269
C	0.769787	2.097311	-0.273540
H	0.084785	2.839357	-0.698605
H	0.817850	2.257388	0.805355
H	1.761378	2.244161	-0.707344

[MA--Br--Cu(TPMA)]‡

ω-B97XD SCF energy: -3991.10539705 a.u.
ω-B97XD enthalpy: -3990.627647 a.u.
ω-B97XD free energy: -3990.720602 a.u.
ω-B97XD SCF energy in solution: -5437.61686040 a.u.
ω-B97XD enthalpy in solution: -5437.139110 a.u.
ω-B97XD free energy in solution: -5437.232065 a.u.
Imaginary frequency: -596.5536 cm-1

Cartesian coordinates

ATOM	X	Y	Z
Cu	0.616578	-0.182458	-0.112377
N	0.012109	1.715187	-0.912854
N	0.108054	-0.237201	1.950023
N	2.312113	-1.109943	-0.817294
N	2.131238	1.144856	0.742802
C	-0.398377	4.239073	-1.976898
C	0.684406	2.769540	-0.427758
C	2.380485	-2.354700	-1.307993
H	1.431922	-2.866319	-1.430183
C	0.514335	4.048642	-0.943277
C	-1.109017	3.146693	-2.460856
C	4.690806	-0.946314	-0.937959
C	-0.869147	1.897903	-1.902114
H	-1.398198	1.008548	-2.230976
C	3.445825	-0.408606	-0.641009

C	3.586834	-2.954360	-1.642205
C	3.282139	1.015482	-0.153879
H	4.209749	1.373457	0.315743
H	3.092777	1.653088	-1.025768
C	1.577695	2.501788	0.767289
H	2.369063	3.261391	0.839261
H	0.963856	2.593205	1.670537
C	1.063252	0.251180	2.758791
C	0.862532	0.403967	4.122915
C	2.373959	0.600559	2.084409
H	2.961292	1.291905	2.705722
H	2.965267	-0.315253	1.967739
C	-1.074456	-0.586205	2.466116
H	-1.818973	-0.952638	1.765345
C	-0.366642	0.031849	4.664721
C	-1.352102	-0.467624	3.823327
C	4.762572	-2.238695	-1.449663
C	-3.643719	-1.824460	-1.088941
C	-3.884814	-3.149578	-0.456480
H	-4.960815	-3.376602	-0.480195
H	-3.367091	-3.947958	-0.993763
H	-3.572043	-3.145941	0.590221
C	-3.859631	-0.605707	-0.298470
O	-3.943842	-0.572008	0.915485
O	-3.905715	0.493441	-1.071919
C	-4.018384	1.727114	-0.366174
H	-4.908008	1.732274	0.267589
H	-3.133362	1.890505	0.256566
H	-4.090413	2.499237	-1.131760
H	5.724287	-2.680329	-1.689121
H	5.589527	-0.361103	-0.772761
H	3.596486	-3.962837	-2.038957
H	1.080352	4.881193	-0.537816
H	-0.549932	5.227755	-2.397916
H	-1.832749	3.251223	-3.261101
H	1.650704	0.807656	4.750373
H	-0.550371	0.143660	5.728391
H	-2.328084	-0.754537	4.197066
H	-3.731174	-1.722818	-2.165864
Br	-1.119636	-1.553234	-1.004489

MA-Cl

ω-B97XD SCF energy: -767.17513876 a.u.
ω-B97XD enthalpy: -767.054346 a.u.
ω-B97XD free energy: -767.097172 a.u.
ω-B97XD SCF energy in solution: -767.34145890 a.u.
ω-B97XD enthalpy in solution: -767.220666 a.u.
ω-B97XD free energy in solution: -767.263492 a.u.

Cartesian coordinates

ATOM	X	Y	Z
C	0.826494	0.248901	0.527173
C	1.669309	1.485859	0.291449
H	2.680254	1.335366	0.677043

H	1.716661	1.719179	-0.774136
H	1.216238	2.337925	0.808715
C	-0.587328	0.406777	-0.023184
O	-1.420274	-0.470850	0.540827
C	-2.763456	-0.439246	0.056177
H	-2.785497	-0.635204	-1.018458
H	-3.288908	-1.223545	0.599510
H	-3.217525	0.535428	0.251206
O	-0.910387	1.222842	-0.850376
H	0.768044	-0.012338	1.585113
Cl	1.569759	-1.193323	-0.280135

[MA--Cl--Cu(TPMA)]‡

ω-B97XD SCF energy: -1879.84386130 a.u.
ω-B97XD enthalpy: -1879.365626 a.u.
ω-B97XD free energy: -1879.456901 a.u.
ω-B97XD SCF energy in solution: -3323.60665415 a.u.
ω-B97XD enthalpy in solution: -3323.128419 a.u.
ω-B97XD free energy in solution: -3323.219694 a.u.
Imaginary frequency: -751.7870 cm-1

Cartesian coordinates

ATOM	X	Y	Z
Cu	-0.517145	-0.081159	0.242452
N	0.121735	1.855641	-0.404212
N	0.084812	-1.548355	-1.162500
N	-2.302264	-0.253515	1.253625
N	-1.910734	0.302327	-1.407451
C	0.601267	4.425518	-1.318511
C	-0.444903	2.283739	-1.541999
C	-2.466683	-0.811850	2.459831
H	-1.557162	-1.116388	2.966564
C	-0.235699	3.568689	-2.027890
C	1.199437	3.971190	-0.148542
C	-4.667816	-0.003753	1.059987
C	0.928388	2.676758	0.276473
H	1.372827	2.262155	1.176174
C	-3.381053	0.151602	0.561749
C	-3.719978	-0.988776	3.029922
C	-3.111478	0.837018	-0.761945
H	-3.992647	0.772677	-1.416897
H	-2.933044	1.900672	-0.563925
C	-1.265614	1.263073	-2.306153
H	-1.994793	1.762314	-2.960280
H	-0.583613	0.701548	-2.954772
C	-0.803574	-1.758503	-2.147837
C	-0.541508	-2.625064	-3.199468
C	-2.117079	-1.012702	-2.023685
H	-2.611208	-0.931291	-3.002691
H	-2.784876	-1.584707	-1.368765
C	1.261372	-2.183090	-1.192037
H	1.956114	-1.952573	-0.389407
C	0.677600	-3.298876	-3.224670
C	1.596168	-3.071401	-2.207912

C	-4.839782	-0.579385	2.315308
C	3.280280	-0.640194	2.485841
C	3.422461	-2.067527	2.877526
H	4.455402	-2.256952	3.204164
H	2.759414	-2.317696	3.709039
H	3.217969	-2.727198	2.031103
C	3.746331	-0.216954	1.157287
O	3.956310	-0.971533	0.225864
O	3.870790	1.118170	1.070704
C	4.251573	1.612681	-0.212118
H	5.194106	1.165160	-0.534994
H	3.477301	1.389105	-0.952044
H	4.362541	2.689812	-0.090666
H	-5.835374	-0.709208	2.726907
H	-5.520780	0.323881	0.474528
H	-3.809463	-1.444318	4.009156
H	-0.715939	3.890703	-2.946349
H	0.780759	5.434135	-1.676534
H	1.857319	4.605703	0.434229
H	-1.276850	-2.769648	-3.984548
H	0.907568	-3.983571	-4.034648
H	2.563404	-3.559972	-2.195667
H	3.261800	0.123331	3.256275
Cl	0.987806	-0.440576	1.887629

MAc•

ω-B97XD SCF energy: -267.63127737 a.u.
ω-B97XD enthalpy: -267.547097 a.u.
ω-B97XD free energy: -267.584056 a.u.
ω-B97XD SCF energy in solution: -267.75048593 a.u.
ω-B97XD enthalpy in solution: -267.666306 a.u.
ω-B97XD free energy in solution: -267.703265 a.u.

Cartesian coordinates

ATOM	X	Y	Z
C	1.785687	-0.574903	0.000179
C	0.517597	0.123445	-0.000570
O	-0.530251	-0.728166	-0.000303
C	-1.810385	-0.104418	0.000081
H	-1.936254	0.520311	-0.888392
H	-2.535843	-0.917744	-0.000517
H	-1.936358	0.518978	0.889485
O	0.396245	1.335351	0.000332
H	1.828986	-1.657247	0.000178
H	2.694127	0.013477	0.000871

MAc-Br

ω-B97XD SCF energy: -2839.12016882 a.u.
ω-B97XD enthalpy: -2839.029744 a.u.
ω-B97XD free energy: -2839.071081 a.u.
ω-B97XD SCF energy in solution: -2842.02695131 a.u.
ω-B97XD enthalpy in solution: -2841.936526 a.u.

ω-B97XD free energy in solution: -2841.977863 a.u.

Cartesian coordinates

ATOM	X	Y	Z
C	0.252761	0.840492	0.735053
C	-1.101856	0.587496	0.108807
O	-1.577007	-0.613725	0.446419
C	-2.839391	-0.954341	-0.129045
H	-2.771934	-0.951946	-1.219551
H	-3.067518	-1.953617	0.239139
H	-3.606744	-0.242509	0.184529
O	-1.679518	1.381916	-0.591219
H	0.260358	0.565456	1.789191
H	0.522779	1.884091	0.594700
Br	1.624177	-0.236826	-0.134814

[MAc--Br--Cu(TPMA)]‡

ω-B97XD SCF energy: -3951.79322944 a.u.
ω-B97XD enthalpy: -3951.345655 a.u.
ω-B97XD free energy: -3951.435084 a.u.
ω-B97XD SCF energy in solution: -5398.29316197 a.u.
ω-B97XD enthalpy in solution: -5397.845588 a.u.
ω-B97XD free energy in solution: -5397.935017 a.u.
Imaginary frequency: -546.6781 cm-1

Cartesian coordinates

ATOM	X	Y	Z
Cu	0.564256	-0.018578	0.170293
N	-0.439356	-1.521150	-0.980580
N	0.031833	1.885013	-0.596652
N	2.432197	-0.371724	0.954054
N	1.721290	0.032314	-1.663604
C	-1.400167	-3.534142	-2.622281
C	-0.031939	-1.604780	-2.255863
C	2.785231	-0.260592	2.241825
H	1.979757	-0.050669	2.937123
C	-0.481676	-2.607083	-3.106351
C	-1.837213	-3.429211	-1.306663
C	4.712741	-0.778478	0.376324
C	-1.325812	-2.408491	-0.515698
H	-1.633497	-2.270284	0.516203
C	3.375960	-0.632130	0.032039
C	4.099245	-0.406780	2.664457
C	2.889089	-0.810445	-1.390102
H	3.702870	-0.623749	-2.105408
H	2.579411	-1.854670	-1.517125
C	0.878681	-0.495512	-2.741961
H	1.481319	-0.831184	-3.597648
H	0.244407	0.324192	-3.097886
C	0.851400	2.322005	-1.567511
C	0.612971	3.504462	-2.252384
C	2.058895	1.450616	-1.847025
H	2.458565	1.645289	-2.852334
H	2.848458	1.698713	-1.128096

C	-1.052514	2.600041	-0.279147
H	-1.697035	2.188722	0.492397
C	-0.509609	4.258280	-1.914770
C	-1.358335	3.797070	-0.917138
C	5.079497	-0.667831	1.714499
C	-3.176704	0.126843	2.853809
C	-3.721727	0.266288	1.504528
O	-3.816750	1.317230	0.898161
O	-4.056781	-0.924390	0.972885
C	-4.543080	-0.875956	-0.366495
H	-5.427181	-0.237906	-0.434196
H	-3.772316	-0.490681	-1.040868
H	-4.794859	-1.904405	-0.624497
H	6.118031	-0.781191	2.007719
H	5.453424	-0.978494	-0.390937
H	4.340498	-0.309387	3.716440
H	-0.124013	-2.657120	-4.129850
H	-1.768368	-4.326013	-3.266526
H	-2.554809	-4.127741	-0.891727
H	1.290648	3.829374	-3.035317
H	-0.719493	5.187774	-2.434088
H	-2.252238	4.340447	-0.634107
H	-3.283612	-0.818021	3.372852
H	-3.081699	1.035077	3.435422
Br	-0.796007	-0.070336	2.127339

MAc-Cl

ω-B97XD SCF energy: -727.8675324 a.u.
ω-B97XD enthalpy: -727.776935 a.u.
ω-B97XD free energy: -727.817939 a.u.
ω-B97XD SCF energy in solution: -728.0222558 a.u.
ω-B97XD enthalpy in solution: -727.9316584 a.u.
ω-B97XD free energy in solution: -727.9726624 a.u.

Cartesian coordinates

ATOM	X	Y	Z
C	-0.45797	0.09227	-0.03734
O	-1.55108	-0.68449	0.03002
O	-0.47092	1.29332	-0.04497
C	-2.79596	0.01836	0.05236
H	-3.56657	-0.75129	0.41212
H	-2.71414	0.91649	0.76249
H	-3.04379	0.37673	-1.01763
C	0.76702	-0.81004	-0.11984
H	0.71085	-1.58581	0.65903
H	0.7707	-1.31603	-1.10855
Cl	2.29061	0.09916	0.05242

[MAc--Cl--Cu(TPMA)]‡

ω-B97XD SCF energy: -1840.53140099 a.u.
ω-B97XD enthalpy: -1840.083406 a.u.
ω-B97XD free energy: -1840.171706 a.u.

ω-B97XD SCF energy in solution: -3284.28217951 a.u.
ω-B97XD enthalpy in solution: -3283.834185 a.u.
ω-B97XD free energy in solution: -3283.922485 a.u.
Imaginary frequency: -726.3954 cm-1

Cartesian coordinates

ATOM	X	Y	Z
Cu	0.490367	0.034069	0.304107
N	-0.520257	-1.542261	-0.731077
N	-0.071708	1.897211	-0.525056
N	2.384923	-0.279159	1.037647
N	1.589877	0.003172	-1.574536
C	-1.502442	-3.652425	-2.232726
C	-0.162603	-1.680277	-2.016462
C	2.776221	-0.112622	2.307939
H	1.991911	0.126919	3.017719
C	-0.624796	-2.731694	-2.798179
C	-1.886115	-3.493502	-0.905830
C	4.647670	-0.707049	0.408415
C	-1.365321	-2.424832	-0.187207
H	-1.632747	-2.246046	0.849519
C	3.300513	-0.577139	0.099145
C	4.103013	-0.238931	2.696354
C	2.772038	-0.817719	-1.299653
H	3.563810	-0.656561	-2.045459
H	2.468379	-1.868852	-1.373125
C	0.710723	-0.582402	-2.591035
H	1.279938	-0.950341	-3.456398
H	0.050540	0.212704	-2.955678
C	0.707680	2.291669	-1.545928
C	0.438694	3.442433	-2.272548
C	1.908120	1.412935	-1.834548
H	2.266325	1.566895	-2.862451
H	2.723570	1.697373	-1.159198
C	-1.144266	2.625261	-0.196511
H	-1.759550	2.245658	0.614069
C	-0.670335	4.210508	-1.923516
C	-1.476841	3.793988	-0.872593
C	5.054627	-0.539094	1.728851
C	-2.870991	0.237654	3.107423
C	-3.589083	0.267938	1.832871
O	-3.779278	1.269813	1.169148
O	-3.964489	-0.962274	1.437768
C	-4.612746	-1.020488	0.168199
H	-5.512930	-0.401637	0.165294
H	-3.938464	-0.674742	-0.620809
H	-4.870004	-2.068469	0.017037
H	6.101887	-0.638814	1.994697
H	5.365374	-0.939029	-0.371600
H	4.376314	-0.097076	3.735392
H	-0.308609	-2.824571	-3.832272
H	-1.879143	-4.482217	-2.821946
H	-2.568812	-4.186190	-0.427187
H	1.083110	3.732313	-3.096344
H	-0.903247	5.116045	-2.474477
H	-2.359029	4.350278	-0.578003

H	-2.890194	-0.667440	3.702348
H	-2.741754	1.186832	3.611489
Cl	-0.736065	0.058888	2.201507

MeCN•

ω-B97XD SCF energy: -132.03827412 a.u.
ω-B97XD enthalpy: -132.002245 a.u.
ω-B97XD free energy: -132.031066 a.u.
ω-B97XD SCF energy in solution: -132.09883066 a.u.
ω-B97XD enthalpy in solution: -132.062802 a.u.
ω-B97XD free energy in solution: -132.091623 a.u.

Cartesian coordinates

ATOM	X	Y	Z
C	-0.188476	0.000513	-0.000005
N	-1.360619	-0.000217	-0.000019
C	1.196300	-0.000134	0.000008
H	1.738273	-0.938035	0.000056
H	1.739113	0.937279	0.000061

MeCN-Br

ω-B97XD SCF energy: -2703.51828156 a.u.
ω-B97XD enthalpy: -2703.475959 a.u.
ω-B97XD free energy: -2703.509643 a.u.
ω-B97XD SCF energy in solution: -2706.36767085 a.u.
ω-B97XD enthalpy in solution: -2706.325348 a.u.
ω-B97XD free energy in solution: -2706.359032 a.u.

Cartesian coordinates

ATOM	X	Y	Z
C	0.181003	-1.805350	0.000000
N	0.961590	-2.659090	0.000000
C	-0.821383	-0.750123	0.000000
H	-1.444424	-0.817223	0.891837
H	-1.444424	-0.817223	-0.891837
Br	0.000000	1.016597	0.000000

[MeCN--Br--Cu(TPMA)]‡

ω-B97XD SCF energy: -3816.19323054 a.u.
ω-B97XD enthalpy: -3815.793198 a.u.
ω-B97XD free energy: -3815.876435 a.u.
ω-B97XD SCF energy in solution: -5262.63718524 a.u.
ω-B97XD enthalpy in solution: -5262.237153 a.u.
ω-B97XD free energy in solution: -5262.320390 a.u.
Imaginary frequency: -490.9149 cm-1

Cartesian coordinates

ATOM	X	Y	Z
Cu	0.166768	-0.006790	-0.138157
N	0.905169	1.928751	-0.434938

N	-0.962889	-0.312930	1.621690
N	1.322340	-1.595182	-0.826411
N	1.736695	0.021653	1.349890
C	2.189517	4.372365	-0.673286
C	1.761335	2.338559	0.516340
C	0.941008	-2.546394	-1.687230
H	-0.040353	-2.414545	-2.130911
C	2.429642	3.552514	0.425765
C	1.294739	3.949129	-1.649013
C	3.383152	-2.751243	-0.483037
C	0.676265	2.716137	-1.492545
H	-0.030373	2.333122	-2.221528
C	2.525546	-1.688189	-0.233819
C	1.747314	-3.632858	-1.998495
C	2.911866	-0.539478	0.674911
H	3.682124	-0.854228	1.393071
H	3.349406	0.253241	0.056702
C	1.906067	1.430520	1.720209
H	2.866603	1.604934	2.225547
H	1.113655	1.682164	2.434540
C	-0.221053	-0.594727	2.706032
C	-0.787061	-0.732515	3.965580
C	1.258214	-0.810183	2.460244
H	1.835693	-0.632127	3.378477
H	1.413205	-1.858255	2.178588
C	-2.285664	-0.170794	1.754854
H	-2.840608	0.052733	0.849813
C	-2.166577	-0.590728	4.102375
C	-2.930477	-0.307010	2.977444
C	2.989192	-3.737312	-1.383347
Br	-1.654012	-0.038006	-1.729521
C	-3.977657	-0.042472	-2.460089
H	3.643696	-4.575980	-1.597137
H	4.344439	-2.804448	0.017494
H	1.400824	-4.378780	-2.704166
H	3.122814	3.852478	1.204914
H	2.696794	5.327089	-0.765501
H	1.078542	4.555937	-2.520585
H	-0.160631	-0.953084	4.824052
H	-2.633158	-0.699029	5.076089
H	-4.006535	-0.186981	3.026910
C	-4.656241	0.002424	-1.219641
N	-5.134772	0.039508	-0.159073
H	-3.995774	-0.984239	-2.997784
H	-3.981122	0.863102	-3.057159

MeCN-Cl

ω-B97XD SCF energy: -592.26509425 a.u.
ω-B97XD enthalpy: -592.222300 a.u.
ω-B97XD free energy: -592.254690 a.u.
ω-B97XD SCF energy in solution: -592.36136569 a.u.
ω-B97XD enthalpy in solution: -592.318571 a.u.
ω-B97XD free energy in solution: -592.350961 a.u.

Cartesian coordinates

ATOM	X	Y	Z
C	-1.277832	0.107136	0.000000
N	-2.301134	-0.431763	0.000000
C	0.000000	0.813275	0.000000
H	0.075216	1.440685	0.889871
H	0.075216	1.440685	-0.889871
Cl	1.389676	-0.316559	0.000000

[MeCN--Cl--Cu(TPMA)]‡

ω-B97XD SCF energy: -1704.93043382 a.u.
ω-B97XD enthalpy: -1704.530225 a.u.
ω-B97XD free energy: -1704.612289 a.u.
ω-B97XD SCF energy in solution: -3148.62537286 a.u.
ω-B97XD enthalpy in solution: -3148.225164 a.u.
ω-B97XD free energy in solution: -3148.307228 a.u.
Imaginary frequency: -666.0346 cm-1

Cartesian coordinates

ATOM	X	Y	Z
Cu	0.035706	-0.038454	-0.280477
N	0.711049	1.929023	-0.527329
N	-1.330168	-0.362979	1.292991
N	1.383905	-1.551864	-0.742462
N	1.361270	0.124667	1.434208
C	1.902384	4.427039	-0.660172
C	1.384477	2.413891	0.529276
C	1.203167	-2.532328	-1.635570
H	0.293326	-2.471827	-2.223557
C	2.000015	3.658296	0.496239
C	1.197519	3.924605	-1.747813
C	3.438820	-2.562618	-0.068365
C	0.618989	2.666906	-1.639482
H	0.060630	2.220489	-2.455830
C	2.484621	-1.558316	0.028789
C	2.118696	-3.562628	-1.802187
C	2.655384	-0.380467	0.966834
H	3.316861	-0.645937	1.803807
H	3.146011	0.428234	0.412275
C	1.385805	1.550450	1.774583
H	2.239253	1.802249	2.420279
H	0.474106	1.769581	2.342570
C	-0.751066	-0.560310	2.489787
C	-1.496010	-0.670915	3.655257
C	0.756977	-0.707615	2.479786
H	1.177823	-0.485677	3.470841
H	0.999827	-1.752119	2.251338
C	-2.662411	-0.282367	1.217547
H	-3.083684	-0.123797	0.230399
C	-2.885142	-0.591806	3.575235
C	-3.479890	-0.397373	2.335291
C	3.255346	-3.577761	-1.002444
C	-3.367342	-0.314438	-3.209629
H	3.989567	-4.370871	-1.099038

H	4.312624	-2.547369	0.575064
H	1.935660	-4.335337	-2.539742
H	2.543476	4.020335	1.362942
H	2.374526	5.402672	-0.710500
H	1.098767	4.488284	-2.668184
H	-0.999414	-0.820042	4.608636
H	-3.489297	-0.677382	4.472629
H	-4.554976	-0.327616	2.217183
H	-3.228903	-1.272560	-3.698407
C	-4.335681	-0.256995	-2.178580
N	-5.061607	-0.206538	-1.270329
H	-3.259220	0.568445	-3.830004
Cl	-1.422301	-0.200398	-2.042214

$[Cu^{I}L_2]^{+}$

ω-B97XD SCF energy: -1691.98651387 a.u.
ω-B97XD enthalpy: -1691.342207 a.u.
ω-B97XD free energy: -1691.450051 a.u.
ω-B97XD SCF energy in solution: -3135.79994691 a.u.
ω-B97XD enthalpy in solution: -3135.155640 a.u.
ω-B97XD free energy in solution: -3135.263484 a.u.

Cartesian coordinates

ATOM	X	Y	Z
Cu	-0.018531	0.001267	-0.952199
N	0.910457	-1.803984	-0.621194
N	1.105405	1.693279	-0.629770
N	-2.044178	0.105862	-0.630778
N	-0.017231	0.007119	1.266579
C	2.108820	-4.194204	0.112269
C	1.304768	-2.000046	0.649437
C	-2.982650	0.452480	-1.517310
H	-2.629772	0.660956	-2.523417
C	1.917836	-3.182020	1.068887
C	1.667146	-4.015252	-1.207442
C	-3.744364	-0.053778	1.058324
C	1.083633	-2.791740	-1.504938
H	0.717895	-2.598897	-2.509593
C	-2.414630	-0.127524	0.641118
C	-4.333263	0.574463	-1.221597
C	-1.317401	-0.549534	1.611237
H	-1.602904	-0.298992	2.642958
H	-1.232850	-1.642859	1.566112
C	1.114680	-0.838176	1.618042
H	1.034522	-1.212683	2.648524
H	2.019483	-0.218118	1.579870
C	1.077399	2.141279	0.638196
C	1.813128	3.251377	1.055782
C	0.148118	1.413922	1.602953
H	0.495836	1.544674	2.637643
H	-0.839180	1.889221	1.541140
C	1.897123	2.312923	-1.510537
H	1.911999	1.892269	-2.512058
C	2.620944	3.896359	0.102833

C	2.689904	3.412460	-1.212278
C	-4.712548	0.293248	0.099951
O	3.361422	4.943983	0.531438
C	1.742189	3.762797	2.472132
H	0.707351	3.946308	2.779276
H	2.176602	3.044997	3.177676
H	2.296753	4.695680	2.567395
C	3.255276	6.189527	-0.155453
H	3.380791	6.965912	0.600792
H	4.038708	6.294642	-0.910370
H	2.271805	6.296561	-0.624697
C	3.620670	3.979978	-2.250119
H	3.244019	4.915331	-2.677114
H	4.605788	4.179076	-1.817554
H	3.749935	3.271391	-3.072594
O	-5.990488	0.400262	0.529395
C	-4.148325	-0.349019	2.480266
H	-3.775053	-1.324317	2.809478
H	-3.757775	0.407351	3.171032
H	-5.234135	-0.348880	2.572351
C	-7.009851	-0.332191	-0.148129
H	-7.734058	-0.624237	0.613761
H	-7.509270	0.285806	-0.898716
H	-6.598855	-1.230375	-0.620305
C	-5.297661	1.057880	-2.271062
H	-5.917610	0.247228	-2.667708
H	-5.966067	1.821653	-1.861932
H	-4.756501	1.499033	-3.112291
O	2.670731	-5.348139	0.539478
C	3.826758	-5.840156	-0.136173
H	4.448355	-6.313479	0.625413
H	3.557043	-6.582656	-0.891515
H	4.385041	-5.022166	-0.603073
C	2.381559	-3.375490	2.490056
H	3.061693	-2.575889	2.802168
H	1.536466	-3.384396	3.188062
H	2.902763	-4.326902	2.591823
C	1.738104	-5.096141	-2.252220
H	2.746274	-5.209284	-2.664414
H	1.436490	-6.060403	-1.831960
H	1.067163	-4.865633	-3.084083

[Br-Cu^{II}L$_2$]$^+$

ω-B97XD SCF energy: -4263.46469801 a.u.
ω-B97XD enthalpy: -4262.815902 a.u.
ω-B97XD free energy: -4262.928354 a.u.
ω-B97XD SCF energy in solution: -5710.06935243 a.u.
ω-B97XD enthalpy in solution: -5709.420556 a.u.
ω-B97XD free energy in solution: -5709.533008 a.u.

Cartesian coordinates

ATOM	X	Y	Z
N	1.954681	-0.672368	0.254001
N	-1.547447	-1.367162	0.251301

N	-0.400899	2.019403	0.259992
N	0.002121	-0.001754	-1.455480
C	4.460716	-1.540828	-0.518910
C	2.171417	-1.067146	-1.008927
C	-0.895190	2.900678	1.131271
H	-1.077263	2.513515	2.130163
C	3.407597	-1.518029	-1.455710
C	4.252563	-1.096170	0.797875
C	-0.385342	3.705831	-1.444457
C	2.966281	-0.684033	1.123425
H	2.723639	-0.337804	2.124358
C	-0.161312	2.407623	-1.000658
C	-1.175700	4.222462	0.808544
C	0.438692	1.338430	-1.887731
H	0.191696	1.498999	-2.944697
H	1.530895	1.377076	-1.798275
C	0.944694	-1.047383	-1.894818
H	1.206482	-0.905493	-2.951036
H	0.432561	-2.013339	-1.812182
C	-2.008111	-1.343592	-1.007209
C	-3.030413	-2.174478	-1.451008
C	-1.374929	-0.293421	-1.894379
H	-1.383106	-0.594430	-2.949781
H	-1.953998	0.634321	-1.816044
C	-2.064209	-2.239274	1.118981
H	-1.633430	-2.212579	2.116199
C	-3.575492	-3.078240	-0.517241
C	-3.074354	-3.135698	0.794499
C	-0.893789	4.626939	-0.507430
C	3.615861	-1.980002	-2.874348
H	2.893160	-2.754576	-3.152597
H	3.506427	-1.151017	-3.583497
H	4.618151	-2.388774	-2.998269
C	5.351252	-0.976513	1.820725
H	5.634809	-1.945219	2.244001
H	6.245362	-0.524343	1.380778
H	5.025015	-0.341778	2.648315
O	5.660749	-1.950041	-0.978468
C	6.392786	-2.940544	-0.256721
H	6.923992	-3.527901	-1.006803
H	7.117386	-2.482061	0.420101
H	5.718673	-3.594168	0.305741
C	-0.084827	4.120911	-2.861196
H	0.945537	3.875208	-3.139683
H	-0.752849	3.620216	-3.571829
H	-0.223024	5.195167	-2.979982
C	-1.820785	5.118739	1.831724
H	-1.116554	5.845395	2.248995
H	-2.657028	5.671416	1.392708
H	-2.207569	4.523791	2.662792
O	-1.142339	5.871866	-0.964524
C	-0.625778	6.997674	-0.254745
H	-0.411257	7.755577	-1.009286
H	-1.358936	7.392605	0.452302
H	0.298032	6.737625	0.271627
O	-4.541322	-3.902485	-0.973407

C	-5.766647	-4.016388	-0.249794
H	-6.538373	-4.210757	-0.995535
H	-5.735363	-4.846585	0.459455
H	-5.996388	-3.084854	0.277112
C	-3.549750	-2.105280	-2.863533
H	-3.826040	-1.081799	-3.138135
H	-2.798072	-2.453675	-3.581672
H	-4.429533	-2.738165	-2.975750
C	-3.522945	-4.151520	1.811216
H	-4.494833	-3.900498	2.247836
H	-3.600630	-5.145100	1.359451
H	-2.800787	-4.207926	2.629460
Cu	0.002987	-0.006589	0.642237
Br	0.001914	-0.008944	2.995274

[MMA--Br--Cu(L$_2$)]‡

ω-B97XD SCF energy: -4609.72443778 a.u.
ω-B97XD enthalpy: -4608.929683 a.u.
ω-B97XD free energy: -4609.063032 a.u.
ω-B97XD SCF energy in solution: -6056.45992776 a.u.
ω-B97XD enthalpy in solution: -6055.665173 a.u.
ω-B97XD free energy in solution: -6055.798522 a.u.
Imaginary frequency: -910.4924 cm-1

Cartesian coordinates

ATOM	X	Y	Z
Cu	-0.767256	-0.300366	-0.175129
N	-0.235561	0.221701	1.862888
N	-0.376764	1.285948	-1.514471
N	-2.434847	-1.469422	-0.381698
N	-2.302229	1.154044	0.388601
C	0.480914	1.179339	4.356230
C	-0.786959	1.345413	2.334674
C	-2.491981	-2.633761	-1.035335
H	-1.555520	-2.982352	-1.460564
C	-0.459990	1.880112	3.580414
C	1.037450	-0.021028	3.885496
C	-4.787115	-1.616305	0.062589
C	0.637934	-0.437763	2.623076
H	1.039233	-1.348488	2.188032
C	-3.560903	-0.960589	0.144672
C	-3.655242	-3.372905	-1.197401
C	-3.411111	0.346922	0.901028
H	-4.351116	0.915715	0.888121
H	-3.194627	0.111563	1.950328
C	-1.748492	2.056962	1.399697
H	-2.550297	2.552911	1.965401
H	-1.197239	2.848975	0.877688
C	-1.363065	2.190558	-1.623182
C	-1.246530	3.339490	-2.399591
C	-2.629561	1.850060	-0.859687
H	-3.231855	2.748024	-0.665799
H	-3.242413	1.174783	-1.469290
C	0.775396	1.506502	-2.147113

H	1.550313	0.759952	-2.001020
C	-0.022680	3.546739	-3.068195
C	1.029034	2.629500	-2.925704
C	-4.820442	-2.850628	-0.612539
Br	1.099249	-1.736145	-0.655903
C	3.586775	-1.650666	-0.354386
C	4.094967	-2.170443	-1.662284
H	5.194879	-2.153698	-1.655889
H	3.779870	-3.205386	-1.819610
H	3.759404	-1.552152	-2.496111
C	3.552993	-0.175872	-0.218331
O	3.725011	0.599541	-1.140263
O	3.257661	0.229058	1.028325
C	2.998453	1.622847	1.168118
H	3.871713	2.213063	0.880901
H	2.145211	1.910978	0.546087
H	2.760832	1.772055	2.221736
C	3.793841	-2.496230	0.864787
H	4.867975	-2.534385	1.099629
H	3.276352	-2.094392	1.736787
H	3.461224	-3.522192	0.684784
O	0.089278	4.688271	-3.782880
C	-2.375532	4.329927	-2.531024
H	-3.302955	3.841389	-2.847202
H	-2.572423	4.837099	-1.579143
H	-2.125004	5.094443	-3.265734
C	0.547206	4.618848	-5.131907
H	0.040876	5.425665	-5.663968
H	1.627609	4.769242	-5.195105
H	0.280230	3.659605	-5.586830
C	2.410029	2.839187	-3.487898
H	2.462276	2.612364	-4.558017
H	2.730335	3.876351	-3.347909
H	3.120078	2.189618	-2.970090
O	-6.023990	-3.453953	-0.713058
C	-6.034930	-1.042697	0.683226
H	-5.881254	-0.804481	1.740912
H	-6.345233	-0.122694	0.174379
H	-6.856285	-1.754781	0.609110
C	-6.153919	-4.821477	-0.326995
H	-7.145476	-4.919467	0.117517
H	-6.081790	-5.485226	-1.192013
H	-5.396727	-5.093290	0.415179
C	-3.637374	-4.623639	-2.035495
H	-3.691733	-5.532832	-1.428228
H	-4.478832	-4.634194	-2.735027
H	-2.713982	-4.673823	-2.618281
O	0.765104	1.687530	5.578210
C	2.125659	1.948346	5.912955
H	2.111013	2.787193	6.610101
H	2.592248	1.087638	6.398565
H	2.700934	2.226419	5.022892
C	-1.075123	3.163495	4.074162
H	-0.979769	3.964221	3.332825
H	-2.142990	3.033973	4.286637
H	-0.592653	3.488579	4.995554

C	1.982516	-0.870753	4.691002
H	2.999363	-0.463810	4.691544
H	1.649481	-0.954445	5.729903
H	2.034406	-1.878463	4.270051

$[Cu^{I}L_3]^{+}$

ω-B97XD SCF energy: -1514.50964069 a.u.
ω-B97XD enthalpy: -1513.914694 a.u.
ω-B97XD free energy: -1514.012492 a.u.
ω-B97XD SCF energy in solution: -2958.25055400 a.u.
ω-B97XD enthalpy in solution: -2957.655607 a.u.
ω-B97XD free energy in solution: -2957.753405 a.u.

Cartesian coordinates

ATOM	X	Y	Z
Cu	0.000000	0.000000	1.170651
N	0.237705	2.018174	0.839857
N	1.628937	-1.214945	0.839857
N	-1.866642	-0.803228	0.839857
N	0.000000	0.000000	-1.099507
C	0.196378	4.719510	-0.017313
C	0.434502	2.344763	-0.453253
C	-2.636761	-1.494182	1.694700
H	-2.313590	-1.490272	2.730940
C	0.409418	3.646528	-0.914504
C	0.000000	4.361223	1.335671
C	-3.362695	-1.468698	-0.914504
C	0.024381	3.030593	1.694700
H	-0.133818	2.748764	2.730940
C	-2.247875	-0.796092	-0.453253
C	-3.776930	-2.180612	1.335671
C	-1.417925	0.045171	-1.411786
H	-1.632555	-0.253005	-2.450764
H	-1.741790	1.087771	-1.305888
C	0.748082	1.205373	-1.411786
H	0.597168	1.540337	-2.450764
H	1.812932	0.964549	-1.305888
C	1.813374	-1.548671	-0.453253
C	2.953277	-2.177830	-0.914504
C	0.669843	-1.250544	-1.411786
H	1.035387	-1.287332	-2.450764
H	-0.071142	-2.052319	-1.305888
C	2.612380	-1.536411	1.694700
H	2.447408	-1.258492	2.730940
C	3.989026	-2.529823	-0.017313
C	3.776930	-2.180612	1.335671
C	-4.185404	-2.189686	-0.017313
H	-0.177615	5.104620	2.101614
H	0.560472	3.826048	-1.972045
H	-4.331923	-2.706129	2.101614
H	-3.593691	-1.427641	-1.972045
H	4.509538	-2.398491	2.101614
H	3.033219	-2.398407	-1.972045
N	-5.295462	-2.852485	-0.432478

N	5.118056	-3.159762	-0.432478
N	0.177406	6.012247	-0.432478
C	-0.046659	7.078810	0.528711
H	0.731204	7.089907	1.301867
H	-0.021776	8.038620	0.013214
H	-1.025036	6.982005	1.014929
C	0.392410	6.330664	-1.832842
H	-0.386173	5.892570	-2.469776
H	0.364529	7.412114	-1.963820
H	1.370752	5.975186	-2.179001
C	6.153758	-3.498997	0.528711
H	5.774438	-4.178195	1.301867
H	6.972537	-4.000452	0.013214
H	6.559112	-2.603295	1.014929
C	5.286311	-3.505169	-1.832842
H	5.296202	-2.611850	-2.469776
H	6.236815	-4.021748	-1.963820
H	4.489287	-4.174699	-2.179001
C	-5.678721	-2.825495	-1.832842
H	-6.601343	-3.390366	-1.963820
H	-5.860039	-1.800487	-2.179001
H	-4.910029	-3.280720	-2.469776
C	-6.107100	-3.579812	0.528711
H	-6.505642	-2.911713	1.301867
H	-6.950761	-4.038168	0.013214
H	-5.534076	-4.378710	1.014929

[Br-Cu^{II}L$_3$]$^+$

ω-B97XD SCF energy: -4085.98600240 a.u.
ω-B97XD enthalpy: -4085.387011 a.u.
ω-B97XD free energy: -4085.489462 a.u.
ω-B97XD SCF energy in solution: -5532.52028641 a.u.
ω-B97XD enthalpy in solution: -5531.921295 a.u.
ω-B97XD free energy in solution: -5532.023746 a.u.

Cartesian coordinates

ATOM	X	Y	Z
Br	0.005355	-0.006436	3.131133
Cu	0.004479	-0.004297	0.776719
N	1.974799	-0.593554	0.384090
N	-1.489103	-1.419797	0.383278
N	-0.478154	1.997474	0.389138
N	0.003087	0.000092	-1.355602
C	4.588326	-1.215493	-0.472050
C	2.226870	-0.923303	-0.892747
C	-1.012505	2.880627	1.246032
H	-1.121095	2.527615	2.267144
C	3.486765	-1.224319	-1.364710
C	4.299855	-0.878395	0.872649
C	-0.678826	3.628734	-1.354876
C	3.006910	-0.578545	1.241010
H	2.755558	-0.316115	2.264295
C	-0.312099	2.385495	-0.885540
C	-1.397642	4.151448	0.879974

C	0.367012	1.364362	-1.770562
H	0.135047	1.531718	-2.831470
H	1.451321	1.465470	-1.648552
C	1.002383	-0.994618	-1.777930
H	1.262773	-0.868560	-2.837963
H	0.546939	-1.984650	-1.663519
C	-1.909403	-1.463570	-0.891077
C	-2.809298	-2.395747	-1.362063
C	-1.359818	-0.365642	-1.774548
H	-1.385823	-0.651388	-2.835268
H	-1.988772	0.523761	-1.656180
C	-1.988203	-2.326157	1.237609
H	-1.625415	-2.249098	2.258186
C	-3.351818	-3.356080	-0.471316
C	-2.901098	-3.289381	0.869163
C	-1.242142	4.575010	-0.462165
H	3.612646	-1.470529	-2.411817
H	-0.522082	3.864193	-2.400411
H	-1.817026	4.802875	1.634830
H	5.074041	-0.844707	1.627290
H	-3.255076	-3.981907	1.621180
H	-3.092042	-2.373589	-2.407254
N	-1.614809	5.811337	-0.874336
N	5.846098	-1.506733	-0.885788
N	-4.247207	-4.286731	-0.882932
C	6.945945	-1.492935	0.066312
H	6.794212	-2.230991	0.862846
H	7.871844	-1.741675	-0.451549
H	7.067909	-0.502736	0.520615
C	6.095656	-1.856746	-2.273806
H	5.816355	-1.038907	-2.949359
H	7.158776	-2.053318	-2.409379
H	5.545396	-2.759738	-2.565808
C	-4.777535	-5.254554	0.065059
H	-5.314076	-4.759812	0.883310
H	-5.477841	-5.912285	-0.448912
H	-3.979851	-5.875331	0.489427
C	-4.701246	-4.302583	-2.263052
H	-3.872232	-4.488419	-2.957091
H	-5.431885	-5.100593	-2.391952
H	-5.184446	-3.356273	-2.535276
C	-2.186773	6.753269	0.075538
H	-1.480314	6.988719	0.880285
H	-2.429290	7.681065	-0.441899
H	-3.109933	6.361515	0.518330
C	-1.419510	6.208336	-2.258465
H	-1.986559	5.566242	-2.943600
H	-1.770729	7.231132	-2.391532
H	-0.359466	6.176270	-2.539019

[MMA--Br--Cu(L_3)]‡

ω-B97XD SCF energy: -4432.24277149 a.u.
ω-B97XD enthalpy: -4431.498665 a.u.
ω-B97XD free energy: -4431.625314 a.u.

ω-B97XD SCF energy in solution: -5878.90846846 a.u.
ω-B97XD enthalpy in solution: -5878.164362 a.u.
ω-B97XD free energy in solution: -5878.291011 a.u.
Imaginary frequency: -728.0029 cm-1

Cartesian coordinates

ATOM	X	Y	Z
Cu	0.454659	-0.385821	-0.222583
N	-0.133683	1.504439	-1.021635
N	-0.019661	-0.438135	1.834395
N	2.151945	-1.283840	-0.927976
N	1.989827	0.975336	0.636633
C	-0.534157	4.073947	-2.123281
C	0.530583	2.572094	-0.551838
C	2.258990	-2.533147	-1.409253
H	1.322192	-3.062910	-1.547476
C	0.379918	3.844740	-1.066792
C	-1.238776	2.940688	-2.592512
C	4.541066	-1.112761	-1.006219
C	-0.999923	1.707970	-2.023696
H	-1.532555	0.824956	-2.364401
C	3.291389	-0.591701	-0.742535
C	3.458796	-3.133009	-1.719976
C	3.125883	0.839303	-0.271755
H	4.059817	1.210813	0.176970
H	2.916228	1.461160	-1.150346
C	1.418146	2.320438	0.652901
H	2.196385	3.094484	0.731350
H	0.793162	2.400853	1.549582
C	0.917966	0.078742	2.646119
C	0.729124	0.266038	4.000173
C	2.230664	0.429786	1.973544
H	2.820163	1.117255	2.599039
H	2.817768	-0.488151	1.852710
C	-1.193061	-0.782511	2.383877
H	-1.942734	-1.175640	1.703258
C	-0.499742	-0.110076	4.597066
C	-1.476364	-0.643473	3.725732
C	4.667914	-2.425296	-1.522893
C	-3.801220	-1.968359	-1.258585
C	-4.060841	-3.301174	-0.629658
H	-5.143249	-3.498150	-0.629139
H	-3.578181	-4.101564	-1.197085
H	-3.718480	-3.326780	0.405968
C	-3.979140	-0.795361	-0.371851
O	-4.100182	-0.861802	0.837146
O	-3.944907	0.371593	-1.038360
C	-3.935934	1.536204	-0.217212
H	-4.831616	1.578595	0.406825
H	-3.048114	1.538080	0.422567
H	-3.904662	2.380013	-0.906287
H	5.412687	-0.498274	-0.816679
H	3.447482	-4.143800	-2.105923
H	0.959672	4.655148	-0.641576
H	-1.959539	3.011031	-3.396694
H	1.530196	0.699248	4.586933

H	-2.455593	-0.940507	4.077400
Br	-1.308337	-1.767060	-1.098997
N	5.876800	-2.970707	-1.805722
N	-0.727971	0.045189	5.926854
N	-0.722020	5.309800	-2.653923
C	5.960025	-4.328783	-2.319013
H	5.427750	-4.428457	-3.272185
H	7.005782	-4.582206	-2.490710
H	5.547636	-5.052998	-1.606063
C	7.092463	-2.209996	-1.573047
H	7.213556	-1.959366	-0.511787
H	7.952686	-2.805643	-1.877495
H	7.101827	-1.282566	-2.158359
C	0.304551	0.596843	6.785248
H	0.567591	1.621018	6.491695
H	-0.060255	0.627103	7.811763
H	1.213076	-0.018099	6.767868
C	-2.004867	-0.356424	6.493712
H	-2.190846	-1.426138	6.340400
H	-1.996857	-0.165648	7.566692
H	-2.834689	0.209985	6.054295
C	0.035557	6.441556	-2.149970
H	-0.252710	7.339422	-2.696179
H	-0.163839	6.616161	-1.085490
H	1.114258	6.294925	-2.286401
C	-1.669349	5.496617	-3.739981
H	-2.684302	5.209438	-3.439493
H	-1.688969	6.549130	-4.021968
H	-1.386566	4.913182	-4.624753
C	-4.039403	-1.825509	-2.730769
H	-5.121616	-1.836792	-2.928404
H	-3.637523	-0.891034	-3.124472
H	-3.596210	-2.664996	-3.273647

$[Cu^{I}L_4]^{+}$

ω-B97XD SCF energy: -1127.16941781 a.u.
ω-B97XD enthalpy: -1126.525386 a.u.
ω-B97XD free energy: -1126.607271 a.u.
ω-B97XD SCF energy in solution: -2570.77978082 a.u.
ω-B97XD enthalpy in solution: -2570.135749 a.u.
ω-B97XD free energy in solution: -2570.217634 a.u.

Cartesian coordinates

ATOM	X	Y	Z
Cu	-0.000097	0.000408	-0.229966
N	0.003521	0.001790	1.970045
N	2.190596	0.120311	-0.038247
N	-1.200253	1.833806	-0.036351
N	-0.990513	-1.954377	-0.035310
C	-2.180220	-2.111564	-0.912352
H	-1.855137	-1.947770	-1.942733
H	-2.859787	-1.291326	-0.669803
C	-0.985218	1.014667	2.344949
H	-0.811179	1.393858	3.364198

H	-1.971437	0.543782	2.357834
C	2.920467	-0.830326	-0.916808
H	2.616710	-0.627634	-1.946748
H	2.548424	-1.828923	-0.676722
C	-0.378445	-1.361386	2.344089
H	-0.790235	-1.401931	3.364781
H	0.521901	-1.980960	2.352980
C	2.620260	1.517582	-0.280549
H	1.991720	2.161642	0.341033
H	3.654034	1.662401	0.067822
C	-0.744699	2.940029	-0.918001
H	-0.770420	2.572921	-1.947010
H	0.306600	3.118231	-0.680327
C	-0.993928	2.203630	1.381730
H	-1.762172	2.912381	1.723497
H	-0.035189	2.728921	1.444740
C	-1.408167	-1.961581	1.384569
H	-2.341286	-1.392816	1.453064
H	-1.637484	-2.981508	1.725906
C	1.375613	0.352707	2.342027
H	1.460928	1.442333	2.349791
H	1.617564	0.018161	3.363122
C	2.408619	-0.238543	1.380861
H	2.383605	-1.331116	1.448923
H	3.406763	0.073618	1.720650
C	-2.625863	1.506934	-0.273749
H	-3.266807	2.330178	0.076023
H	-2.867190	0.640872	0.349090
C	0.003293	-3.026370	-0.277324
H	-0.388291	-3.993088	0.073546
H	0.876419	-2.803747	0.342704
C	-1.512074	4.257965	-0.815658
H	-1.473515	4.683490	0.191735
H	-1.057033	4.984265	-1.495499
H	-2.562446	4.156046	-1.104110
C	-2.943002	1.192230	-1.729501
H	-2.956057	2.090858	-2.352181
H	-2.210169	0.494574	-2.150356
H	-3.932893	0.732182	-1.800121
C	-2.936428	-3.436137	-0.810896
H	-3.798052	-3.402728	-1.484161
H	-2.324486	-4.292616	-1.108733
H	-3.316071	-3.620258	0.198720
C	0.429018	-3.143714	-1.734761
H	1.320372	-3.773405	-1.809135
H	-0.345483	-3.602326	-2.355518
H	0.668059	-2.161103	-2.156995
C	4.445518	-0.823967	-0.813594
H	4.849163	-1.585043	-1.487788
H	4.881437	0.135538	-1.107333
H	4.793668	-1.063176	0.195841
C	2.504162	1.945471	-1.737342
H	1.532671	1.659666	-2.156191
H	2.601585	3.032417	-1.812094
H	3.287088	1.504832	-2.360519

$[Br\text{-}Cu^{II}L_4]^+$

ω-B97XD SCF energy: -3698.63906492 a.u.
ω-B97XD enthalpy: -3697.989838 a.u.
ω-B97XD free energy: -3698.074841 a.u.
ω-B97XD SCF energy in solution: -5145.03727414 a.u.
ω-B97XD enthalpy in solution: -5144.388047 a.u.
ω-B97XD free energy in solution: -5144.473050 a.u.

Cartesian coordinates

ATOM	X	Y	Z
N	0.000301	0.001692	2.177963
N	1.954837	1.111112	0.346337
N	-1.940172	1.135091	0.346510
N	-0.012973	-2.247399	0.346906
C	-0.982227	-2.888300	-0.581565
H	-0.657266	-2.657018	-1.596374
H	-1.935586	-2.369066	-0.444031
C	-1.308160	0.511900	2.652833
H	-1.213898	0.885341	3.680963
H	-2.013689	-0.320391	2.684378
C	2.995300	0.591416	-0.580911
H	2.632220	0.753179	-1.596334
H	3.024648	-0.493372	-0.439381
C	0.212917	-1.386469	2.652973
H	-0.156700	-1.491546	3.681478
H	1.286428	-1.581458	2.684195
C	1.770722	2.584854	0.217426
H	0.874252	2.850745	0.786443
H	2.612240	3.095746	0.708583
C	-2.013147	2.293989	-0.582900
H	-1.975521	1.896003	-1.597358
H	-1.087539	2.861641	-0.446380
C	-1.831420	1.604820	1.738858
H	-2.797656	1.956313	2.126531
H	-1.154659	2.465618	1.752537
C	-0.472728	-2.386872	1.740162
H	-1.556617	-2.231175	1.755580
H	-0.293571	-3.399067	2.128517
C	1.096381	0.880107	2.652147
H	0.728879	1.907516	2.681279
H	1.370693	0.614213	3.681495
C	2.305446	0.784153	1.739863
H	2.710943	-0.232981	1.755880
H	3.093721	1.444736	2.126894
C	-3.123940	0.237622	0.220992
H	-3.986461	0.710642	0.713751
H	-2.903877	-0.670561	0.790843
C	1.354685	-2.826199	0.219490
H	1.374267	-3.811408	0.708884
H	2.032843	-2.184863	0.791175
C	-3.213787	3.219484	-0.402013
H	-3.231282	3.696997	0.582895
H	-3.157781	4.015656	-1.149813
H	-4.166625	2.702214	-0.548833

C	-3.502628	-0.155373	-1.199810
H	-3.923463	0.682786	-1.761291
H	-2.645073	-0.539332	-1.756432
H	-4.270303	-0.933758	-1.152106
C	-1.185451	-4.390468	-0.401078
H	-1.907490	-4.738090	-1.145519
H	-0.262685	-4.958374	-0.552915
H	-1.585994	-4.644135	0.585628
C	1.884345	-2.954953	-1.201488
H	2.940909	-3.235750	-1.153605
H	1.365409	-3.733619	-1.766469
H	1.792945	-2.017794	-1.754572
C	4.396748	1.169672	-0.401887
H	5.060307	0.717163	-1.144346
H	4.425136	2.252203	-0.557651
H	4.816918	0.954567	0.585800
C	1.619046	3.107031	-1.204050
H	0.853952	2.558995	-1.757951
H	1.333334	4.162317	-1.156741
H	2.553534	3.047376	-1.767898
Cu	0.000023	0.000849	0.070127
Br	-0.000774	0.000149	-2.285134

[MMA--Br--Cu(L_4)]‡

ω-B97XD SCF energy: -4044.90361402 a.u.
ω-B97XD enthalpy: -4044.108847 a.u.
ω-B97XD free energy: -4044.216196 a.u.
ω-B97XD SCF energy in solution: -5491.43389956 a.u.
ω-B97XD enthalpy in solution: -5490.639133 a.u.
ω-B97XD free energy in solution: -5490.746482 a.u.
Imaginary frequency: -496.8001 cm-1

Cartesian coordinates

ATOM	X	Y	Z
N	0.155259	0.017463	2.312222
N	1.856856	1.171408	0.219773
N	-1.991534	1.239117	0.726385
N	-0.139597	-2.171969	0.384561
C	-1.233710	-2.759988	-0.424586
H	-1.035541	-2.522471	-1.468976
H	-2.148638	-2.222572	-0.152347
C	-1.076378	0.534465	2.935037
H	-0.875468	0.894203	3.954436
H	-1.788777	-0.287654	3.031445
C	2.760948	0.666305	-0.846585
H	2.274009	0.858215	-1.803864
H	2.794427	-0.421652	-0.735246
C	0.396966	-1.388982	2.683870
H	0.163134	-1.554354	3.745379
H	1.461899	-1.599608	2.564077
C	1.695379	2.648721	0.165188
H	0.908319	2.914482	0.877349
H	2.616913	3.128496	0.528344
C	-2.177614	2.433065	-0.137362

H	-2.283388	2.076225	-1.163070
H	-1.237267	2.991973	-0.104446
C	-1.689945	1.655759	2.108963
H	-2.591147	2.016525	2.625192
H	-0.996210	2.501785	2.058103
C	-0.418548	-2.339767	1.820131
H	-1.487254	-2.158818	1.976877
H	-0.222439	-3.369545	2.153119
C	1.317348	0.864927	2.634550
H	0.975649	1.896211	2.748263
H	1.755651	0.573940	3.599953
C	2.378136	0.785949	1.546751
H	2.757372	-0.238172	1.470009
H	3.228782	1.417230	1.840495
C	-3.189394	0.356433	0.728928
H	-3.977018	0.814421	1.346959
H	-2.906285	-0.573562	1.230822
C	1.177313	-2.779522	0.060939
H	1.230857	-3.790557	0.493803
H	1.944168	-2.187129	0.571001
C	-3.334775	3.359195	0.232417
H	-3.213333	3.804189	1.224943
H	-3.374677	4.179044	-0.490797
H	-4.302862	2.850159	0.202060
C	-3.757374	0.018297	-0.642872
H	-4.237055	0.879704	-1.115771
H	-2.989183	-0.354315	-1.323746
H	-4.523206	-0.754427	-0.521034
C	-1.458116	-4.262803	-0.276790
H	-2.253124	-4.564581	-0.964813
H	-0.569480	-4.841420	-0.546334
H	-1.761988	-4.548559	0.735661
C	1.515678	-2.844392	-1.422053
H	2.544876	-3.200847	-1.530794
H	0.865512	-3.529621	-1.972219
H	1.431610	-1.862851	-1.893042
C	4.182669	1.224014	-0.845147
H	4.739392	0.766469	-1.668201
H	4.207292	2.307282	-0.997497
H	4.720773	0.996403	0.080395
C	1.334654	3.213580	-1.200738
H	0.475275	2.699535	-1.637724
H	1.088430	4.273701	-1.086996
H	2.164631	3.145738	-1.909228
Cu	-0.114175	0.120834	0.159625
Br	-0.445839	0.141953	-2.229105
C	-0.938073	-0.802079	-4.573499
C	0.434658	-1.204139	-5.005111
C	-1.786418	-1.885900	-4.028015
C	-1.575784	0.382762	-5.226690
H	0.386196	-1.611993	-6.025895
H	1.107735	-0.342482	-5.025971
H	0.844102	-1.982075	-4.358979
O	-1.370566	-2.982605	-3.701726
O	-3.073212	-1.524615	-3.903848
H	-1.874186	0.115357	-6.251601

H	-2.469667	0.713670	-4.696671
H	-0.865264	1.211017	-5.297973
C	-3.938565	-2.514734	-3.353655
H	-3.895346	-3.435972	-3.938808
H	-3.657998	-2.734618	-2.319085
H	-4.937701	-2.082194	-3.389745

$[Cu^{I}L_5]^{+}$

ω-B97XD SCF energy: -891.34053933 a.u.
ω-B97XD enthalpy: -890.878772 a.u.
ω-B97XD free energy: -890.944536 a.u.
ω-B97XD SCF energy in solution: -2334.87195140 a.u.
ω-B97XD enthalpy in solution: -2334.410184 a.u.
ω-B97XD free energy in solution: -2334.475948 a.u.

Cartesian coordinates

ATOM	X	Y	Z
Cu	-0.000907	0.002375	-0.623937
C	1.294517	-2.629815	-1.399418
H	2.235390	-2.087066	-1.290371
H	0.930879	-2.495736	-2.420905
H	1.482960	-3.700902	-1.230314
C	2.950587	0.604414	-0.633700
H	3.007711	0.217565	-1.653910
H	3.026962	-0.236552	0.058403
H	3.806114	1.275679	-0.462037
C	-0.954166	-2.855310	-0.630720
H	-1.720238	-2.496068	0.059267
H	-0.802382	-3.931137	-0.452792
H	-1.316791	-2.717656	-1.652133
C	-2.002270	2.254005	-0.630476
H	-3.011976	2.657128	-0.457264
H	-1.698270	2.497372	-1.651158
H	-1.312874	2.743113	0.060525
N	0.002578	-0.002453	1.613775
N	0.297457	-2.102118	-0.451028
N	1.672204	1.310471	-0.449204
N	-1.971079	0.793582	-0.447034
C	-2.928703	0.190066	-1.390548
H	-2.921857	-0.896202	-1.282212
H	-2.636577	0.440297	-2.413113
H	-3.951656	0.556424	-1.215714
C	0.022129	-1.425030	1.960156
H	-1.010859	-1.779201	2.020107
H	0.463553	-1.597898	2.953572
C	0.797253	-2.255760	0.933036
H	1.847978	-1.948372	0.937372
H	0.776802	-3.314868	1.235230
C	1.557399	1.814432	0.937284
H	0.766225	2.570541	0.945021
H	2.485469	2.324475	1.240184
C	-1.238338	0.692761	1.963734
H	-1.026453	1.764067	2.021323
H	-1.606876	0.399893	2.958689

C	1.627420	2.440411	-1.394176
H	0.683327	2.978014	-1.287806
H	1.698136	2.059956	-2.415885
H	2.456054	3.143858	-1.221275
C	1.226353	0.723495	1.960291
H	1.161440	1.186720	2.956708
H	2.047748	0.003201	2.011532
C	-2.348679	0.439016	0.939371
H	-2.608337	-0.624253	0.943814
H	-3.254434	0.986244	1.244755

[Br-Cu^{II}L$_5$]$^+$

ω-B97XD SCF energy: -3462.81516241 a.u.
ω-B97XD enthalpy: -3462.349364 a.u.
ω-B97XD free energy: -3462.420433 a.u.
ω-B97XD SCF energy in solution: -4909.13744332 a.u.
ω-B97XD enthalpy in solution: -4908.671645 a.u.
ω-B97XD free energy in solution: -4908.742714 a.u.

Cartesian coordinates

ATOM	X	Y	Z
Cu	-0.113567	-0.000264	-0.000039
N	1.987584	0.003362	0.003126
N	0.129478	2.042787	0.779978
N	0.134754	-1.697220	1.378526
N	0.137552	-0.345430	-2.158922
C	-0.736354	-1.393681	-2.718138
H	-1.777786	-1.114363	-2.556123
H	-0.552115	-2.341962	-2.209484
H	-0.550108	-1.521756	-3.793612
C	2.448060	-1.259393	0.630900
H	3.487325	-1.158067	0.970213
H	2.440413	-2.041286	-0.131342
C	-0.747274	3.047580	0.150532
H	-1.787703	2.761127	0.306545
H	-0.558677	3.083614	-0.924099
H	-0.567943	4.043251	0.579573
C	2.449151	0.091591	-1.404098
H	3.488978	-0.251470	-1.484755
H	2.439873	1.142175	-1.701428
C	-0.178221	1.993449	2.220926
H	-0.050834	2.982054	2.684523
H	0.479222	1.284830	2.730568
H	-1.211468	1.663646	2.348399
C	-0.744298	-1.659794	2.561974
H	-1.784136	-1.660281	2.233896
H	-0.563852	-0.745535	3.130568
H	-0.559938	-2.527546	3.210604
C	1.547505	-1.655761	1.791682
H	1.875028	-2.624100	2.197614
H	1.634833	-0.928529	2.604913
C	1.551811	-0.718671	-2.328256
H	1.642514	-1.786169	-2.104109
H	1.879963	-0.585443	-3.369535

C	2.444315	1.179231	0.784156
H	2.434423	0.910704	1.842483
H	3.483733	1.424538	0.529414
C	1.542985	2.381622	0.544311
H	1.634947	2.722569	-0.491619
H	1.866694	3.217505	1.181653
C	-0.165534	-2.921460	0.614412
H	0.494967	-3.006147	-0.251990
H	-1.197763	-2.871286	0.261466
H	-0.036855	-3.816699	1.239404
C	-0.167458	0.926925	-2.838102
H	-0.041007	0.832213	-3.925996
H	0.492592	1.721146	-2.480695
H	-1.199706	1.205996	-2.616157
Br	-2.463882	-0.002897	-0.002586

[MMA--Br--Cu(L_5)]‡

ω-B97XD SCF energy: -3809.07611895 a.u.
ω-B97XD enthalpy: -3808.464274 a.u.
ω-B97XD free energy: -3808.556945 a.u.
ω-B97XD SCF energy in solution: -5255.51763100 a.u.
ω-B97XD enthalpy in solution: -5254.905786 a.u.
ω-B97XD free energy in solution: -5254.998457 a.u.
Imaginary frequency: -520.4314 cm-1

Cartesian coordinates

ATOM	X	Y	Z
Cu	-0.955238	-0.306898	-0.209813
N	-2.897405	0.647243	-0.091864
N	-0.356109	1.659356	-1.066141
N	-1.964542	-1.750144	-1.435236
N	-1.197410	-0.423771	2.005508
C	-0.814682	-1.713602	2.599954
H	0.238968	-1.903569	2.388957
H	-1.404848	-2.519076	2.157301
H	-0.974586	-1.711819	3.688400
C	-3.853420	-0.324301	-0.656119
H	-4.771637	0.176047	-0.995156
H	-4.149542	-1.015596	0.136301
C	0.902951	2.211483	-0.539865
H	1.727234	1.530277	-0.752890
H	0.830416	2.326033	0.543850
H	1.119898	3.192080	-0.987879
C	-3.171711	0.932391	1.329265
H	-4.250250	1.055354	1.503858
H	-2.705440	1.887761	1.580765
C	-0.210909	1.472867	-2.517828
H	0.038362	2.420250	-3.019010
H	-1.136787	1.085759	-2.951192
H	0.587300	0.750343	-2.703110
C	-1.221614	-2.137490	-2.648952
H	-0.287426	-2.620705	-2.360326
H	-0.980924	-1.248307	-3.235224
H	-1.814621	-2.826324	-3.267624

C	-3.234717	-1.099810	-1.814453
H	-3.957302	-1.840502	-2.188642
H	-3.019381	-0.420956	-2.645418
C	-2.626380	-0.162890	2.239569
H	-3.163560	-1.099582	2.058250
H	-2.815807	0.109717	3.289389
C	-2.828379	1.882970	-0.895004
H	-3.003430	1.623202	-1.941789
H	-3.626957	2.581799	-0.607922
C	-1.472386	2.565014	-0.751878
H	-1.335842	2.910082	0.277932
H	-1.448173	3.462819	-1.388969
C	-2.208680	-2.958307	-0.628281
H	-2.783040	-2.710153	0.267061
H	-1.249809	-3.378739	-0.317532
H	-2.765465	-3.712045	-1.204270
C	-0.349530	0.625232	2.590113
H	-0.462239	0.665829	3.684469
H	-0.609458	1.603105	2.177900
H	0.693416	0.410020	2.343374
Br	1.241016	-1.257231	-0.231817
C	3.743079	-1.311922	0.395803
C	4.367779	-1.490930	-0.949814
C	3.701252	0.075532	0.909714
C	3.768069	-2.458068	1.356419
H	5.459966	-1.558132	-0.834143
H	4.029361	-2.419126	-1.418254
H	4.155950	-0.644649	-1.605033
O	3.916216	1.063687	0.235551
O	3.383559	0.138690	2.217394
H	4.781564	-2.564379	1.771288
H	3.085027	-2.308428	2.193985
H	3.521300	-3.393886	0.847523
C	3.384677	1.449613	2.778909
H	4.361358	1.922073	2.652197
H	2.627353	2.077013	2.299498
H	3.158902	1.316120	3.836434

$[Cu^{I}L_6]^{+}$

ω-B97XD SCF energy: -930.65009642 a.u.
ω-B97XD enthalpy: -930.157817 a.u.
ω-B97XD free energy: -930.227658 a.u.
ω-B97XD SCF energy in solution: -2374.19413157 a.u.
ω-B97XD enthalpy in solution: -2373.701852 a.u.
ω-B97XD free energy in solution: -2373.771693 a.u.

Cartesian coordinates

ATOM	X	Y	Z
Cu	-0.064480	-0.315348	-0.074493
N	-1.232106	1.295173	0.900649
C	-0.779956	2.640518	0.490190
H	-1.253875	2.879420	-0.467307
H	-1.140044	3.387967	1.214166
C	0.736393	2.778719	0.319979

H	1.261461	2.317925	1.165614
H	0.973264	3.847271	0.374857
C	1.285384	2.268606	-1.017251
H	0.594695	2.570115	-1.812048
H	2.245558	2.762465	-1.235378
N	1.462609	0.802396	-1.119474
C	2.704330	0.390225	-0.435243
H	3.580644	0.579707	-1.074114
H	2.829326	1.011009	0.455428
C	2.679475	-1.080424	-0.036667
H	3.632013	-1.344239	0.448505
H	2.593292	-1.706018	-0.930164
N	1.537264	-1.397205	0.843531
C	1.310665	-2.850349	0.859904
H	2.197114	-3.393491	1.221754
H	1.069656	-3.198856	-0.147315
C	-2.006288	-2.550405	-0.590165
H	-1.291358	-3.005037	-1.280130
H	-3.016252	-2.906046	-0.844895
N	-1.912106	-1.084458	-0.681729
C	-2.863281	-0.471538	0.269181
H	-2.754616	-0.993815	1.225089
H	-3.900886	-0.624867	-0.066782
C	-2.612608	1.020772	0.460044
H	-2.783217	1.540269	-0.486164
H	-3.349652	1.418465	1.174004
C	-1.121468	1.148081	2.357304
H	-0.093066	1.333305	2.674026
H	-1.385783	0.130548	2.656564
H	-1.780964	1.854325	2.886267
C	1.514578	0.419154	-2.539067
H	0.558805	0.650334	-3.015547
H	1.688454	-0.654996	-2.635414
H	2.316184	0.952399	-3.073969
C	1.796648	-0.942680	2.217627
H	0.928805	-1.164635	2.842933
H	1.964498	0.136140	2.238733
C	-2.205419	-0.675836	-2.065788
H	-1.503294	-1.170206	-2.741313
H	-2.083236	0.403015	-2.182328
H	-3.230714	-0.951272	-2.357720
H	2.678500	-1.443049	2.646719
H	-1.766030	-2.873024	0.425625
H	0.470298	-3.080427	1.519481

$[Br\text{-}Cu^{II}L_6]^+$

ω-B97XD SCF energy: -3502.10368323 a.u.
ω-B97XD enthalpy: -3501.605598 a.u.
ω-B97XD free energy: -3501.678192 a.u.
ω-B97XD SCF energy in solution: -4948.44295180 a.u.
ω-B97XD enthalpy in solution: -4947.944867 a.u.
ω-B97XD free energy in solution: -4948.017461 a.u.

Cartesian coordinates

ATOM	X	Y	Z
Cu	-0.094356	-0.036347	-0.092818
Br	-0.895972	-0.119599	2.218465
N	-1.525208	1.465845	-0.984031
C	-1.103914	2.646250	-0.200906
H	-1.335457	2.442858	0.848704
H	-1.672984	3.534605	-0.513656
C	0.372869	2.905134	-0.375589
H	0.672233	3.780939	0.210918
H	0.596220	3.141333	-1.418231
N	1.179495	1.720422	0.037024
C	2.355769	1.652274	-0.870752
H	2.885762	2.613730	-0.808547
H	1.971308	1.561908	-1.893994
C	3.344474	0.523933	-0.620119
H	3.709418	0.530182	0.410818
H	4.223896	0.736300	-1.238185
C	2.837315	-0.847905	-1.038739
H	2.506726	-0.791598	-2.082675
H	3.662293	-1.575256	-0.999219
N	1.702112	-1.362320	-0.241646
C	1.212549	-2.609679	-0.866009
H	1.238470	-2.490788	-1.952684
H	1.877809	-3.449522	-0.623017
C	-0.193142	-2.915444	-0.403972
H	-0.228888	-3.046046	0.680048
H	-0.543118	-3.851314	-0.861397
N	-1.120364	-1.812860	-0.744792
C	-2.414711	-2.121720	-0.094629
H	-2.278415	-2.143715	0.985502
H	-2.787134	-3.090556	-0.453347
C	-2.944927	1.223217	-0.668679
H	-3.538263	2.133093	-0.835629
H	-3.034242	0.916100	0.375956
C	-1.383691	1.719830	-2.429628
H	-1.864709	0.919672	-2.992474
H	-0.332136	1.747546	-2.722929
H	-1.856611	2.670636	-2.714463
C	1.622533	1.950721	1.433538
H	0.759044	2.192291	2.051084
H	2.349461	2.773434	1.460155
H	2.069406	1.055480	1.856739
C	2.154076	-1.678159	1.132474
H	2.543271	-0.789124	1.621623
H	2.946055	-2.439244	1.103127
H	1.319318	-2.029565	1.737300
C	-1.321660	-1.747605	-2.206007
H	-0.442524	-1.336478	-2.708834
H	-2.174167	-1.104454	-2.421397
H	-1.533499	-2.743231	-2.618298
H	-3.147436	-1.354252	-0.330997
H	-3.343268	0.442388	-1.318320

[MMA--Br--Cu(L_6)]‡

ω-B97XD SCF energy: -3848.36524979 a.u.
ω-B97XD enthalpy: -3847.722650 a.u.
ω-B97XD free energy: -3847.819416 a.u.
ω-B97XD SCF energy in solution: -5294.83208105 a.u.
ω-B97XD enthalpy in solution: -5294.189481 a.u.
ω-B97XD free energy in solution: -5294.286247 a.u.
Imaginary frequency: -803.4894 cm-1

Cartesian coordinates

ATOM	X	Y	Z
Cu	-0.089041	0.012925	0.050205
Br	-0.980507	0.253707	2.308233
N	-1.631132	1.684832	-1.086429
C	-1.000489	2.819397	-0.403883
H	-1.207206	2.724573	0.667330
H	-1.437770	3.774833	-0.741609
C	0.495446	2.861704	-0.639328
H	0.910784	3.786436	-0.219684
H	0.700134	2.894022	-1.711513
N	1.211590	1.690355	-0.054930
C	2.376062	1.411308	-0.942973
H	2.953498	2.343668	-1.034695
H	1.972501	1.184406	-1.937162
C	3.323856	0.291035	-0.528578
H	3.649574	0.407745	0.509234
H	4.232240	0.417117	-1.128317
C	2.808569	-1.115520	-0.808381
H	2.528617	-1.173876	-1.866635
H	3.619943	-1.844581	-0.650109
N	1.629426	-1.496739	-0.015044
C	1.028841	-2.731044	-0.549866
H	1.074367	-2.691026	-1.642062
H	1.606567	-3.616366	-0.242748
C	-0.409765	-2.885996	-0.091294
H	-0.474049	-2.997189	0.994762
H	-0.834404	-3.801070	-0.530579
N	-1.235698	-1.718196	-0.463375
C	-2.555661	-1.875985	0.177711
H	-2.423628	-2.018022	1.250142
H	-3.073539	-2.751727	-0.237899
C	-3.028816	1.602239	-0.652999
H	-3.573848	2.538801	-0.854127
H	-3.067008	1.392560	0.419437
C	-1.577445	1.845733	-2.542545
H	-2.181253	1.071573	-3.020658
H	-0.555297	1.737843	-2.914352
H	-1.968225	2.824983	-2.864515
C	1.684463	2.076578	1.293730
H	0.851255	2.482173	1.866621
H	2.478238	2.832914	1.215640
H	2.059124	1.211964	1.838644
C	2.006818	-1.709183	1.392092
H	2.445011	-0.805447	1.813941
H	2.739591	-2.526528	1.480986
H	1.125784	-1.940817	1.990123
C	-1.419230	-1.646031	-1.923219

H	-0.489716	-1.366361	-2.426921
H	-2.167944	-0.886680	-2.145434
H	-1.766081	-2.608503	-2.326434
H	-3.157129	-0.984942	0.004088
H	-3.537310	0.796588	-1.189426
C	-1.693193	-1.084880	4.445146
C	-3.176671	-0.995745	4.291669
C	-1.061407	-2.334441	3.972231
C	-1.035132	-0.284731	5.522723
H	-3.655405	-1.477375	5.157798
H	-3.507512	0.046077	4.272240
H	-3.523129	-1.510122	3.394215
O	-1.564743	-3.105237	3.172310
O	0.146463	-2.544053	4.520877
H	-1.198374	-0.777130	6.493049
H	0.042327	-0.199727	5.374923
H	-1.474140	0.714758	5.581303
C	0.751749	-3.801462	4.223204
H	0.113312	-4.620738	4.562177
H	0.923957	-3.911181	3.149193
H	1.698098	-3.805672	4.762315

$[Cu^{I}L_{7}]^{+}$

ω-B97XD SCF energy: -891.34525004 a.u.
ω-B97XD enthalpy: -890.883375 a.u.
ω-B97XD free energy: -890.951220 a.u.
ω-B97XD SCF energy in solution: -2334.87612921 a.u.
ω-B97XD enthalpy in solution: -2334.414254 a.u.
ω-B97XD free energy in solution: -2334.482099 a.u.

Cartesian coordinates

ATOM	X	Y	Z
Cu	-0.035532	0.401885	0.108087
N	1.738426	1.290303	-0.518975
N	-1.058633	-1.330441	-0.939590
N	-1.947196	1.036739	0.552095
C	1.625505	1.874284	-1.865707
H	1.296777	1.109345	-2.573947
H	2.586074	2.287358	-2.208973
H	0.884787	2.677289	-1.851809
C	2.124714	2.346250	0.433414
H	2.182249	1.943632	1.446790
H	1.368642	3.134543	0.422872
H	3.099087	2.784852	0.169322
C	2.733047	0.198359	-0.528595
H	2.560823	-0.388650	-1.436193
H	3.754405	0.603046	-0.600231
C	2.632048	-0.698084	0.703591
H	3.379118	-1.502770	0.623008
H	2.887850	-0.126353	1.600353
C	1.004971	-2.363696	-0.022843
H	1.402066	-3.302879	0.393118
H	1.537474	-2.189139	-0.961638
C	-0.485832	-2.530564	-0.314432

H	-0.631084	-3.423365	-0.941873
H	-1.016162	-2.716302	0.623650
C	-0.825261	-1.306845	-2.385432
H	-1.195069	-0.369134	-2.808742
H	-1.327061	-2.144232	-2.895819
H	0.245990	-1.366183	-2.596398
C	-2.477554	-1.108831	-0.622596
H	-2.717925	-1.631378	0.306722
H	-3.136631	-1.530997	-1.395125
C	-2.789759	0.378729	-0.471380
H	-2.606965	0.890565	-1.421989
H	-3.856796	0.508154	-0.232480
C	-2.340895	0.623726	1.911002
H	-3.397997	0.857442	2.108865
H	-1.720834	1.150815	2.639606
H	-2.184909	-0.448327	2.047173
C	-2.091736	2.499367	0.437778
H	-1.779785	2.823868	-0.558162
H	-1.456049	2.986571	1.180872
H	-3.133274	2.813483	0.603515
N	1.274359	-1.236154	0.887026
C	1.055291	-1.622303	2.285226
H	1.773513	-2.386988	2.619614
H	0.045848	-2.021134	2.411445
H	1.150341	-0.743278	2.927875

[Br-Cu^{II}L$_7$]$^+$

ω-B97XD SCF energy: -3462.79843157 a.u.
ω-B97XD enthalpy: -3462.331105 a.u.
ω-B97XD free energy: -3462.401686 a.u.
ω-B97XD SCF energy in solution: -4909.12722762 a.u.
ω-B97XD enthalpy in solution: -4908.659901 a.u.
ω-B97XD free energy in solution: -4908.730482 a.u.

Cartesian coordinates

ATOM	X	Y	Z
Cu	0.020012	-0.058429	-0.062902
N	1.359592	-1.648675	-0.599722
N	1.747135	1.212459	-0.415288
N	-0.982540	1.761889	-0.427888
N	-1.932312	-0.935528	-0.734982
C	1.452410	-2.685917	0.453208
H	1.709425	-2.218366	1.403411
H	2.201618	-3.439659	0.177649
H	0.481313	-3.167287	0.574764
C	0.959080	-2.293143	-1.864083
H	0.806065	-1.548147	-2.649254
H	0.031852	-2.841353	-1.709727
H	1.725274	-3.006329	-2.195215
C	2.691282	-1.016126	-0.783613
H	3.193374	-0.996033	0.184615
H	3.313104	-1.627114	-1.450110
C	2.558427	0.392147	-1.334722
H	3.554360	0.834929	-1.479853

H	2.060628	0.376835	-2.310850
C	2.495813	1.501100	0.827711
H	1.879944	2.098661	1.498217
H	3.425396	2.039826	0.599620
H	2.721896	0.581249	1.364050
C	1.290692	2.474046	-1.050668
H	1.928036	2.739379	-1.902040
H	1.387143	3.284451	-0.325693
C	-0.157316	2.349845	-1.504321
H	-0.544835	3.331796	-1.810862
H	-0.223191	1.682975	-2.372459
C	-1.040355	2.638065	0.762552
H	-1.736336	2.215258	1.486169
H	-1.369877	3.644279	0.471258
H	-0.073446	2.692811	1.256514
C	-2.366567	1.477781	-0.880530
H	-2.390838	1.444045	-1.972379
H	-3.039474	2.286400	-0.575569
C	-2.819705	0.160016	-0.283613
H	-2.759670	0.204620	0.808082
H	-3.862515	-0.050629	-0.561227
C	-2.149719	-1.182690	-2.174984
H	-3.223102	-1.226883	-2.405790
H	-1.709209	-2.135431	-2.463383
H	-1.690839	-0.401169	-2.785027
C	-2.273427	-2.153833	0.027143
H	-2.070566	-1.983922	1.086254
H	-1.661421	-2.989349	-0.320006
H	-3.330262	-2.417572	-0.116112
Br	-0.185743	-0.297502	2.354280

[MMA--Br--Cu(L7)]‡

ω-B97XD SCF energy: -3809.06221457 a.u.
ω-B97XD enthalpy: -3808.450303 a.u.
ω-B97XD free energy: -3808.544012 a.u.
ω-B97XD SCF energy in solution: -5255.51663555 a.u.
ω-B97XD enthalpy in solution: -5254.904724 a.u.
ω-B97XD free energy in solution: -5254.998433 a.u.
Imaginary frequency: -463.8756 cm-1

Cartesian coordinates

ATOM	X	Y	Z
Cu	-0.113335	0.383257	0.324321
N	1.296360	-1.476267	-0.692988
N	1.709269	1.483140	-0.082363
N	-0.961587	1.727071	-1.116381
N	-2.170531	-0.479459	0.208703
C	1.234934	-2.769646	0.000171
H	1.195132	-2.607531	1.080070
H	2.108690	-3.395894	-0.242269
H	0.337727	-3.311282	-0.305943
C	1.160520	-1.702108	-2.133356
H	1.168291	-0.758012	-2.683864
H	0.207905	-2.198153	-2.338198

H	1.968599	-2.337780	-2.531426
C	2.583570	-0.847019	-0.372451
H	2.722283	-0.911005	0.711340
H	3.417191	-1.397523	-0.841530
C	2.656315	0.604048	-0.812172
H	3.679459	0.978175	-0.670720
H	2.447973	0.679551	-1.881972
C	2.358387	2.003985	1.138650
H	1.629642	2.552490	1.738693
H	3.193824	2.668674	0.877198
H	2.730340	1.175580	1.741393
C	1.315116	2.616918	-0.949717
H	2.177124	2.982057	-1.524710
H	1.001986	3.439959	-0.303067
C	0.181336	2.226994	-1.892129
H	-0.098720	3.087567	-2.517169
H	0.506954	1.431307	-2.569456
C	-1.700745	2.843483	-0.504474
H	-2.425037	2.475835	0.222169
H	-2.228930	3.432589	-1.268508
H	-1.015861	3.500309	0.032508
C	-1.853072	0.844071	-1.881783
H	-1.230962	0.090898	-2.377692
H	-2.399524	1.395178	-2.662711
C	-2.846341	0.165308	-0.943582
H	-3.563038	0.899001	-0.567547
H	-3.432590	-0.570210	-1.507918
C	-2.044182	-1.926195	-0.021685
H	-3.033905	-2.400703	-0.087012
H	-1.500895	-2.373702	0.812064
H	-1.505223	-2.102596	-0.954806
C	-2.950549	-0.272669	1.443996
H	-2.944765	0.785911	1.716707
H	-2.502860	-0.851662	2.252412
H	-3.988161	-0.608181	1.307629
Br	0.336093	-0.342218	2.555482
C	-0.246684	-1.705261	4.656575
C	-1.281845	-0.835180	5.290844
C	-0.748774	-2.822305	3.822376
C	1.090557	-1.820485	5.315795
H	-1.605636	-1.295967	6.236225
H	-0.872483	0.150195	5.528720
H	-2.163826	-0.727632	4.658134
O	-1.875557	-2.886760	3.365504
O	0.185191	-3.759414	3.602287
H	1.004731	-2.475148	6.195934
H	1.839813	-2.257019	4.654011
H	1.435391	-0.843102	5.664319
C	-0.235146	-4.875893	2.820391
H	-1.109036	-5.352704	3.269493
H	-0.486208	-4.560036	1.803641
H	0.611679	-5.560730	2.806681

$[Cu^{I}L_8]^{+}$

ω-B97XD SCF energy: -968.74944587 a.u.
ω-B97XD enthalpy: -968.249541 a.u.
ω-B97XD free energy: -968.316676 a.u.
ω-B97XD SCF energy in solution: -2412.30289406 a.u.
ω-B97XD enthalpy in solution: -2411.802989 a.u.
ω-B97XD free energy in solution: -2411.870124 a.u.

Cartesian coordinates

ATOM	X	Y	Z
Cu	-0.000026	-0.000232	-0.297226
N	-1.917786	0.488016	-0.875493
N	0.096000	1.862688	0.804594
N	1.917862	-0.488669	-0.875171
N	-0.096147	-1.862036	0.805132
C	1.395612	2.479428	0.471386
C	2.589134	1.516794	0.575511
C	2.855542	0.641655	-0.654766
C	2.244269	-1.627105	0.015208
C	1.053461	-2.568295	0.210711
C	-1.395815	-2.479501	0.473343
C	-2.589333	-1.516760	0.576154
C	-2.855200	-0.642475	-0.654855
H	1.572340	3.352563	1.119095
H	1.336786	2.854168	-0.556118
H	2.511963	0.904847	1.482135
H	3.489343	2.126160	0.714745
H	2.807248	1.276639	-1.545728
H	3.882631	0.247415	-0.604959
H	2.556244	-1.223699	0.982144
H	3.099340	-2.192922	-0.384131
H	0.744436	-2.975119	-0.756170
H	1.367011	-3.422719	0.830068
H	-1.572321	-3.351412	1.122743
H	-1.337281	-2.856127	-0.553487
H	-2.512573	-0.904222	1.482420
H	-3.489579	-2.126069	0.715422
H	-2.806138	-1.278033	-1.545364
H	-3.882460	-0.248560	-0.605956
C	2.006323	-0.910764	-2.285065
H	1.667211	-0.098401	-2.931644
H	3.038821	-1.178372	-2.557745
H	1.362911	-1.774944	-2.461479
C	-2.006051	0.909452	-2.285594
H	-1.666868	0.096761	-2.931719
H	-3.038507	1.176949	-2.558554
H	-1.362593	1.773518	-2.462399
C	0.066166	-1.758284	2.258688
H	0.995904	-1.237881	2.499652
H	-0.755705	-1.186323	2.692819
H	0.087674	-2.752110	2.732908
C	-0.066017	1.761404	2.258329
H	-0.995888	1.241704	2.500332
H	0.755749	1.189955	2.693322
H	-0.087157	2.756018	2.730929
C	-1.053631	2.568205	0.209375
H	-0.744534	2.974306	-0.757794

H	-1.367420	3.423154	0.827895
C	-2.244389	1.626798	0.014346
H	-2.556322	1.223774	0.981452
H	-3.099452	2.192386	-0.385324

[Br-Cu^{II}L$_8$]$^+$

ω-B97XD SCF energy: -3540.21551240 a.u.
ω-B97XD enthalpy: -3539.709377 a.u.
ω-B97XD free energy: -3539.780873 a.u.
ω-B97XD SCF energy in solution: -4986.56476382 a.u.
ω-B97XD enthalpy in solution: -4986.058628 a.u.
ω-B97XD free energy in solution: -4986.130124 a.u.

Cartesian coordinates

ATOM	X	Y	Z
N	0.999800	-1.817907	-0.695923
N	-1.784148	-1.166550	-0.171236
N	-0.999803	1.817847	-0.696001
N	1.784161	1.166573	-0.171295
C	-0.084684	-2.752746	-1.062878
C	-2.946859	0.535537	-1.682497
C	-1.865212	1.590333	-1.872686
C	0.084642	2.752737	-1.062958
C	1.283566	2.563728	-0.156569
C	1.865266	-1.590457	-1.872587
C	1.773651	-2.411727	0.414829
H	0.262459	-3.792937	-0.996978
H	-0.355373	-2.582785	-2.107559
H	-3.654698	0.823196	-0.900920
H	-3.532696	0.521158	-2.608444
H	-2.333182	2.541572	-2.169482
H	-1.214711	1.278124	-2.698745
H	-0.262534	3.792917	-0.997050
H	0.355312	2.582794	-2.107645
H	1.019596	2.794804	0.878303
H	2.086156	3.253596	-0.453493
H	2.333243	-2.541714	-2.169318
H	1.214794	-1.278296	-2.698686
H	2.520692	-1.712477	0.780887
H	2.271945	-3.333361	0.082539
H	1.115107	-2.630112	1.255305
C	-1.773785	2.411589	0.414704
H	-2.272200	3.333142	0.082369
H	-2.520741	1.712225	0.780740
H	-1.115318	2.630089	1.255206
C	2.423139	0.882622	-1.482913
H	3.249483	1.595304	-1.620731
H	1.690202	1.084791	-2.269951
C	2.946901	-0.535630	-1.682452
H	3.654755	-0.823232	-0.900871
H	3.532734	-0.521296	-2.608402
C	-2.423113	-0.882702	-1.482874
H	-3.249472	-1.595379	-1.620627
H	-1.690179	-1.084951	-2.269896

C	-2.794163	-1.074543	0.908206
H	-3.598976	-1.799029	0.724808
H	-2.314453	-1.272952	1.865007
H	-3.226490	-0.078469	0.957198
C	2.794156	1.074722	0.908178
H	3.598958	1.799197	0.724693
H	2.314419	1.273265	1.864937
H	3.226501	0.078671	0.957334
C	-1.283564	-2.563707	-0.156441
H	-2.086165	-3.253585	-0.453312
H	-1.019549	-2.794742	0.878430
Cu	0.000015	0.000003	0.080468
Br	0.000006	0.000061	2.502446

[MMA--Br--Cu(L$_8$)]‡

ω-B97XD SCF energy: -3886.47471765 a.u.
ω-B97XD enthalpy: -3885.823910 a.u.
ω-B97XD free energy: -3885.918384 a.u.
ω-B97XD SCF energy in solution: -5332.95250215 a.u.
ω-B97XD enthalpy in solution: -5332.301694 a.u.
ω-B97XD free energy in solution: -5332.396169 a.u.
Imaginary frequency: -1241.2860 cm-1

Cartesian coordinates

ATOM	X	Y	Z
N	0.944568	-1.970656	-0.857169
N	-1.867085	-1.240992	-0.372119
N	-0.946791	1.822873	-0.282996
N	1.775113	0.910988	0.310555
C	-0.162475	-2.699977	-1.490988
C	-2.874696	0.805113	-1.557542
C	-1.773770	1.859330	-1.500086
C	0.215136	2.718163	-0.425276
C	1.346273	2.314774	0.506950
C	1.943845	-1.576733	-1.863507
C	1.556683	-2.820072	0.175406
H	0.095186	-3.758266	-1.651555
H	-0.338900	-2.274223	-2.481992
H	-3.609595	0.944341	-0.759730
H	-3.425932	0.986802	-2.487199
H	-2.223815	2.858579	-1.620716
H	-1.103441	1.703472	-2.353730
H	-0.064911	3.761822	-0.216205
H	0.545960	2.691765	-1.466627
H	1.041771	2.418068	1.552110
H	2.197236	2.996700	0.356414
H	2.442040	-2.471862	-2.271778
H	1.405584	-1.103510	-2.693802
H	2.339584	-2.279155	0.704795
H	1.993129	-3.727677	-0.270114
H	0.813475	-3.107824	0.920357
C	-1.730009	2.231711	0.893664
H	-2.126936	3.251098	0.766590
H	-2.562645	1.550024	1.058753

H	-1.108718	2.188698	1.788563
C	2.471395	0.787884	-0.993730
H	3.311969	1.499831	-0.999003
H	1.780985	1.105554	-1.782048
C	2.999257	-0.596978	-1.362023
H	3.596034	-1.026335	-0.552752
H	3.703375	-0.450674	-2.189062
C	-2.388310	-0.641035	-1.628852
H	-3.214765	-1.274705	-1.986853
H	-1.596954	-0.692816	-2.382771
C	-2.949932	-1.317271	0.629837
H	-3.817925	-1.850197	0.215665
H	-2.587229	-1.836251	1.516109
H	-3.261792	-0.321918	0.940351
C	2.700818	0.578772	1.410869
H	3.645574	1.129768	1.295897
H	2.244386	0.856402	2.360386
H	2.910781	-0.489488	1.431512
C	-1.426830	-2.630578	-0.648697
H	-2.232255	-3.184805	-1.154077
H	-1.260231	-3.112877	0.317650
Cu	-0.097169	-0.205293	0.221526
Br	-0.231453	-0.671502	2.614103
C	0.204696	0.258433	4.964758
C	1.520902	-0.387576	5.258363
C	0.258060	1.662050	4.497279
C	-1.001272	-0.220993	5.708905
H	1.829613	-0.122196	6.280711
H	1.440266	-1.476782	5.211657
H	2.301550	-0.046368	4.577341
O	1.234696	2.184494	3.986834
O	-0.897098	2.316202	4.690612
H	-0.964798	0.160285	6.740307
H	-1.930191	0.132768	5.259796
H	-1.013551	-1.313009	5.759875
C	-0.884731	3.704692	4.362294
H	-0.105122	4.223839	4.924475
H	-0.705838	3.852460	3.293660
H	-1.869681	4.079816	4.636708

$[Cu^{I}L_{9}]^{+}$

ω-B97XD SCF energy: -967.53231998 a.u.
ω-B97XD enthalpy: -967.053777 a.u.
ω-B97XD free energy: -967.115322 a.u.
ω-B97XD SCF energy in solution: -2411.08281894 a.u.
ω-B97XD enthalpy in solution: -2410.604276 a.u.
ω-B97XD free energy in solution: -2410.665821 a.u.

Cartesian coordinates

ATOM	X	Y	Z
Cu	0.000028	0.000163	-0.726655
N	1.935309	-0.634618	-0.826425
N	-0.309899	-1.460675	0.896515
N	-1.935317	0.634764	-0.826342

N	0.309873	1.460422	0.896671
C	2.138641	-1.496412	0.365101
C	0.892508	-2.292924	0.753664
C	-1.530370	-2.252990	0.647545
C	-2.816146	-1.459547	0.398748
C	-2.868137	-0.525278	-0.815427
C	-2.138685	1.496322	0.365331
C	-0.892523	2.292721	0.754003
C	0.369925	0.681811	2.144755
C	-0.369902	-0.682219	2.144699
C	1.530321	2.252810	0.647823
C	2.816148	1.459462	0.398981
C	2.868205	0.525355	-0.815308
H	2.435160	-0.869986	1.203145
H	2.968922	-2.195618	0.190823
H	0.688279	-3.036398	-0.022070
H	1.112871	-2.852037	1.677486
H	-1.714240	-2.958329	1.474739
H	-1.334690	-2.855916	-0.245166
H	-3.145552	-0.944301	1.306354
H	-3.596015	-2.209954	0.221302
H	-2.658756	-1.100659	-1.723300
H	-3.899648	-0.147512	-0.903925
H	-2.435181	0.869729	1.203256
H	-2.968974	2.195553	0.191186
H	-0.688289	3.036318	-0.021609
H	-1.112855	2.851685	1.677925
H	-0.024909	1.267657	2.990358
H	1.421873	0.509255	2.373231
H	0.024975	-1.268168	2.990211
H	-1.421838	-0.509692	2.373247
H	1.714136	2.958060	1.475105
H	1.334643	2.855832	-0.244822
H	3.145531	0.944107	1.306533
H	3.595999	2.209919	0.221662
H	2.658893	1.100867	-1.723114
H	3.899706	0.147559	-0.903799
C	-2.171021	1.414777	-2.057157
H	-1.964974	0.792183	-2.930470
H	-3.211103	1.771644	-2.109526
H	-1.500258	2.276268	-2.085073
C	2.170964	-1.414420	-2.057385
H	1.964980	-0.791648	-2.930586
H	3.211019	-1.771359	-2.109804
H	1.500133	-2.275851	-2.085468

[Br-Cu^{II}L$_9$]$^+$

ω-B97XD SCF energy: -3539.00248393 a.u.
ω-B97XD enthalpy: -3538.518133 a.u.
ω-B97XD free energy: -3538.584187 a.u.
ω-B97XD SCF energy in solution: -4985.34662253 a.u.
ω-B97XD enthalpy in solution: -4984.862272 a.u.
ω-B97XD free energy in solution: -4984.928326 a.u.

Cartesian coordinates

ATOM	X	Y	Z
N	-1.903492	1.095446	0.179245
N	-0.035826	-0.535432	1.776374
N	1.853886	-0.846211	-0.710087
N	-0.892938	-1.669847	-0.771923
C	-2.266150	0.528098	1.501399
C	-1.038226	0.355475	2.385620
C	1.278009	-0.335795	2.432738
C	2.466489	-1.046271	1.783893
C	2.857217	-0.621022	0.367393
C	1.500534	-2.274880	-0.840800
C	0.150894	-2.414713	-1.511969
C	-1.252880	-2.368140	0.489884
C	-0.466746	-1.940820	1.754254
C	-2.070678	-1.535062	-1.668826
C	-3.217845	-0.681593	-1.145900
C	-2.903880	0.784864	-0.876651
H	-2.765448	-0.428743	1.366037
H	-2.986591	1.183591	2.007308
H	-0.563524	1.328131	2.541609
H	-1.351530	-0.017935	3.372750
H	1.218315	-0.640971	3.489063
H	1.471791	0.741064	2.410212
H	2.377948	-2.134761	1.866402
H	3.333482	-0.799660	2.407746
H	3.072057	0.449960	0.358130
H	3.779662	-1.152735	0.091342
H	1.475480	-2.735919	0.144371
H	2.264506	-2.809617	-1.419820
H	0.197149	-2.007070	-2.525048
H	-0.121784	-3.475471	-1.603959
H	-1.126975	-3.451082	0.358093
H	-2.315954	-2.216600	0.661601
H	-1.093098	-2.169704	2.628952
H	0.417361	-2.567832	1.855040
H	-2.452821	-2.536484	-1.917428
H	-1.704309	-1.088386	-2.598874
H	-3.712851	-1.147739	-0.288462
H	-3.979433	-0.685379	-1.933882
H	-2.528441	1.250553	-1.794328
H	-3.847091	1.290507	-0.624024
C	2.446388	-0.382696	-1.988550
H	2.717548	0.667353	-1.902052
H	3.335299	-0.980121	-2.230287
H	1.719639	-0.477148	-2.798090
C	-1.887086	2.574187	0.305103
H	-1.585834	3.024434	-0.639198
H	-2.890477	2.926730	0.579400
H	-1.169411	2.885116	1.061746
Cu	0.049447	0.233562	-0.293469
Br	1.161536	2.309861	-0.504415

[MMA--Br--Cu(L$_9$)]‡

ω-B97XD SCF energy: -3885.26251653 a.u.
ω-B97XD enthalpy: -3884.633001 a.u.
ω-B97XD free energy: -3884.722071 a.u.
ω-B97XD SCF energy in solution: -5331.73780658 a.u.
ω-B97XD enthalpy in solution: -5331.108291 a.u.
ω-B97XD free energy in solution: -5331.197361 a.u.
Imaginary frequency: -437.9173 cm-1

Cartesian coordinates

ATOM	X	Y	Z
N	-2.259319	0.914358	0.544048
N	0.247149	-0.387338	1.481276
N	1.421717	-0.241385	-1.441074
N	-1.070520	-1.630258	-0.829034
C	-2.127526	0.254171	1.867052
C	-0.694044	0.288787	2.385562
C	1.632890	0.041486	1.777169
C	2.705794	-0.418094	0.788824
C	2.623268	0.112456	-0.643433
C	1.288150	-1.704097	-1.591408
C	-0.147596	-2.099663	-1.879331
C	-0.922407	-2.404761	0.424317
C	0.082630	-1.847739	1.467095
C	-2.451884	-1.704332	-1.357606
C	-3.536207	-1.081287	-0.487017
C	-3.434128	0.417998	-0.221742
H	-2.462363	-0.778161	1.791455
H	-2.788162	0.740289	2.597688
H	-0.368044	1.328537	2.483120
H	-0.669313	-0.156603	3.393214
H	1.922780	-0.289461	2.787688
H	1.626999	1.136055	1.778144
H	2.833991	-1.505803	0.810781
H	3.650870	-0.023896	1.180144
H	2.676033	1.202184	-0.609544
H	3.515315	-0.239355	-1.186306
H	1.626806	-2.191416	-0.678947
H	1.938857	-2.069184	-2.398370
H	-0.467207	-1.652970	-2.825209
H	-0.214668	-3.191809	-2.000986
H	-0.630410	-3.439472	0.192430
H	-1.904944	-2.479362	0.886896
H	-0.231971	-2.213301	2.456725
H	1.059604	-2.294465	1.290113
H	-2.717294	-2.754196	-1.560497
H	-2.447393	-1.183237	-2.320759
H	-3.677431	-1.637770	0.444515
H	-4.478073	-1.221527	-1.030163
H	-3.424816	0.955200	-1.176378
H	-4.349739	0.723177	0.307803
C	1.565416	0.375596	-2.774717
H	1.646788	1.457233	-2.667935
H	2.461730	-0.009957	-3.282568
H	0.689090	0.157592	-3.389683
C	-2.492146	2.359029	0.769039
H	-2.530602	2.881422	-0.186853

H	-3.441827	2.505391	1.302975
H	-1.679201	2.787742	1.353148
Cu	-0.398859	0.449310	-0.462353
Br	0.359278	2.758148	-0.656867
C	1.958215	4.719925	-0.644799
C	1.886700	5.120575	0.794282
C	3.113502	3.868101	-1.014870
C	1.353882	5.630364	-1.667197
H	2.534589	5.994450	0.957878
H	0.868365	5.409122	1.069033
H	2.237739	4.320844	1.448253
O	3.796547	3.254624	-0.215978
O	3.313644	3.816206	-2.341597
H	2.005122	6.506922	-1.800431
H	1.246473	5.147079	-2.639015
H	0.378292	5.992419	-1.331307
C	4.421183	3.023683	-2.765226
H	5.340684	3.354341	-2.277509
H	4.252707	1.969103	-2.527544
H	4.486976	3.163280	-3.843470

$[Cu^{I}(TPMA^{*1})]^{+}$

ω-B97XD SCF energy: -1305.78529795 a.u.
ω-B97XD enthalpy: -1305.331762 a.u.
ω-B97XD free energy: -1305.412618 a.u.
ω-B97XD SCF energy in solution: -2749.45625369 a.u.
ω-B97XD enthalpy in solution: -2749.002718 a.u.
ω-B97XD free energy in solution: -2749.083574 a.u.

Cartesian coordinates

ATOM	X	Y	Z
Cu	-0.839685	-0.061414	-0.915875
N	1.182091	-0.088462	-0.582770
N	-1.821969	1.741104	-0.710827
N	-1.924908	-1.764665	-0.509696
N	-0.841240	0.075235	1.320441
C	3.855684	-0.213698	0.146660
C	1.553753	0.203736	0.676914
C	-2.702291	-2.461531	-1.349111
H	-2.652257	-2.173348	-2.394001
C	2.884867	0.162752	1.092451
C	3.475904	-0.553067	-1.161563
C	-2.759787	-3.086934	1.297973
C	2.123115	-0.459930	-1.457156
H	1.770852	-0.715513	-2.452505
C	-1.944630	-2.076985	0.800451
C	-3.530956	-3.493976	-0.931004
C	-0.996943	-1.316582	1.714507
H	-1.322683	-1.427097	2.760755
H	-0.010775	-1.790499	1.636538
C	0.456742	0.656832	1.633897
H	0.748031	0.450718	2.673023
H	0.362976	1.746631	1.545365
C	-2.146948	2.032423	0.563167

C	-2.661061	3.273834	0.920115
C	-1.983751	0.930521	1.598996
H	-1.945371	1.372813	2.606650
H	-2.883793	0.304409	1.562360
C	-2.013762	2.674367	-1.652911
H	-1.734853	2.394946	-2.663640
C	-2.862979	4.237008	-0.062475
C	-2.535432	3.931028	-1.377915
C	-3.562631	-3.809881	0.421780
H	-4.205250	-4.602251	0.791358
H	-2.762038	-3.303741	2.361443
H	-4.139198	-4.027540	-1.652254
H	-3.266386	5.210441	0.196589
H	-2.900684	3.479737	1.958484
H	-2.671318	4.649697	-2.177845
C	3.289560	0.520924	2.499827
H	2.899637	1.501120	2.792670
H	2.917526	-0.216053	3.221106
H	4.375526	0.545310	2.585655
C	4.439703	-1.071287	-2.195105
H	5.060186	-0.275019	-2.618639
H	5.106932	-1.822693	-1.761911
H	3.897529	-1.539272	-3.021009
O	5.132247	-0.288498	0.581356
C	6.156268	0.396459	-0.138651
H	6.885333	0.719586	0.605594
H	6.646454	-0.265309	-0.856828
H	5.752138	1.273350	-0.654543

[Br-Cu^{II}(TPMA^{*1})]$^{+}$

ω-B97XD SCF energy: -3877.25888364 a.u.
ω-B97XD enthalpy: -3876.800833 a.u.
ω-B97XD free energy: -3876.885894 a.u.
ω-B97XD SCF energy in solution: -5323.72151156 a.u.
ω-B97XD enthalpy in solution: -5323.263461 a.u.
ω-B97XD free energy in solution: -5323.348522 a.u.

Cartesian coordinates

ATOM	X	Y	Z
Cu	0.756420	-0.081649	0.437448
N	-1.316955	-0.108259	0.208815
N	1.739839	1.785453	0.328391
N	1.833737	-1.717359	-0.363946
N	0.588721	0.319721	-1.627135
C	-4.027815	-0.078065	-0.333686
C	-1.769326	0.417504	-0.939543
C	2.673782	-2.516422	0.302093
H	2.762948	-2.319201	1.365972
C	-3.118807	0.468965	-1.263564
C	-3.560256	-0.667049	0.854630
C	2.321017	-2.882779	-2.388431
C	-2.188717	-0.634927	1.071564
H	-1.753073	-1.058289	1.972293
C	1.650147	-1.895617	-1.680784

C	3.374293	-3.535297	-0.331208
C	0.622523	-0.984686	-2.313060
H	0.806044	-0.859878	-3.388723
H	-0.366566	-1.442321	-2.197685
C	-0.699634	1.008812	-1.832462
H	-0.987612	0.970370	-2.890540
H	-0.559193	2.064596	-1.572135
C	2.014502	2.188834	-0.921160
C	2.569237	3.432674	-1.185660
C	1.734344	1.168170	-2.000416
H	1.570065	1.649465	-2.973764
H	2.610778	0.517694	-2.098997
C	2.018075	2.589677	1.359997
H	1.777562	2.190982	2.340810
C	2.861789	4.272836	-0.113727
C	2.585483	3.844974	1.179794
C	3.195627	-3.718345	-1.697506
Br	0.961964	-0.531039	2.730690
H	3.731176	-4.502085	-2.223450
H	2.159030	-3.000855	-3.454826
H	4.044623	-4.166113	0.240775
H	3.300364	5.249685	-0.289403
H	2.773690	3.735630	-2.207378
H	2.801121	4.468900	2.039314
C	-3.601319	1.091197	-2.548203
H	-3.168623	2.085635	-2.698969
H	-3.333661	0.473471	-3.413878
H	-4.686301	1.190160	-2.538980
C	-4.445478	-1.390064	1.835964
H	-5.037602	-0.705177	2.450459
H	-5.134985	-2.061480	1.315242
H	-3.836860	-1.994476	2.512993
O	-5.325453	-0.048469	-0.690538
C	-6.317287	0.384026	0.241347
H	-7.096532	0.861239	-0.353985
H	-6.746107	-0.460769	0.784449
H	-5.902096	1.111359	0.945791

$[Cu^{I}(TPMA^{*2})]^{+}$

ω-B97XD SCF energy: -1498.88603890 a.u.
ω-B97XD enthalpy: -1498.337101 a.u.
ω-B97XD free energy: -1498.431630 a.u.
ω-B97XD SCF energy in solution: -2942.62808748 a.u.
ω-B97XD enthalpy in solution: -2942.079150 a.u.
ω-B97XD free energy in solution: -2942.173679 a.u.

Cartesian coordinates

ATOM	X	Y	Z
Cu	-0.020186	0.738228	-0.938320
N	1.687649	-0.360642	-0.625712
N	0.112982	2.775426	-0.652634
N	-1.819576	-0.176847	-0.575273
N	0.020320	0.752887	1.291453
C	3.924392	-1.845873	0.068286

C	2.152273	-0.333212	0.636163
C	-2.816425	-0.355463	-1.448174
H	-2.634434	0.005391	-2.456527
C	3.279065	-1.053957	1.034285
C	3.423295	-1.915424	-1.240788
C	-3.179404	-1.176033	1.134109
C	2.307771	-1.138280	-1.519394
H	1.873812	-1.154759	-2.515140
C	-2.002656	-0.563931	0.699762
C	-4.036266	-0.938299	-1.135308
C	-0.832725	-0.369051	1.657955
H	-1.200322	-0.274546	2.689519
H	-0.218546	-1.278011	1.626497
C	1.427792	0.579319	1.620095
H	1.560273	0.210298	2.646797
H	1.906769	1.565934	1.579528
C	-0.052668	3.134104	0.635045
C	0.156369	4.440594	1.061659
C	-0.530574	2.062661	1.602089
H	-0.320619	2.376237	2.637091
H	-1.620806	1.990189	1.505750
C	0.478406	3.710515	-1.539242
H	0.602941	3.372000	-2.562614
C	0.530536	5.408776	0.135845
C	0.693193	5.037916	-1.193457
C	-4.201157	-1.373914	0.188543
O	-5.347931	-1.935266	0.632104
C	-3.358280	-1.632897	2.559406
H	-2.551536	-2.305665	2.869047
H	-3.368329	-0.783899	3.252663
H	-4.305119	-2.160195	2.671377
C	-5.859378	-3.085151	-0.040229
H	-6.309735	-3.714286	0.729030
H	-6.623867	-2.807695	-0.770125
H	-5.055437	-3.638776	-0.536063
C	-5.127843	-1.012104	-2.168910
H	-5.249518	-2.022330	-2.573305
H	-6.086470	-0.703115	-1.741262
H	-4.902895	-0.347622	-3.007403
O	4.988860	-2.570522	0.479537
C	6.222206	-2.451101	-0.227583
H	7.011239	-2.564495	0.517278
H	6.325117	-3.235794	-0.981331
H	6.309584	-1.467903	-0.701293
C	3.807934	-0.982861	2.444136
H	3.975227	0.053049	2.756961
H	3.108473	-1.436930	3.155716
H	4.752605	-1.519768	2.522800
C	3.989286	-2.832141	-2.291949
H	4.912332	-2.439534	-2.730943
H	4.208907	-3.816556	-1.867937
H	3.270526	-2.967590	-3.104536
H	0.023905	4.693337	2.108797
H	0.696315	6.434254	0.449500
H	0.987067	5.755549	-1.950620

[Br-Cu^{II}(TPMA^{*2})]$^{+}$

ω-B97XD SCF energy: -4070.36207378 a.u.
ω-B97XD enthalpy: -4069.807833 a.u.
ω-B97XD free energy: -4069.904826 a.u.
ω-B97XD SCF energy in solution: -5516.89551275 a.u.
ω-B97XD enthalpy in solution: -5516.341272 a.u.
ω-B97XD free energy in solution: -5516.438265 a.u.

Cartesian coordinates

ATOM	X	Y	Z
Cu	0.013709	0.694106	0.474758
N	-1.752859	-0.408588	0.292777
N	-0.067909	2.695873	-0.239664
N	1.842107	-0.285862	0.210929
N	-0.022341	0.365380	-1.605254
C	-4.043741	-1.876310	-0.193564
C	-2.215486	-0.541324	-0.958741
C	2.856753	-0.299554	1.077078
H	2.683950	0.239028	2.004697
C	-3.363701	-1.261615	-1.264785
C	-3.548316	-1.770365	1.117787
C	3.129015	-1.603606	-1.323936
C	-2.399719	-1.009717	1.293796
H	-1.960488	-0.873731	2.278252
C	1.977516	-0.913183	-0.966774
C	4.064724	-0.941177	0.834400
C	0.749062	-0.868203	-1.849599
H	1.006715	-0.954170	-2.912710
H	0.101996	-1.717657	-1.600526
C	-1.432007	0.214543	-2.010420
H	-1.497390	-0.271318	-2.992007
H	-1.860674	1.218236	-2.116257
C	0.170863	2.811416	-1.554348
C	0.067862	4.026955	-2.215473
C	0.609353	1.536730	-2.238267
H	0.397298	1.567124	-3.315560
H	1.693438	1.431531	-2.117824
C	-0.400412	3.778533	0.470248
H	-0.568846	3.609127	1.529416
C	-0.279449	5.157441	-1.479266
C	-0.514451	5.033613	-0.114826
C	4.185144	-1.622881	-0.389200
Br	0.057289	1.086568	2.790262
O	5.303758	-2.270387	-0.769513
C	3.246519	-2.317071	-2.645892
H	2.425208	-3.026700	-2.792409
H	3.231124	-1.607992	-3.481822
H	4.185084	-2.867614	-2.698605
C	5.922729	-3.203399	0.116592
H	6.349738	-3.980693	-0.518317
H	6.720935	-2.730757	0.693290
H	5.186268	-3.649860	0.791838
C	5.184237	-0.810706	1.833627
H	5.348819	-1.734360	2.396939

H	6.122272	-0.546349	1.336011
H	4.952339	-0.023985	2.555602
O	-5.133523	-2.599295	-0.517769
C	-6.350817	-2.418072	0.206196
H	-7.153392	-2.578409	-0.514809
H	-6.441841	-3.146680	1.014788
H	-6.421088	-1.402400	0.607670
C	-3.875669	-1.372123	-2.677463
H	-3.971303	-0.387733	-3.147521
H	-3.203767	-1.976888	-3.298037
H	-4.853746	-1.851899	-2.690674
C	-4.147862	-2.490713	2.296705
H	-5.073513	-2.021979	2.644536
H	-4.368454	-3.532967	2.046515
H	-3.445193	-2.487705	3.133609
H	0.257900	4.090399	-3.281991
H	-0.367761	6.121800	-1.968859
H	-0.786038	5.890235	0.491121

$[Cu^{I}(TPMA^{Ph})]^{+}$

ω-B97XD SCF energy: -1343.66987764 a.u.
ω-B97XD enthalpy: -1343.225540 a.u.
ω-B97XD free energy: -1343.305191 a.u.
ω-B97XD SCF energy in solution: -2787.34718548 a.u.
ω-B97XD enthalpy in solution: -2786.902848 a.u.
ω-B97XD free energy in solution: -2786.982499 a.u.

Cartesian coordinates

ATOM	X	Y	Z
Cu	0.211912	0.017157	-0.372843
N	1.661350	-0.323442	1.361367
N	-0.906084	0.755710	1.207654
N	0.351922	-2.016927	-0.477115
N	1.779597	1.174019	-1.022000
C	1.251327	0.671500	2.341207
H	1.693915	1.629447	2.042117
H	1.626535	0.449919	3.352465
C	-0.259208	0.848570	2.380164
C	-0.931098	1.117327	3.565159
H	-0.386651	1.172592	4.502164
C	-2.309130	1.313534	3.524271
H	-2.857912	1.535054	4.433913
C	-2.971701	1.222394	2.308791
H	-4.041465	1.384495	2.238663
C	-2.237168	0.931144	1.157944
C	-2.872182	0.781500	-0.173192
C	-2.276552	1.355388	-1.303698
H	-1.392777	1.978203	-1.185008
C	-2.844316	1.181692	-2.561566
H	-2.387737	1.645681	-3.430609
C	-4.011514	0.433392	-2.702482
H	-4.456972	0.299515	-3.683118
C	-4.614746	-0.129322	-1.580744
H	-5.526897	-0.707883	-1.686145

C	-4.050539	0.046482	-0.320440
H	-4.514041	-0.411480	0.548945
C	1.393146	-1.704545	1.727913
H	0.529063	-1.703508	2.403536
H	2.226652	-2.163034	2.282470
C	1.035800	-2.581235	0.535185
C	1.355012	-3.934810	0.532744
H	1.917332	-4.358570	1.358737
C	0.941916	-4.731314	-0.529733
H	1.179044	-5.790078	-0.547733
C	0.223845	-4.147023	-1.566603
H	-0.119226	-4.726330	-2.416025
C	-0.043331	-2.786893	-1.500268
H	-0.593664	-2.282700	-2.287984
C	2.948546	-0.084462	0.729784
H	3.226240	-0.999402	0.192035
H	3.749023	0.110199	1.460663
C	2.900198	1.047209	-0.286270
C	3.996455	1.880639	-0.478794
H	4.880978	1.760453	0.138560
C	3.945602	2.859243	-1.465934
H	4.791488	3.518658	-1.630389
C	2.792152	2.979410	-2.231687
H	2.704246	3.727299	-3.011257
C	1.735492	2.118417	-1.970883
H	0.811856	2.178976	-2.538099

[Br-Cu^{II}(TPMA^{Ph})]$^{+}$

ω-B97XD SCF energy: -3915.13072131 a.u.
ω-B97XD enthalpy: -3914.682128 a.u.
ω-B97XD free energy: -3914.765893 a.u.
ω-B97XD SCF energy in solution: -5361.60513152 a.u.
ω-B97XD enthalpy in solution: -5361.156538 a.u.
ω-B97XD free energy in solution: -5361.240303 a.u.

Cartesian coordinates

ATOM	X	Y	Z
Cu	0.546436	-0.229026	-0.611033
N	1.015142	-2.243421	0.056350
N	-0.520501	-0.304611	1.476871
N	-1.151277	-1.154981	-1.223507
N	2.464266	0.037265	-0.027779
C	0.724042	-2.352595	1.502385
H	1.575320	-1.924371	2.041271
H	0.641533	-3.407657	1.795253
C	-0.511572	-1.577582	1.893474
C	-1.543701	-2.135891	2.628760
H	-1.501582	-3.173323	2.943935
C	-2.633297	-1.325796	2.950519
H	-3.460890	-1.723935	3.528805
C	-2.640053	-0.004961	2.534223
H	-3.456793	0.659645	2.793157
C	-1.557932	0.484843	1.790918
C	-1.503065	1.885539	1.320255

C	-0.311229	2.606822	1.430704
H	0.555254	2.134404	1.884874
C	-0.242872	3.917690	0.977776
H	0.682637	4.476630	1.074585
C	-1.359292	4.513515	0.396261
H	-1.301579	5.533652	0.030633
C	-2.549695	3.800404	0.283231
H	-3.419939	4.262388	-0.171723
C	-2.625942	2.493221	0.752789
H	-3.554436	1.935796	0.655911
C	0.167688	-3.130096	-0.757990
H	0.027123	-4.107304	-0.277880
H	0.676185	-3.307140	-1.711937
C	-1.168386	-2.487824	-1.065860
C	-2.328697	-3.224672	-1.251360
H	-2.318713	-4.301144	-1.115735
C	-3.494927	-2.556946	-1.615625
H	-4.416459	-3.109715	-1.766314
C	-3.464099	-1.177371	-1.784944
H	-4.349764	-0.623642	-2.073690
C	-2.267013	-0.506814	-1.577883
H	-2.165273	0.567451	-1.695089
C	2.458767	-2.374440	-0.200721
H	2.603322	-2.538099	-1.274034
H	2.895733	-3.233192	0.326002
C	3.165103	-1.090564	0.179596
C	4.466442	-1.057149	0.657795
H	5.009402	-1.981624	0.823932
C	5.055985	0.179271	0.910227
H	6.073049	0.232730	1.284614
C	4.328342	1.340335	0.675996
H	4.756662	2.320099	0.851280
C	3.028474	1.228196	0.202172
H	2.409709	2.090542	-0.023841
Br	0.410887	1.623914	-2.033537

$[Cu^{I}(BPED)]^{+}$

ω-B97XD SCF energy: -1038.91268343 a.u.
ω-B97XD enthalpy: -1038.519920 a.u.
ω-B97XD free energy: -1038.587679 a.u.
ω-B97XD SCF energy in solution: -2482.48910206 a.u.
ω-B97XD enthalpy in solution: -2482.096339 a.u.
ω-B97XD free energy in solution: -2482.164098 a.u.

Cartesian coordinates

ATOM	X	Y	Z
Cu	-0.007369	-0.091412	-0.662950
N	-1.968994	-0.137627	-0.882640
N	-0.526996	-1.172171	1.290389
N	0.560540	1.572480	0.810115
N	1.950483	-0.161505	-0.905466
C	-2.648825	0.627351	-1.752203
H	-2.057418	1.123301	-2.514086
C	-4.026073	0.783953	-1.698409

H	-4.528001	1.412602	-2.424733
C	-4.729723	0.123359	-0.697955
H	-5.806651	0.227494	-0.616536
C	-4.029557	-0.672391	0.202286
H	-4.546357	-1.202125	0.995929
C	-2.650229	-0.789632	0.080672
C	-1.853700	-1.704713	0.989747
H	-2.432985	-1.921242	1.901165
H	-1.720295	-2.658298	0.465390
C	-0.577271	-0.081365	2.273639
H	-0.586170	-0.477143	3.301522
H	-1.519482	0.458395	2.134018
C	0.591897	0.888329	2.110763
H	0.582908	1.615427	2.937629
H	1.535435	0.338452	2.185727
C	1.897852	1.935645	0.345494
H	2.492691	2.430901	1.128817
H	1.783894	2.659144	-0.470359
C	2.658859	0.744559	-0.202659
C	4.032987	0.621736	-0.035700
H	4.573281	1.362749	0.544391
C	4.698625	-0.451636	-0.618507
H	5.770871	-0.564337	-0.496850
C	3.967181	-1.375820	-1.355279
H	4.441957	-2.225959	-1.831214
C	2.596955	-1.193305	-1.471259
H	1.984029	-1.886732	-2.036606
C	0.403978	-2.228075	1.686947
H	0.092930	-2.733085	2.614941
H	1.400326	-1.805717	1.838893
H	0.477332	-2.970347	0.887799
C	-0.343256	2.722541	0.818455
H	-0.010129	3.510390	1.512153
H	-1.346052	2.402768	1.112987
H	-0.411829	3.142824	-0.188389

[Br-Cu^{II}(BPED)]$^{+}$

ω-B97XD SCF energy: -3610.36999034 a.u.
ω-B97XD enthalpy: -3609.972982 a.u.
ω-B97XD free energy: -3610.045204 a.u.
ω-B97XD SCF energy in solution: -5056.74422829 a.u.
ω-B97XD enthalpy in solution: -5056.347220 a.u.
ω-B97XD free energy in solution: -5056.419442 a.u.

Cartesian coordinates

ATOM	X	Y	Z
Cu	-0.014881	0.299617	0.153611
N	-1.406989	-1.237098	-0.320009
N	-1.669210	1.489451	-0.365707
N	1.042155	1.531128	-1.260089
N	1.679336	-0.792326	-0.090324
C	-1.351651	-2.509349	0.086351
C	-2.441829	-3.364582	0.003036
C	-3.634986	-2.869416	-0.511500

C	-3.695514	-1.542436	-0.928567
C	-2.556037	-0.758048	-0.820295
C	-2.488283	0.673721	-1.288979
C	-1.114833	2.685575	-1.040840
C	0.030664	2.318865	-1.982695
C	1.773855	0.563947	-2.090291
C	2.376153	-0.504711	-1.202583
C	3.570473	-1.148313	-1.493132
C	4.045575	-2.113639	-0.609978
C	3.328308	-2.387061	0.549932
C	2.150534	-1.691705	0.782179
C	-2.491708	1.885933	0.798041
C	1.974356	2.397134	-0.512225
H	-0.403157	-2.841366	0.495262
H	-2.355271	-4.389050	0.345696
H	-4.511765	-3.504923	-0.580138
H	-4.612450	-1.122012	-1.327777
H	-3.491176	1.106449	-1.395436
H	-2.026246	0.682901	-2.281238
H	-1.901101	3.220691	-1.590932
H	-0.755623	3.354701	-0.254856
H	0.461936	3.235159	-2.407430
H	-0.335685	1.723988	-2.824242
H	1.065658	0.094602	-2.783425
H	2.556765	1.047054	-2.691666
H	4.123236	-0.889638	-2.390176
H	4.977963	-2.629217	-0.815322
H	3.681006	-3.109974	1.276031
H	1.571976	-1.811953	1.692679
H	-2.894488	0.989729	1.273667
H	-1.864616	2.395598	1.528568
H	-3.315551	2.536281	0.475771
H	1.418357	3.042057	0.169346
H	2.638653	1.784209	0.099298
H	2.568576	3.012349	-1.201985
Br	0.270487	0.760854	2.473022

$[Cu^{I}(N[3,2,3])]^{+}$

ω-B97XD SCF energy: -969.94984486 a.u.
ω-B97XD enthalpy: -969.426430 a.u.
ω-B97XD free energy: -969.497704 a.u.
ω-B97XD SCF energy in solution: -2413.50704843 a.u.
ω-B97XD enthalpy in solution: -2412.983634 a.u.
ω-B97XD free energy in solution: -2413.054908 a.u.

Cartesian coordinates

ATOM	X	Y	Z
Cu	-0.027122	0.299526	-0.042988
N	-1.681168	1.369796	-0.751115
N	1.682914	1.299177	0.801713
N	1.015594	-1.317454	-1.072881
N	-1.039541	-1.473383	0.999162
C	2.826605	1.172098	-0.133398
C	3.259084	-0.247323	-0.494497

C	2.383159	-0.974422	-1.511931
C	1.051743	-2.361040	-0.033063
C	-0.328326	-2.680639	0.533256
C	-2.488728	-1.558602	0.726570
C	-3.187729	-0.210098	0.569900
C	-2.885598	0.504477	-0.750915
H	3.689804	1.704108	0.299867
H	2.552412	1.703302	-1.052400
H	3.429124	-0.851715	0.401999
H	4.246561	-0.157459	-0.961732
H	2.283189	-0.332642	-2.394211
H	2.902808	-1.889750	-1.841589
H	1.702722	-2.013885	0.773180
H	1.495055	-3.290211	-0.429653
H	-0.929640	-3.173654	-0.233541
H	-0.213731	-3.413772	1.344386
H	-2.984805	-2.142998	1.517691
H	-2.628112	-2.114144	-0.206445
H	-2.985415	0.437720	1.429628
H	-4.265607	-0.404524	0.598403
H	-2.747689	-0.246234	-1.537542
H	-3.751515	1.118096	-1.047429
C	0.256114	-1.776825	-2.244284
H	0.297666	-1.010940	-3.022099
H	0.664789	-2.713486	-2.656615
H	-0.792881	-1.935355	-1.986164
C	-1.402913	1.775376	-2.141725
H	-1.191377	0.891536	-2.748064
H	-2.259362	2.308664	-2.582542
H	-0.530849	2.433985	-2.164766
C	-0.812742	-1.270555	2.435373
H	0.258375	-1.257112	2.643823
H	-1.232844	-0.312451	2.753445
H	-1.273961	-2.071438	3.035294
C	2.054335	0.789184	2.130913
H	1.231124	0.959795	2.828349
H	2.254668	-0.282475	2.092354
H	2.952087	1.297428	2.516370
C	1.389312	2.735556	0.945104
H	1.128290	3.158306	-0.028146
H	0.550863	2.873523	1.631266
H	2.259997	3.282632	1.339271
C	-1.960824	2.586143	0.034088
H	-2.083330	2.343907	1.091373
H	-1.131154	3.286627	-0.063776
H	-2.876278	3.081422	-0.323834

[Br-Cu^{II}(N[3,2,3])]$^{+}$

ω-B97XD SCF energy: -3541.40084102 a.u.
ω-B97XD enthalpy: -3540.873571 a.u.
ω-B97XD free energy: -3540.951407 a.u.
ω-B97XD SCF energy in solution: -4987.75188260 a.u.
ω-B97XD enthalpy in solution: -4987.224613 a.u.
ω-B97XD free energy in solution: -4987.302449 a.u.

Cartesian coordinates

ATOM	X	Y	Z
N	0.002973	-1.827437	-0.659398
N	-2.459959	-0.367396	-0.898306
N	3.565782	0.598578	-0.779412
N	-0.648086	1.953882	0.142826
C	-0.896552	-2.027201	-1.820694
H	-0.578771	-1.340892	-2.611892
H	-0.793574	-3.045263	-2.217776
C	-2.452543	2.055740	-1.654210
H	-3.203519	2.384884	-0.930122
H	-2.661296	2.628708	-2.564323
C	-0.002973	-3.026933	0.205406
H	-1.025234	-3.269252	0.500651
H	0.560571	-2.826374	1.114636
H	0.432501	-3.880557	-0.330282
C	3.908563	1.230513	0.489957
H	3.304656	0.813330	1.301614
H	3.707781	2.305539	0.435444
H	4.972979	1.094592	0.749247
C	-1.431068	2.630635	1.199473
H	-1.097253	2.268311	2.172072
H	-2.493645	2.408293	1.097091
H	-1.286414	3.717052	1.135835
C	1.378604	-1.547301	-1.166245
H	1.350264	-0.571991	-1.667899
H	1.620093	-2.304025	-1.928920
C	-2.634108	0.588147	-2.020034
H	-3.631606	0.434426	-2.455959
H	-1.902488	0.329418	-2.791880
C	-2.336007	-1.749411	-1.430256
H	-2.657185	-2.442404	-0.648789
H	-3.008820	-1.892862	-2.285232
C	2.479255	-1.525950	-0.112478
H	2.143287	-0.991232	0.781952
H	2.729295	-2.545427	0.198367
C	-1.045294	2.432702	-1.205535
H	-0.314230	2.033014	-1.919142
H	-0.941334	3.526903	-1.223110
C	-3.606167	-0.296045	0.035174
H	-4.534768	-0.590848	-0.470825
H	-3.722135	0.717868	0.417901
H	-3.430110	-0.960708	0.884337
C	3.726595	-0.852773	-0.693324
H	4.611372	-1.123865	-0.094000
H	3.906902	-1.244660	-1.701856
C	0.786077	2.281065	0.340297
H	1.075462	2.007927	1.355226
H	1.408978	1.719218	-0.364816
H	0.948088	3.357480	0.192698
C	4.363663	1.170785	-1.857629
H	4.065062	0.732774	-2.815053
H	4.189506	2.250102	-1.908151
H	5.446761	1.006424	-1.722739
Cu	-0.745339	-0.106668	0.251643

Br	-0.120846	-0.408564	2.471962

[Cu^{I}(PMDTA)-MeCN]$^{+}$

ω-B97XD SCF energy: -850.82938461 a.u.
ω-B97XD enthalpy: -850.424563 a.u.
ω-B97XD free energy: -850.497131 a.u.
ω-B97XD SCF energy in solution: -2294.35145721 a.u.
ω-B97XD enthalpy in solution: -2293.946636 a.u.
ω-B97XD free energy in solution: -2294.019204 a.u.

Cartesian coordinates

ATOM	X	Y	Z
Cu	0.310532	0.027790	-0.222607
N	-0.382252	-1.927223	-0.735272
N	-1.288577	-0.069112	1.354276
N	-0.572203	1.903529	-0.716114
C	-1.351627	-1.930656	-1.840731
C	0.741500	-2.810455	-1.084434
C	-1.003367	-2.386853	0.523564
C	-1.962233	-1.355414	1.115687
C	-0.694166	-0.012818	2.693004
C	-2.121651	1.111875	1.080309
C	-1.291641	2.266580	0.522789
C	-1.492303	1.831654	-1.861375
C	0.462399	2.911197	-1.000027
H	-0.862015	-1.575656	-2.750614
H	-2.185014	-1.260318	-1.622602
H	-1.751600	-2.940083	-2.023385
H	1.486169	-2.791880	-0.285042
H	1.210412	-2.452923	-2.004387
H	0.407264	-3.847850	-1.237862
H	-1.537417	-3.338012	0.368951
H	-0.194514	-2.582487	1.235429
H	-2.393447	-1.762212	2.041848
H	-2.798839	-1.194810	0.430972
H	-0.000260	-0.846280	2.828434
H	-1.461311	-0.058560	3.481799
H	-0.125533	0.912966	2.810650
H	-2.894679	0.834719	0.359035
H	-2.645893	1.455342	1.984404
H	-1.944279	3.137270	0.351403
H	-0.541441	2.567763	1.261145
H	-2.269467	1.085984	-1.683751
H	-0.936280	1.535117	-2.753955
H	-1.974502	2.803185	-2.050247
H	1.178952	2.945239	-0.175815
H	0.023455	3.911360	-1.135810
H	0.996117	2.635514	-1.912864
N	2.229282	0.096075	0.170599
C	3.369267	0.126211	0.352657
C	4.807995	0.162470	0.582147
H	5.237755	1.045971	0.103039
H	5.009816	0.203115	1.655731
H	5.272332	-0.734004	0.163131

[Br-Cu^{II}(PMDTA)-MeCN]$^{+}$

ω-B97XD SCF energy: -3422.28278402 a.u.
ω-B97XD enthalpy: -3421.872861 a.u.
ω-B97XD free energy: -3421.947930 a.u.
ω-B97XD SCF energy in solution: -4868.59917348 a.u.
ω-B97XD enthalpy in solution: -4868.189250 a.u.
ω-B97XD free energy in solution: -4868.264319 a.u.

Cartesian coordinates

ATOM	X	Y	Z
N	0.402663	-2.001127	0.661333
N	2.140299	-0.001162	-0.370087
N	0.405227	2.000767	0.661647
C	0.484749	-2.120681	2.133880
C	-0.660512	-2.896628	0.158538
C	1.697924	-2.368224	0.039392
C	2.711149	-1.241941	0.190319
C	2.257519	-0.001780	-1.845722
C	2.712831	1.239213	0.189547
C	1.700610	2.366504	0.039144
C	0.488117	2.119787	2.134188
C	-0.657130	2.897632	0.159524
H	-0.476319	-1.851252	2.571248
H	1.243738	-1.444616	2.535281
H	0.740056	-3.149483	2.419555
H	-0.787332	-2.741956	-0.913641
H	-1.598690	-2.647432	0.656027
H	-0.407950	-3.943914	0.369175
H	2.086778	-3.293354	0.485065
H	1.509101	-2.569932	-1.017699
H	3.650065	-1.508809	-0.311757
H	2.943878	-1.072139	1.245231
H	1.757066	-0.871943	-2.267907
H	3.317737	-0.005403	-2.131489
H	1.763423	0.871903	-2.268052
H	2.946237	1.069456	1.244311
H	3.651617	1.504995	-0.313339
H	2.090595	3.291243	0.484643
H	1.511436	2.568442	-1.017844
H	1.246529	1.442740	2.535036
H	-0.473073	1.851307	2.571871
H	0.744725	3.148209	2.420065
H	-0.784670	2.743247	-0.912614
H	-0.403167	3.944580	0.370151
H	-1.595360	2.649558	0.657468
Cu	0.091717	0.000167	0.182845
N	-1.765077	0.001279	1.520728
C	-2.882000	0.001112	1.217422
C	-4.255070	0.000913	0.741712
H	-4.779120	-0.891222	1.093197
H	-4.779026	0.893471	1.092259
H	-4.217378	0.000349	-0.353279
Br	-1.240903	0.000953	-1.851671

[Cu^{I}(BPMPA)-MeCN]$^{+}$

ω-B97XD SCF energy: -1077.00292092 a.u.
ω-B97XD enthalpy: -1076.606369 a.u.
ω-B97XD free energy: -1076.684555 a.u.
ω-B97XD SCF energy in solution: -2520.59780663 a.u.
ω-B97XD enthalpy in solution: -2520.201255 a.u.
ω-B97XD free energy in solution: -2520.279441 a.u.

Cartesian coordinates

ATOM	X	Y	Z
Cu	-0.277160	0.980711	-0.113763
N	0.209535	-1.066798	0.746718
N	-2.064298	-0.036809	-0.455994
N	1.306372	0.430006	-1.350529
N	-0.252499	2.656275	0.842794
C	-3.032486	0.349239	-1.297615
C	-4.162657	-0.415443	-1.548952
C	-4.288728	-1.639941	-0.902168
C	-3.283232	-2.046583	-0.032176
C	-2.186324	-1.216567	0.174574
C	-1.089742	-1.593277	1.153755
C	0.745562	-1.748851	-0.433121
C	1.675622	-0.856324	-1.226670
C	2.821664	-1.352645	-1.836086
C	3.602290	-0.499510	-2.609035
C	3.214384	0.828603	-2.743382
C	2.062560	1.249202	-2.092163
C	1.179845	-0.964329	1.850771
C	-0.260917	3.653556	1.423682
C	-0.276308	4.910927	2.159627
H	-4.917384	-0.058955	-2.240401
H	-5.153190	-2.272217	-1.076628
H	-3.344888	-2.999759	0.483096
H	-1.084286	-2.685399	1.288449
H	-1.331324	-1.152706	2.128923
H	-0.096854	-2.009080	-1.085281
H	1.251852	-2.691291	-0.183424
H	3.095067	-2.394607	-1.705360
H	4.501205	-0.866154	-3.093784
H	3.792166	1.529970	-3.334198
H	2.090870	-0.518753	1.433056
H	0.212270	4.777210	3.128287
H	0.255805	5.679347	1.592868
H	-1.308664	5.232598	2.319772
H	1.723896	2.278182	-2.159941
H	-2.885714	1.308348	-1.783864
H	0.778576	-0.236965	2.567207
C	1.529290	-2.261320	2.585871
H	0.627025	-2.686037	3.042775
H	1.907313	-3.011095	1.880299
C	2.579313	-2.012778	3.668624
H	2.822095	-2.937759	4.198441
H	3.506491	-1.619999	3.236639

H	2.220721	-1.287983	4.408044

[Br-Cu^{II}(BPMPA)-MeCN]$^{+}$

ω-B97XD SCF energy: -3648.45769822 a.u.
ω-B97XD enthalpy: -3648.057264 a.u.
ω-B97XD free energy: -3648.141061 a.u.
ω-B97XD SCF energy in solution: -5094.84619615 a.u.
ω-B97XD enthalpy in solution: -5094.445762 a.u.
ω-B97XD free energy in solution: -5094.529559 a.u.

Cartesian coordinates

ATOM	X	Y	Z
C	2.335209	1.158584	0.817358
C	3.654861	1.582868	0.794462
H	3.906000	2.596823	1.087084
C	4.639522	0.683491	0.393345
H	5.680180	0.989722	0.366338
C	4.274538	-0.607840	0.029648
H	5.012811	-1.337247	-0.281597
C	2.932450	-0.957612	0.069928
H	2.577271	-1.949856	-0.186092
C	1.194293	2.016974	1.308500
H	1.021714	1.781270	2.364734
H	1.448163	3.080566	1.252693
C	-1.273776	1.981103	1.297502
H	-1.558872	3.036617	1.237815
H	-1.103333	1.751959	2.355519
C	-2.384757	1.089227	0.797187
C	-3.716284	1.474019	0.767464
H	-3.999408	2.478773	1.062767
C	-4.671265	0.547664	0.356172
H	-5.720435	0.822668	0.323723
C	-4.265434	-0.730379	-0.011239
H	-4.979831	-1.479521	-0.331221
C	-2.913970	-1.040680	0.037508
H	-2.527584	-2.020589	-0.220298
C	-0.034680	2.282440	-0.812880
H	-0.903930	1.869671	-1.332740
H	0.841879	1.883635	-1.331278
C	-0.046706	3.808360	-0.907962
Cu	-0.000757	-0.418882	0.373044
N	-0.031931	1.692600	0.557809
N	1.990184	-0.087535	0.450967
N	-2.000508	-0.144897	0.429245
H	-0.926599	4.226455	-0.405907
H	0.833616	4.238813	-0.417249
C	-0.058809	4.238417	-2.376676
H	-0.945055	3.854628	-2.892970
H	-0.066393	5.328095	-2.461719
H	0.825641	3.866032	-2.904307
N	0.023819	-0.606164	-2.098036
C	0.071086	-1.641784	-2.612684
C	0.132359	-2.974895	-3.193459
H	0.061230	-3.700758	-2.376723

H	-0.694490	-3.124492	-3.892002
H	1.079072	-3.113384	-3.721360
Br	0.030787	-2.753430	0.742331

[Cu^{I}(TMEDA)]$^{+}$

ω-B97XD SCF energy: -892.54916927 a.u.
ω-B97XD enthalpy: -892.064946 a.u.
ω-B97XD free energy: -892.136543 a.u.
ω-B97XD SCF energy in solution: -2336.08377001 a.u.
ω-B97XD enthalpy in solution: -2335.599547 a.u.
ω-B97XD free energy in solution: -2335.671144 a.u.

Cartesian coordinates

ATOM	X	Y	Z
Cu	0.000011	-0.000410	-0.000223
N	-1.590375	-1.053875	1.035145
N	1.589815	1.053930	1.035623
C	-2.780405	-0.239549	0.722259
C	2.780026	0.239645	0.723393
C	-1.408199	-1.131877	2.491274
C	1.742027	2.416926	0.504086
C	-1.742519	-2.416980	0.503791
C	1.407047	1.132152	2.491657
N	-1.589772	1.054028	-1.035466
N	1.590331	-1.053791	-1.035129
C	-2.779883	0.239450	-0.723519
C	2.780361	-0.239386	-0.722390
C	-1.742301	2.416886	-0.503603
C	1.408134	-1.131974	-2.491264
C	-1.406886	1.132641	-2.491482
C	1.742552	-2.416834	-0.503649
H	-3.705327	-0.803841	0.918836
H	-2.784758	0.620078	1.399207
H	2.784043	-0.619982	1.400355
H	3.704826	0.803977	0.920456
H	-2.272088	-1.603564	2.984443
H	-1.273577	-0.128553	2.902274
H	-0.515732	-1.722498	2.715031
H	1.820357	2.398954	-0.585462
H	0.865270	3.008995	0.774610
H	2.636677	2.909787	0.915255
H	-2.637104	-2.909826	0.915104
H	-1.820940	-2.399111	-0.585744
H	-0.865678	-3.008922	0.774328
H	1.272338	0.128881	2.902764
H	0.514469	1.722765	2.714988
H	2.270714	1.603963	2.985116
H	-2.783495	-0.620179	-1.400474
H	-3.704766	0.803557	-0.920830
H	3.705270	-0.803655	-0.919081
H	2.784581	0.620237	-1.399352
H	-2.637146	2.909555	-0.914551
H	-1.820442	2.398588	0.585944
H	-0.865736	3.009238	-0.774135

H	1.273462	-0.128702	-2.902382
H	0.515697	-1.722670	-2.714939
H	2.272046	-1.603682	-2.984376
H	-2.270505	1.604576	-2.984887
H	-1.272118	0.129473	-2.902827
H	-0.514262	1.723282	-2.714554
H	1.820776	-2.398938	0.585906
H	0.865847	-3.008924	-0.774307
H	2.637267	-2.909606	-0.914777

[Br-Cu^{II}(TMEDA)]$^{+}$

ω-B97XD SCF energy: -3463.99511590 a.u.
ω-B97XD enthalpy: -3463.505417 a.u.
ω-B97XD free energy: -3463.579682 a.u.
ω-B97XD SCF energy in solution: -4910.32192008 a.u.
ω-B97XD enthalpy in solution: -4909.832221 a.u.
ω-B97XD free energy in solution: -4909.906486 a.u.

Cartesian coordinates

ATOM	X	Y	Z
N	2.393025	0.566908	-0.578836
N	0.760891	-1.871796	-0.475769
N	-2.393016	-0.566916	-0.578956
N	-0.760856	1.871792	-0.475800
C	2.967114	-0.772338	-0.799484
C	-2.799022	-1.440606	-1.688146
C	-2.967054	0.772345	-0.799646
C	-2.187993	1.843889	-0.066338
C	2.799066	1.440593	-1.688019
C	2.932451	1.114462	0.681708
H	4.016235	-0.805031	-0.471017
H	2.977000	-0.979413	-1.873063
H	-3.891921	-1.447489	-1.815127
H	-2.343414	-1.101615	-2.623372
H	-4.016199	0.805066	-0.471258
H	-2.976847	0.979434	-1.873225
H	-2.206563	1.678125	1.013982
H	-2.640171	2.825032	-0.267341
H	3.891970	1.447481	-1.814955
H	2.343499	1.101589	-2.623260
H	2.487754	2.087254	0.891347
H	4.024186	1.231989	0.613151
H	2.684559	0.460752	1.517397
C	-2.932514	-1.114436	0.681570
H	-4.024251	-1.231924	0.612972
H	-2.487865	-2.087243	0.891242
H	-2.684631	-0.460722	1.517259
C	-0.636401	2.147979	-1.924288
H	-1.236614	3.023346	-2.205591
H	-0.965928	1.290324	-2.515612
C	0.636463	-2.147993	-1.924260
H	1.236675	-3.023365	-2.205545
H	0.965998	-1.290347	-2.515590
C	0.097414	-2.952556	0.284866

H	0.613302	-3.905624	0.113338
H	0.109898	-2.705098	1.347234
H	-0.934198	-3.051922	-0.048857
C	-0.097421	2.952565	0.284855
H	-0.613309	3.905627	0.113299
H	-0.109949	2.705116	1.347225
H	0.934206	3.051940	-0.048823
C	2.188013	-1.843907	-0.066250
H	2.640205	-2.825044	-0.267252
H	2.206533	-1.678173	1.014075
Cu	0.000031	0.000008	-0.119284
Br	-0.000062	-0.000005	2.294932
H	0.406145	2.349678	-2.163490
H	-0.406079	-2.349685	-2.163480
H	2.485528	2.468567	-1.491409
H	-2.485497	-2.468580	-1.491516

$[Cu^{I}(bpy)]^{+}$

ω-B97XD SCF energy: -1187.68036542 a.u.
ω-B97XD enthalpy: -1187.333591 a.u.
ω-B97XD free energy: -1187.407480 a.u.
ω-B97XD SCF energy in solution: -2631.30491842 a.u.
ω-B97XD enthalpy in solution: -2630.958144 a.u.
ω-B97XD free energy in solution: -2631.032033 a.u.

Cartesian coordinates

ATOM	X	Y	Z
Cu	0.000011	0.000013	-0.001035
N	-1.587013	-0.934728	0.945367
N	1.588046	-0.945339	-0.934597
N	-1.588127	0.933921	-0.946033
N	1.587085	0.946186	0.933939
C	-2.800983	0.523861	-0.530382
C	2.800395	0.531271	0.524495
C	2.800938	-0.530170	-0.524151
C	-2.800356	-0.524959	0.530884
C	3.967647	1.073143	1.060327
H	4.943363	0.738630	0.730248
C	2.618282	2.482494	2.452228
H	2.500171	3.248922	3.209458
C	-2.621035	2.451948	-2.481458
H	-2.503775	3.209322	-3.247873
C	3.874313	2.059429	2.034749
H	4.774048	2.490503	2.461029
C	2.620817	-2.481453	-2.452019
H	2.503490	-3.247914	-3.209337
C	-3.967563	-1.060637	1.073005
H	-4.943306	-0.730328	0.738795
C	-1.504434	1.871745	-1.895048
H	-0.500249	2.160776	-2.188137
C	3.968739	-1.071806	-1.059024
H	4.944111	-0.737084	-0.728147
C	-3.876597	2.033853	-2.057607
H	-4.776806	2.459799	-2.488023

C	1.504268	-1.894456	-1.872312
H	0.500056	-2.187124	-2.161679
C	-1.502175	-1.872529	1.894291
H	-0.497627	-2.161315	2.186387
C	1.502335	1.895265	1.871586
H	0.497814	2.187716	2.160107
C	-3.874141	-2.035217	2.059126
H	-4.773838	-2.461390	2.490385
C	3.876416	-2.058118	-2.033514
H	4.776587	-2.488999	-2.459068
C	-2.618071	-2.453009	2.481772
H	-2.499896	-3.210363	3.248069
C	-3.968833	1.059257	-1.071393
H	-4.944174	0.728717	-0.736249

[Br-Cu^{II}(bpy)]$^{+}$

ω-B97XD SCF energy: -3759.13482060 a.u.
ω-B97XD enthalpy: -3758.784654 a.u.
ω-B97XD free energy: -3758.863186 a.u.
ω-B97XD SCF energy in solution: -5205.55739230 a.u.
ω-B97XD enthalpy in solution: -5205.207226 a.u.
ω-B97XD free energy in solution: -5205.285758 a.u.

Cartesian coordinates

ATOM	X	Y	Z
Cu	-0.000043	-0.587018	-0.000340
Br	0.000415	-2.953229	-0.000946
N	0.713634	0.852760	1.456582
C	2.017647	1.144164	1.314228
C	2.647218	2.067309	2.145407
C	1.908073	2.691612	3.143897
C	0.560863	2.382428	3.285536
C	0.006182	1.454683	2.413345
N	1.955860	-0.430955	-0.497412
C	2.718174	0.411542	0.224486
C	4.075965	0.551551	-0.047149
C	4.641449	-0.185065	-1.082097
C	3.842109	-1.052530	-1.816149
C	2.499008	-1.155091	-1.481822
N	-1.955927	-0.431867	0.496801
C	-2.718291	0.411363	-0.224215
C	-4.076026	0.551217	0.047756
C	-4.641418	-0.186326	1.082093
C	-3.842045	-1.054556	1.815199
C	-2.498995	-1.156899	1.480594
N	-0.713880	0.853618	-1.456166
C	-2.017865	1.144947	-1.313379
C	-2.647492	2.068895	-2.143617
C	-1.908432	2.694116	-3.141601
C	-0.561249	2.385020	-3.283678
C	-0.006508	1.456418	-2.412436
H	0.049144	2.847623	-4.050414
H	1.040687	1.177763	-2.478431
H	-2.383494	3.413266	-3.800503

H	-3.698065	2.303696	-2.025425
H	-4.696195	1.216794	-0.539519
H	-5.698979	-0.087359	1.303027
H	-4.246008	-1.656697	2.620372
H	-1.829203	-1.846929	1.982083
H	-1.041040	1.176022	2.478945
H	-0.049602	2.844317	4.052647
H	2.383089	3.410111	3.803542
H	3.697808	2.302192	2.027526
H	4.696098	1.216535	0.540836
H	5.699054	-0.085989	-1.302775
H	4.246138	-1.653920	-2.621850
H	1.829256	-1.844580	-1.984093

[AN--Br--Cu(TPMA)]‡

ω-B97XD SCF energy: -3855.50293737 a.u.
ω-B97XD enthalpy: -3855.072592 a.u.
ω-B97XD free energy: -3855.159404 a.u.
ω-B97XD SCF energy in solution: -5301.95836042 a.u.
ω-B97XD enthalpy in solution: -5301.528015 a.u.
ω-B97XD free energy in solution: -5301.614827 a.u.
Imaginary frequency: -498.4846 cm-1

Cartesian coordinates

ATOM	X	Y	Z
Cu	0.170093	0.017538	-0.135830
N	0.920770	1.950484	-0.418842
N	-0.951153	-0.303966	1.630127
N	1.325669	-1.576123	-0.823384
N	1.753780	0.032727	1.360201
C	2.219802	4.387100	-0.653382
C	1.782758	2.351542	0.530701
C	0.938263	-2.524721	-1.683903
H	-0.042435	-2.385429	-2.127297
C	2.458456	3.561714	0.441729
C	1.318844	3.972933	-1.627325
C	3.378364	-2.746277	-0.480021
C	0.693366	2.743215	-1.472663
H	-0.018203	2.366886	-2.200400
C	2.527907	-1.677136	-0.230858
C	1.736666	-3.617048	-1.995135
C	2.922351	-0.531509	0.678833
H	3.695936	-0.851358	1.391536
H	3.359973	0.260571	0.059769
C	1.927278	1.439463	1.731914
H	2.888917	1.612331	2.236218
H	1.136526	1.691950	2.447886
C	-0.207309	-0.584729	2.713053
C	-0.771277	-0.724003	3.973599
C	1.272236	-0.800181	2.466792
H	1.848316	-0.627127	3.387123
H	1.425084	-1.847876	2.182422
C	-2.274192	-0.166226	1.765160
H	-2.830514	0.054908	0.860147

C	-2.150817	-0.585966	4.112581
C	-2.917104	-0.304998	2.988563
C	2.977824	-3.729899	-1.379950
Br	-1.652618	-0.006359	-1.725210
C	-3.985014	-0.110777	-2.515431
H	3.626439	-4.573259	-1.593342
H	4.339239	-2.805995	0.020625
H	1.385246	-4.360990	-2.700529
H	3.156361	3.854426	1.219435
H	2.732749	5.338964	-0.743996
H	1.103251	4.584164	-2.495977
H	-0.142909	-0.943161	4.831053
H	-2.615703	-0.695447	5.087002
H	-3.993533	-0.189282	3.039910
C	-4.635264	-0.079584	-1.252505
N	-5.103096	-0.065708	-0.186867
H	-3.966198	0.840169	-3.040181
C	-4.047106	-1.364414	-3.338006
H	-3.322365	-1.317504	-4.153949
H	-3.846130	-2.249342	-2.729148
H	-5.047893	-1.473092	-3.777046

[MMA--Cl--Cu(TPMA)]‡

ω-B97XD SCF energy: -1919.15469417 a.u.
ω-B97XD enthalpy: -1918.646938 a.u.
ω-B97XD free energy: -1918.741378 a.u.
ω-B97XD SCF energy in solution: -3362.92976910 a.u.
ω-B97XD enthalpy in solution: -3362.422013 a.u.
ω-B97XD free energy in solution: -3362.516453 a.u.
Imaginary frequency: -844.5997 cm-1

Cartesian coordinates

ATOM	X	Y	Z
Cu	-0.496797	-0.096315	0.264164
N	0.134149	1.858947	-0.363264
N	0.098806	-1.558523	-1.150103
N	-2.304180	-0.264268	1.242081
N	-1.879998	0.313333	-1.412644
C	0.620880	4.438295	-1.246955
C	-0.411854	2.293862	-1.508046
C	-2.486680	-0.834554	2.439832
H	-1.584257	-1.144851	2.956011
C	-0.197995	3.583691	-1.979610
C	1.195570	3.977835	-0.067553
C	-4.666518	-0.010950	1.016430
C	0.921030	2.678837	0.340657
H	1.345229	2.258418	1.247224
C	-3.372220	0.148714	0.538846
C	-3.748216	-1.016417	2.989985
C	-3.083562	0.847446	-0.774135
H	-3.958791	0.796296	-1.438560
H	-2.901356	1.907721	-0.561862
C	-1.218487	1.277869	-2.293277
H	-1.934323	1.782711	-2.958221

H	-0.525263	0.719299	-2.932628
C	-0.775874	-1.750391	-2.151137
C	-0.506289	-2.610518	-3.206359
C	-2.084986	-0.994786	-2.040913
H	-2.564691	-0.904736	-3.026583
H	-2.765534	-1.567400	-1.399739
C	1.267271	-2.208280	-1.165603
H	1.949750	-1.993907	-0.348237
C	0.705138	-3.298300	-3.218118
C	1.608749	-3.091550	-2.183717
C	-4.857214	-0.599207	2.263154
C	3.342061	-0.565293	2.554117
C	3.479432	-2.003570	2.928482
H	4.523752	-2.203813	3.211449
H	2.850348	-2.245039	3.789225
H	3.231760	-2.660231	2.093282
C	3.733762	-0.214132	1.169828
O	3.916222	-1.027532	0.283383
O	3.835851	1.111202	0.978458
C	4.132781	1.511622	-0.357859
H	5.070305	1.065167	-0.696235
H	3.327048	1.208433	-1.032882
H	4.215273	2.597794	-0.327356
H	-5.858852	-0.732770	2.658644
H	-5.510557	0.322938	0.421603
H	-3.852356	-1.481720	3.963190
H	-0.661836	3.911414	-2.904482
H	0.803445	5.450467	-1.593262
H	1.837891	4.610926	0.533922
H	-1.230762	-2.739766	-4.004139
H	0.940618	-3.978052	-4.030708
H	2.569533	-3.592307	-2.159186
Cl	0.994798	-0.460289	1.922046
C	3.418113	0.466480	3.632197
H	4.464482	0.579937	3.952769
H	3.069422	1.442882	3.293127
H	2.836884	0.155755	4.504491

[PhCh$_2$--Cl--Cu(TPMA)]‡

ω-B97XD SCF energy: -1843.71308220 a.u.
ω-B97XD enthalpy: -1843.226478 a.u.
ω-B97XD free energy: -1843.315275 a.u.
ω-B97XD SCF energy in solution: -3287.44591892 a.u.
ω-B97XD enthalpy in solution: -3286.959315 a.u.
ω-B97XD free energy in solution: -3287.048112 a.u.
Imaginary frequency: -571.1683 cm-1

Cartesian coordinates

ATOM	X	Y	Z
Cu	-0.800749	-0.039895	0.143170
N	-1.519769	1.922500	0.412693
N	0.363087	-0.353422	-1.609018
N	-2.071381	-1.587420	0.737797
N	-2.342942	0.071201	-1.434996

C	-2.777095	4.376022	0.673731
C	-2.334871	2.369412	-0.555476
C	-1.761734	-2.553769	1.609601
H	-0.796308	-2.453419	2.095334
C	-2.989073	3.590763	-0.456148
C	-1.923751	3.913132	1.668547
C	-4.155097	-2.665119	0.298761
C	-1.317171	2.675071	1.499256
H	-0.643927	2.255965	2.240646
C	-3.249130	-1.632564	0.094708
C	-2.619712	-3.612228	1.879120
C	-3.558767	-0.462812	-0.817589
H	-4.309460	-0.746928	-1.569309
H	-3.998784	0.335224	-0.207952
C	-2.451140	1.489438	-1.783874
H	-3.381017	1.706995	-2.329586
H	-1.618605	1.729648	-2.455424
C	-0.350103	-0.577642	-2.723950
C	0.251053	-0.688369	-3.970399
C	-1.842923	-0.757273	-2.534123
H	-2.379227	-0.558243	-3.473566
H	-2.031550	-1.804717	-2.270664
C	1.692863	-0.243347	-1.692673
H	2.214857	-0.064979	-0.756832
C	1.636466	-0.576865	-4.058703
C	2.370718	-0.352424	-2.900995
C	-3.836254	-3.668936	1.208891
C	3.157454	-0.068010	2.600092
H	-4.529729	-4.484015	1.388742
H	-5.095922	-2.680029	-0.241964
H	-2.332412	-4.373045	2.595447
H	-3.651095	3.921501	-1.249998
H	-3.275405	5.334622	0.775308
H	-1.733338	4.491795	2.565029
H	-0.352848	-0.861776	-4.855375
H	2.131063	-0.661910	-5.020939
H	3.449694	-0.255837	-2.917400
C	3.945117	-0.036658	1.411379
C	4.398836	-1.231409	0.810649
C	4.250884	1.189034	0.779577
C	5.145769	-1.197835	-0.357103
H	4.163505	-2.182502	1.280057
C	4.995253	1.216697	-0.390146
H	3.897869	2.115417	1.224188
C	5.451520	0.025192	-0.959544
H	5.501995	-2.123829	-0.797867
H	5.232020	2.167440	-0.857773
H	6.051876	0.050345	-1.864423
H	2.956518	0.848848	3.142230
H	3.032787	-0.997103	3.144685
Cl	0.830195	-0.132895	1.701289

[PhCh$_2$--Br--Cu(TPMA)]‡
ω-B97XD SCF energy: -3954.97452040 a.u.

ω-B97XD enthalpy: -3954.488273 a.u.
ω-B97XD free energy: -3954.578786 a.u.
ω-B97XD SCF energy in solution: -5401.45702190 a.u.
ω-B97XD enthalpy in solution: -5400.970774 a.u.
ω-B97XD free energy in solution: -5401.061287 a.u.
Imaginary frequency: -398.9936 cm-1

Cartesian coordinates

ATOM	X	Y	Z
Cu	-0.767433	-0.032269	0.185473
N	-1.491778	1.930346	0.441527
N	0.435397	-0.343495	-1.549615
N	-2.037074	-1.589209	0.761140
N	-2.271458	0.069965	-1.411545
C	-2.762308	4.381075	0.667181
C	-2.288466	2.371422	-0.544843
C	-1.741416	-2.558174	1.635368
H	-0.782981	-2.460272	2.135172
C	-2.948254	3.590830	-0.463889
C	-1.927482	3.924966	1.680547
C	-4.116127	-2.663174	0.290089
C	-1.312981	2.688668	1.528591
H	-0.650866	2.276134	2.283573
C	-3.205805	-1.631871	0.100992
C	-2.604823	-3.615773	1.889872
C	-3.499465	-0.461437	-0.814641
H	-4.237261	-0.743504	-1.579569
H	-3.947965	0.337494	-0.212444
C	-2.376550	1.486465	-1.771214
H	-3.295773	1.697136	-2.336984
H	-1.530793	1.725423	-2.426433
C	-0.261579	-0.575894	-2.673235
C	0.355880	-0.687238	-3.911372
C	-1.755103	-0.762956	-2.500863
H	-2.282293	-0.570492	-3.446618
H	-1.942204	-1.809691	-2.233763
C	1.765707	-0.226679	-1.616293
H	2.274587	-0.044212	-0.673651
C	1.741724	-0.567571	-3.981919
C	2.459440	-0.335384	-2.815536
C	-3.811892	-3.669244	1.202725
Br	0.936235	-0.127248	1.849167
C	3.452784	-0.075162	2.709826
H	-4.509151	-4.483532	1.371120
H	-5.049181	-2.675464	-0.263974
H	-2.328329	-4.378369	2.608524
H	-3.594424	3.916395	-1.272768
H	-3.265719	5.338356	0.754922
H	-1.756348	4.507548	2.578322
H	-0.235398	-0.867357	-4.803489
H	2.249113	-0.652593	-4.937473
H	3.538014	-0.233260	-2.817241
C	4.181960	-0.042025	1.484725
C	4.600636	-1.235959	0.856391
C	4.465418	1.184957	0.843909
C	5.295762	-1.200417	-0.342691

H	4.380545	-2.188425	1.330492
C	5.157548	1.214517	-0.357163
H	4.138091	2.111347	1.307843
C	5.582817	0.023817	-0.951998
H	5.626281	-2.126460	-0.803085
H	5.378757	2.166651	-0.829720
H	6.143996	0.050642	-1.881671
H	3.275146	0.840920	3.262062
H	3.344915	-1.006857	3.254311

[STY--Cl--Cu(TPMA)]‡

ω-B97XD SCF energy: -1883.02229988 a.u.
ω-B97XD enthalpy: -1882.505889 a.u.
ω-B97XD free energy: -1882.598762 a.u.
ω-B97XD SCF energy in solution: -3326.76860960 a.u.
ω-B97XD enthalpy in solution: -3326.252199 a.u.
ω-B97XD free energy in solution: -3326.345072 a.u.
Imaginary frequency: -718.4246 cm-1

Cartesian coordinates

ATOM	X	Y	Z
Cu	0.874109	-0.091898	-0.088741
N	1.429848	1.323603	-1.553355
N	-0.133602	0.760110	1.588840
N	2.207818	-1.662466	0.258775
N	2.519308	0.979090	0.941956
C	2.471986	3.147114	-3.358390
C	2.278063	2.276099	-1.136467
C	1.903565	-2.963266	0.187324
H	0.900547	-3.189811	-0.160677
C	2.827158	3.202778	-2.013776
C	1.584751	2.164929	-3.783273
C	4.385989	-2.225689	1.054939
C	1.089307	1.268001	-2.845330
H	0.396597	0.475877	-3.112646
C	3.428874	-1.292957	0.677067
C	2.810825	-3.956702	0.532066
C	3.720769	0.193667	0.655984
H	4.543050	0.436304	1.345066
H	4.056626	0.458400	-0.353678
C	2.555068	2.318620	0.353012
H	3.507712	2.830144	0.554504
H	1.763964	2.910007	0.828575
C	0.673811	1.251037	2.541764
C	0.177499	1.925861	3.648839
C	2.154218	0.982185	2.359768
H	2.753070	1.702643	2.936360
H	2.375046	-0.014461	2.759945
C	-1.455973	0.915466	1.705219
H	-2.056008	0.497135	0.901901
C	-1.200566	2.082505	3.775219
C	-2.032556	1.568684	2.788262
C	4.072702	-3.579548	0.976887
C	-3.307345	-1.735799	-1.518425

H	4.804427	-4.327646	1.263785
H	5.360746	-1.896595	1.400639
H	2.527323	-5.000050	0.455768
H	3.519209	3.955484	-1.649840
H	2.885618	3.860559	-4.063851
H	1.284985	2.084910	-4.821830
H	0.856763	2.317962	4.399113
H	-1.615018	2.602784	4.632761
H	-3.109936	1.670327	2.840072
C	-3.936886	-0.699612	-0.752193
C	-4.479523	-0.929106	0.529906
C	-4.000905	0.611143	-1.275472
C	-5.076051	0.103513	1.241647
H	-4.448263	-1.924408	0.961288
C	-4.586119	1.640432	-0.556492
H	-3.576467	0.805457	-2.256699
C	-5.132745	1.390696	0.704854
H	-5.509733	-0.096767	2.216974
H	-4.631694	2.638597	-0.980870
H	-5.610237	2.193029	1.259380
C	-3.301947	-3.173649	-1.121864
H	-2.992332	-3.311219	-0.081026
H	-4.310538	-3.600208	-1.227227
H	-2.627406	-3.749632	-1.758619
H	-3.108661	-1.511507	-2.562056
Cl	-0.849538	-1.156479	-1.074222

[STY--Br--Cu(TPMA)]‡

ω-B97XD SCF energy: -3994.28349789 a.u.
ω-B97XD enthalpy: -3993.767416 a.u.
ω-B97XD free energy: -3993.862600 a.u.
ω-B97XD SCF energy in solution: -5440.77894008 a.u.
ω-B97XD enthalpy in solution: -5440.262858 a.u.
ω-B97XD free energy in solution: -5440.358042 a.u.
Imaginary frequency: -513.8592 cm-1

Cartesian coordinates

ATOM	X	Y	Z
Cu	0.846306	-0.128923	-0.105120
N	1.380898	1.289464	-1.576626
N	-0.200752	0.708912	1.564968
N	2.198320	-1.677374	0.263199
N	2.448750	0.971490	0.927199
C	2.408987	3.124352	-3.378361
C	2.206966	2.259541	-1.155095
C	1.920227	-2.984820	0.201458
H	0.924730	-3.234479	-0.152140
C	2.748438	3.192452	-2.030147
C	1.543821	2.124861	-3.807945
C	4.381802	-2.190374	1.079261
C	1.054106	1.223084	-2.871821
H	0.376196	0.419146	-3.142085
C	3.409478	-1.280251	0.686265
C	2.844481	-3.956661	0.561824

C	3.670421	0.211221	0.653529
H	4.482054	0.478742	1.345638
H	4.005655	0.475497	-0.356415
C	2.464987	2.311882	0.336725
H	3.405098	2.841072	0.549973
H	1.656244	2.887360	0.801871
C	0.593690	1.218724	2.519290
C	0.081368	1.889396	3.621270
C	2.078563	0.974080	2.344804
H	2.663944	1.707506	2.918476
H	2.315158	-0.016825	2.749975
C	-1.526482	0.839631	1.676474
H	-2.116701	0.404508	0.874336
C	-1.299829	2.021666	3.741618
C	-2.118327	1.487628	2.754372
C	4.095397	-3.550855	1.011851
Br	-0.951508	-1.277205	-1.157431
C	-3.591309	-1.772135	-1.590039
H	4.839350	-4.281950	1.310848
H	5.347354	-1.838792	1.428523
H	2.581686	-5.005884	0.493016
H	3.422526	3.959234	-1.662003
H	2.817341	3.841966	-4.082648
H	1.256117	2.035054	-4.849076
H	0.750600	2.296733	4.372423
H	-1.726984	2.538323	4.595099
H	-3.197568	1.569193	2.800888
C	-4.149414	-0.719288	-0.792229
C	-4.680480	-0.945307	0.495600
C	-4.151667	0.604979	-1.286237
C	-5.208917	0.102194	1.238841
H	-4.696982	-1.950057	0.905613
C	-4.668426	1.648143	-0.535977
H	-3.733549	0.797944	-2.270530
C	-5.206840	1.401797	0.729771
H	-5.636633	-0.096195	2.217305
H	-4.666510	2.656156	-0.939309
H	-5.632293	2.216157	1.308655
C	-3.646412	-3.216207	-1.215203
H	-3.321819	-3.385832	-0.183531
H	-4.675259	-3.595295	-1.305006
H	-3.012378	-3.814107	-1.873412
H	-3.398740	-1.538851	-2.633313

[Me--Br--Cu(TPMA)]‡

ω-B97XD SCF energy: -3723.97809215 a.u.
ω-B97XD enthalpy: -3723.580238 a.u.
ω-B97XD free energy: -3723.660789 a.u.
Imaginary frequency: -103.27 cm-1

Cartesian coordinates

ATOM	X	Y	Z
Cu	-0.69288	0.21468	-0.03706
N	-0.11434	-1.24282	-1.51009
N	-0.42606	-0.60151	1.91372

N	-2.27843	1.47308	-0.41981
N	-2.35628	-1.23014	0.08143
C	0.30045	-3.16421	-3.4618
C	-0.86308	-2.35483	-1.53191
C	-2.24927	2.81013	-0.34674
H	-1.27519	3.25246	-0.16725
C	-0.69085	-3.33652	-2.50036
C	1.08423	-2.01629	-3.42593
C	-4.63539	1.55804	-0.78917
C	0.83943	-1.0769	-2.43257
H	1.42016	-0.16382	-2.34468
C	-3.44924	0.85119	-0.64353
C	-3.39111	3.58598	-0.49363
C	-3.39139	-0.65618	-0.77963
H	-4.37937	-1.09939	-0.58656
H	-3.12747	-0.89387	-1.81718
C	-1.85849	-2.51981	-0.40054
H	-2.67901	-3.187	-0.70184
H	-1.34038	-3.00681	0.43368
C	-1.4839	-1.29043	2.37217
C	-1.44742	-1.97495	3.5786
C	-2.72335	-1.2508	1.50107
H	-3.39295	-2.09009	1.73917
H	-3.27281	-0.32626	1.71423
C	0.69927	-0.57143	2.63433
H	1.53163	-0.01898	2.20841
C	-0.27778	-1.93766	4.33547
C	0.81471	-1.22755	3.85476
C	-4.60538	2.94778	-0.71588
C	3.77715	1.66994	-0.03778
H	-5.5202	3.52062	-0.8272
H	-5.56733	1.0286	-0.95835
H	-3.32182	4.66544	-0.42657
H	-1.31899	-4.22176	-2.49866
H	0.4551	-3.91632	-4.22877
H	1.86652	-1.84226	-4.15592
H	-2.31663	-2.52829	3.9195
H	-0.22235	-2.46466	5.28255
H	1.75033	-1.18244	4.39981
Br	1.192	1.67048	-0.16524
H	4.04243	1.98026	-1.02683
H	3.95131	2.34379	0.77492
H	3.75446	0.62885	0.20823

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