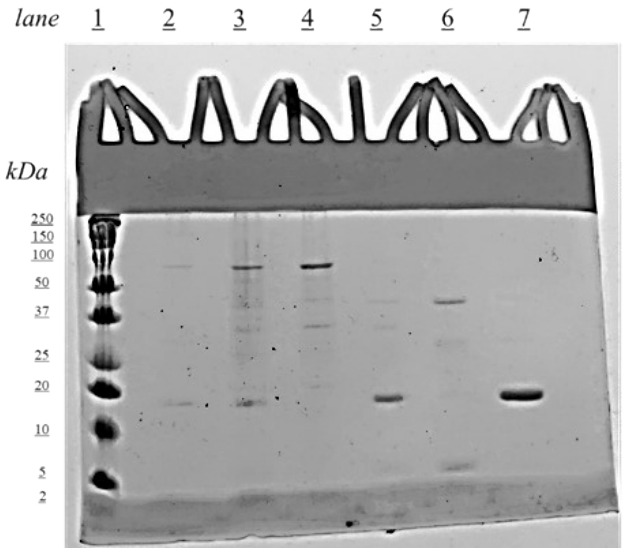
Supplementary Information

Contents



Samples:

1) Biorad molecular marker
2) Supernatant in spheroplast buffer
3) Supernatant in MQ H_2O
4) Flow-through from anion exchange column
5) Crude protein fractions from anion exchange column
6) First peak from SEC
7) Pure *Bl*AA10 – second peak in SEC

Figure S1. SDS PAGE Electrophoresis of *Bl*AA10 enzyme.

Gel electrophoresis was carried out using a 12% SDS-PAGE gel to confirm purity of *Bl*AA10 enzyme (lane 7) showing single band slightly under 20 kDa.

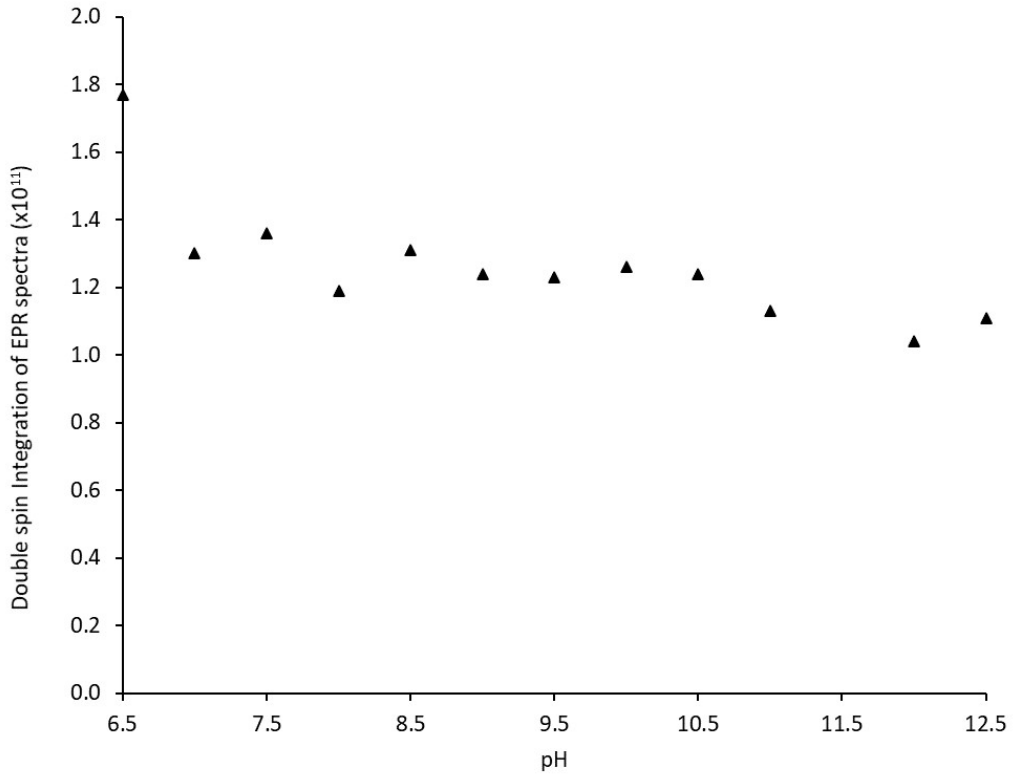


Figure S2 Spin quantification by double-integration of EPR spectra of *Bl*AA10 collected at varying pH.

The first derivative spectra were integrated twice with the maximum value of the resulting curve reporting on the total area under each absorption spectrum. Experimental conditions (such as microwave power) can affect signal intensity and as such were fixed between experiments. However, other factors such as slightly differing sample alignment in the EPR cavity along with variations in concentration due to altering pH were not able to be controlled for introducing some uncertainty in these values. Notwithstanding these caveats, however, the data shows a relatively consistent double-integration spin quantification (albeit with a slight downward trend likely due to diluting samples slightly with NaOH with increasing pH) indicating no redox processes occurred throughout the experiment.

Table S1. Singular Values obtained from SVD analysis of the pH titration EPR spectra

Principal Component	Singular Value
1	59
2	20
3	10

Singular Value Decomposition (SVD) was carried out in MATLAB R2020a by importing the EPR pH titration data set as a matrix (A) using the function:

$$A = \left[\begin{pmatrix} a & \cdots & b \\ \vdots & \ddots & \vdots \\ y & \cdots & z \end{pmatrix}\right]$$

Whereby the dataset is copied inside the square brackets.

A series of singular values were obtained using the functions:

$s = svd(A)$

$[U,S,V] = svd(A)$

The latter performs a singular value decomposition of matrix A, such that $A = U \times S \times V'$. It was possible to obtain abstract spectra from the U ($m \times m$) matrix by the function:

$G = U(1{:}m, n)$

Where G contains the generated abstract spectrum, m is the rank of the U matrix (in this case 1024 due to the selected scan width of the EPR spectrum) and n is the selected principal component (in this case 1-3).

From the SVD analysis, three large non-zero singular values were obtained (Table S1) with their corresponding abstract spectra containing relatively little noise. In the absence of noiseless data, other non-zero singular values were generated. However, subsequent values were disregarded due to their comparatively small singular values and noisy abstract spectra. It was determined that there were 3 major principal components within the dataset.

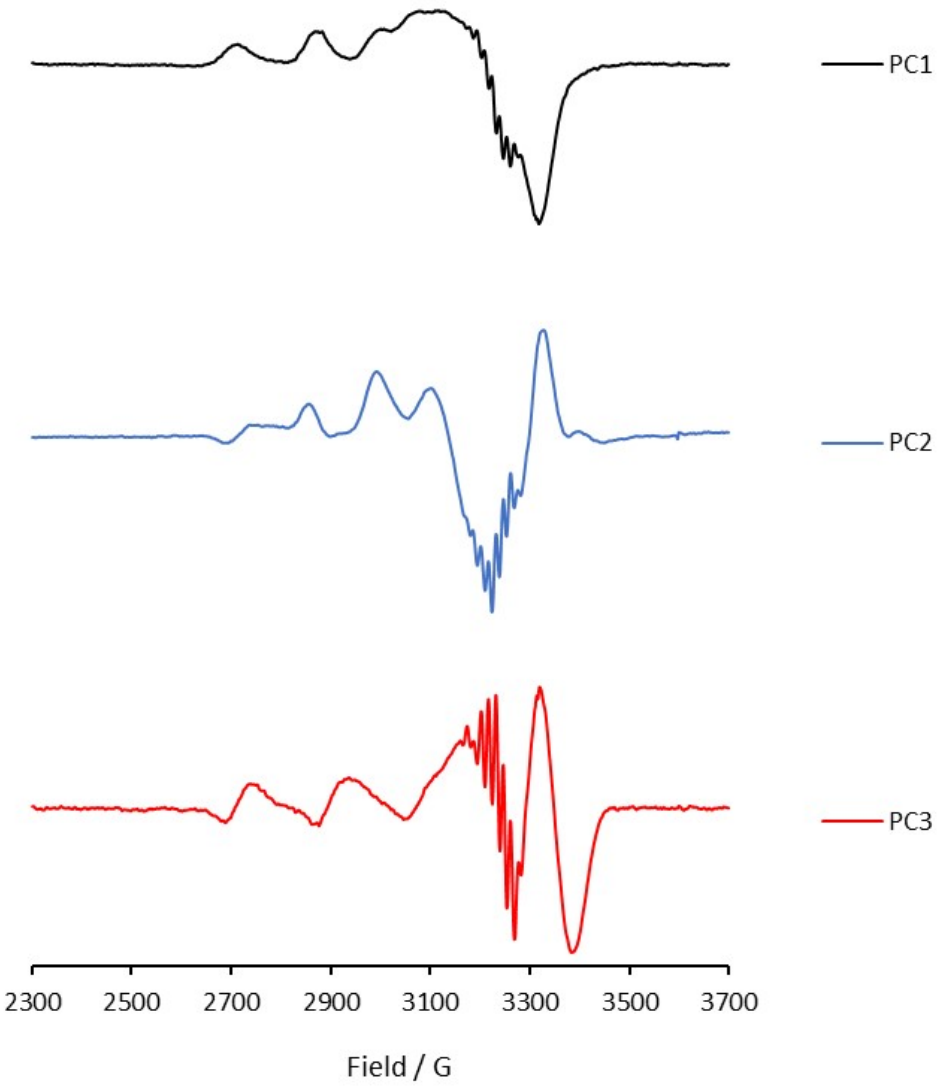


Figure S3. Singular Value Decomposition (SVD) abstract EPR spectra of the three large principal components.

PC3 (red) appears to somewhat resemble species **3** formed at high pH notable by the low field hyperfine peaks and overshoot feature. However, the abstract spectra of both PC1 and PC2 do not seem to match the spectra obtained for species **1** & **2** suggesting the SVD analysis struggled to separate these two species. This would likely improve with increasing number of data sets by performing the pH titration with smaller incremental steps.

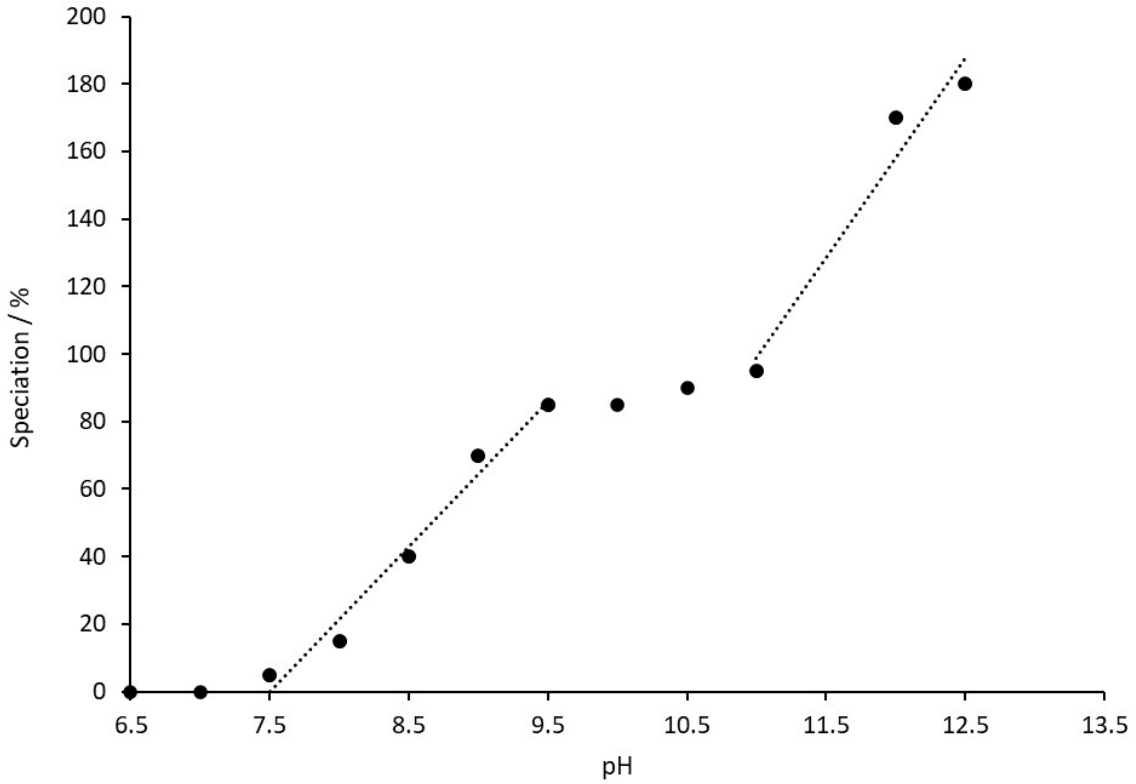


Figure S4. pH titration speciation plot. Speciation determined by comparative weighting of each species within the EPR spectra ranging from pH 6.5-12.5 with 0% representing all species 1, 100% being all species 2, and 200% being all species 3.

The speciation of the sample at each pH value was determined by assuming the spectrum collected at pH 6.5 describes 100% species **1**. Each spectrum was intensity-normalised to a maximum value of 1, to remove error from sample-cavity alignment between experiment and the slightly varying sample concentration from adjusting the pH. A percentage of the intensity of species **1** was then subtracted from each 'mixed' EPR spectrum and to determine the relative ratio of species **1**: species **2**. Speciation was determined when no shoulders corresponding to the 'subtracted spectrum' were present, yielding a flat baseline between peaks within the parallel region of the spectrum. By pH 10.5, there was no/negligible signal intensity corresponding to species 1 and the spectrum was assumed to be $\approx$ 100% species **2**. Subsequent speciation between pH 10.5-12.5 were derived using the same method, but now by subtracting species **3** intensity from the mixed spectra assuming the spectrum at pH 12.5 $\approx$ 100% species **3**.

Assumptions were made on basis that each of the species at pH 6.5, 10.5 and 12.5 could be well described using a single set of spin Hamiltonian parameters in their respective simulations.

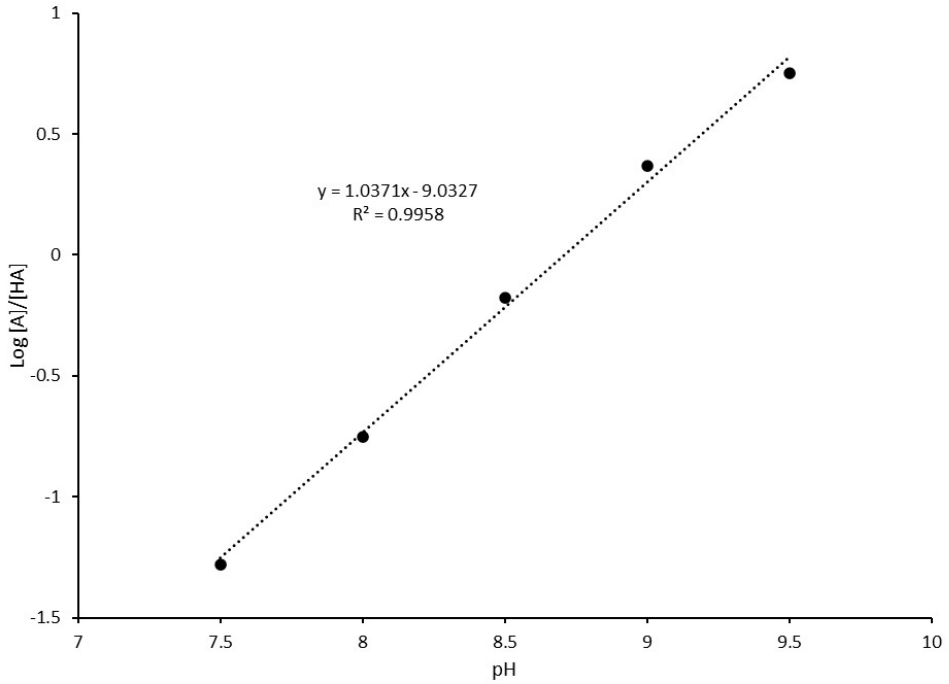


Figure S5 pH titration regression analysis to determine pKa1 and proton stoichiometry.

$$pH = pK_a - log\frac{[A^-]}{[HA]}$$

At 50% of each species, $$-log\frac{[A]}{[HA]} = 0, \ \therefore \ pH = pK_a$$

$$log\frac{[A^-][H^+]}{[HA]} = 1.037 \times pH - 9.033$$

At 50% of each species:

$$0 = 1.037 \times pH - 9.033$$

$$pH = pKa = \frac{9.033}{1.037} = 8.71$$

The proton stoichiometry is reported by the gradient. Here, this is 1.037. Since the value needs to be an integer number, it was assumed a single proton was involved in the first deprotonation process.

The same process was performed on the second deprotonation step to find an approximate pKa2 of 11.5 and proton stoichiometry of 1.3. Again, this was adjudged to be a single deprotonation event. Due to the comparatively few data points in this part of the titration, the value of pKa2 is expected to carry more error than pKa1.

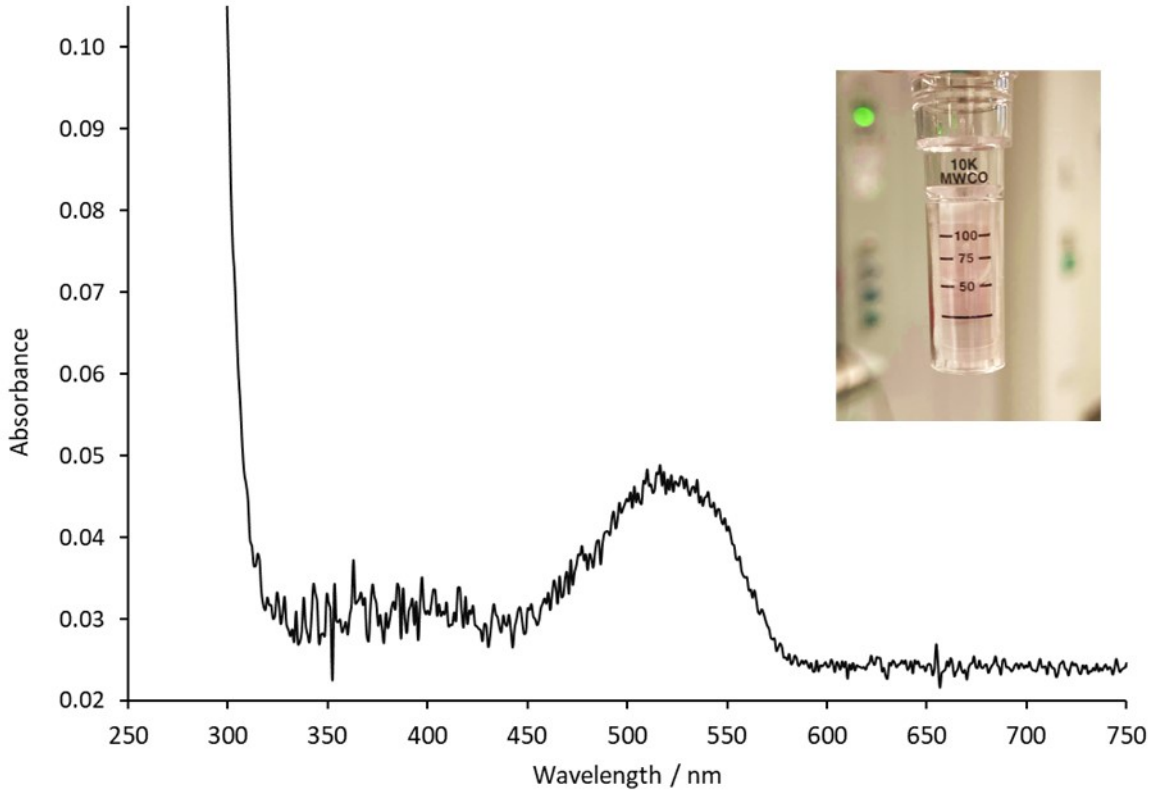


Figure S6. UV-Visible spectrum of *Bl*AA10 (*ca.* 10 µM) in MES, CHES, HEPES and CAPS, each at 5 mM (pH 12.5). Insert showing 10 kDa mass cut—off centrifugal filter containing *Bl*AA10 (*ca. 10* µM) MES, CHES, HEPES and CAPS, each at 5 mM (pH 12.5) with a pale pink colour.

The addition of NaOH to the *Bl*AA10 enzyme afforded a colour change of the solution to from colourless to pale pink when approaching pH $>$ 12. A UV/Visible spectrum was collected of *Bl*AA10 at a concentration of 10 µM and pH 12.5. The absorption band centred at 520 nm has a molar absorptivity $\varepsilon \approx$ 2500 M^{-1} cm^{-1}. The absorption band is centred in the cyan/green region of the electromagnetic spectrum, giving rise to a complementary colour of red/pink; in accordance with the appearance of the sample in the centrifugal concentrator.

DFT Geometry optimisations

Initial atomic coordinates to model species **1**, **2** and **3** were generated from the crystallographic structure of the similar enzyme *Ba*AA10 (PDB 5IJU, resolution 1.7 Å) from the Carbohydrate-Active enZymes (CAZy) database.[1] In all models the crystallographic coordinates were truncated to include the Cu(II) ion and 9 residues deemed to be key in the active site geometry: His28, Glu68, Gln92, Ala123, Pro124, His125, Thr127, Trp187 and Phe196 (numbering starting at the first histidine is position 28; His 28 and His 125 are analogous to His32 and His121 in BlLPMO10A). Hydrogen atoms were added to appropriate positions as were not attainable from the crystallographic coordinate file. The following modifications were made to reduce the size of the computational models, thus decreasing computational cost/time:

His28 and His125 were truncated at the carbonyl carbon, which was replaced by a methyl group, Glu68 and Gln92 were truncated with methyl substitution of the Cγ, the nitrogen of the amide bond between Ala123 and Thr122 was replaced by methyl groups, Trp187 and Phe196 were truncated with methyl substitution of the Cβ, Thr127 was truncated with methyl substitution of the Cα and the methyl group of Cβ was removed. For the species **1** model, two water molecules were retained with Cu-O distances fixed to 1.9 and 2.2 Å in keeping with the crystallographic coordinates. These Cu-O constraints were lifted for models **2** and **3**. Upon optimisation, the proton attached to the water nearest the Glu side chain was deprotonated by the carboxylate group. For the species **2** model, the proton shared by the ligating hydroxide and glutamate was removed and a proton from the additional water molecule was transferred to the $-NH_2$ group. For the species **3** model, the $-NH_3^+$ proton was transferred back to the hydroxide and an additional proton was removed from the $-NH_2$ group, giving an $-NH^-$ (azanide) group. By significantly truncating these models, certain structural constraints needed to be applied in order prevent atomic movement that would otherwise be impossible if the remainder of the proteins structure was imposed. In order to account for this, numerous atoms were kept frozen throughout the optimisations denoted by asterisks in figure S7.

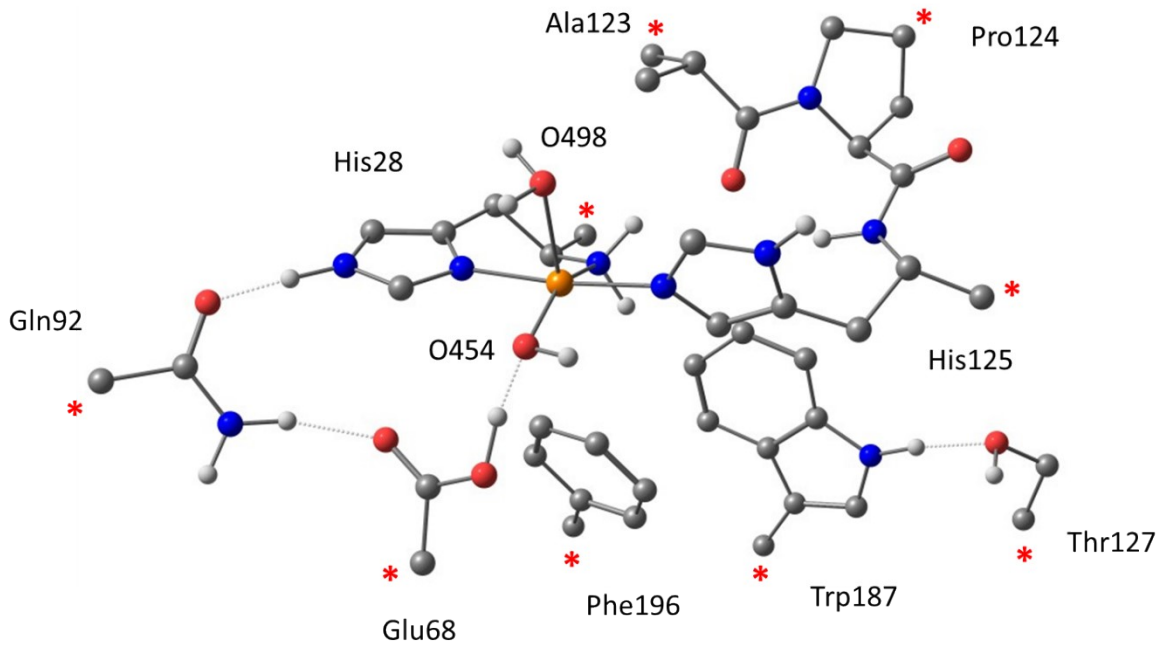


Figure S7. DFT model used to describe species 1. Residue numbers correspond to the labels from the crystal structure (PDB 5IJU) with His28 being the first amino acid in the polypeptide chain. Atoms kept frozen throughout the calculation are denoted by a red asterisk. Hydrogens connected to carbon atoms are omitted from the figure for clarity. Analogous positions were also frozen for models 2 and 3.

Geometry optimisations were performed using ORCA 4.2.0 program at the DFT level of theory. Optimisations of all models were performed using the spin-unrestricted, generalised gradient approximation (GGA) functional uBP86. Ahlrichs's Def-2-TZVP basis set was used to treat the copper and the first coordination sphere nitrogen atoms and oxygen atoms. On all remaining atoms a Def2-SVP basis set was used. Solvation effects were accounted for using the polarizable continuum model with water as the desired solvent (CPCM(water)), as implemented by ORCA 4.2.0. To assess the validity of the optimised geometries, the atomic positions were compared against the crystallographic coordinates, with the copper ion the origin of both models as in figure S8.

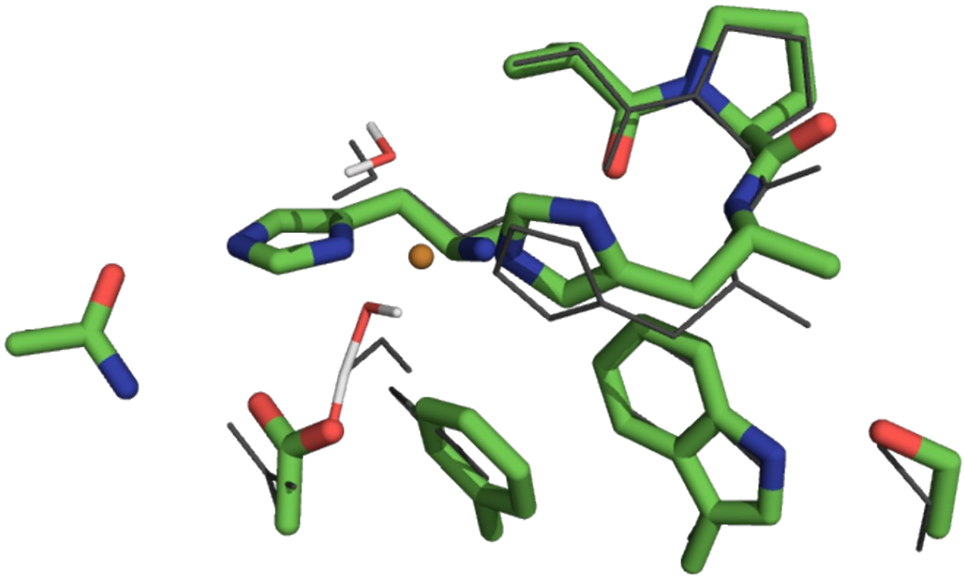


Figure S8. Comparison on the DFT optimised coordinates of model 1 (sticks coloured according to atom type) against the crystallographic coordinates of *Ba*AA10 (PDB 5IJU) (grey wires). Both models were aligned using the copper ion as the origin.

DFT EPR property calculations

EPR property calculations were performed on the optimized geometries of **1**, **2** and **3** using the ORCA 4.2.0 program at the DFT level of theory. The cartesian reference system was oriented as such that the NH2-Cu(II)-O axis was aligned with the y-axis and the N-Cu(II)-N axis was oriented along x. The integration grid size was kept large (AngularGrid = 7 for all atoms and IntAcc = 7 for the Cu(II) ion) to ensure that the core density was correctly described. Solvation effects were accounted for in the property calculations by implementing the conductor-like polarized continuum model (CPCM) with a dielectric constant of 80.0 and a refractive index of 1.33 (water). The hyperfine coupling calculations included the Fermi-contact, spin dipolar and spin orbit contributions. The hybrid functional, uB3LYP, was used for these calculations with and adjusted fraction (38%) of Hartree-Fock exchange following studies showing improvements in the EPR property calculations.[2] The copper ions were described using the core-property "CP-PPP" basis set having shown good accuracy with EPR calculations on d-block metals.[3] The IGLO-III basis set was applied to all ligating atoms and the ring atoms of the imidazole groups due to increased flexibility in the core region, making it more suited for EPR properties calculations with respect to the Def2-TZVP basis set. All remaining atoms were treated with Ahlrich's def2-SVP basis set.

Table S2. EPR spin Hamiltonian parameters derived *via* simulation and DFT for species 1, 2 and 3.

		Species **1**		Species **2**		Species **3**	
		Simulation	DFT	Simulation	DFT	Simulation	DFT
g-factors	g_1	2.030	2.049	2.044	2.070	2.038	2.037
	g_2	2.125	2.081	2.069	2.079	2.062	2.070
	g_3	2.260	2.216	2.233	2.244	2.180	2.188
Cu HFC / MHz	$\lvert A_1 \rvert$	60	110	50	94	70	15
	$\lvert A_2 \rvert$	90	29	66	4	90	140
	A_3	-445	-598	-554	-582	-614	-496
Principal N SHFC / MHz	N1	40	36	N/A	1	33	43
	N2	40	47	40	40	35	44
	N3	32	44	40	40	35	39

Time Dependent-DFT (TD-DFT)

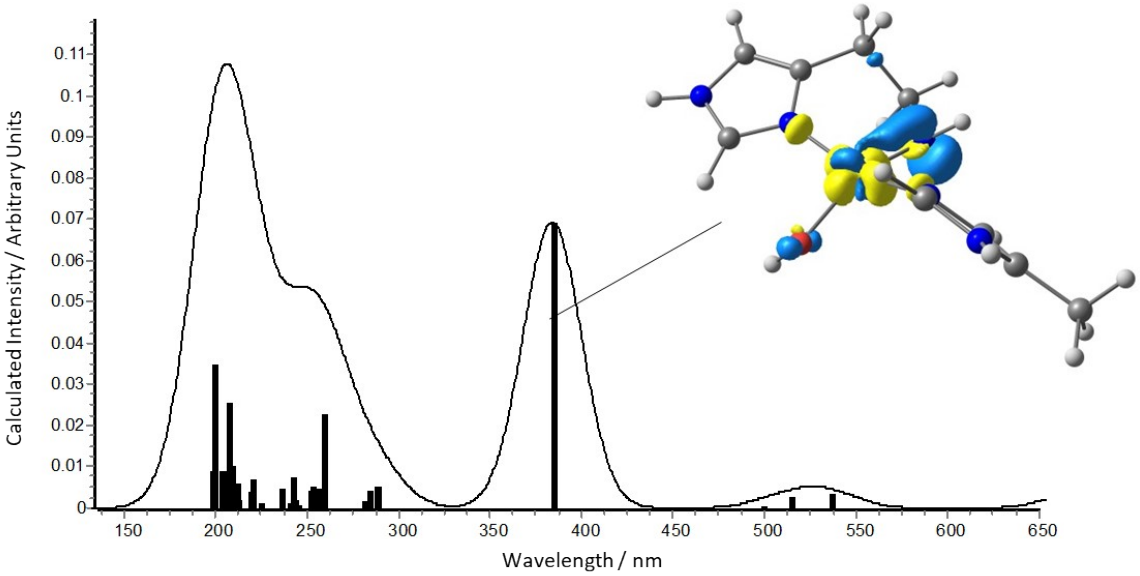


Figure S9. TD-DFT UV/vis spectrum of truncated model of species 3 and transition density of the proposed LMCT transition from the azanide (blue) to the metal (yellow). Spectrum generated by Gaussian broadening of the TD-DFT vectors.

A TD-DFT calculation was performed on truncated coordinates of species **3** (model size reduced to lower computational cost) using the hybrid exchange-correlation functional, CAM-B3LYP, to provide more accurate energies of charge transfer excitations in which standard B3LYP significantly underestimates.[4] All atoms were treated with the def2-TZVP basis set with the inclusion of dispersion correction using the D3(BJ) scheme. Solvation effects were modelled using the conductor-like polarisable continuum model (CPCM) using water as the desired solvent. To improve the speed of these calculations, the RIJCOSX approximation was employed with the auxiliary basis set, def2/J. A total of 30 roots were calculated for the spectrum and a Gaussian broadening scheme was applied to produce the calculated spectrum. The vectors calculated at wavelengths < 300 nm showed to be π-π* transitions from the imidazole groups and would be expected to make up part of the large 280 nm absorption band synonymous with a proteins UV-Visible absorption profile. The vectors calculated at wavelengths > 500 nm belonged to d-d transitions (albeit considerably blue shifted). Finally, the vector calculated at 385 nm was considerably more intense than those in the d-d region and the transition density showed that this transition occurs via density from the azanide nitrogen to the copper as a formal LMCT transition (albeit significantly blue-shifted as with the d-d values). These bands appear to be considerably blue shifted compared to the experimental data. However, calculating exact energies with TD-DFT is known to be problematic in open-shell transition metal complexes due to heavy spin contaminations of excited states.[5] Notwithstanding this caveat, however, the calculation does reveal that for the proposed Cu(II)-azanide species that an intense LMCT band is expect to appear between the d-d region and the protein's characteristic band at 280 nm

DFT cartesian coordinates

Species 1

Single point energy uB3LYP (38%HFX): -4415.903404286993 Hartree's

N	0.000000000	-2.106299000	0.000000000	C	-4.177704000	-0.674004000	0.065444000
C	1.285261000	-2.847226000	-0.152034000	C	-2.930088000	-0.819181000	-0.520022000
C	1.122078000	-4.350704000	0.041703000	N	-3.964911000	0.129792000	1.174747000
C	2.336038000	-2.287052000	0.820419000	C	-2.648652000	0.446659000	1.245175000
C	2.845544000	-0.947966000	0.407208000	N	-1.997756000	-0.113122000	0.222818000
C	4.138269000	-0.453258000	0.327257000	C	-8.957055000	-5.259243000	-3.500860000
N	1.982180000	0.060670000	0.000000000	C	-8.595048000	-5.747141000	-4.902956000
C	2.724471000	1.133715000	-0.290291000	O	-7.977147000	-4.360466000	-2.938994000
N	4.031509000	0.855908000	-0.104730000	C	-3.066742000	-5.816685000	-6.614897000
C	1.631917000	1.915757000	-5.298686000	C	-3.756518000	-5.390754000	-5.358724000
C	1.606374000	1.912440000	-3.778504000	C	-5.122775000	-5.268517000	-5.136719000
O	2.622213000	1.682122000	-3.103618000	C	-3.121457000	-5.032139000	-4.114885000
O	0.413896000	2.127533000	-3.263347000	C	-4.166982000	-4.718600000	-3.175313000
C	7.366924000	3.807846000	-2.235129000	C	-1.775105000	-4.921238000	-3.712727000
C	6.123790000	2.996081000	-1.944977000	N	-5.369813000	-4.874719000	-3.830946000
N	5.285393000	2.768311000	-2.972645000	C	-3.880113000	-4.342045000	-1.848153000
O	5.929856000	2.577606000	-0.777208000	C	-1.493909000	-4.497629000	-2.412103000
C	-1.237577000	-3.314669000	4.017779000	C	-2.530154000	-4.232100000	-1.478554000
C	-2.326742000	-3.718388000	3.015369000	C	0.654185000	-3.672477000	-6.185474000
O	-2.245557000	-3.386867000	1.806101000	C	0.174375000	-2.654386000	-5.179963000
C	-0.784796000	-1.872228000	3.752311000	C	-1.165963000	-2.215792000	-5.164509000
N	-3.370718000	-4.462920000	3.473447000	C	1.061682000	-2.130257000	-4.213566000
C	-4.372727000	-5.030393000	2.541718000	C	-1.613004000	-1.286190000	-4.211669000
C	-5.498029000	-4.004295000	2.244676000	C	0.623948000	-1.190203000	-3.268833000
O	-6.558380000	-3.991514000	2.885384000	C	-0.717473000	-0.766831000	-3.264858000
C	-4.908392000	-6.251818000	3.304949000	Cu	0.000000000	0.000000000	0.000000000
C	-4.868706000	-5.803219000	4.777582000	O	-0.062899000	1.700025000	-0.846144000
C	-3.566685000	-4.974428000	4.854900000	O	0.133766000	0.900513000	2.002794000
N	-5.231319000	-3.148614000	1.218215000	H	0.937252000	2.670457000	-5.713171000
C	-6.157546000	-2.073320000	0.828242000	H	1.286244000	0.917746000	-5.642701000
C	-7.522375000	-2.600893000	0.368845000	H	7.355898000	4.711777000	-1.594650000
C	-5.513642000	-1.231457000	-0.291537000	H	7.457620000	4.112504000	-3.294201000

H	5.501788000	3.155806000	-3.892369000
H	4.381152000	2.268454000	-2.883026000
H	-0.029686000	-1.562411000	4.501599000
H	-1.634247000	-1.162349000	3.795137000
H	-0.325872000	-1.774204000	2.749604000
H	-1.667611000	-3.358953000	5.038394000
H	-4.224551000	-7.108200000	3.136930000
H	-5.920548000	-6.537875000	2.964384000
H	-5.743952000	-5.160508000	4.990465000
H	-4.859422000	-6.646591000	5.494132000
H	-3.635754000	-4.138403000	5.578310000
H	-2.702258000	-5.608840000	5.142787000
H	-3.864934000	-5.294688000	1.592874000
H	-9.018824000	-6.115604000	-2.798768000
H	-8.447209000	-4.895176000	-5.597785000
H	-7.674248000	-6.362188000	-4.888057000
H	-9.415336000	-6.376732000	-5.306071000
H	-8.111062000	-3.479499000	-3.342798000
H	-2.382209000	-5.028729000	-6.999499000
H	-2.439634000	-6.720426000	-6.453806000
H	-5.951177000	-5.437580000	-5.833694000
H	-0.959938000	-5.146987000	-4.413863000
H	-0.443246000	-4.367808000	-2.125658000
H	-4.683663000	-4.154429000	-1.120978000
H	-2.285359000	-3.952182000	-0.442045000
H	1.118293000	-4.546685000	-5.682197000
H	-0.176229000	-4.041652000	-6.818446000
H	-1.875583000	-2.626351000	-5.899595000
H	2.112617000	-2.461984000	-4.206464000
H	-2.666568000	-0.966990000	-4.210047000
H	1.335196000	-0.765472000	-2.544520000
H	-1.045018000	-0.007958000	-2.540812000
H	-0.554931000	-2.458342000	0.801229000
H	1.624751000	-2.647667000	-1.188349000
H	2.056037000	-4.878231000	-0.237294000
H	3.186700000	-2.991328000	0.887664000
H	1.887069000	-2.248630000	1.839636000
H	5.102806000	-0.921532000	0.546896000
H	2.335610000	2.081927000	-0.660864000
H	-4.236695000	-3.072281000	0.949144000
H	-6.325517000	-1.421568000	1.717072000
H	-8.188473000	-1.744850000	0.140760000
H	-6.219383000	-0.411500000	-0.542515000
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H	-6.320622000	-4.719417000	-3.431948000
H	-3.792661000	-6.050094000	-7.418589000
H	1.428961000	-3.245579000	-6.857440000
H	8.255801000	3.213779000	-1.943812000
H	2.659130000	2.080103000	-5.669793000
H	-9.952172000	-4.762834000	-3.503324000
H	0.908759000	-4.587282000	1.103907000
H	0.298392000	-4.772965000	-0.559476000
C	-0.049322000	-4.304750000	3.955766000
H	0.733518000	-4.005084000	4.679757000
H	-0.365215000	-5.340431000	4.192215000
H	0.398585000	-4.309316000	2.942947000
H	-0.584157000	-2.303455000	-0.822216000
H	-7.428870000	-3.218953000	-0.548658000
H	-7.988307000	-3.209102000	1.164688000

Species 2

Single point energy uB3LYP (38%HFX): -4415.403254849613 Hartree's

N	28.395404000	2.179706000	75.635634000	C	27.478423000	-1.036725000	74.497215000
C	27.811571000	3.496969000	76.083355000	N	29.522981000	-1.834849000	74.353654000
C	28.544004000	4.658001000	75.421022000	C	29.313074000	-1.406179000	75.625907000
C	27.877057000	3.610779000	77.619221000	N	28.076110000	-0.925080000	75.744045000
C	26.841106000	2.891959000	78.435160000	C	26.540957000	0.049601000	66.553510000
C	25.971636000	3.512244000	79.320212000	C	25.237999000	0.404003000	65.839996000
N	26.586223000	1.515216000	78.492020000	O	26.347946000	-0.677501000	67.780772000
C	25.603850000	1.335639000	79.387336000	C	23.034995000	4.172974000	69.639914000
N	25.208756000	2.524186000	79.900007000	C	24.137895000	3.163669000	69.751562000
C	21.657999000	0.989999000	78.099997000	C	24.189391000	1.905975000	69.158240000
C	22.781287000	0.111559000	78.666636000	C	25.359927000	3.287999000	70.515736000
O	22.955070000	0.087729000	79.929129000	C	26.094261000	2.060769000	70.343405000
O	23.481864000	-0.524468000	77.823315000	C	25.900683000	4.301478000	71.340944000
C	23.453002000	2.661002000	84.412001000	N	25.351987000	1.243493000	69.514896000
C	23.396775000	2.354310000	82.921147000	C	27.330557000	1.839174000	70.982309000
N	22.892789000	1.168528000	82.534492000	C	27.126764000	4.076978000	71.976527000
O	23.834279000	3.197247000	82.097541000	C	27.832514000	2.855943000	71.808236000
C	32.489747000	1.804847000	75.165148000	C	22.458000000	4.792022000	73.872074000
C	31.675255000	1.557910000	73.896161000	C	23.282112000	3.643830000	74.411169000
O	30.414506000	1.557445000	73.879677000	C	23.923959000	2.736101000	73.541217000
C	32.067780000	0.869360000	76.301614000	C	23.448963000	3.459422000	75.802236000
N	32.378155000	1.385363000	72.756372000	C	24.713253000	1.684059000	74.039670000
C	31.724643000	1.364034000	71.427906000	C	24.214147000	2.396294000	76.304581000
C	31.283034000	-0.071723000	71.054050000	C	24.850022000	1.501623000	75.426774000
O	31.999896000	-0.830925000	70.387896000	Cu	27.373532000	-0.073807000	77.488236000
C	32.832591000	1.875332000	70.498405000	O	26.039517000	-1.364684000	77.732942000
C	34.104999000	1.306000000	71.147000000	O	29.157404000	0.728152000	77.652753000
C	33.853637000	1.457586000	72.643923000	H	21.566210000	0.876066000	77.004209000
N	30.046874000	-0.424785000	71.503088000	H	21.874603000	2.053791000	78.333413000
C	29.526651000	-1.790111000	71.319179000	H	24.516303000	2.680652000	84.726421000
C	29.291002000	-2.135003000	69.835995000	H	22.904017000	1.927588000	85.031403000
C	28.245528000	-1.969751000	72.154566000	H	22.560320000	0.499823000	83.230873000
C	28.378199000	-1.605172000	73.603843000	H	22.845357000	0.891254000	81.523605000

H	32.682306000	1.073007000	77.201581000	H	28.017445000	5.608303000	75.633908000
H	32.230087000	-0.191075000	76.017772000	H	27.762385000	4.684833000	77.864649000
H	31.003217000	0.989444000	76.581409000	H	28.906205000	3.344725000	77.944287000
H	33.550844000	1.593536000	74.940841000	H	25.849456000	4.570279000	79.574681000
H	32.839175000	2.984381000	70.517349000	H	25.129121000	0.385284000	79.652887000
H	32.687382000	1.539103000	69.455253000	H	29.638916000	0.179986000	72.231160000
H	34.200037000	0.236383000	70.879374000	H	30.303267000	-2.495578000	71.696741000
H	35.027473000	1.829041000	70.829644000	H	28.988305000	-3.197899000	69.750386000
H	34.337181000	0.660917000	73.241403000	H	27.935603000	-3.032530000	72.057203000
H	34.210710000	2.440765000	73.014921000	H	27.419484000	-1.367878000	71.721937000
H	30.833891000	2.022218000	71.461282000	H	26.444151000	-0.728851000	74.321006000
H	27.088553000	0.970112000	66.842448000	H	30.388044000	-2.262549000	74.013894000
H	24.672278000	-0.510856000	65.565065000	H	30.062319000	-1.440198000	76.420353000
H	24.590562000	1.039443000	66.476992000	H	29.152607000	1.272858000	78.463150000
H	25.455411000	0.960353000	64.905187000	H	25.127761000	-0.980657000	77.872525000
H	25.884607000	-1.514262000	67.575312000	H	24.513957000	2.690804000	80.687925000
H	22.522375000	4.336690000	70.613517000	H	25.690415000	0.382006000	69.035129000
H	23.416410000	5.165036000	69.316621000	H	22.266543000	3.850630000	68.910179000
H	23.458572000	1.422085000	68.498050000	H	21.691283000	5.123910000	74.599774000
H	25.357292000	5.247262000	71.491094000	H	23.042389000	3.675027000	84.583167000
H	27.550754000	4.863850000	72.617706000	H	20.690844000	0.749236000	78.589118000
H	27.891257000	0.905744000	70.831282000	H	27.208815000	-0.531015000	65.877193000
H	28.788041000	2.701363000	72.333118000	H	29.580073000	4.748419000	75.806468000
H	23.101758000	5.670104000	73.646515000	H	28.594094000	4.527621000	74.324168000
H	21.947272000	4.516931000	72.927033000	C	32.394498000	3.296120000	75.535720000
H	23.808229000	2.848429000	72.453431000	H	33.028117000	3.510175000	76.418980000
H	22.951190000	4.149748000	76.502727000	H	32.728442000	3.946734000	74.702290000
H	25.207764000	1.002954000	73.328386000	H	31.352248000	3.576718000	75.789870000
H	24.302122000	2.242548000	77.386927000	H	27.683340000	1.613456000	75.160184000
H	25.408985000	0.650036000	75.848803000	H	28.487218000	-1.510256000	69.393795000
H	29.207308000	2.225705000	74.970940000	H	30.224161000	-1.988242000	69.263890000
H	26.751032000	3.492615000	75.764815000	H	28.775015000	1.575655000	76.515717000

Species 3

Single point energy uB3LYP (38%HFX): -4414.815119531047 Hartree's

N	0.000000000	-1.938135000	0.000000000	C	-4.064333000	-0.154887000	0.738706000
C	1.240492000	-2.690738000	-0.046188000	C	-2.857416000	-0.647698000	0.265013000
C	0.991023000	-4.176505000	0.233300000	N	-3.721635000	0.836122000	1.649364000
C	2.342901000	-2.132572000	0.910903000	C	-2.361263000	0.935660000	1.686066000
C	2.851549000	-0.818822000	0.415186000	N	-1.823280000	0.046347000	0.859639000
C	4.143345000	-0.380175000	0.153431000	C	-8.817712000	-4.710922000	-2.547817000
N	1.974356000	0.176907000	0.000000000	C	-9.113530000	-5.117550000	-3.989370000
C	2.708427000	1.176426000	-0.500934000	O	-8.271811000	-3.385129000	-2.426137000
N	4.024367000	0.873710000	-0.421514000	C	-3.732152000	-5.557309000	-6.074339000
C	1.483186000	1.913459000	-5.309096000	C	-4.325528000	-4.899112000	-4.867840000
C	1.471590000	2.332830000	-3.824413000	C	-5.539046000	-4.225614000	-4.769100000
O	2.591557000	2.440757000	-3.221391000	C	-3.729951000	-4.836900000	-3.553122000
O	0.342767000	2.510674000	-3.283615000	C	-4.639379000	-4.111371000	-2.708250000
C	7.518436000	3.538220000	-2.703036000	C	-2.512845000	-5.309997000	-3.012327000
C	6.140784000	2.966173000	-2.429703000	N	-5.724456000	-3.745451000	-3.481271000
N	5.296969000	2.849261000	-3.469503000	C	-4.350104000	-3.861248000	-1.351963000
O	5.853123000	2.631152000	-1.253449000	C	-2.228093000	-5.052378000	-1.668275000
C	-1.038899000	-2.919202000	4.271800000	C	-3.129215000	-4.327946000	-0.846127000
C	-2.208289000	-3.341004000	3.370546000	C	0.126307000	-3.627455000	-5.964013000
O	-2.192215000	-3.122714000	2.140317000	C	-0.217743000	-2.598341000	-4.912058000
C	-0.553702000	-1.521896000	3.856943000	C	-1.560813000	-2.378786000	-4.536352000
N	-3.269396000	-3.969821000	3.951323000	C	0.787244000	-1.839246000	-4.271768000
C	-4.365981000	-4.520263000	3.121763000	C	-1.890265000	-1.422362000	-3.562100000
C	-5.463392000	-3.452215000	2.870872000	C	0.459570000	-0.875940000	-3.303054000
O	-6.500253000	-3.408448000	3.551128000	C	-0.882150000	-0.658452000	-2.952457000
C	-4.894465000	-5.679638000	3.975652000	Cu	0.000000000	0.000000000	0.000000000
C	-4.725433000	-5.152697000	5.409803000	O	-0.389619000	1.874310000	-0.650852000
C	-3.384013000	-4.400057000	5.362755000	H	0.550030000	2.226426000	-5.817112000
N	-5.207199000	-2.587642000	1.851623000	H	1.536464000	0.805043000	-5.355475000
C	-6.100529000	-1.457627000	1.551199000	H	7.654747000	4.444451000	-2.079134000
C	-7.494176000	-1.909759000	1.102709000	H	7.688901000	3.797726000	-3.765099000
C	-5.465412000	-0.574275000	0.457075000	H	5.604658000	3.174431000	-4.387864000

H	4.280394000	2.581487000	-3.372037000
H	0.311963000	-1.215284000	4.479204000
H	-1.355761000	-0.765935000	3.976918000
H	-0.252491000	-1.509390000	2.789921000
H	-1.401696000	-2.869991000	5.318372000
H	-4.261068000	-6.574421000	3.805384000
H	-5.941606000	-5.933412000	3.727808000
H	-5.549723000	-4.450332000	5.638364000
H	-4.721273000	-5.952270000	6.175375000
H	-3.358555000	-3.530633000	6.049707000
H	-2.537215000	-5.069246000	5.624819000
H	-3.946991000	-4.842120000	2.147539000
H	-8.055818000	-5.383307000	-2.102617000
H	-9.857761000	-4.434848000	-4.450964000
H	-8.193854000	-5.104735000	-4.607739000
H	-9.534060000	-6.143800000	-4.017907000
H	-8.922749000	-2.750850000	-2.788232000
H	-2.745623000	-5.117742000	-6.338835000
H	-3.553378000	-6.641411000	-5.905637000
H	-6.295730000	-4.042171000	-5.542418000
H	-1.798987000	-5.861680000	-3.644161000
H	-1.282736000	-5.410861000	-1.236253000
H	-5.051950000	-3.317249000	-0.704895000
H	-2.849589000	-4.106025000	0.194539000
H	1.210489000	-3.633960000	-6.192105000
H	-0.155268000	-4.651081000	-5.632752000
H	-2.361878000	-2.970372000	-5.005889000
H	1.843162000	-2.004657000	-4.544836000
H	-2.943961000	-1.285028000	-3.271573000
H	1.248905000	-0.289840000	-2.809556000
H	-1.122220000	0.112064000	-2.203728000
H	-0.564587000	-2.291138000	0.786724000
H	1.657773000	-2.596930000	-1.079636000
H	1.924176000	-4.777454000	0.190213000
H	3.195674000	-2.839555000	0.988467000
H	1.898845000	-2.039668000	1.927289000
H	5.116617000	-0.852523000	0.324638000
H	2.324659000	2.061717000	-1.017100000
H	-4.230768000	-2.556788000	1.512686000
H	-6.210929000	-0.853866000	2.481542000
H	-8.143503000	-1.021101000	0.967821000
H	-6.121424000	0.309448000	0.316197000
H	-5.472005000	-1.129619000	-0.502938000
H	-2.654324000	-1.447706000	-0.455915000
H	-4.375997000	1.410045000	2.186303000
H	-1.812156000	1.669356000	2.283689000
H	0.054777000	2.071978000	-1.516242000
H	4.786897000	1.523657000	-0.769602000
H	-6.632934000	-3.392624000	-3.114417000
H	-4.390876000	-5.458577000	-6.959625000
H	-0.420005000	-3.438614000	-6.912280000
H	8.281071000	2.803349000	-2.376889000
H	2.365556000	2.320166000	-5.842874000
H	-9.736073000	-4.796326000	-1.923205000
H	0.537940000	-4.306988000	1.237282000
H	0.274692000	-4.579903000	-0.505884000
C	0.102311000	-3.963466000	4.215665000
H	0.922595000	-3.662257000	4.897552000
H	-0.246039000	-4.971966000	4.517911000
H	0.512567000	-4.035397000	3.189035000
H	-7.452517000	-2.451052000	0.134214000
H	-7.952216000	-2.566013000	1.864306000
O	0.644523000	3.026240000	1.350747000
H	1.280061000	2.340145000	1.630071000
H	0.217768000	2.566455000	0.475477000

Truncated Species 3 for TD-DFT

Single point energy uB3LYP (38%HFX): -2341.605057235535 Hartree's

N	0.000000000	-1.938134958	0.000000000	H	1.657773148	-2.596929941	-1.079635890
C	1.240492015	-2.690738250	-0.046188178	H	3.195674419	-2.839555064	0.988467117
C	2.342901048	-2.132572142	0.910902962	H	1.898845135	-2.039668197	1.927288941
C	2.851549395	-0.818821887	0.415186119	H	5.116617466	-0.852523069	0.324638071
C	4.143345145	-0.380175223	0.153431239	H	2.324659250	2.061716896	-1.017099840
N	1.974356083	0.176907129	0.000000000	H	-6.121424519	0.309448038	0.316197165
C	2.708427058	1.176426113	-0.500934001	H	-5.472005498	-1.129619327	-0.502937995
N	4.024367049	0.873710268	-0.421514021	H	-2.654323976	-1.447706184	-0.455914776
C	-5.465412479	-0.574274793	0.457075261	H	-4.375997393	1.410045169	2.186303213
C	-4.064333161	-0.154887006	0.738706039	H	-1.812156376	1.669356308	2.283689289
C	-2.857416383	-0.647698136	0.265013025	H	0.054777254	2.071978172	-1.516242046
N	-3.721635328	0.836122279	1.649363992	H	4.786897177	1.523656878	-0.769602053
C	-2.361262970	0.935659990	1.686066138	H	1.004395352	-3.702462707	0.248891111
N	-1.823280211	0.046346931	0.859638916	H	-5.819682889	-1.169608194	1.285610726
Cu	0.000000000	0.000000000	0.000000000				
O	-0.389618921	1.874310361	-0.650852032				
H	-0.564587145	-2.291137988	0.786724112				

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