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SUPLEMENTARY MATERIALS

of the manuscript

From 7-azaindole to adenine: molecular recognition aspects on mixed-ligand Cu(II) complexes with deaza-adenine ligands

Corresponding author: Alicia Domínguez-Martín.

Corresponding author Institution: Department of Inorganic Chemistry, Faculty of Pharmacy, University of Granada, E-18071 Granada, Spain.
E-mail: adominguez@ugr.es
Telephone number: +34 958 243 853.

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S1. Experimental methods

Computational details

DFT calculations, at the B3LYP[1] and unrestricted M06-L/6-31G* theoretical levels for the isolated ligands and copper complexes, respectively, have been performed with the Gaussian09 program,[2] using the 6-31G* basis set, for the isolated ligands and the 6-31+G** one for the copper complexes.[3] All structures were fully optimized at the following theoretical levels: B3LYP/6-31+G**//B3LYP/6-31+G** for the isolated ligands and M06-L/6-31G*//M06-L/6-31G* for the copper(II) complexes. The most stable spin multiplicities for the mono- and dinuclear copper complexes studied were doublet and triplet, respectively. The local stability of all structures was checked through the eigen values of the matrix of second derivatives (Hessian); all energetic minima presented no imaginary frequencies. Solvent effect was taken into account by means of the self consistent reaction field method (SCRF), selecting PCM algorithm with water as solvent.[4]

In order to corroborate the above mentioned theoretical levels and model systems, we performed additional calculations for the most stable Ia-3p9 complex with MIDA, consisted in the following tests: (i) Calculations improving the basis set (6-311++G**); (ii) Calculations with the inclusion of one water molecule coordinated to copper (similar to the crystallographic data); (iii) Calculations including the PCM solvation method; (iv) Calculations with geometrical optimizations starting from different geometries (variation in the dihedral angles between the chelating ligand and the deaza-adenine) in order to explore the potential energy surface (PES) in this region. All these additional calculation tests yielded similar geometries to those obtained at the gas phase and with standard theoretical levels above mentioned.

X-Ray Structure Determinations

Measured crystals were prepared under inert conditions immersed in perfluoropolyether as protecting oil for manipulation. Suitable crystals were mounted on MiTeGen Micromounts™ and these samples were used for data collection. Data were collected with Bruker X8 KappaAPEXII (**1**, **3** and **10**, 100 K), Bruker X8 Proteum (**2**, **7**, **9**) diffractometers, whereas those of **4**, **5**, **6** and **8** were collected at the ESRF synchrotron BM16 beam line (Grenoble, France). The data were processed with APEX2 (**1**, **2**, **3**, **7**, **9** and **10**)[5] and HKL2000 (**4**-**6** and **8**)[6] programs and corrected for absorption using SADABS.[7] The structures were solved by direct methods[8] which revealed the position of all non-hydrogen atoms. These atoms were refined on F^2 by a full-matrix least-squares procedure using anisotropic displacement parameters.[8] All hydrogen atoms were located in difference Fourier maps and included as fixed contributions riding on attached atoms with isotropic thermal displacement parameters 1.2 times those of the respective atom. Geometric calculations were carried out with PLATON[9] and drawings were produced with

PLATON[9] and MERCURY.[10] Additional crystal data and more information about the X-ray structural analyses are shown in Supplementary material S3 to S13. Crystallographic data for the structural analysis have been deposited with the Cambridge Crystallographic Data Centre, CCDC No. 881136 – 881145 from 1 to 10 respectively. Copies of this information may be obtained free of charge on application to CCDC, 12 Union Road, Cambridge CB2 1EZ, UK (fax: 44 1223 336 033; e-mail: deposit@ccdc.cam.ac.uk or http://www.ccdc.cam.ac.uk).

Other Physical methods

Analytical data were obtained in a Thermo-Scientific (Flash 2000) elemental micro-analyser. Infrared spectra were recorded by using KBr pellets on a Jasco FT-IR 410 or a Jasco FT-IR 6300 spectrometer. TG analyses were carried out in air-dry flow (100 mL/min) by a Shimadzu thermo-balance TGA-DTG-50H instrument, coupled with a FT-IR Nicolet Magma 550 spectrometer. A series of FT-IR spectra (20-30 per sample) of the evolved gasses were time-spaced recorded during the TG experiment. Diffuse reflectance (electronic) spectra were recorded in a Varian Cary-5E spectrophotometer. X-band EPR measurements were carried out on a Bruker ELEXSYS 500 spectrometer with a maximum available microwave power of 200 mW and equipped with a super-high-Q resonator ER-4123-SHQ. For Q-band studies, EPR spectra were recorded on a Bruker EMX system equipped with an ER-510-QT resonator. The magnetic field was calibrated by a NMR probe and the frequency inside the cavity was determined with a Hewlett-Packard 5352B microwave frequency counter. Computer simulation: WINEPR-Simfonia, version 1.5, Bruker Analytische Messtechnik GmbH).

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S2. Table S-1: *Gas phase Relative Gibbs Energies (ΔG_r) and selected geometrical parameters for the different mono- and di-nuclear Cu(II) complexes of deaza-adenines with chelant ligans calculated at the UM06-L/6-31+G*//UM06-L/6-31+G* theoretical level.*

Compound[a]	Nomenclature	NC[b]	NP[c]	ΔG_{rel} (Kcal/mol)	Cu···N (Å)	O···HN (Å)	<O-Cu-N-C (º)
Ia-3p9	Cu(MIDA)(H7azain)	3	9	0.0	1.988	1.799	0.2
Ia-9p3	Cu(MIDA)(H7azain)	9	3	3.5	1.934	1.746	1.8
Ib-3p9	Cu(NBzIDA)(H7azain)	3	9	0.0	1.989	1.795	1.1
Ib-9p3	Cu(NBzIDA)(H7azain)	9	3	3.2	1.935	1.746	1.0
IIa-3p7	Cu(MIDA)(H4abim)	3	7	10.2	1.973		60.3
IIa-3p9	Cu(MIDA)(H4abim)	3	9	0.0	1.983	1.813	0.1
IIa-7p3	Cu(MIDA)(H4abim)	7	3	9.0	1.947		1.5
IIa-7p9	Cu(MIDA)(H4abim)	7	9	3.4	1.959		0.0
IIa-9p3	Cu(MIDA)(H4abim)	9	3	2.7	1.938	1.759	1.5
IIa-9p7	Cu(MIDA)(H4abim)	9	7	10.8	1.969		30.4
IIc-3p7	Cu(CBIDA)(H4abim)	3	7	10.0	1.979		63.3
IIc-3p9	Cu(CBIDA)(H4abim)	3	9	0.0	1.983	1.813	0.6
IIc-7p3	Cu(CBIDA)(H4abim)	7	3	8.7	1.947		1.3
IIc-7p9	Cu(CBIDA)(H4abim)	7	9	3.4	1.960		0.9
IIc-9p3	Cu(CBIDA)(H4abim)	9	3	3.0	1.938	1.763	0.4
IIc-9p7	Cu(CBIDA)(H4abim)	9	7	10.6	1.976		23.5
IId-3p7	Cu(H_2EDTA)(H4abim)	3	7	1.1	1.991		65.2
IId-3p9	Cu(H_2EDTA)(H4abim)	3	9	0.0	1.996	1.948	17.8
IId-7p3	Cu(H_2EDTA)(H4abim)	7	3	5.3	1.965		7.9
IId-9p3	Cu(H_2EDTA)(H4abim)	9	3	3.0	1.955	1.887	10.4
IId-9p7	Cu(H_2EDTA)(H4abim)	9	7	2.6	1.972		65.5
IIIa-1p7	Cu(MIDA)(H5abim)	1	7	0.0	1.975		2.0
IIIa-1p9	Cu(MIDA)(H5abim)	1	9	0.6	1.978		0.9
IIIa-7p1	Cu(MIDA)(H5abim)	7	1	1.5	1.942		2.0
IIIa-7p9	Cu(MIDA)(H5abim)	7	9	1.2	1.966		0.7
IIIa-9p1	Cu(MIDA)(H5abim)	9	1	3.1	1.947		1.6
IIIa-9p7	Cu(MIDA)(H5abim)	9	7	0.5	1.964		0.2
IIIb-1p7	Cu(NBzIDA)(H5abim)	1	7	0.0	1.976		0.2
IIIb-1p9	Cu(NBzIDA)(H5abim)	1	9	0.3	1.978		0.4
IIIb-7p1	Cu(NBzIDA)(H5abim)	7	1	1.4	1.943		1.5
IIIb-7p9	Cu(NBzIDA)(H5abim)	7	9	1.4	1.968		0.5
IIIb-9p1	Cu(NBzIDA)(H5abim)	9	1	3.1	1.948		1.7
IIIb-9p7	Cu(NBzIDA)(H5abim)	9	7	0.7	1.965		1.2
IVa-1p3	Cu(MIDA)(H7deaA)	1	3	16.2	2.018	1.760	13.9
IVa-1p9	Cu(MIDA)(H7deaA)	1	9	2.8	2.001	1.754	20.7
IVa-3p1	Cu(MIDA)(H7deaA)	3	1	29.1	2.014		93.5
IVa-3p9	Cu(MIDA)(H7deaA)	3	9	0.0	1.975	1.810	0.5
IVa-9p1	Cu(MIDA)(H7deaA)	9	1	24.7	1.945		35.0
IVa-9p3	Cu(MIDA)(H7deaA)	9	3	3.3	1.933	1.770	1.9
IVb-1p3	Cu(NBzIDA)(H7deaA)	1	3	16.0	2.021	1.753	11.1
IVb-1p9	Cu(NBzIDA)(H7deaA)	1	9	2.3	1.999	1.757	21.6
IVb-3p1	Cu(NBzIDA)(H7deaA)	3	1	29.4	2.017		92.4
IVb-3p9	Cu(NBzIDA)(H7deaA)	3	9	0.0	1.977	1.805	0.8
IVb-9p1	Cu(NBzIDA)(H7deaA)	9	1	24.7	1.945		33.9
IVb-9p3	Cu(NBzIDA)(H7deaA)	9	3	3.4	1.934	1.766	0.6
Va-7,9p1	Cu_2(MIDA)$_2$(H5abim)	7,9	1	0.0	1.960 1.963	- -	7.8 8.6

Va-1,9p7	$Cu_2(MIDA)_2(H5abim)$	1,9	7	1.2	1.981 1.970	- -	0.6 0.6
Va-1,7p9	$Cu_2(MIDA)_2(H5abim)$	1,7	9	1.3	1.989 2.006	- -	4.3 44.0
Vb-7,9p1	$Cu_2(NBzIDA)_2(H5abim)$	7,9	1	0.0	1.962 1.965	- -	2.3 2.7
Vb-1,9p7	$Cu_2(NBzIDA)_2(H5abim)$	1,9	7	0.6	1.982 1.971	- -	0.2 1.3

[a]. The latin numbers refer to the deaza-adenine ligand (i.e. I is 7-azaindole; II is 4-azabenzimidazole; III is 5-azabenzimidazole and IV is 7-deaza-adenine. V refers to the dinuclear possibility calculations with 5-benzimidazole.

The letters ‘a’, ‘b’, ‘c’ and ‘d’ refers to the chelating ligands used in the model systems: N-methyl-iminodiacetate(2-) (MIDA), N-benzyl-iminodiacetate(2-) (NBzIDA), N-(p-chloro-benzyl)-iminodiacetate(2-) (CBIDA) and ethylenediamino-tetraacetate(2-) (H_2EDTA), respectively.

Notation for the N atom coordinated to Cu and the N atom protonated, i.e. 9p3: coordination at N9 and protonation at the N3 of the deaza-adenine ligand.

[b]. Nitrogen atom numbering, according to the conventional numbering of purines, to which the deaza-adenine is coordinated to copper (see Scheme 1 for atom numbering).

[c]. Protonated nitrogen atom numbering (see Scheme 1 for atom numbering).

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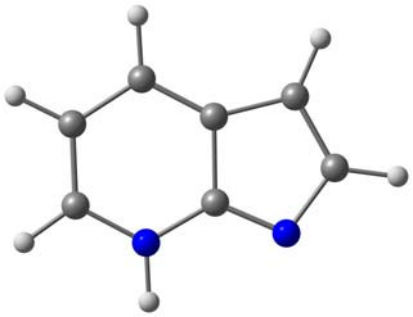
S3. Optimized geometries and Total Calculated Gibbs Free Energies:

NOTE: The latin numbers refer to the deaza-adenine ligand (i.e. I is 7-azaindole; II is 4-azabenzimidazole; III is 5-azabenzimidazole and IV is 7-deaza-adenine. Moreover, to possibilities are calculated per each nucleobase: gas phase and condering the solvent effect (s).

For the isolate ligands, the number after the letter 'p' refers to the location of the tautomerizable proton. For the metal complexes, the previous numbering criteria (see notes 'a' in Table S1) was followed.

B3LYP/6-31+G** Free Energy: -379.780081

I-p3



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N	-1.397938200119	1.691819126442	-0.124746351335
C	-0.178036042900	2.298148152621	-0.106555192832
C	-0.101434301317	3.755654904795	-0.092411483245
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C	1.893281508177	2.748042449857	-0.080976773878
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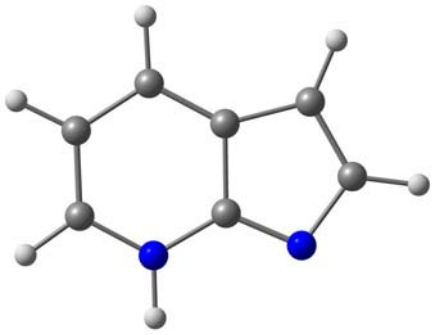
PCM-B3LYP/6-31+G** Free Energy: -379.792695

Is-p3



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C	-0.102851059709	3.745357706433	-0.092520247334
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C	1.901139191576	2.751810798588	-0.080861009682
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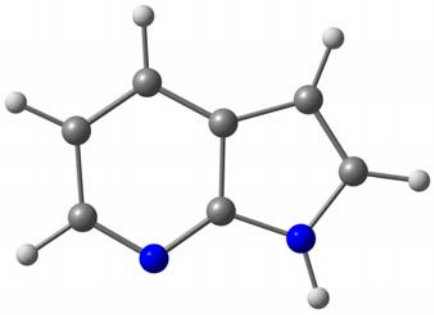
B3LYP/6-31+G** Free Energy: -379.800047

I-p9



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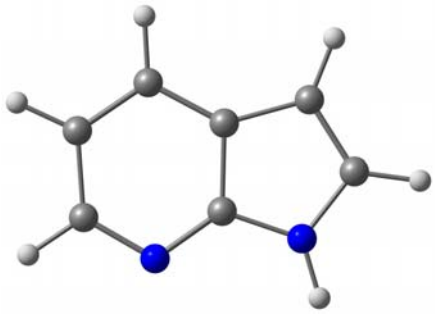
PCM-B3LYP/6-31+G** Free Energy: -379.808126

Is-p9



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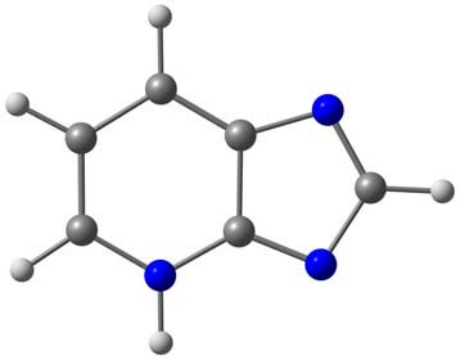
B3LYP/6-31+G** Free Energy: -395.842544



II-p3

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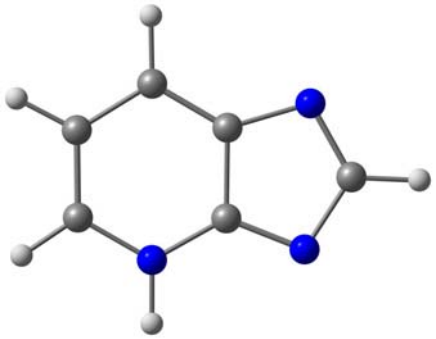
PCM-B3LYP/6-31+G** Free Energy: -395.859562



IIs-p3

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C	-1.258240363141	4.515599513395	-0.097463342460
N	1.234486088184	4.043151541241	-0.075968681596
C	1.810253315079	2.833611978129	-0.081056173563
N	0.994694822496	1.733599581452	-0.099560004008
H	-3.504285736331	1.921042208898	-0.144433423499
H	-1.211199530395	5.600316903988	-0.087059522548
H	2.888410533876	2.717706051569	-0.070937387693
H	-3.426513281897	4.416561502053	-0.120801212463
H	-1.504903566383	0.704745538863	-0.134861754461

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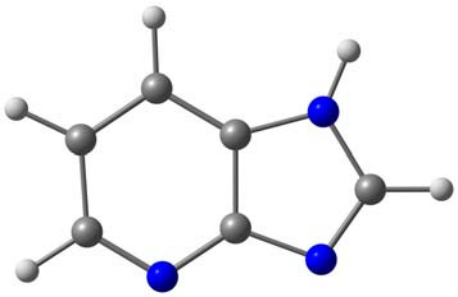
B3LYP/6-31+G** Free Energy: -395.851615

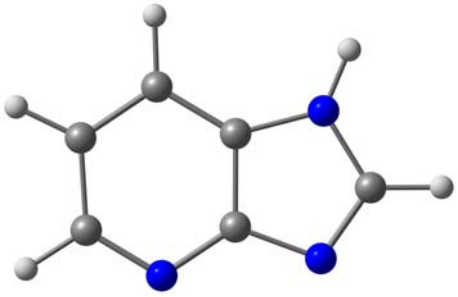
II-p7



C	-2.501028488815	3.870691975586	-0.116215163223
C	-2.513205260167	2.460053498839	-0.129242198708
N	-1.422623934151	1.689638217377	-0.125019573102
C	-0.257409275801	2.346090445645	-0.106960221002
C	-0.149842001368	3.763440380086	-0.092877634732
C	-1.290615413775	4.561918127194	-0.097380668691
N	1.209384271624	4.012262018679	-0.076503930034
C	1.832311359171	2.780926953043	-0.081303849230
N	1.004071354526	1.768764708563	-0.099163376477
H	-3.466263064080	1.935921283460	-0.143875157669
H	-1.251270131002	5.647230978724	-0.087053142855
H	2.911611511913	2.701437464338	-0.070812880336
H	-3.441908719450	4.411351622051	-0.120988213967
H	1.666191846965	4.911687988692	-0.063510931983

PCM-B3LYP/6-31+G** Free Energy: -395.868994

IIs-p7



C	-2.500550719490	3.869620276740	-0.116220429092
C	-2.518443118981	2.460127316789	-0.129299647278
N	-1.425246643382	1.685748076636	-0.125077422294
C	-0.257742399053	2.344340936248	-0.106968555499
C	-0.148550645513	3.759868906123	-0.092887382030
C	-1.288637240216	4.559505400222	-0.097374670072
N	1.208578534738	4.006897466268	-0.076559216945
C	1.834077114974	2.789576882706	-0.081207388335
N	1.002909732325	1.767402959146	-0.099178372786
H	-3.473333522260	1.940284326041	-0.143925449280
H	-1.243693689779	5.643550090139	-0.086995572692
H	2.912994039927	2.715274436617	-0.070686434405
H	-3.440235160658	4.411468916898	-0.120976804333
H	1.667277773669	4.907749671823	-0.063549596919

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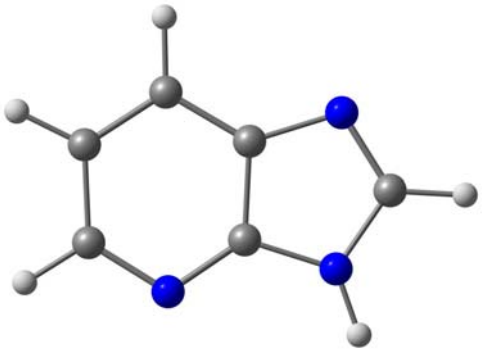
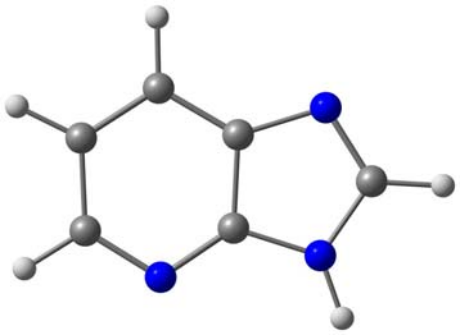
B3LYP/6-31+G** Free Energy: -395.857872



II-p9

C	-2.49623	3.86082	-0.11625
C	-2.53104	2.46740	-0.12939
N	-1.45238	1.64423	-0.12574
C	-0.29748	2.33329	-0.10746
C	-0.11628	3.71009	-0.09297
C	-1.26034	4.51434	-0.09745
N	1.22106	4.02459	-0.07625
C	1.84114	2.86294	-0.08048
N	0.96316	1.81357	-0.09916
H	1.18529	0.83048	-0.10586
H	-3.48844	1.95011	-0.14406
H	-1.18125	5.59431	-0.08673
H	2.91349	2.71869	-0.07073
H	-3.41909	4.43136	-0.12060

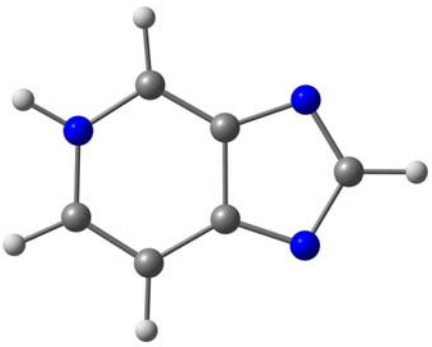
PCM-B3LYP/6-31+G** Free Energy: -395.869303



IIs-p9

C	-2.490121755364	3.864919405420	-0.116153777873
C	-2.541145374803	2.457746222289	-0.129560295168
N	-1.460366075983	1.659416258100	-0.125687189978
C	-0.302975585014	2.318876997086	-0.107667434407
C	-0.119729178468	3.724743274682	-0.092896256302
C	-1.262489390979	4.528811165419	-0.097373705514
N	1.234997960242	4.030406369241	-0.076058267192
C	1.837281391938	2.858829614616	-0.080541592965
N	0.973474265305	1.794772731245	-0.099242206110
H	1.226785461585	0.815757355629	-0.105584479992
H	-3.504390932945	1.954622629378	-0.144125892889
H	-1.198571841693	5.612473297379	-0.086799962246
H	2.908546958058	2.710602218268	-0.070785384979
H	-3.419685904564	4.424242460740	-0.120653554374

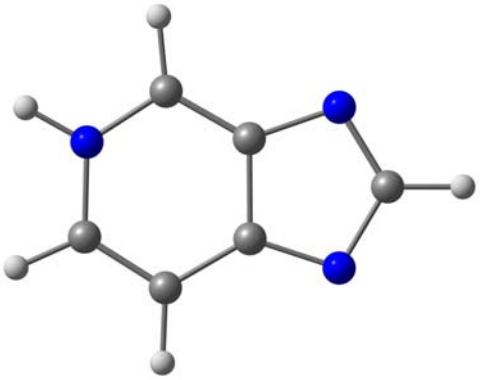
B3LYP/6-31+G** Free Energy: -395.838506



III-p1

N	-2.427274394840	3.783931855724	-0.116244289130
C	-2.568217978760	2.416834186138	-0.130223200875
C	-1.466698487784	1.593728053243	-0.126352399699
C	-0.191937853560	2.198834790608	-0.107608521613
C	-0.085884720616	3.651384778533	-0.093208440651
C	-1.223217969123	4.424510730607	-0.097907855367
N	1.237514088977	3.995373686794	-0.076352000384
C	1.833450769092	2.797021640772	-0.081153799023
N	1.043562579724	1.678951742995	-0.099573328403
H	-3.587265401331	2.052051415006	-0.144117909734
H	2.914001499716	2.706542737461	-0.070791152481
H	-1.588355253847	0.516402219143	-0.137477979738
H	-1.235609368558	5.507902999168	-0.088115051643
H	-3.266365174950	4.347054338459	-0.119777924967

PCM-B3LYP/6-31+G** Free Energy: -395.859672



IIIs-p1

N	-2.425195745606	3.782269348772	-0.116238474108
C	-2.568761213766	2.420959595670	-0.130190605865
C	-1.466377133602	1.596023718401	-0.126327083759
C	-0.194768741301	2.204123934236	-0.107588900024
C	-0.088869011757	3.645518589038	-0.093293547734
C	-1.230159620864	4.422219596951	-0.098001698162
N	1.241176192075	3.991232566771	-0.076352756745
C	1.842343657044	2.793379181438	-0.081095019873
N	1.053004230531	1.680761839588	-0.099458148350
H	-3.587521947587	2.057730021905	-0.144067838423
H	2.923799708592	2.705535482042	-0.070698843984
H	-1.594373875159	0.519582136334	-0.137509491587
H	-1.249614786556	5.504829376554	-0.088289955510
H	-3.266979375912	4.346359787456	-0.119791489597

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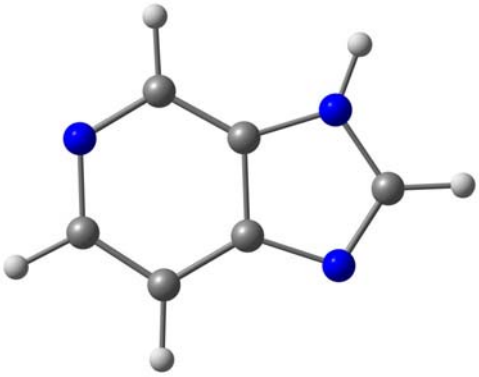
B3LYP/6-31+G** Free Energy: -395.850557

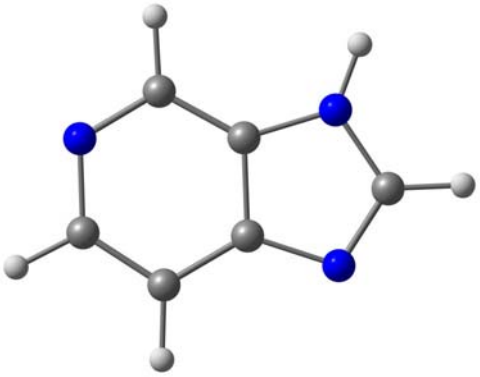
III-p7



N	-2.493768872664	3.815058424405	-0.116655857627
C	-2.552375143682	2.462819432232	-0.129639026081
C	-1.445972882570	1.617591290390	-0.125913589058
C	-0.188059042484	2.231545673470	-0.107263802320
C	-0.131944040825	3.644124056059	-0.093754198001
C	-1.300580848986	4.409427222294	-0.098855817110
N	1.222046523776	3.941499610168	-0.077006571760
C	1.886526712593	2.737663414078	-0.081141077688
N	1.091702329894	1.694973131353	-0.098917639701
H	-3.555090082812	2.043603696038	-0.143862910023
H	2.967878080433	2.692412713009	-0.070353526443
H	-1.553006739599	0.538218339573	-0.136901072081
H	-1.285285730780	5.497684735004	-0.088737339956
H	1.645178411046	4.857136173340	-0.064243196199

PCM-B3LYP/6-31+G** Free Energy: -395.864878

IIIs-p7



N	-2.492732009374	3.815746587038	-0.116639793072
C	-2.554373828135	2.460596875076	-0.129679860229
C	-1.449027420421	1.614585880592	-0.125971638545
C	-0.189621638300	2.227712190987	-0.107314354430
C	-0.129891075691	3.641245879471	-0.093759791245
C	-1.295226238063	4.410217911210	-0.098794457106
N	1.220206665126	3.938183572353	-0.077056586758
C	1.886432628668	2.746243814277	-0.081062993075
N	1.090462519643	1.694112483677	-0.098937005651
H	-3.556217635681	2.039531827329	-0.143911402907
H	2.967371404633	2.707316537247	-0.070221669308
H	-1.564296494853	0.535829876115	-0.137037847786
H	-1.270672029776	5.496964412089	-0.088594848859
H	1.644833816896	4.855470062781	-0.064263375044

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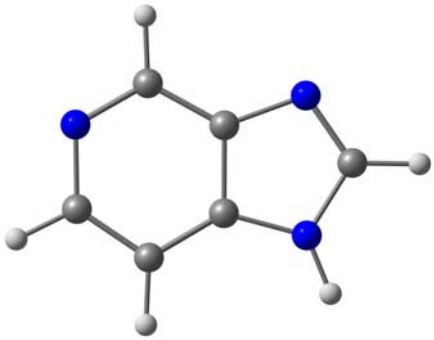
B3LYP/6-31+G** Free Energy: -395.850983

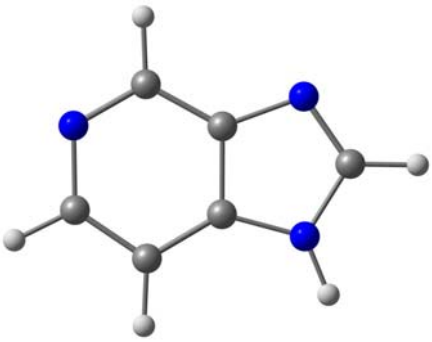
III-p9



N	-2.471198626404	3.810371402047	-0.116449234726
C	-2.564127734780	2.461202196456	-0.129780137657
C	-1.481877582585	1.583219998713	-0.126620183227
C	-0.223330279039	2.188352785946	-0.108037637701
C	-0.095287695031	3.595476827276	-0.093811731500
C	-1.261802130146	4.371755660099	-0.098776897347
N	1.245024690426	3.965181905426	-0.076540047110
C	1.897974644913	2.833091404498	-0.080155898355
N	1.075912400337	1.721319572859	-0.098861710586
H	1.375945020934	0.758085745681	-0.104586201752
H	-3.575879381006	2.063726693547	-0.143902727979
H	2.975495213127	2.734066742891	-0.069903411061
H	-1.627958109089	0.507780049097	-0.137992329865
H	-1.210140404802	5.457889039686	-0.088284504627

PCM-B3LYP/6-31+G** Free Energy: -395.865750

IIIs-p9



N	-2.473442396576	3.811456418617	-0.116462850331
C	-2.563966165758	2.458091109564	-0.129807024569
C	-1.479208086223	1.584991893359	-0.126576019889
C	-0.221806860716	2.192597157258	-0.107982797494
C	-0.096319737643	3.601177441122	-0.093770166109
C	-1.261978910432	4.376521287333	-0.098735246252
N	1.245536563010	3.967393984398	-0.076514531620
C	1.896206790500	2.825541918132	-0.080243436882
N	1.072948264814	1.725795219070	-0.098851350647
H	1.373561481626	0.760499980227	-0.104588471469
H	-3.573365788151	2.055751314601	-0.143949841976
H	2.972439137353	2.719009636954	-0.070073316175
H	-1.618121920785	0.509566255701	-0.137873528913
H	-1.213732343135	5.463126408010	-0.088274066163

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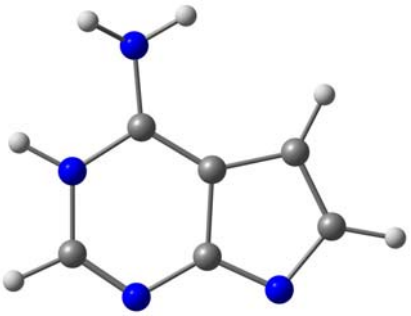
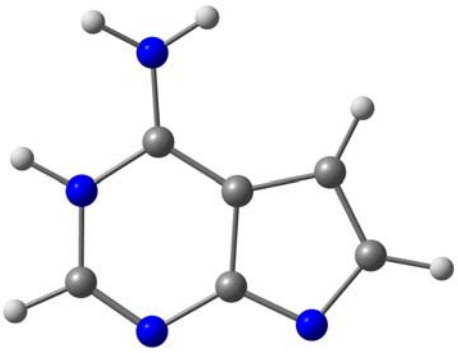
B3LYP/6-31+G** Free Energy: -451.177401



IV-p1

N	1.863670709684	-0.489733264458	-0.011711185635
C	1.253119212892	-1.738018883086	0.002907532809
N	-0.027834253224	-1.919622117798	0.010600520953
C	-0.797163352939	-0.788230586914	0.011885376413
C	-0.227725263419	0.559607353840	0.000078903987
C	1.146822172972	0.680243950324	-0.019221974572
C	-1.349812916426	1.434256673527	-0.014899071666
C	-2.447120441119	0.579065466090	-0.006207357741
N	-2.125647175454	-0.758037213892	0.005550228629
H	1.938565281008	-2.579716417610	0.004875919434
N	1.859531981796	1.860702483124	0.016529552967
H	-3.489966110514	0.875526146448	-0.008141837478
H	1.303053055153	2.692209679640	-0.126255655632
H	2.744272775362	1.890478382296	-0.474124992469
H	-1.366269115358	2.516393767091	-0.018647266971
H	2.872407439334	-0.451942418435	0.052731417014

PCM-B3LYP/6-31+G** Free Energy: -451.207461



IVs-p1

N	1.857988286068	-0.487881282078	-0.029472099498
C	1.257871699337	-1.731283354872	0.004549912134
N	-0.027091355142	-1.920540841192	0.026121246021
C	-0.793490679972	-0.782609899227	0.015305931051
C	-0.239972609902	0.551145837431	-0.018271156973
C	1.149154030680	0.684330708158	-0.044705572633
C	-1.361460258213	1.427955133296	-0.022060056000
C	-2.462815078617	0.577976336882	0.009210275682
N	-2.133956298186	-0.760560360464	0.031222395801
H	1.947574863786	-2.567592161516	0.011191769049
N	1.828388943592	1.852651495056	-0.047056664967
H	-3.505618851930	0.875989010411	0.017338911135
H	1.315158422391	2.708125514248	-0.199629763255
H	2.817219686672	1.883928847870	-0.251833714436
H	-1.369969585910	2.509777545782	-0.041968466347
H	2.870922785342	-0.458229529783	-0.033992836760

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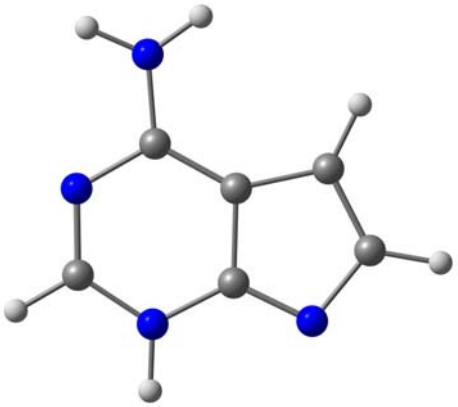
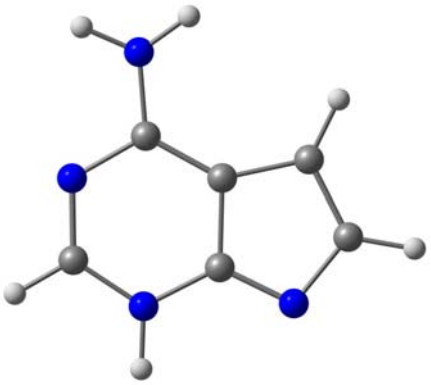
B3LYP/6-31+G** Free Energy: -451.195568



IV-p3

N	1.917742833090	-0.488865240623	-0.056817670817
C	1.334433057278	-1.664438663357	-0.022554809593
N	-0.004479220018	-1.849623198091	0.008514883781
C	-0.839833301447	-0.755891112698	0.006164105994
C	-0.257107787777	0.554990181641	-0.027262490656
C	1.140603454984	0.637375548044	-0.059464596798
C	-1.387960837358	1.425567070733	-0.019730345368
C	-2.489351321868	0.576796256863	0.016105179396
N	-2.162183194936	-0.767126304428	0.032243769849
H	1.948791279568	-2.559017379163	-0.020063304462
N	1.823637474313	1.812587439045	-0.073712978963
H	-3.532694196537	0.868220270212	0.032912597603
H	1.339258775419	2.682912719845	-0.219756016243
H	2.822235663255	1.782214970143	-0.211208927869
H	-1.401852500106	2.507077499246	-0.032109935220
H	-0.406458673833	-2.779638720528	0.032707001999

PCM-B3LYP/6-31+G** Free Energy: -451.213864

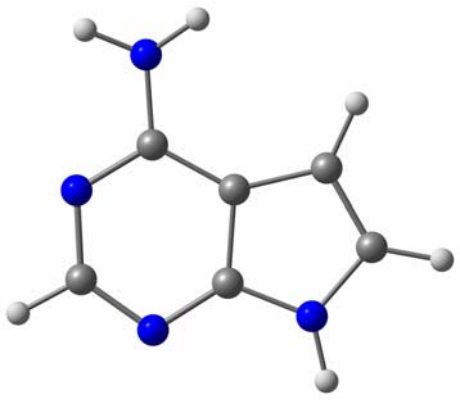


IVs-p3

N	1.918365080733	-0.493587095941	-0.077818864241
C	1.331315789588	-1.670736276594	-0.028360192577
N	-0.003669959181	-1.855546512535	0.015703835633
C	-0.836724141871	-0.759827800380	0.009747928575
C	-0.259281363528	0.545358217239	-0.043018739860
C	1.144404565224	0.636486147047	-0.086287207614
C	-1.385544801021	1.424988126951	-0.034389758468
C	-2.491568829082	0.584986975758	0.021010054086
N	-2.167139719207	-0.762779930700	0.048654620555
H	1.941700870292	-2.566848160705	-0.021428779714
N	1.812971705948	1.807460642590	-0.138090863250
H	-3.533580396303	0.882927608281	0.043296689384
H	1.329303489663	2.691433606547	-0.145760439559
H	2.821677038277	1.805278868898	-0.165804448447
H	-1.387975833148	2.506332135508	-0.064043755355
H	-0.389471992391	-2.792785214946	0.052556383909

B3LYP/6-31+G** Free Energy: -451.213371

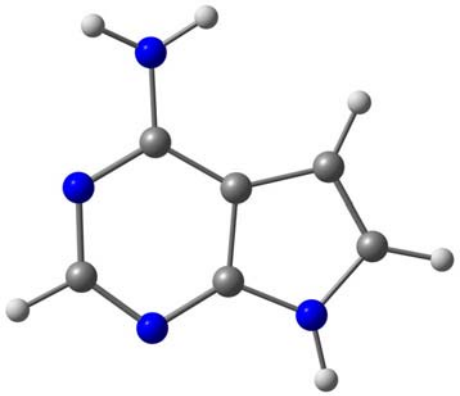
IV-p9



N	1.910555389330	-0.474539317187	-0.041385054618
C	1.290741774522	-1.668696573902	-0.015185309809
N	-0.018836450814	-1.913761098820	0.002039953395
C	-0.749642116664	-0.788920899726	-0.003136504932
C	-0.254683241423	0.533915230044	-0.020976877294
C	1.155732499855	0.634532934450	-0.043025948991
C	-1.389281439548	1.415439121845	-0.010974984764
C	-2.505175648069	0.615021724154	0.009544221817
N	-2.118520808365	-0.716491455963	0.013252059451
H	1.945195827941	-2.536638258409	-0.010650480088
N	1.810835860257	1.836973628301	-0.027530723762
H	-3.551008098467	0.884233945398	0.025069185510
H	1.317383301690	2.673847859783	-0.296208926534
H	2.801876387652	1.806392271794	-0.218563125412
H	-1.395258476821	2.496273942346	-0.009150720537
H	-2.728285667035	-1.519736169174	0.032840422043

PCM-B3LYP/6-31+G** Free Energy: -451.227360

IVs-p9



N	1.915095071828	-0.481397881309	-0.042807940846
C	1.293373811921	-1.674986748002	-0.015671478115
N	-0.016576435808	-1.920380013533	0.006191136217
C	-0.753352662775	-0.792745849180	0.001681215228
C	-0.252158900429	0.528555085094	-0.021000054669
C	1.158897203693	0.635063450954	-0.045552450086
C	-1.382677510334	1.414895640525	-0.015541282631
C	-2.500849191552	0.616209714269	0.008623676021
N	-2.118924911794	-0.716287886654	0.018632205485
H	1.947430574861	-2.543887560144	-0.014041348402
N	1.806106602499	1.833590810902	-0.034440170579
H	-3.547021577869	0.883888962915	0.019920260882
H	1.302068134038	2.678141682578	-0.259721832782
H	2.796995306079	1.830495165291	-0.231847634066
H	-1.381688414774	2.495547249359	-0.025634447193
H	-2.745088005520	-1.508854938019	0.037167331524

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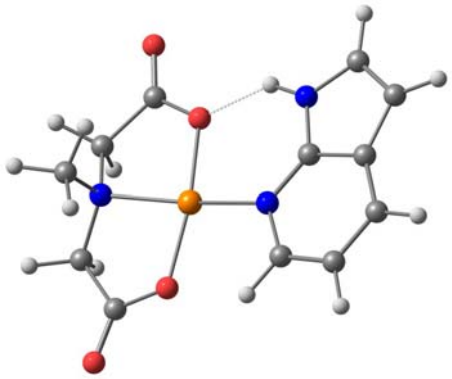
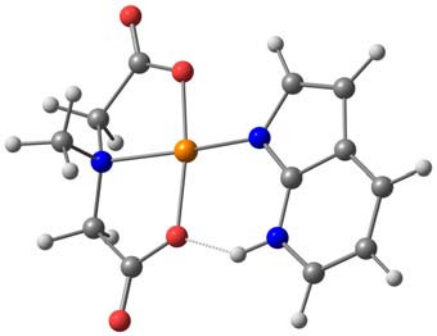
UM06l/6-31G* Free Energy: -2570.272040

Ia-3p9



Cu	-0.606744259690	-0.138854346417	-0.152092447739
O	-0.292242224217	1.743695244542	-0.225329307155
O	-1.316332376480	3.744774304277	-0.302873832616
O	-1.315456224357	-1.888538789923	-0.234582429204
O	-3.244705531539	-3.037174561955	-0.382398020679
N	-2.500001361334	0.408320862055	0.238733449872
C	3.957082026217	-1.693642521441	0.136844672004
N	2.352769242148	1.464847699399	-0.078582914761
C	4.518970378956	0.860387274667	0.056124387274
C	1.565357032854	-2.030833759097	0.027625705290
H	0.693313307375	-2.677924158514	0.002367688286
C	2.857902987283	-2.544091521689	0.115616859871
H	2.986657172246	-3.621650224369	0.164475988316
C	3.722467820582	-0.321339575948	0.067508585164
C	2.364763170269	0.106450212816	-0.019900567743
N	1.293828929612	-0.709659538682	-0.035882816825
C	3.651641900513	1.916744244654	-0.034186064043
H	3.849570406658	2.980060220099	-0.072229655547
C	-2.676811803036	1.770023103362	-0.283087698455
H	-3.446723477968	2.327448870623	0.267526159704
H	-3.006504468341	1.700999683004	-1.327092681874
C	-1.342411896332	2.530502454840	-0.257158751894
C	-3.359462250293	-0.649108659543	-0.315422442922
H	-3.587717513670	-0.397091686243	-1.358364234422
H	-4.314923337917	-0.725960022737	0.221178493772
C	-2.617423107455	-1.998075475001	-0.300143741751
C	-2.512078242571	0.391491660110	1.707149628704
H	-2.254857349881	-0.612362254981	2.060424421903
H	-3.503740102722	0.665596807585	2.097061229399
H	-1.771581775369	1.103651815334	2.086388628574
H	4.969370579309	-2.089186346705	0.204021429832
H	1.485768321469	2.007900273522	-0.152029421763
H	5.598195027512	0.921497712048	0.107344701633

UM06l/6-31G* Free Energy: -2570.266459



Ia-9p3

Cu	0.692794820011	-0.194562228567	-0.082285131858
O	1.589942887677	-1.860048217530	-0.141469212447
O	3.638994302098	-2.757156147032	-0.402116253839
O	0.129442666587	1.648597188823	-0.130527837464
O	0.900418527776	3.753450958611	-0.337241851984
N	2.509855198171	0.589825084741	0.188941305728
C	-4.671725134883	-0.631852799341	0.049640957371
N	-1.101140970253	-0.911010846667	0.014555632902
C	-2.796994471003	-2.463163901436	0.087066222628
C	-3.716788719160	1.587259811650	-0.047872696534
H	-3.777310917799	2.668915774258	-0.090420336727
C	-4.825065006435	0.758325943246	-0.000572892299
H	-5.813017912637	1.207855786769	-0.004628605347
C	-3.391277497333	-1.173947700124	0.051587990583
C	-2.278986591639	-0.268154801786	0.003781656424
N	-2.470936958820	1.068411860597	-0.044058573436
C	-1.437427161674	-2.253848227112	0.058946480946
H	-0.630258773994	-2.978033271251	0.065682508810
C	3.451931661301	-0.374272699681	-0.402647317059
H	4.445258185096	-0.316962586217	0.063065813911
H	3.572197176088	-0.130018789297	-1.465452038150
C	2.885599646185	-1.806316227116	-0.299385115557
C	2.482951899091	1.949458175529	-0.367639403136
H	2.745781273949	1.893302967617	-1.431359447280
H	3.216492693433	2.609485670123	0.115456553928
C	1.072639087997	2.552348309019	-0.261521269696
C	2.620039136385	0.612540802729	1.653008816738
H	1.822628394631	1.237182323191	2.069232471966
H	3.593348023225	1.016395092496	1.969755740737
H	2.512601513977	-0.405942770592	2.039616060621
H	-5.550723348302	-1.273569839962	0.085079732222
H	-1.615947173155	1.658002577939	-0.084224013599
H	-3.303618456361	-3.418929273654	0.126259051185

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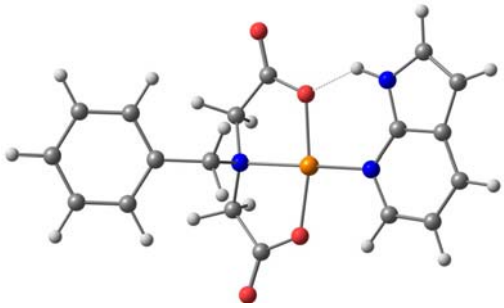

UM06l/6-31G* Free Energy: -2801.220389

Ib-3p9

Cu	0.613582570087	0.358242626205	0.507034756501
O	0.663149391302	-1.543624477315	0.734574481834
O	-0.603939579536	-3.325159312766	1.267241923617
O	0.178900688017	2.202627800045	0.440612789325
O	-1.514185143451	3.651973783867	0.757513093042
N	-1.360668320107	0.109674891008	0.771768774967
C	5.129151410012	1.083239243676	-1.051740014621
N	3.176521579750	-1.730923796404	-0.122419920068
C	5.300922900428	-1.518955608295	-0.842466815139
C	2.923971846547	1.833927719848	-0.403526483039
H	2.191959027098	2.620864597171	-0.245809271375
C	4.212991215805	2.109945265284	-0.855515513944
H	4.485068125057	3.143542918152	-1.049904030030
C	4.716177241882	-0.220738835468	-0.783093795385
C	3.378127894899	-0.401456749409	-0.323732729905
N	2.483000990586	0.586496211831	-0.134368867953
C	4.336577430663	-2.401987969955	-0.434182676538
H	4.374418766736	-3.479045622809	-0.335205970072
C	-1.537828126162	-1.127303117749	1.538977486244
H	-2.534614763714	-1.567199611566	1.408553650447
H	-1.423991553669	-0.885054861164	2.603416163715
C	-0.438194506243	-2.125708435817	1.152678029164
C	-1.847830606124	1.357888435508	1.371982512170
H	-1.672906065005	1.301337384113	2.454119876857
H	-2.924261607088	1.507292058952	1.220759254359
C	-1.033241605617	2.534531085896	0.808026696694
C	-1.781914316197	-0.039605738987	-0.656700424427
H	-1.429571976053	0.864016295509	-1.171552932598
H	-1.212776094700	-0.891140510466	-1.053730861429
H	6.137726532592	1.293190020723	-1.404478266631
H	2.286609120896	-2.110213112939	0.219209578296
H	6.308381600005	-1.768460881523	-1.148835314040
C	-3.252429689092	-0.236905878044	-0.863857880376
C	-4.100641443258	0.864115147866	-1.025273176663
C	-3.800946008996	-1.523817303354	-0.881280905782
C	-5.470430621268	0.682351945885	-1.190127604132
C	-5.170605353178	-1.706764128623	-1.046179390268
C	-6.006991371256	-0.603263929753	-1.198720863691
H	-3.677500375053	1.870116882541	-1.027577210546
H	-3.142856020757	-2.387828852118	-0.771963955316
H	-6.119076333432	1.546797088292	-1.317796590409
H	-5.584220450018	-2.713249944985	-1.061418106737
H	-7.077819402771	-0.745717722912	-1.331609495398

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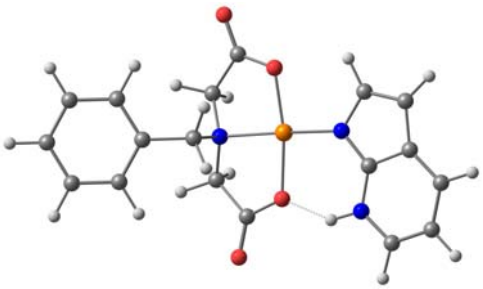
UM06l/6-31G* Free Energy: -2801.215273



Ib-9p3

Cu	-0.546038328909	0.511141717559	0.436485340249
O	0.013944036334	2.321919313517	0.312797379414
O	1.822581886914	3.630002991609	0.619651626235
O	-0.753556193775	-1.393500254795	0.689614186828
O	0.369783498932	-3.249121768413	1.294226232543
N	1.386671384440	0.116610490537	0.739048545768
C	-5.695399381216	-0.264924442222	-0.930333122181
N	-2.363378959206	0.799189969815	-0.161945791204
C	-4.246298200736	1.918420150232	-0.862745740226
C	-4.395838994714	-2.190995757395	-0.260744727222
H	-4.260906261183	-3.247022736098	-0.055655831481
C	-5.592805694574	-1.639083690444	-0.685425832378
H	-6.448243516988	-2.292760623155	-0.823689189635
C	-4.579760663385	0.543277181363	-0.741766286283
C	-3.365153076839	-0.082243720610	-0.301633942221
N	-3.308323407571	-1.413349402591	-0.077048466950
C	-2.921463646082	2.019212914341	-0.505229225068
H	-2.285361734945	2.896539077705	-0.463513620645
C	1.941235706169	1.342839506828	1.328873793159
H	3.031092088580	1.408449505919	1.220810840813
H	1.716425713671	1.328423226646	2.403324584030
C	1.239821797997	2.562583573843	0.698536994249
C	1.454659318399	-1.115707367482	1.532007614317
H	1.337476642296	-0.844832745065	2.589254344146
H	2.418714473860	-1.630681896531	1.432674927161
C	0.293643636004	-2.044239212898	1.145085502971
C	1.835980397607	-0.089672830247	-0.673297730527
H	1.231027138904	-0.917562025722	-1.067342743181
H	1.547718664483	0.819279496888	-1.217633249624
H	-6.642118087142	0.157328834195	-1.263746709055
H	-2.394257235958	-1.790608595287	0.243672494747
H	-4.896033981658	2.726919218691	-1.172415907292
C	3.298793538626	-0.369791120479	-0.835263369666
C	4.207578303118	0.683305287369	-0.988021688939
C	3.779606099561	-1.683388437693	-0.818540616753
C	5.569818346846	0.428017187811	-1.111584749427
C	5.141898717143	-1.939810720746	-0.942446563301
C	6.038629701395	-0.883720997488	-1.087354425438
H	3.837439145359	1.709716523094	-1.013663905732
H	3.074295980805	-2.510213688842	-0.715906432748
H	6.266005086786	1.255690939355	-1.232584519117
H	5.502712432791	-2.966554753277	-0.931611993901
H	7.103822627957	-1.083603319415	-1.188133026747

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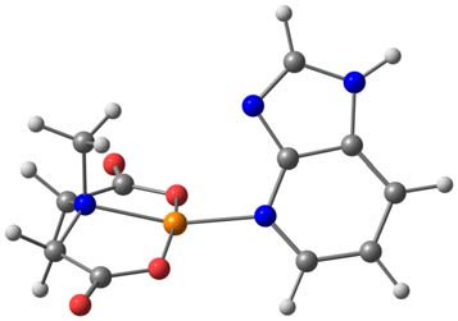

UM06l/6-31G* Free Energy: -2586.317789

IIa-3p7

Cu	-0.593974760411	-0.153635740528	-0.124877663996
O	-1.328470060991	-1.788244238491	0.477973094699
O	-3.285142609495	-2.885279511888	0.662738941340
O	-0.208657014197	1.678379703048	-0.386422234882
O	-1.196369769771	3.638160928567	-0.888195928152
N	-2.407877043499	0.252712293314	-0.843543727180
C	3.795972697475	-2.069705677611	0.209666131017
N	0.779837790914	-2.341439741709	-1.741888038308
N	2.719242556195	-3.476301600396	-1.635610180579
H	3.408413767008	-4.180579057432	-1.857041691873
C	2.224032977923	-0.334264765127	0.845388136859
H	1.968035678038	0.540652028860	1.438156187132
C	3.469278747673	-0.957350408640	0.979520815204
H	4.180662383519	-0.561704401494	1.698440751260
C	2.821298478371	-2.484397349786	-0.686836477573
C	1.588082261992	-1.805692012362	-0.774314085671
N	1.282703431045	-0.750135025928	-0.008468294129
C	1.487801162245	-3.332655735550	-2.223085802720
H	1.164223805186	-3.998563016144	-3.014136969638
C	-3.339235072140	-0.628374575748	-0.120439297273
H	-4.214755205807	-0.886022679301	-0.732072970535
H	-3.703836258383	-0.091212039752	0.763779380996
C	-2.622800652590	-1.904528586242	0.369886870323
C	-2.588610708794	1.707096450673	-0.705953988570
H	-3.086671092762	1.903210679303	0.251331673216
H	-3.231653768094	2.115491632779	-1.497407458352
C	-1.228950398487	2.437352695334	-0.683304922367
C	-2.270108456976	-0.150928872569	-2.248374943158
H	-1.494848395700	0.456991301657	-2.726993245877
H	-3.218248554381	-0.014361642236	-2.791091242304
H	-1.970255113328	-1.203243262456	-2.296510136286
H	4.758306198225	-2.567287772117	0.308205317340

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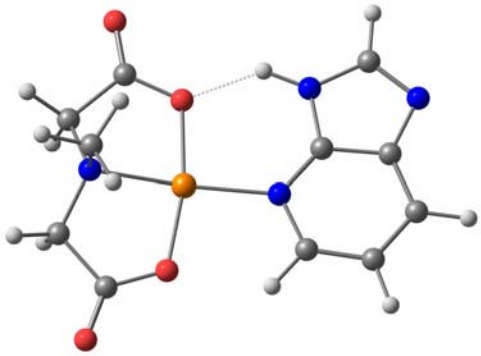

UM06l/6-31G* Free Energy: -2586.334088

IIa-3p9

Cu	-0.606641032327	-0.138823523783	-0.154042158486
O	-0.284079260120	1.744567800257	-0.187437088768
O	-1.311299944761	3.742582996656	-0.286911793022
O	-1.294470828352	-1.892751695321	-0.258084622920
O	-3.215101991423	-3.046706182712	-0.466053910925
N	-2.504147752435	0.398985429044	0.197366299231
C	4.000131727454	-1.600142666372	0.101992289075
N	2.353132359400	1.506568114133	-0.041858422572
N	4.515854885587	0.872027284436	0.078880136976
C	1.611043462570	-2.005590416646	-0.011226929386
H	0.758669718692	-2.678532194386	-0.047850633028
C	2.919992215875	-2.478666092873	0.063567306700
H	3.079651195253	-3.552889698400	0.088703571713
C	3.705466102129	-0.241872194162	0.061910560882
C	2.344962111909	0.142869217903	-0.014190898976
N	1.294546523974	-0.691414888452	-0.046224011935
C	3.671903015545	1.873885906148	0.014848487405
H	3.956212564352	2.919796212129	0.005307416799
C	-2.667576108851	1.764507241014	-0.320447307319
H	-3.455032732874	2.316657239312	0.210068367237
H	-2.965238554311	1.702267452444	-1.374439725603
C	-1.336509996952	2.528369930054	-0.248428833967
C	-3.341668939148	-0.659187941278	-0.389777167173
H	-3.539383341122	-0.401198486324	-1.437496804144
H	-4.312355635075	-0.743904745986	0.117176176004
C	-2.594585098295	-2.006126875851	-0.360725952237
C	-2.559419040076	0.371673458989	1.664859744990
H	-2.310749566324	-0.634150491053	2.018545816706
H	-3.562734752350	0.640958261196	2.026880551625
H	-1.832196384829	1.082692632079	2.070873705227
H	5.027834953411	-1.951841098157	0.158927851294
H	1.496768122891	2.072021015498	-0.103168021800

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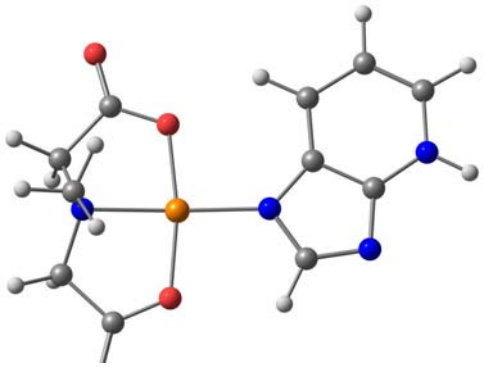

UM06l/6-31G* Free Energy: -2586.319718

IIa-7p3

Cu	-0.721622180281	-0.158707841578	-0.029679503268
O	-0.309800388760	1.700028866199	-0.121321397401
O	-1.270723145426	3.723363567246	-0.338268160483
O	-1.465264329068	-1.905359532586	-0.039001849153
O	-3.432106685490	-2.991298477244	-0.198012075369
N	-2.592182731892	0.454440749202	0.303776321186
N	4.626203806546	-0.723817798591	-0.065194412624
N	1.121797191063	-0.784146193157	0.013244529598
N	2.826404345104	-2.332172235505	0.032344406295
C	4.005250519999	1.568140421801	-0.144399011448
H	4.322933936222	2.604763471055	-0.194101351157
C	4.975940694555	0.586465965518	-0.124997778882
H	6.039414054529	0.794126881246	-0.156022864855
C	3.324031447148	-1.093762000154	-0.023999264758
C	2.307029665428	-0.094754597124	-0.041722034354
C	2.637567248145	1.248084890916	-0.102232237752
H	1.858550967500	2.009101974855	-0.119750238650
C	1.502216053259	-2.078924506103	0.048116772728
H	0.753530481018	-2.863756732123	0.085476095502
C	-2.695569183943	1.800131719585	-0.278762104017
H	-3.462634039759	2.408300341425	0.220284524271
H	-2.991650650124	1.698498941541	-1.330299805740
C	-1.328575043589	2.510832956331	-0.233883407179
C	-3.463644048180	-0.600663023177	-0.235222818322
H	-3.648902065806	-0.385371979208	-1.294976838125
H	-4.438855519092	-0.627306411755	0.270175608660
C	-2.765886080788	-1.973515904391	-0.139591931564
C	-2.648967679187	0.498697517376	1.769286042713
H	-2.436085666718	-0.497524727991	2.170549675409
H	-3.642380866952	0.820677037719	2.116699468917
H	-1.896076007693	1.201708671674	2.140840944874
H	5.334364902130	-1.450560012815	-0.051908305276

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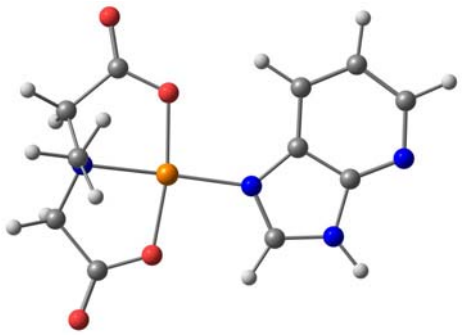
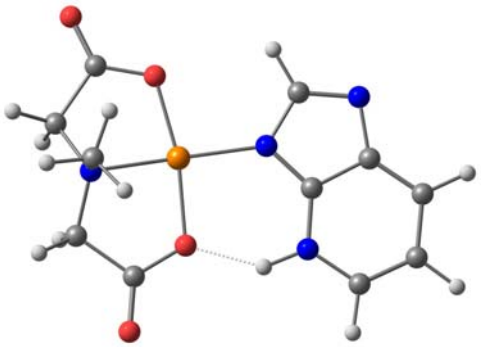


UM06l/6-31G* Free Energy: -2586.328729

IIa-7p9

Cu	-0.710716118248	-0.106419462103	-0.042414145593
O	-0.337106631131	1.748084159832	-0.153305886586
O	-1.348420861616	3.742894508355	-0.406479473617
O	-1.398970433020	-1.876993435084	-0.026605364393
O	-3.329879736361	-3.024159292545	-0.182762288276
N	-2.595997692349	0.454038711417	0.275086236667
N	4.707240282895	-0.749602638324	0.000373505261
N	1.145418033195	-0.731375947448	0.015262673530
N	2.785163180634	-2.227204064971	0.049386095164
H	3.254934552777	-3.121681202830	0.071256910992
C	4.041475760603	1.586890276713	-0.071174245708
H	4.380905674628	2.619033523783	-0.106313616229
C	4.995065920226	0.556745403487	-0.041179949097
H	6.057073292960	0.800615175093	-0.051952486656
C	3.404825291776	-0.988948347915	0.011384858082
C	2.355426637200	-0.052855390818	-0.013871367350
C	2.680782601761	1.301670564597	-0.057486909656
H	1.904532831466	2.063536170620	-0.084306969560
C	1.448818758044	-2.018905962005	0.046879850249
H	0.700778237194	-2.802930005234	0.065750509560
C	-2.726310749751	1.787493188820	-0.332163532349
H	-3.512144765914	2.384616694397	0.150064568773
H	-3.009701680233	1.660813382263	-1.384401642091
C	-1.376169404149	2.531961126334	-0.285901874106
C	-3.432778131074	-0.634035095191	-0.254328881424
H	-3.617197128665	-0.439913584806	-1.318290730608
H	-4.410356007386	-0.681661919039	0.244579210732
C	-2.698399040159	-1.984805282510	-0.134714107389
C	-2.667384482593	0.522048678874	1.739444891287
H	-2.431713857312	-0.460790546443	2.160647689275
H	-3.672328173232	0.822616731608	2.071680484407
H	-1.937750162246	1.251916881144	2.105214986606



UM06l/6-31G* Free Energy: -2586.329764

IIa-9p3

Cu	0.718303254458	-0.237592562264	-0.129073189326
O	1.577652145547	-1.917458870021	-0.193345348768
O	3.613244046842	-2.847721905509	-0.443297737795
O	0.172653735323	1.609962867431	-0.183388030208
O	0.972656576184	3.703808811794	-0.383178052020
N	2.542479929673	0.519725116690	0.139898854567
C	-4.636078327637	-0.614573729846	0.003603245301
N	-1.098140766427	-0.906837722704	-0.032953996554
N	-2.849600094581	-2.401339500120	0.040445229256
C	-3.694613421079	1.619046905239	-0.096666689730
H	-3.770916196330	2.699578929482	-0.139943513282
C	-4.793017965069	0.778045856806	-0.047525930168
H	-5.783600869499	1.221603943026	-0.050968704133
C	-3.346519732661	-1.124519787603	0.003702423031
C	-2.251465490936	-0.215433003870	-0.045132695580
N	-2.438713996978	1.118196906759	-0.093998514494
C	-1.542072072914	-2.211148446208	0.012725983310
H	-0.813348024605	-3.015390396097	0.024422292688
C	3.466000565478	-0.462001972987	-0.453525049136
H	4.461448712681	-0.420806438685	0.008906278198
H	3.586476721530	-0.221736933935	-1.517207477901
C	2.875725515543	-1.884737186038	-0.346183975877
C	2.531113437847	1.878037125445	-0.421835000460
H	2.787732234563	1.814244455257	-1.486649216102
H	3.275927502775	2.529491571689	0.055228579635
C	1.129751324266	2.500657031353	-0.311536909941
C	2.660749045576	0.545787168403	1.603559188804
H	1.874569314990	1.182850076069	2.022306161492
H	3.641104975592	0.937364948670	1.913202631741
H	2.542157049199	-0.469804674438	1.994504268104
H	-5.499636995810	-1.275076519922	0.040549570957
H	-1.583063133639	1.707934935867	-0.135919674414

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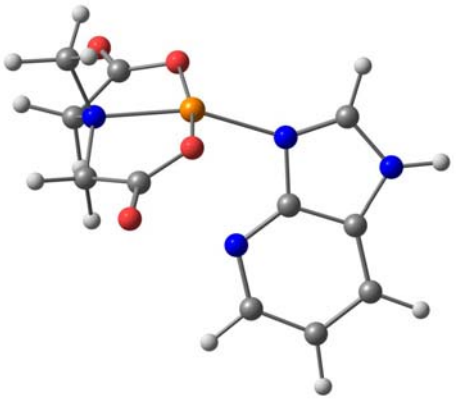
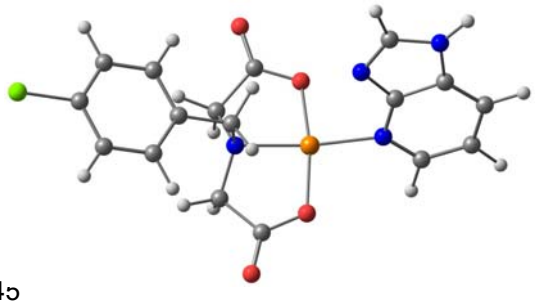


UM06l/6-31G* Free Energy: -2586.315500

IIa-9p7

Cu	-0.720976257530	-0.306482953517	-0.632419827594
O	-1.431831742506	-1.973112869357	-0.083187655320
O	-2.866310273833	-2.825190706368	1.431025602208
O	-0.379892370509	1.452270140831	-1.263801161440
O	-0.717204997562	3.581910760530	-0.609530822064
N	-2.320021665389	0.497891017597	0.245650012662
C	4.312036670594	-0.018041007111	0.640879364943
N	1.175739595802	-0.867991448164	-0.872547932219
N	3.302946801278	-1.352541024624	-1.301023314098
H	4.096520406794	-1.760217541043	-1.774474197104
C	2.470351209631	0.995716937883	1.859835527874
H	2.126960147993	1.614930221082	2.687387082334
C	3.847401798406	0.773435917273	1.684428899539
H	4.550178480113	1.226583043991	2.378363761505
C	3.324994464461	-0.540085889992	-0.185222252912
C	1.973675683048	-0.247694616290	0.069429489430
N	1.516475636935	0.497243375049	1.072687817248
C	1.999036946184	-1.511118254765	-1.664733333037
H	1.704061948458	-2.109750864566	-2.516211357647
C	-2.601054862522	-0.445540368072	1.338914243969
H	-3.630235683852	-0.351249150429	1.711867293002
H	-1.921824503737	-0.213581351654	2.169805868383
C	-2.314231002857	-1.890966416149	0.876585832329
C	-1.834286860310	1.842275241139	0.595904211027
H	-1.236376246496	1.759004641288	1.512222953751
H	-2.659319803573	2.541234143014	0.791846825662
C	-0.912245540694	2.381809497801	-0.518491500148
C	-3.425241882000	0.555259180002	-0.714023108190
H	-3.125046270879	1.154658235809	-1.579368130824
H	-4.318205815619	1.006667526359	-0.255366849952
H	-3.670467625283	-0.457862699975	-1.049186706083
H	5.372535615436	-0.207700717568	0.491069362765



UM06l/6-31G* Free Energy: -3276.859737

IIc-3p7

N	3.189708640143	0.350690622802	-0.076209307445
N	4.172928380311	-2.689053168252	-1.467356819779
N	2.235019305687	-1.690924220096	-0.913098773052
C	5.588826805768	0.502914812569	-0.220299427881
H	6.470785875046	1.111328023633	-0.043137311051
C	4.330874966465	1.023304962571	0.102529074674
C	3.291189941804	-0.872912709844	-0.610673492080
C	4.525521253309	-1.461020349520	-0.955370005575
C	5.715187942684	-0.774382125700	-0.758140820594
C	2.803902911803	-2.758845822994	-1.414535474380
H	2.274183369472	-3.635692219814	-1.767196249453
H	6.687605475046	-1.192181143083	-1.009441425626
Cu	1.353355316301	0.797803685135	0.511337584122
O	1.292453461857	-0.577437107578	1.821240901079
O	-0.170717596128	-1.677771841462	3.134522047901
O	1.159493558698	2.352454025626	-0.553212340190
O	-0.389320773661	3.830954457555	-1.252397523002
N	-0.626109740837	0.892287644854	0.743706130924
C	-0.886497376028	0.356982496569	2.086027128016
H	-1.918327053433	0.004092807743	2.208259048683
H	-0.730722739494	1.172155776376	2.804453522542
C	0.133083780624	-0.757794257241	2.392616981904
C	-1.003455878125	2.284209595396	0.469286827380
H	-0.908878114105	2.848541438612	1.405707704949
H	-2.045178184386	2.380469934949	0.137464036227
C	-0.029247499100	2.896140842840	-0.557757412937
C	-1.045616490066	-0.047585107129	-0.339995082221
H	-0.659738972133	0.374862273555	-1.277606320354
H	-0.503228662609	-0.985656081781	-0.160151383945
C	-2.522808834679	-0.282039518451	-0.427725954962
C	-3.328119616027	0.521906188368	-1.240802692500
C	-3.126466399170	-1.300000129648	0.318817947341
C	-4.703640418261	0.327545934306	-1.306376069753
C	-4.500023967930	-1.509170054535	0.266811160106
C	-5.276401985169	-0.688708452230	-0.546977092972
H	-2.869341208353	1.309297987988	-1.840671654220
H	-2.509495231529	-1.939975719177	0.951453364480
H	-5.327241516075	0.951175639586	-1.941228671715
H	-4.967285867194	-2.300833788999	0.846312209208
H	4.230227405400	2.024505041980	0.514861986179
Cl	-6.999757758032	-0.945678689521	-0.623582041435
H	4.794527492109	-3.407451685957	-1.810248308591

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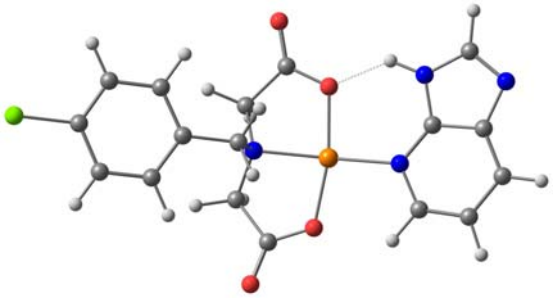
UM06l/6-31G* Free Energy: -3276.875629



IIc-3p9

N	-2.291861984708	-0.111706717967	-0.443736195928
N	-2.675458915605	-3.625067262728	-1.030894643757
N	-3.979829585360	-1.783243436821	-0.999659832116
H	-4.789174091859	-1.151520778980	-1.050168140422
C	-0.098018278454	-1.093852334571	-0.179778224518
H	0.950381122646	-0.914579665339	0.041113126195
C	-0.969611825940	-0.006224510505	-0.180641166101
C	-2.718660258060	-1.357200777923	-0.702706875694
C	-1.911302020521	-2.520110379301	-0.726158786699
C	-0.554939386653	-2.380710092106	-0.454060315492
C	-3.883705876936	-3.137998893201	-1.181645474176
H	-4.759235243221	-3.726817589404	-1.429857681551
H	0.111162205201	-3.240605923581	-0.457457553513
Cu	-3.437228919771	1.506687029807	-0.407705336911
O	-5.088743479498	0.620229958380	-0.808340844305
O	-7.268463286685	0.997472517406	-1.219519522746
O	-2.030709347230	2.706336635547	0.003746154089
O	-1.592314301879	4.893869217458	0.307565020331
N	-4.504829738244	3.170377832233	-0.731792403098
C	-5.906805542282	2.830315215048	-0.466689291295
H	-6.609759053534	3.512736986144	-0.960840761477
H	-6.076883327087	2.913449051512	0.614387652956
C	-6.162342311995	1.375550402340	-0.885146301625
C	-3.882029134828	4.207886284423	0.100494466845
H	-4.278255942109	4.104784352015	1.118880214829
H	-4.117870080331	5.223220935130	-0.242080233465
C	-2.362424091935	3.966437721389	0.139726228386
C	-4.230906331901	3.367830203077	-2.189334288072
H	-3.138577225946	3.417846524729	-2.288648437502
H	-4.567345809335	2.450042402710	-2.690108277861
C	-4.879927801748	4.574057745003	-2.794482096556
C	-4.227052963930	5.811470030128	-2.791620275981
C	-6.157774091026	4.489107409015	-3.356930841954
C	-4.833446908178	6.942274070219	-3.326693739051
C	-6.779818872364	5.609135499948	-3.896848712274
C	-6.108932248375	6.828991075894	-3.873783702751
H	-3.224323526438	5.890630649033	-2.368926340908
H	-6.673422094985	3.527778975403	-3.380023104693
H	-4.323998237689	7.902021011615	-3.326885441666
H	-7.771060938541	5.540627541964	-4.336619072363
H	-0.627777289492	1.003767269976	0.028680460536
Cl	-6.875492420947	8.238301817105	-4.551437913940

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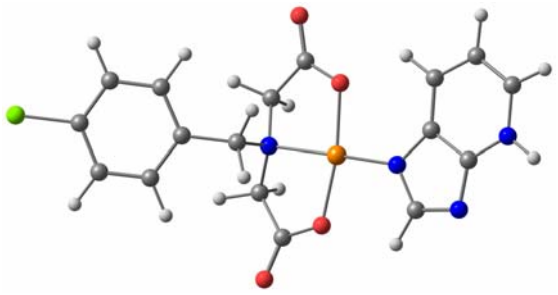

UM06l/6-31G* Free Energy: -3276.861758

IIc-7p3

N	6.203716699022	-0.253151362190	-1.117041967582
N	2.939420529503	0.616941265376	-0.181584051980
N	4.806845910811	1.712246168437	-0.964730811320
C	5.216896604512	-2.315548255062	-0.470434735522
H	5.329860133516	-3.387143954702	-0.340779262743
C	6.298023325798	-1.595465262022	-0.938491236723
C	5.052883178306	0.405024474395	-0.840348432280
C	3.925930102698	-0.320852024852	-0.355048272959
C	3.995758940587	-1.690325939649	-0.166393554607
C	3.524987727694	1.775508211891	-0.552341173549
H	2.964112481840	2.703923674614	-0.513750329825
H	3.132515982282	-2.242688459449	0.202359171602
Cu	1.120411739707	0.444798017624	0.490379506735
O	1.170496968067	-1.444717777226	0.776458185990
O	-0.100979292401	-3.163568246235	1.482409819433
O	0.726811465323	2.300493164749	0.314197710528
O	-0.942675624041	3.785066504026	0.610600985126
N	-0.830151821478	0.255923633156	0.871272976541
C	-0.964051474464	-0.936109747130	1.716161169063
H	-1.974460138509	-1.363990060089	1.688951378844
H	-0.764366146531	-0.637165081581	2.753282694860
C	0.093350708037	-1.974510178210	1.296440520031
C	-1.247002341734	1.549850976096	1.425670018642
H	-0.987316837021	1.555874014381	2.492249390116
H	-2.329481678404	1.714607796606	1.350933475748
C	-0.458230113489	2.672215493262	0.722222559356
C	-1.347154626092	0.035145156603	-0.512716353634
H	-1.014932929545	0.899047224598	-1.103489764764
H	-0.822833761544	-0.850306308676	-0.896217822348
C	-2.831590574559	-0.139727719306	-0.609241011679
C	-3.670420342126	0.967547028477	-0.775148966577
C	-3.407132716620	-1.411075804197	-0.514900638488
C	-5.051242392655	0.817341625191	-0.838119952432
C	-4.785814670823	-1.580920190969	-0.576006565760
C	-5.595707897717	-0.459972093932	-0.736118025863
H	-3.234934837744	1.964318734340	-0.860835816240
H	-2.764270351687	-2.284824278101	-0.396829520275
H	-5.701532150779	1.677889580866	-0.969788413458
H	-5.231252670345	-2.569586877349	-0.505740485109
H	7.254803196112	-2.041977792590	-1.183901613078
Cl	-7.325333536094	-0.660418040847	-0.820092729631
H	6.994112232580	0.281901709676	-1.461822054241

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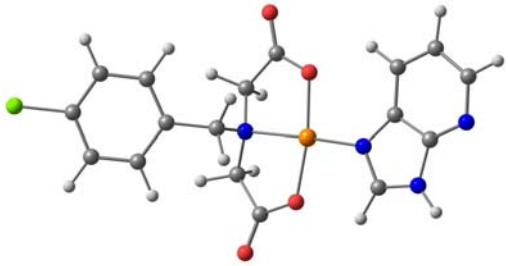
UM06l/6-31G* Free Energy: -3276.870285



IIc-7p9

N	-1.390695949931	-1.720501398703	-0.497018516369
N	2.078047711760	-1.398788794743	0.243757801729
N	0.632829563418	-3.023411505378	-0.201563973158
H	0.266523686666	-3.951060015390	-0.364580292904
C	-0.981008772800	0.655718732169	-0.191751871958
H	-1.417194812690	1.651429501204	-0.189467711082
C	-1.804743384691	-0.448304781186	-0.463901599657
C	-0.097568598488	-1.847062679663	-0.241674438930
C	0.828989413471	-0.828375985145	0.044560972027
C	0.373883330092	0.488712315311	0.071561891300
C	1.913487376590	-2.702800237229	0.091355257195
H	2.721833598290	-3.417611496967	0.190797003610
H	1.052372440856	1.311546189015	0.286922233009
Cu	3.815713732760	-0.621697933108	0.710022665313
O	3.264720633670	1.195986881707	0.779745937076
O	4.068568489837	3.268395206061	1.140393140607
O	4.675495519558	-2.321901673152	0.714771221125
O	6.692424521660	-3.278005618492	1.016371060835
N	5.662087601988	0.112945136862	0.856752974873
C	5.517903665739	1.399987321787	1.548348425719
H	6.368593604701	2.071179048771	1.375311725298
H	5.473658030105	1.198980684423	2.626500318489
C	4.191272858793	2.056667238512	1.119151406414
C	6.455579626587	-0.939944306145	1.503391419013
H	6.299436275591	-0.860368418599	2.586965459274
H	7.532091482874	-0.831457896180	1.319920113945
C	5.944776491897	-2.316754629736	1.036641169937
C	6.000405447067	0.276745562474	-0.589683189646
H	5.889315677534	-0.717285684980	-1.043021317312
H	5.220842574915	0.923817241290	-1.013403618439
C	7.362933729309	0.838128699974	-0.857049883811
C	8.469260836654	-0.006777640715	-0.994714722682
C	7.555968157879	2.220180698779	-0.955103190497
C	9.741512819157	0.508484350815	-1.216145965219
C	8.820651336600	2.753696292068	-1.176207634770
C	9.904116747287	1.888520196559	-1.303045058639
H	8.332292901480	-1.087568290071	-0.934275564055
H	6.700349508918	2.890836667007	-0.862038698122
H	10.599539141962	-0.149091013819	-1.326107889193
H	8.968363009035	3.827319036935	-1.255257704526
H	-2.864277075408	-0.296712582709	-0.668355907568
Cl	11.493255114304	2.544718085410	-1.586070842118

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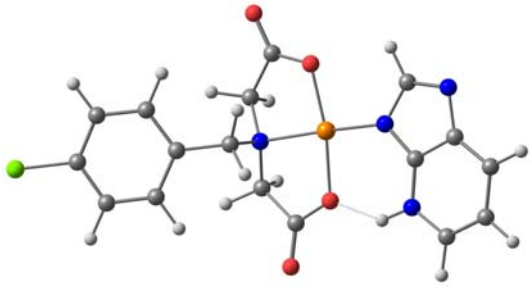
UM06l/6-31G* Free Energy: -3276.870826



IIc-9p3

N	-1.301460784491	-0.036649823518	-0.204794608765
N	-2.220124469295	-3.398941931567	-0.857370229277
N	-3.267940993643	-1.350126838840	-0.761479399189
C	0.721733128060	-1.273513973605	-0.008831221919
H	1.788629648941	-1.260265776977	0.190447383596
C	0.028567381523	-0.076132560007	0.035947032315
C	-1.962355067587	-1.175709162893	-0.490787467565
C	-1.297455643166	-2.433686828135	-0.548313259933
C	0.066677152279	-2.478087525049	-0.303225734965
C	-3.343267734419	-2.711319977499	-0.966594827407
H	-4.303610318499	-3.155216522729	-1.209063910322
H	0.611849470142	-3.418822801189	-0.337890035999
Cu	-4.684649931772	-0.028194747891	-0.800216254411
O	-6.093372327518	-1.213906520449	-1.249138248002
O	-8.300752526711	-1.221291727308	-1.702569604600
O	-3.512343850885	1.440880172147	-0.350384441375
O	-3.489281405847	3.671253869020	-0.044415051013
N	-6.011220963891	1.417518678837	-1.146664969407
C	-7.318077013814	0.802811398735	-0.873347607771
H	-8.147888886735	1.346343182177	-1.341973971947
H	-7.478837189384	0.827642178632	0.212256986191
C	-7.280269029613	-0.669703940311	-1.331182259344
C	-5.608672625102	2.569505637179	-0.332081144146
H	-6.009625773396	2.425695636290	0.679470193974
H	-6.012431005371	3.517481060779	-0.709987210668
C	-4.075961832521	2.623600533066	-0.237098250011
C	-5.783748612648	1.645336932203	-2.607573890359
H	-4.727810173962	1.929177419646	-2.711899917611
H	-5.912713453288	0.668038167184	-3.090883023598
C	-6.677836650685	2.672425115579	-3.230746857921
C	-6.297147083998	4.017462847583	-3.278304917043
C	-7.920276168126	2.305565828169	-3.759432150743
C	-7.134221476282	4.980921973054	-3.829930160651
C	-8.770614189235	3.255067722348	-4.314397975613
C	-8.367757802737	4.587741841335	-4.342029712319
H	-5.324607500007	4.316224546232	-2.883575212299
H	-8.225967917855	1.258350253378	-3.739692457639
H	-6.835676522477	6.024969565000	-3.869573688402
H	-9.734123315999	2.968496306595	-4.726929911104
H	0.495310921214	0.876213644524	0.260611491658
Cl	-9.423160755768	5.785241978290	-5.039468483344
H	-1.865311663481	0.836552989020	-0.178837674838

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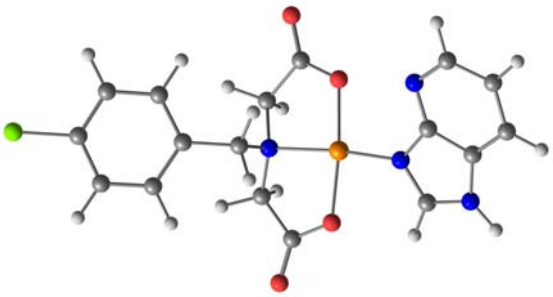

UM06l/6-31G* Free Energy: -3276.858796

IIc-9p7

N	-3.672363254200	-1.763796072512	-0.650765570751
N	-4.902384838401	1.515715213950	-0.577463071943
N	-2.981692722099	0.495967013083	-0.117601436309
C	-5.988726130226	-1.935804774260	-1.358419200921
H	-6.785325434970	-2.597404058728	-1.688724856486
C	-4.722681398111	-2.471196258241	-1.063638224632
C	-3.902730640915	-0.462503408272	-0.517958861357
C	-5.128213096540	0.173324079596	-0.808561762072
C	-6.217827630457	-0.571065423391	-1.240496867733
C	-3.614523842502	1.651967159972	-0.174322038393
H	-3.142077901106	2.602154004418	0.044695025616
H	-7.181906168740	-0.124730767651	-1.474949999649
Cu	-1.139098732487	0.418818773431	0.591118284267
O	-0.889287584775	2.264037772762	0.163850296642
O	0.667027862322	3.891053545692	0.139969523612
O	-1.109803322239	-1.325187331059	1.314286960795
O	0.283426170915	-2.822193128495	2.259544972910
N	0.836374287578	0.412644222205	0.901513343445
C	1.223531503878	1.802190707926	1.174324459626
H	2.277576267402	1.999868158611	0.941031015955
H	1.092576855409	1.981452627883	2.248990982902
C	0.292720736740	2.764524192625	0.415779989835
C	1.070261880318	-0.582155168208	1.956177767023
H	0.929314428038	-0.082433985710	2.922979704832
H	2.092546870864	-0.980576948467	1.941490303182
C	0.022176036272	-1.707381982684	1.840441615919
C	1.285170611104	-0.058250426350	-0.443239670143
H	0.771351887306	-1.013092635762	-0.619046435345
H	0.893628248936	0.668769742385	-1.167731463632
C	2.767160639447	-0.215845100569	-0.595386592182
C	3.390643762598	-1.426869460924	-0.276276214041
C	3.557044462941	0.849106689907	-1.040686659651
C	4.768734498870	-1.574773646306	-0.386004425272
C	4.936599879926	0.720111140625	-1.157340559831
C	5.529665805357	-0.494576687307	-0.824669193054
H	2.785999713127	-2.270887082554	0.058915010907
H	3.083490088179	1.794856631890	-1.308596658577
H	5.250975942328	-2.516901498566	-0.139876354469
H	5.548240418536	1.547618069113	-1.506496155754
H	-4.553242546008	-3.541843440283	-1.175516650844
Cl	7.257926077538	-0.669339595852	-0.969950540910
H	-5.558424692158	2.274231136099	-0.698013793510

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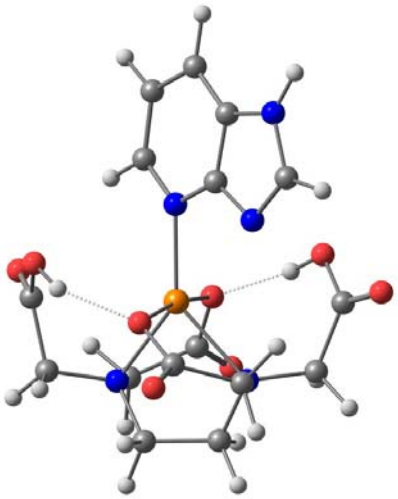

UM06l/6-31G* Free Energy: -3136.584470

IId-3p7

N	2.394797455437	-0.756692950501	0.772109803957
C	3.661325146052	-1.058621260996	0.907030466006
H	4.033241043994	-1.981729497344	1.334927784781
N	4.514036077874	-0.093080351848	0.437664880212
C	3.727228525799	0.919677487707	-0.064858292784
C	3.955808070009	2.135496889640	-0.691568608693
H	4.954060464642	2.523164554744	-0.883602201995
C	2.816272078994	2.837582192195	-1.075271320899
H	2.907014829012	3.800816053952	-1.568503625394
C	1.539035152482	2.315762603189	-0.846377336925
H	0.648366006013	2.862073326064	-1.150611237815
N	1.326233415507	1.140822581543	-0.240592141389
C	2.411163056846	0.465058625536	0.158143963418
Cu	-0.407000560067	0.186123178198	-0.023653733050
N	-0.992474836034	-1.913366260576	0.154062140809
C	-0.471217043568	-2.229300044802	1.501172640349
H	0.576137840699	-2.533782732648	1.384441889208
H	-1.020126381516	-3.070123205273	1.952513031184
C	-0.481874595190	-1.036062749112	2.465453969642
O	-0.346063691339	0.137601368934	1.894772892392
O	-0.591230735473	-1.218905919708	3.665233850024
C	-0.484706068713	-2.850368928762	-0.870404793925
H	-1.056256826262	-2.671576945570	-1.790982678699
H	-0.641946779973	-3.893964953356	-0.558011177255
C	1.001051343263	-2.662245886192	-1.158046501150
O	1.313558514525	-1.619886166546	-1.939737824514
H	0.507970622650	-1.092933700650	-2.189248389109
O	1.848315336369	-3.412147857906	-0.728403388355
C	-2.469733815777	-1.918927307962	0.120808447681
H	-2.866049960043	-2.819223035266	0.620261172109
H	-2.782345755616	-1.973715228323	-0.929457856612
C	-3.067376305188	-0.683414106254	0.767354546771
H	-4.165014087028	-0.716403235727	0.660980686072
H	-2.846492199128	-0.664746880749	1.840675704145
N	-2.520035150876	0.545771998576	0.169088407671
C	-2.963678797826	0.742427450373	-1.226108632645
H	-2.909543925143	1.816609232020	-1.442695560406
H	-4.004905490243	0.415377799932	-1.363486832938
C	-2.046470367556	0.022821111253	-2.224676026798
O	-0.774213042006	0.093812832339	-1.914148347594
O	-2.500042776296	-0.532384078263	-3.211428255423
C	-2.749273994569	1.720418422269	1.033315848197
H	-2.696825305793	1.386908637591	2.074527927427
H	-3.739189506221	2.166327950985	0.855173001885
C	-1.673561566716	2.758208859800	0.738511571382
O	-0.616199456971	2.775511395580	1.559093125823
H	-0.570697516172	1.940061468589	2.089171424643
O	-1.752752694419	3.516677574218	-0.205125571653
H	5.522580251556	-0.141815310894	0.428983160235

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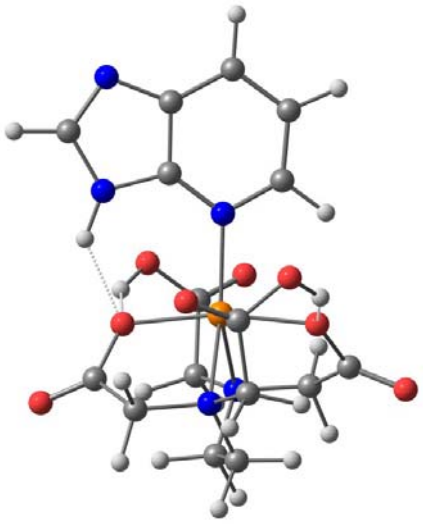
UM06l/6-31G* Free Energy: -3136.586274



IId-3p9

N	2.661358014489	-0.618007556157	1.364133165933
C	3.988704256892	-0.757249942549	1.682298796031
H	4.289567225152	-1.188313751831	2.630143896025
N	4.813252196485	-0.336015230761	0.756987873057
C	3.983279880053	0.126377678759	-0.241624259952
C	4.260387170910	0.707282620928	-1.473450058966
H	5.283971152996	0.863989727041	-1.805576757595
C	3.165659787159	1.077799449092	-2.248728366539
H	3.306070447505	1.543359750433	-3.220004705902
C	1.864527000162	0.859100036745	-1.801017173216
H	1.007878980163	1.128142358764	-2.411333559144
N	1.563802196542	0.289745827450	-0.614535262678
C	2.627661666868	-0.043940927940	0.125744832734
H	1.836316538444	-0.791889834633	1.933473578459
Cu	-0.341343690502	-0.016232023711	-0.103654602021
N	-1.838830055916	-1.555782708840	0.157903749511
C	-1.547450229842	-2.117282906747	1.491410551250
H	-0.841394760784	-2.946417845503	1.355182563157
H	-2.455586965577	-2.517282500454	1.965369960242
C	-0.880946461806	-1.099582513160	2.415819194615
O	-0.040735546719	-0.286822174482	1.799539878431
O	-1.093462027027	-1.088085496317	3.613616364498
C	-1.711188797721	-2.547730771191	-0.931077574508
H	-2.219736720032	-2.144876008165	-1.812691591063
H	-2.183533980374	-3.503762224031	-0.659590888584
C	-0.229232106136	-2.784674607783	-1.204257930008
O	0.286943235243	-2.165296027182	-2.272008005904
H	-0.316932328612	-1.442520246457	-2.567542590448
O	0.449595859104	-3.481724705442	-0.481655535502
C	-3.147036675270	-0.877470424097	0.124365373329
H	-3.931966841348	-1.520879590763	0.555024493266
H	-3.417405988252	-0.701932176620	-0.923306742676
C	-3.097611457919	0.433990213039	0.887186475595
H	-4.077152988397	0.935954624222	0.816293835329
H	-2.913820200754	0.243441382711	1.952040350157
N	-2.021510001932	1.307665437118	0.385451181527
C	-2.357224519605	1.883480090871	-0.933305207970
H	-1.735651047956	2.777596516171	-1.073518555447
H	-3.410222008819	2.199980618203	-0.974351049685
C	-2.060988231257	0.921434408299	-2.087363198450
O	-0.998978863245	0.169199526103	-1.903355547234
O	-2.759866194284	0.899524358286	-3.084440086467
C	-1.673791866590	2.339781539893	1.383202521407
H	-1.693862097339	1.868059353285	2.372704320114
H	-2.401007162969	3.165929005243	1.376377391115
C	-0.289025782461	2.899473587042	1.076603777216
O	0.735267894406	2.312175933386	1.713097755674
H	0.436185878681	1.480714211387	2.151554042910
O	-0.114259781810	3.802729940342	0.291198328377

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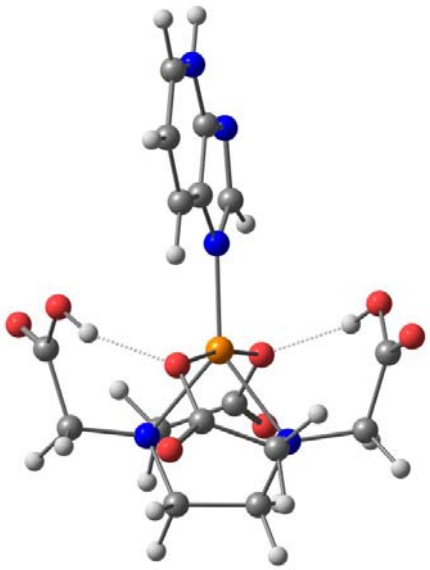
UM06l/6-31G* Free Energy: -3136.577850



IId-7p3

N	1.454688266806	-0.072823798204	-0.737266516380
C	1.830474727518	-0.043167315267	-2.032379916544
H	1.085089756431	-0.022858521599	-2.820169981269
N	3.151564770568	-0.043481910490	-2.297158116639
C	3.657155873957	-0.075832369829	-1.063017021803
N	4.962039232967	-0.092583103267	-0.703649447768
C	5.325478351559	-0.127330826146	0.603021822726
H	6.390859733111	-0.137440507172	0.801863662590
C	4.363350618947	-0.147884185117	1.592470173187
H	4.688684284557	-0.175665628035	2.627332118210
C	2.994057061290	-0.132054898993	1.280325348531
C	2.644504699581	-0.094538828305	-0.057439305205
Cu	-0.405724605659	-0.043007710460	-0.105591616841
N	-1.952277368287	1.509016298001	0.092574551791
C	-2.343230292328	1.726010076991	-1.315727696540
H	-1.680543042766	2.499085868689	-1.727073955906
H	-3.375576841753	2.100385002663	-1.390754531934
C	-2.186950637241	0.468767233812	-2.180606538262
O	-1.149089161892	-0.273363066699	-1.870870704900
O	-2.970164900247	0.230712917366	-3.083083404068
C	-1.506259091972	2.755395510703	0.746669153551
H	-1.482809343667	2.573273788628	1.827877091543
H	-2.204606933004	3.582197787760	0.546804516898
C	-0.122345801228	3.154086917286	0.248788961635
O	0.910263402519	2.600614816161	0.901462935183
H	0.594635985652	1.900046798576	1.525628173530
O	0.042502000177	3.910164114605	-0.680825095462
C	-3.036501530129	0.888863096894	0.875412144705
H	-3.984601040070	1.435329100421	0.733623832166
H	-2.776760872437	0.971733507072	1.938162510114
C	-3.237072143296	-0.565655610995	0.500378935143
H	-4.024136471828	-1.001949853955	1.138182825636
H	-3.585176143598	-0.646400009873	-0.536213238200
N	-1.983641360157	-1.334328473799	0.623273245232
C	-1.605558889121	-1.548714927447	2.035909028208
H	-0.958909133477	-2.435233526467	2.074324962282
H	-2.489147817129	-1.753486598419	2.658545413998
C	-0.816745619284	-0.373788460059	2.623555224677
O	-0.008763733504	0.210988443639	1.767998478486
O	-0.933272809861	-0.063115045558	3.796015542967
C	-2.086491757663	-2.600432111273	-0.133036735753
H	-2.614744640112	-2.386005646850	-1.068938580322
H	-2.659303056207	-3.352450012324	0.429960560115
C	-0.694735799006	-3.152664023384	-0.416177574648
O	-0.130272678863	-2.753864528446	-1.562957534976
H	-0.659334637721	-2.028349092670	-1.979152640761
O	-0.123541479768	-3.892220275403	0.353657618873
H	2.235741766543	-0.142382619203	2.059361457290
H	5.662461101149	-0.076660793564	-1.437787135028

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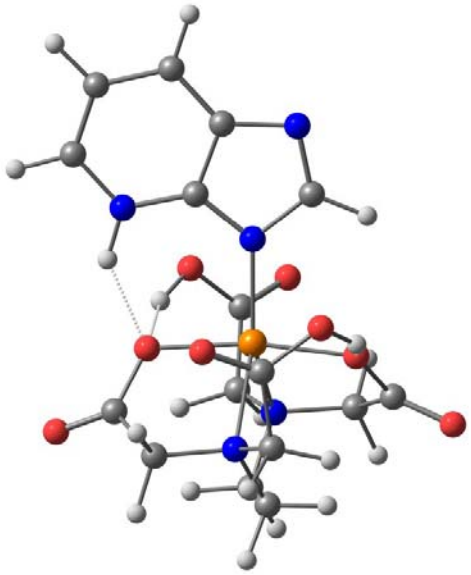
UM06l/6-31G* Free Energy: -3136.581466



IId-9p3

N	1.417982414397	0.015600126256	-0.867296422723
C	1.819288357673	-0.111228431412	-2.179912637971
H	1.068792048855	-0.215972350697	-2.956413955698
N	3.117473525609	-0.100398231281	-2.421050301366
C	3.657700447593	0.040810140919	-1.170851389254
C	4.962613036059	0.117597163799	-0.713294249525
H	5.801684060977	0.066793003303	-1.403599118812
C	5.170102230951	0.262071908982	0.667264538943
H	6.175646811192	0.325654034780	1.070728141738
C	4.104792429412	0.327598971831	1.545324224812
H	4.218446578757	0.440444213255	2.617258149172
N	2.830844275729	0.251962626178	1.091280824040
C	2.591146597100	0.111464115066	-0.227364981868
Cu	-0.393707434956	-0.046097200524	-0.135002880077
N	-2.158156158695	1.258035329147	0.048414596254
C	-2.651986355304	1.269416231934	-1.346986590221
H	-2.139917828098	2.085987641782	-1.873142448136
H	-3.731525600202	1.479353922574	-1.383888865443
C	-2.352827908552	-0.032171691138	-2.100586258343
O	-1.202721426406	-0.585049183707	-1.794358977300
O	-3.137737911891	-0.471291984948	-2.922528982799
C	-1.913627989180	2.625852258586	0.550739519539
H	-1.790810216640	2.564420796007	1.639612786273
H	-2.765492626095	3.287478623473	0.333712427085
C	-0.662208452750	3.215602177927	-0.086595611442
O	0.498622419861	2.847508411792	0.482049098239
H	0.340180628491	2.183933315722	1.195187148427
O	-0.697680578485	3.946865256689	-1.046917249833
C	-3.093754207507	0.557869418387	0.950112123009
H	-4.121763220864	0.934768917385	0.816645699665
H	-2.800695664762	0.788670029570	1.982758443228
C	-3.069815236647	-0.942458978574	0.730309567877
H	-3.747571297958	-1.427244775778	1.452891599027
H	-3.440993640124	-1.189644083347	-0.271002112603
N	-1.700016410684	-1.463414602684	0.859797617294
C	-1.233280235348	-1.457660195090	2.258740106826
H	-0.475431755849	-2.245017373083	2.357307518369
H	-2.052692824422	-1.682712248527	2.957032205788
C	-0.559655062619	-0.144812342459	2.660005962079
O	0.132621573645	0.426540793018	1.687812890294
O	-0.632282324931	0.284616080397	3.795564789757
C	-1.540987216499	-2.770157515863	0.190212737161
H	-2.178950929255	-2.771611140543	-0.699009943558
H	-1.853854342601	-3.599578530527	0.843076297685
C	-0.072614058285	-2.958146871176	-0.181156850410
O	0.233938274148	-2.847442909683	-1.477133619067
H	-0.469235440371	-2.332932933353	-1.939910962712
O	0.770781914169	-3.194976208771	0.657818525203
H	2.016188731519	0.308929274498	1.714451871541

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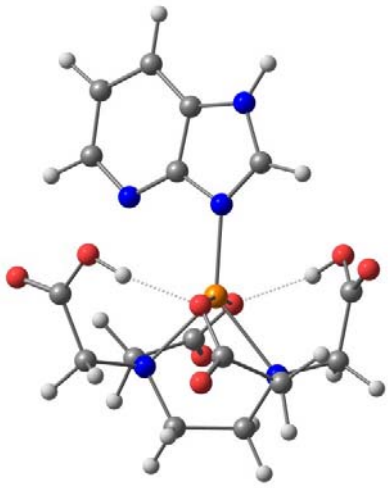
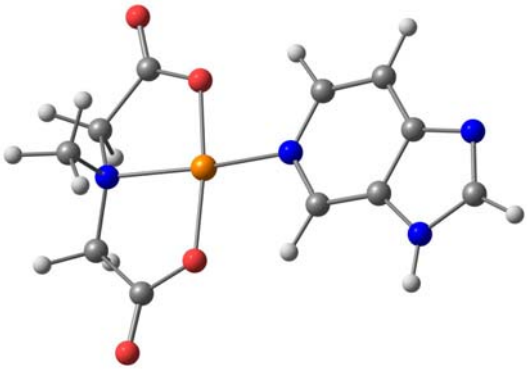
UM06l/6-31G* Free Energy: -3136.582103



IId-9p7

N	1.219569047714	1.110344144207	-0.517427079772
C	1.530769011278	2.258886701924	-1.074462376815
H	0.806797993811	2.982192578773	-1.433245716319
N	2.875821990731	2.463811816982	-1.101971016558
C	3.479695518054	1.366973591332	-0.516280912893
C	4.786483090982	0.971020514039	-0.261492591656
H	5.651237430529	1.575244261374	-0.527202461758
C	4.917671190829	-0.266799638558	0.357910620068
H	5.905313862113	-0.657534899059	0.588049397279
C	3.783345757803	-1.027555965453	0.692225504840
H	3.901981244786	-2.000695132781	1.167021571253
N	2.527318672024	-0.648340878571	0.461314306105
C	2.413912045083	0.527999348613	-0.144980108941
Cu	-0.462792405505	0.170957315978	-0.096295189830
N	-2.531523845225	0.652645734625	0.259783651421
C	-3.111365461064	0.711008073025	-1.095671017503
H	-3.034444943437	1.748263097934	-1.443503737039
H	-4.173873470132	0.425551388381	-1.089210475737
C	-2.336568717202	-0.162221807173	-2.093409530288
O	-1.038449359017	-0.145784815532	-1.911231093866
O	-2.916720622913	-0.777157371666	-2.972394283537
C	-2.589416514375	1.930864366339	0.993992614024
H	-2.490260827369	1.715221199792	2.061912651691
H	-3.546030457395	2.450383195029	0.831127934784
C	-1.451233235069	2.825151500420	0.512610684570
O	-0.402509421611	2.960918795151	1.330275419446
H	-0.345862967961	2.175740699902	1.933920295633
O	-1.488555682141	3.389954529286	-0.563300339026
C	-3.046094600252	-0.475381772169	1.052780375685
H	-4.149322323782	-0.490288204827	1.048925015520
H	-2.728887674137	-0.334325041096	2.092128824813
C	-2.536134785251	-1.801588161294	0.513859723425
H	-2.900542122793	-2.620191960734	1.156814922285
H	-2.949856551839	-1.974108502186	-0.487677086820
N	-1.062055978024	-1.843676964731	0.403653645425
C	-0.409233742336	-2.018285933565	1.718860143131
H	0.624939840729	-2.335216387002	1.530230240636
H	-0.904011311556	-2.804740029136	2.308774854907
C	-0.339635345303	-0.722579324166	2.533370087368
O	-0.206667991615	0.363259644606	1.808780526984
O	-0.387046007454	-0.747023127826	3.750781157937
C	-0.674447629552	-2.907696607659	-0.547606308514
H	-1.330864506311	-2.821628672371	-1.423239252245
H	-0.818021345716	-3.901748953223	-0.097922293105
C	0.781918411308	-2.794052449321	-0.990024644596
O	1.031150781807	-1.873712757799	-1.930794101392
H	0.209806579335	-1.371714674421	-2.174394365144
O	1.654038539049	-3.499180430065	-0.536728782574
H	3.331389838410	3.283312964657	-1.476907403278



UM06l/6-31G* Free Energy: -2586.321077

IIIa-1p7

Cu	0.840435055447	-0.065308369470	-0.129846632426
O	1.304468440146	-1.899969237106	-0.113216116994
O	3.077584259505	-3.283247216247	-0.223713609066
O	0.715076804458	1.824156471929	-0.263043002631
O	1.970458414752	3.677265918589	-0.500860420069
N	2.783362728883	0.259732861985	0.196553814039
C	-1.927885870216	0.707240705140	-0.080365853359
N	-5.221929232005	-0.744421193399	0.115134284075
N	-4.385602305595	1.339655672202	-0.040311719056
H	-4.374508467545	2.347569190569	-0.105064124383
C	-1.618672057012	-1.615207390592	0.050024380481
H	-0.868146656647	-2.401300596346	0.067673570697
N	-1.110504098403	-0.357778977835	-0.038349007350
C	-3.293756002678	0.498828538105	-0.022561577533
C	-3.846534372128	-0.798649746025	0.074829596365
C	-2.972795237673	-1.887220578725	0.111732423027
C	-5.490252816160	0.536778437775	0.043932690960
H	-6.488681091180	0.959776177462	0.048765444671
C	3.483003987532	-0.927251494576	-0.318035490056
H	4.441903910465	-1.093948546170	0.191553678323
H	3.700139766880	-0.764879754149	-1.381169070676
C	2.581126389704	-2.172421328775	-0.197492686090
C	3.088722598717	1.562403538491	-0.413868269818
H	3.361957728097	1.395369644276	-1.463254414920
H	3.941179649378	2.056347668187	0.072349793530
C	1.845113320136	2.472186297550	-0.382115648043
C	2.846362215018	0.325742696089	1.661214677222
H	2.207404268041	1.141151513175	2.016165453087
H	3.876694546463	0.502934952305	2.004571962685
H	2.487638414845	-0.618843810637	2.083169518074
H	-1.445670214342	1.680009942443	-0.157348597464
H	-3.336158076900	-2.908218986132	0.183078952659

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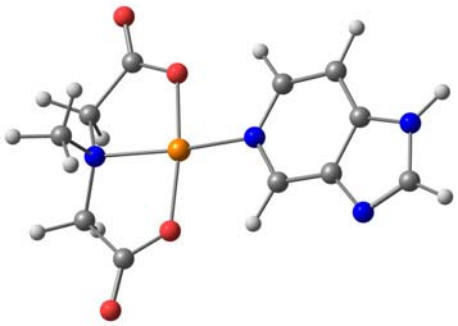
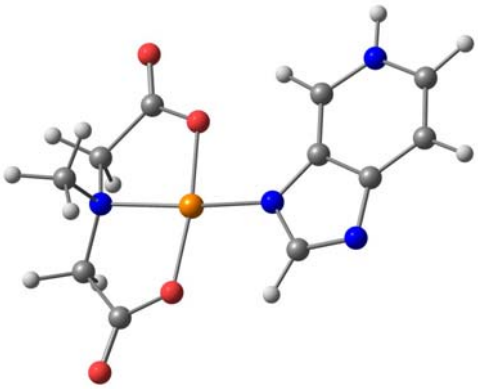


UM06l/6-31G* Free Energy: -2586.320328

IIIa-1p9

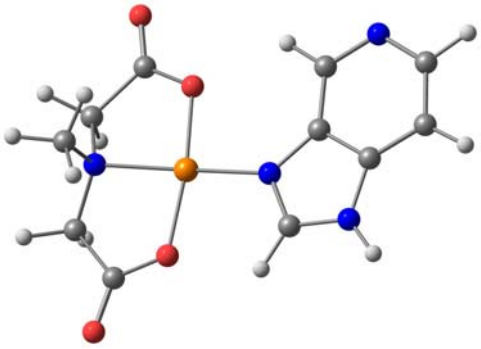
Cu	0.844419624310	-0.054684871795	-0.159355031363
O	1.264843556920	-1.902896722852	-0.132126966205
O	3.000553194596	-3.331816444266	-0.254097273128
O	0.762734572277	1.831107527103	-0.308006181822
O	2.062674870332	3.649538801067	-0.580285017984
N	2.799047614591	0.221137456267	0.144790062293
C	-1.927237262930	0.754788007059	-0.045389592355
N	-5.176718172350	-0.560484388439	0.193399102946
N	-4.320295102475	1.515947837961	0.047027167390
C	-1.622869714925	-1.568300949577	0.051724330747
H	-0.877537856031	-2.359760342999	0.047206235962
N	-1.112423724053	-0.312086817800	-0.032962484978
C	-3.302991587743	0.579172783420	0.038730932549
C	-3.819246091476	-0.733029189097	0.129817746683
C	-2.976024331767	-1.840150048396	0.137691221783
C	-5.405095120225	0.799685307398	0.139178487404
H	-6.413653362340	1.195840981749	0.173177802428
C	3.463833006365	-0.986810903243	-0.366209343510
H	4.422811035966	-1.173883587972	0.136267523025
H	3.676043823935	-0.838052333910	-1.432321050589
C	2.532919701848	-2.208107916490	-0.228920662263
C	3.128929507264	1.510484227720	-0.481135964821
H	3.388377219063	1.326999775518	-1.531223094014
H	3.997020835534	1.988765602117	-0.007129397964
C	1.906713634388	2.449990127437	-0.446482536714
C	2.879683776412	0.299259984404	1.607804545986
H	2.266961992892	1.135051434924	1.961417502429
H	3.918252831892	0.451649258191	1.938304639622
H	2.500320715064	-0.631294469962	2.042867324978
H	-1.452046422118	1.730452462654	-0.123093901977
H	-3.331521450379	-2.864919865194	0.203740545911
H	-5.877155314785	-1.284739723165	0.264170327475



UM06l/6-31G* Free Energy: -2586.318667

IIIa-7p1

Cu	-0.709189098794	-0.164422847403	-0.011795451476
O	-0.219450024847	1.683488687770	-0.058906867443
O	-1.087979486552	3.750627478731	-0.234775235989
O	-1.528252770880	-1.873908350746	-0.067731905647
O	-3.539377268236	-2.867104460618	-0.273733646055
N	-2.554586852296	0.525276342277	0.315934172106
C	4.684480106596	-0.790006294473	-0.034026236963
N	1.107374927593	-0.850483998130	0.031869325916
N	2.785810796282	-2.421490649755	0.036029820128
N	3.931128368245	1.467986545937	-0.080048748148
H	4.172022956464	2.450257647202	-0.113228670154
C	4.950391672139	0.555578235777	-0.074036881428
H	5.950695186032	0.971912996164	-0.103443047126
C	3.339063261657	-1.190884862613	-0.000922429558
C	2.307320586295	-0.193189180719	-0.007552755367
C	2.614318614148	1.147566166123	-0.047619628615
H	1.871671222137	1.943150181316	-0.058602260037
C	1.471552380415	-2.152958547625	0.049383379756
H	0.707758403177	-2.924400383921	0.071782891954
C	-2.596149186338	1.888312642405	-0.232346701829
H	-3.340935585170	2.515978873335	0.276263212505
H	-2.887407323227	1.826796684468	-1.288340860632
C	-1.202180591391	2.539648298716	-0.159873187916
C	-3.465020420802	-0.477573353738	-0.258270862871
H	-3.626185531069	-0.230392087215	-1.314995470629
H	-4.446929427647	-0.472004852756	0.234554598236
C	-2.829147789660	-1.881984186201	-0.185094883660
C	-2.625934370733	0.534522258562	1.781683891740
H	-2.463329418777	-0.480396817247	2.158674968966
H	-3.607316325789	0.892991414627	2.127408652265
H	-1.845863315789	1.192132957277	2.179538335835
H	5.496073306706	-1.511280537423	-0.030214517965



UM06l/6-31G* Free Energy: -2586.319111

IIIa-7p9

Cu	-0.709927457527	-0.092509197336	-0.077513409112
O	-0.338445928776	1.757509135479	-0.184715269247
O	-1.351018689527	3.751903961309	-0.441494078511
O	-1.395534616661	-1.865145298277	-0.084250027230
O	-3.320611011134	-3.017735713407	-0.265993308552
N	-2.601612859401	0.460849191446	0.215980166415
C	4.739755140813	-0.644232493533	0.105201085129
N	1.148247093341	-0.727916637503	0.025564334648
N	2.759672680296	-2.250847786390	0.087816201367
N	3.987048023474	1.667397057079	0.041499522988
C	4.951269425061	0.728925027588	0.084350632974
H	5.971755326807	1.111897084853	0.102812618338
C	3.404317180122	-1.029375197701	0.079819579176
C	2.376106244112	-0.072586133803	0.036333711479
C	2.712385853938	1.285169694626	0.017221471882
H	1.939869520870	2.052513952614	-0.023444105389
C	1.423165820170	-2.016740004554	0.051833612142
H	0.663331399588	-2.789789683066	0.043459978065
C	-2.726029295225	1.795140750554	-0.391018955888
H	-3.518739697498	2.390138992563	0.082339847051
H	-2.995629957365	1.669441141635	-1.446959856261
C	-1.377149443744	2.541037978881	-0.326024312697
C	-3.429744165654	-0.627155790813	-0.326690263053
H	-3.603900970201	-0.428876988573	-1.391585005939
H	-4.412283145933	-0.679394844705	0.161872842494
C	-2.693643767238	-1.976224989822	-0.206134213174
C	-2.693082838075	0.526862130224	1.679371825079
H	-2.457654105957	-0.455000697212	2.103119127364
H	-3.704275303425	0.821180392806	1.997935065037
H	-1.973049294998	1.260863160629	2.055638700523
H	5.564640121536	-1.351742941641	0.139000968692
H	3.191563718304	-3.163429253262	0.111921514101

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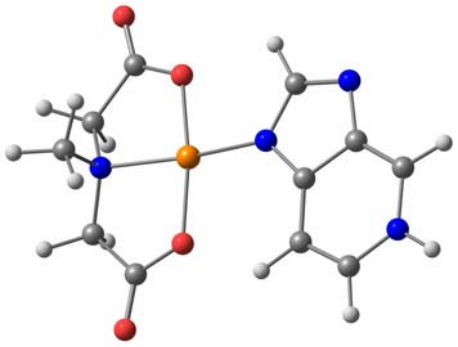
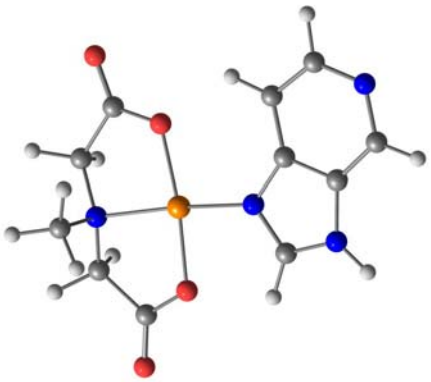


UM06l/6-31G* Free Energy: -2586.316076

IIIa-9p1

Cu	0.732672192217	-0.113055566817	-0.222644370699
O	1.503280373804	-1.848423186386	-0.246928446732
O	3.474984959265	-2.911081715048	-0.483779656673
O	0.297461378958	1.740780774588	-0.331983758925
O	1.221020013207	3.771967631056	-0.622500601895
N	2.611030234942	0.529643485618	0.010410904917
C	-4.625009655960	-0.746642674400	0.051232034919
N	-1.093999687841	-0.767523752241	-0.065339941418
N	-2.739785830213	-2.368677223419	0.087954299447
C	-3.948062806203	1.555047241285	-0.123199549416
H	-4.324695222581	2.569833368608	-0.178776797348
N	-4.901353152492	0.578613922983	-0.026055408700
H	-5.871889297487	0.863530795038	-0.012756496734
C	-3.302114506620	-1.124545272759	0.030003823567
C	-2.279676838380	-0.119726521915	-0.069904503442
C	-2.611832115047	1.240145393290	-0.147237633151
C	-1.447265215134	-2.093004303940	0.024078961154
H	-0.668704751733	-2.849486788088	0.037004741954
C	3.472492245958	-0.521307695159	-0.551838059974
H	4.469025130093	-0.527866262327	-0.089097784449
H	3.608574073768	-0.318631736231	-1.621465902498
C	2.798418847651	-1.901298972431	-0.406975950601
C	2.672049959823	1.867629391812	-0.594885498160
H	2.924401127364	1.754460141737	-1.656569993875
H	3.451730610494	2.492618534571	-0.137848522462
C	1.299641056894	2.561960701234	-0.501648829418
C	2.731975665578	0.595996608025	1.471195423355
H	1.987644035625	1.295657524427	1.865745091922
H	3.735704117890	0.934387749510	1.770061686803
H	2.548809265473	-0.396633422990	1.895428264929
H	-5.464380519227	-1.430062237940	0.124209048725
H	-1.842474690098	2.005100068303	-0.227268575163



UM06l/6-31G* Free Energy: -2586.320150

IIIa-9p7

Cu	0.708853704851	-0.095097452788	-0.076494862976
O	1.381728751007	-1.871810597228	-0.123685014746
O	3.298640518178	-3.032688283305	-0.336438607599
O	0.351625436552	1.762413544230	-0.134180231253
O	1.378024119697	3.754609286144	-0.343690021167
N	2.604058285735	0.437996264122	0.229465923101
C	-4.739517824635	-0.580705625960	0.048663421591
N	-1.151703400321	-0.719984636845	-0.001931416064
N	-2.779962076964	-2.226180740924	0.018441214126
C	-4.035603950569	1.612604101141	0.033104746536
H	-4.352933906891	2.654773854921	0.034114907544
N	-5.040599841203	0.712864869962	0.051273747535
C	-3.409149934936	-0.990950873821	0.028249624495
C	-2.367090698973	-0.047928499185	0.011399334698
C	-2.679861875305	1.310451649914	0.013439579540
C	-1.446542868553	-2.009188588481	-0.002569767266
H	-0.694144188442	-2.789540312852	-0.020383293374
C	3.424205782209	-0.642176817987	-0.340504942427
H	4.407042776364	-0.712733099879	0.145077921009
H	3.598097023309	-0.419669112644	-1.400680031986
C	2.678932558375	-1.988815772767	-0.250699436782
C	2.738790986368	1.786341962490	-0.343281398681
H	3.006783938465	1.685732096743	-1.402300693873
H	3.536537617951	2.362792164700	0.144418193576
C	1.396119171703	2.540810033766	-0.258069965140
C	2.695516167759	0.465814247815	1.694143502890
H	1.977693913948	1.192082436401	2.089213683058
H	3.707513611098	0.748395402747	2.020541490472
H	2.456567299790	-0.525926966896	2.092047036910
H	-5.569389358895	-1.289374121037	0.062738961102
H	-1.901038736607	2.068604867371	-0.006051674209
H	-3.223964001006	-3.133218279837	0.021742069312

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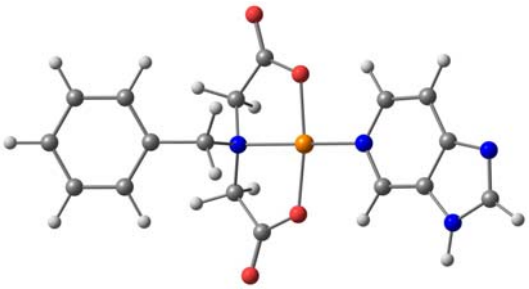
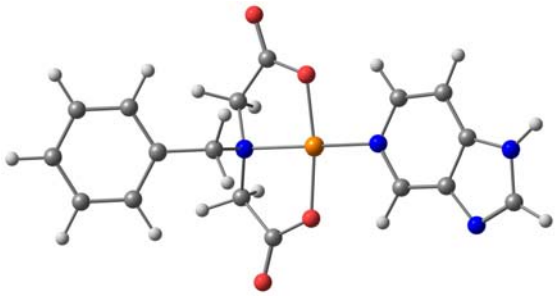


UM06l/6-31G* Free Energy: -2817.269468

IIIb-1p7

Cu	0.884675673877	-0.824882285522	0.206091090038
O	0.838117135515	-2.173364876512	1.541082020574
O	2.188388078189	-3.457267116899	2.806691243882
O	1.279555617092	0.479719341476	-1.122891973178
O	3.007467647591	1.486171532800	-2.158236890999
N	2.847456004700	-0.787661084022	0.562834677798
C	-1.574843307619	0.271050181251	-0.804286236269
N	-5.141840862921	-0.033149316675	-0.377143757273
N	-3.772592329636	1.204419014365	-1.665833235417
H	-3.489514223346	1.883474793004	-2.357880359894
C	-1.904826279451	-1.363588057317	0.846565704656
H	-1.393709923462	-2.049164565894	1.517524306126
N	-1.075625894483	-0.614938951793	0.072874164115
C	-2.947640626504	0.411095908248	-0.898009892868
C	-3.831033514852	-0.353056646546	-0.101587973504
C	-3.283267449491	-1.269414039912	0.798513856013
C	-5.054087568980	0.888766265120	-1.305004946130
H	-5.901840145161	1.380792035260	-1.768799757496
C	3.181877590792	-2.119724149002	1.081859244970
H	4.112679263644	-2.125500244165	1.662995605557
H	3.327710170958	-2.787938663358	0.223287775395
C	1.999073476518	-2.649446515709	1.915037821476
C	3.473482564909	-0.356511548232	-0.693134520983
H	3.578552864448	-1.239990175558	-1.336130657005
H	4.477223266783	0.061286947737	-0.544311511422
C	2.547762930154	0.650434273163	-1.400233849679
C	2.900159987355	0.267621042413	1.620456272094
H	2.438505723557	1.161769043969	1.180104302022
H	2.244617412400	-0.081025390284	2.429720388556
H	-0.846872856426	0.830809583899	-1.388668631239
H	-3.909299482613	-1.886053291794	1.436782987489
C	4.272897769119	0.574387740842	2.136532359876
C	4.796532687737	-0.128590050153	3.227010391000
C	5.058006153839	1.556453902249	1.522841265126
C	6.082302563341	0.137921074143	3.688227365112
C	6.343831610960	1.823606514727	1.983014460776
C	6.857959783973	1.113132006733	3.065431481117
H	4.183841619467	-0.885742685726	3.719529108847
H	4.650227811149	2.118200911735	0.680518867396
H	6.476680787826	-0.413692913713	4.539483917446
H	6.943077237806	2.592205067482	1.498624767766
H	7.862168662157	1.324449273207	3.428352508492



UM06l/6-31G* Free Energy: -2817.268948

IIIb-1p9

Cu	-0.397655886914	0.204703108074	0.552178676002
O	-0.092600369956	2.078974215114	0.457588572983
O	1.523207310327	3.626021428048	0.719740907686
O	-0.365920098620	-1.684818052585	0.743408108669
O	1.016736798251	-3.388764872228	1.252892685642
N	1.584160978939	0.076700977609	0.748176114751
C	-3.031772509330	-0.823110323998	-0.047011933052
N	-6.253889422569	0.225229718640	-0.977474310583
N	-5.305233206748	-1.770216116465	-0.547451649605
C	-2.870929132740	1.509831991684	-0.222672822132
H	-2.194362072812	2.355405347343	-0.127366807068
N	-2.304282451218	0.302144365385	0.033370951315
C	-4.373924769441	-0.758365723210	-0.401149854538
C	-4.949344772367	0.504651075730	-0.666665059696
C	-4.196694378155	1.672154741276	-0.580652664272
C	-6.396851085328	-1.144662972416	-0.887181183015
H	-7.350723842262	-1.618587450230	-1.089237193416
C	2.012316513601	1.356959169994	1.324401252556
H	3.071861308022	1.572305389265	1.136410208734
H	1.878846715687	1.297106022093	2.412329975985
C	1.109211913946	2.482056527753	0.784759208772
C	1.826596999215	-1.147318605756	1.521616307068
H	1.706286065063	-0.901625971924	2.584728126698
H	2.843517271149	-1.537722650226	1.388482161246
C	0.768867095240	-2.201320404536	1.142859805065
C	1.979023350163	-0.065305225573	-0.686502963364
H	1.436533111260	-0.942052892541	-1.065123812205
H	1.580545732438	0.820018945206	-1.200005409740
H	-2.514545814614	-1.754725972692	0.173124807753
H	-4.600130288547	2.662052061707	-0.776121572667
H	-6.973723583725	0.889213740767	-1.224686693057
C	3.451958314964	-0.204971248618	-0.922602904800
C	4.251693642754	0.925993549443	-1.119657931755
C	4.051789718835	-1.468958784928	-0.929354875922
C	5.624386262218	0.796841185023	-1.309311128020
C	5.424226708623	-1.599254123084	-1.118732940439
C	6.212336235135	-0.466030464084	-1.307056234608
H	3.787727775689	1.913906001914	-1.130073579217
H	3.431454763789	-2.356058938919	-0.789731194159
H	6.234925680404	1.684380064520	-1.464429867420
H	5.877925711133	-2.588487957244	-1.124506717477
H	7.285407708299	-0.567716875766	-1.458754569206

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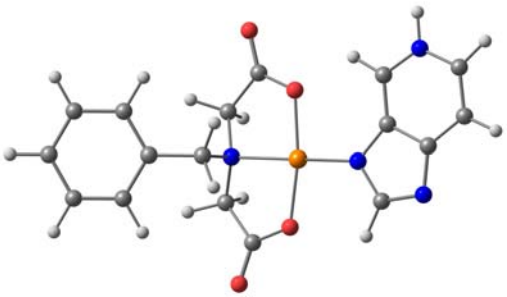
UM06l/6-31G* Free Energy: -2817.267169



IIIb-7p1

Cu	-0.409050645729	0.499668588397	0.217731206938
O	0.324214056419	1.821766395868	1.398109698793
O	-0.204649543651	3.715616773655	2.491453923802
O	-1.437126074528	-0.607425154050	-0.938738924171
O	-3.499044213223	-0.788516681769	-1.829824894666
N	-2.138172204409	1.428985022018	0.574418771287
C	4.601713996105	-1.543381626989	0.661207744515
N	1.198875627262	-0.586472973417	0.106550681461
N	2.569412346719	-2.292715174892	-0.596950476291
N	4.206172947583	0.445515490730	1.908814284431
H	4.573864362784	1.151311567965	2.533798821235
C	5.044138583769	-0.559028562344	1.508648113565
H	6.052083819780	-0.512495308184	1.904525340065
C	3.268721883288	-1.480434329307	0.223570355469
C	2.431419851069	-0.404993227340	0.673069410434
C	2.911464763818	0.563212048943	1.524817174917
H	2.318774078004	1.398065424939	1.894680386144
C	1.360757380990	-1.711030888181	-0.626914190428
H	0.527418387655	-2.102165357309	-1.202760235480
C	-1.800105915421	2.808568421104	0.941669752514
H	-2.593395439609	3.299014353565	1.520339479841
H	-1.670348456575	3.382087739552	0.014704175368
C	-0.464781589316	2.819329326587	1.706625684885
C	-2.949804746006	1.213973230972	-0.630452174966
H	-2.645741138170	1.960550203562	-1.375720428723
H	-4.023177431104	1.349664475251	-0.447342331139
C	-2.649349153422	-0.189438933546	-1.193636164340
C	-2.626512585988	0.632039837494	1.741280581910
H	-2.639546200592	-0.414559812525	1.409007769196
H	-1.854139401079	0.724631429561	2.516696136537
H	5.269855314518	-2.339292859582	0.346562845764
C	-3.967831118787	1.041639021732	2.268342451032
C	-5.135665044005	0.474865558629	1.745949419858
C	-4.074189692969	2.006138594438	3.276056460948
C	-6.384204111923	0.870395115080	2.215907693907
C	-5.322496558135	2.402281464362	3.747029118738
C	-6.479027134609	1.835420544355	3.216306648410
H	-5.058447738327	-0.285796732681	0.967065179125
H	-3.166188212178	2.441541714028	3.697477145055
H	-7.284821866797	0.419556709239	1.803496972369
H	-5.391555904052	3.150909249586	4.534052136288
H	-7.455480831342	2.141603808644	3.587297310685

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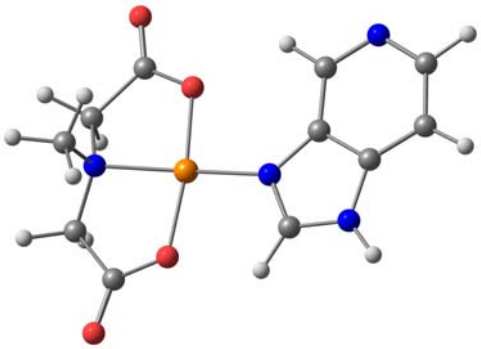

UM06l/6-31G* Free Energy: -2817.267257

IIIb-7p9

Cu	-0.444483707977	0.642098838010	0.158507485985
O	0.167567181915	1.974083343507	1.360028151078
O	-0.535587534471	3.807404766268	2.463546110905
O	-1.341979577990	-0.518116764222	-1.058910859991
O	-3.343564027596	-0.841712449824	-2.038443213553
N	-2.247587824606	1.429187374761	0.462392485245
C	4.627283368026	-1.388866059425	0.612099074346
N	1.217571101270	-0.405965593278	0.048459362301
N	2.527680235898	-2.040646217316	-0.680166745299
N	4.241326429353	0.601653498363	1.955085440434
C	5.020800012227	-0.399277608892	1.504593313168
H	6.039701305725	-0.405068373755	1.892260927741
C	3.310096118313	-1.293150393578	0.178152616320
C	2.472788490429	-0.259561103583	0.631108495766
C	2.981888183743	0.681669158644	1.532112071943
H	2.359117937510	1.495630839047	1.902515077853
C	1.296063958435	-1.471391542874	-0.723404357488
H	0.467600169620	-1.840718463632	-1.317069279207
C	-2.005079924044	2.826935494904	0.841492088142
H	-2.846482288283	3.266440940552	1.391671993334
H	-1.876207921946	3.407953518295	-0.080814641402
C	-0.698965114326	2.911111832332	1.655738341676
C	-3.008540919618	1.165641721812	-0.765632946445
H	-2.757377495171	1.950268917174	-1.491037638181
H	-4.093413532293	1.202823346188	-0.605842778485
C	-2.576391566869	-0.191778949537	-1.350877724100
C	-2.713911924673	0.597843979877	1.614759487048
H	-2.665048973119	-0.445687960049	1.275438491881
H	-1.962272143480	0.726548145279	2.405113496310
H	5.307439135610	-2.172533633093	0.287345067244
H	2.807022839987	-2.866121895323	-1.190516879311
C	-4.084339511025	0.933061647523	2.119210301123
C	-5.212351466033	0.302348359445	1.583207222295
C	-4.256711739671	1.893701400273	3.121760667205
C	-6.487352232179	0.632169006019	2.032741314965
C	-5.531328468263	2.224222022312	3.572077955791
C	-6.648132961672	1.594967582489	3.026680014358
H	-5.083898555706	-0.458731763248	0.811475931894
H	-3.380005887101	2.378528532483	3.554876933443
H	-7.356452944569	0.131983257539	1.609751466396
H	-5.651668131147	2.970730013372	4.354767481968
H	-7.644904898823	1.850386250563	3.381564420956

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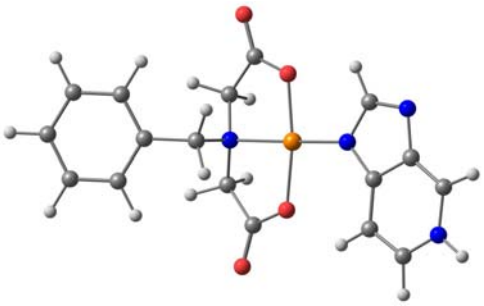

UM06l/6-31G* Free Energy: -2817.264539

IIIb-9p1

Cu	0.913877886266	-0.874893380660	0.113936427996
O	1.147006269873	-2.156773904716	1.504226983897
O	2.748125483915	-3.144680569668	2.744370386212
O	1.048973287974	0.433990125816	-1.275235192807
O	2.551165028957	1.649603649718	-2.429648646697
N	2.860961567715	-0.515243272576	0.371969554847
C	-4.386426889932	-0.519580820920	-0.870082695004
N	-1.027999278412	-1.024274589534	0.103369828903
N	-3.068026533056	-1.871492526178	0.749027242486
C	-3.061885679445	0.930511202628	-2.259472692924
H	-3.121465920819	1.664179043426	-3.055004512339
N	-4.258433196575	0.408091766651	-1.850799959195
H	-5.099237147909	0.734546705471	-2.308896263771
C	-3.237168961213	-0.958093311401	-0.253419815499
C	-1.966477213022	-0.426749012005	-0.663127805797
C	-1.881475312692	0.532971257829	-1.681660668661
C	-1.754565033984	-1.866996146175	0.910480566108
H	-1.234589711936	-2.483625769625	1.637092137939
C	3.422949979578	-1.762716410573	0.904299462832
H	4.378441437909	-1.609656864644	1.421705909551
H	3.612048435340	-2.432903038069	0.055579883706
C	2.384117540110	-2.426534719747	1.829183380802
C	3.364009758532	-0.026657042306	-0.916592646071
H	3.597364346636	-0.899526015690	-1.539959439854
H	4.287032557775	0.558486616961	-0.815632733191
C	2.261061420964	0.787929800488	-1.617156940864
C	2.790604523911	0.565057882573	1.402790486011
H	2.196304478969	1.373016832294	0.955478275386
H	2.211174750888	0.149578472986	2.238212220868
H	-5.388036372756	-0.860465316848	-0.630583187340
H	-0.922163331880	0.939193289410	-1.995277971321
C	4.118865908037	1.073090692860	1.874274537942
C	4.766658766267	0.464217581575	2.954685081440
C	4.739435701400	2.149250614955	1.230666977323
C	6.013137498258	0.915812212358	3.377091841375
C	5.985991755157	2.602098365150	1.652548911257
C	6.624955501486	1.984698078642	2.725363128018
H	4.282416332875	-0.368788204391	3.467543566630
H	4.232659458659	2.637153363116	0.396030319878
H	6.505386008691	0.435074438920	4.220269832649
H	6.456655507837	3.442301050816	1.145412692748
H	7.598263072620	2.340672885884	3.058048692538

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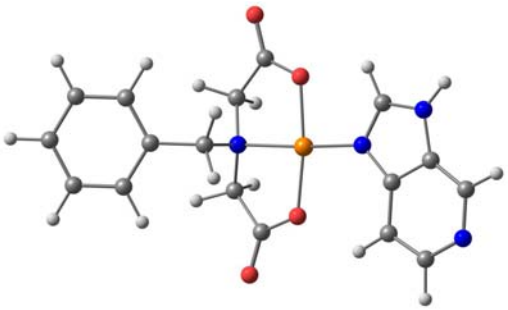

UM06l/6-31G* Free Energy: -2817.268345

IIIb-9p7

Cu	0.853972354943	-0.898947791216	0.243149680210
O	0.974641240840	-2.252006588633	1.579753316536
O	2.479918645547	-3.367245440728	2.829277644950
O	1.067353599235	0.433637243522	-1.091216976221
O	2.655190806392	1.629095244981	-2.149499727814
N	2.799234270017	-0.641346153378	0.575612585148
C	-4.488365453029	-0.325755923348	-0.795276835155
N	-1.108926854758	-0.995313574408	0.216191509644
N	-3.102579090559	-1.780142949874	0.790125528016
C	-3.173588247901	1.080348630850	-2.060612869380
H	-3.170394227113	1.852818058255	-2.828795251389
N	-4.395796568015	0.618368656429	-1.724884176302
C	-3.340367717956	-0.823560237511	-0.184665839685
C	-2.070202679243	-0.337656974331	-0.539802118333
C	-1.969681018215	0.653979575060	-1.514216581339
C	-1.767381044270	-1.843665476086	0.987902802088
H	-1.277833531548	-2.506496605897	1.692534508776
C	3.287992019474	-1.928928601046	1.085816930140
H	4.224089288692	-1.831356353472	1.649755788080
H	3.491274607954	-2.576274135604	0.222942965822
C	2.188434642417	-2.589302237999	1.938557254279
C	3.352796238281	-0.141794944895	-0.689360855932
H	3.553514520942	-1.007301264991	-1.333920013749
H	4.301427597185	0.392271040328	-0.552464856368
C	2.304473552205	0.748756927950	-1.384475301712
C	2.752530055005	0.413722873481	1.634597023075
H	2.198012019272	1.255823188438	1.199149636124
H	2.143065007372	-0.000731245298	2.448992860217
H	-5.487610454636	-0.683130116208	-0.540470170866
H	-1.004239562458	1.053244822954	-1.814935689703
H	-3.791747367866	-2.337620550142	1.273974540582
C	4.090920401926	0.857711778685	2.140731562769
C	4.690984829230	0.207762009821	3.224700727708
C	4.767163816924	1.917234544868	1.526208660374
C	5.945691173069	0.602238514905	3.679137819591
C	6.022141716354	2.312316974947	1.979661839741
C	6.613369779593	1.654014854550	3.055665362718
H	4.162389264503	-0.610048719632	3.717718244037
H	4.297812666488	2.438549367666	0.689977610332
H	6.400053068902	0.090650618005	4.525452370884
H	6.536473388152	3.139956341290	1.495078066415
H	7.593033346725	1.965579358465	3.413277218789

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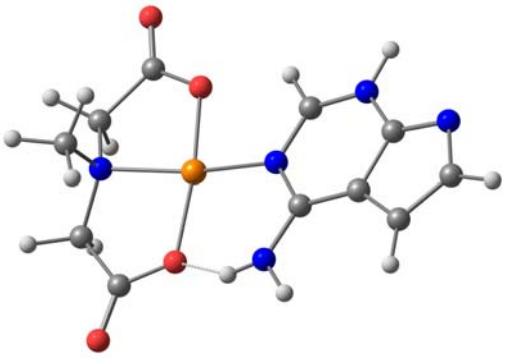
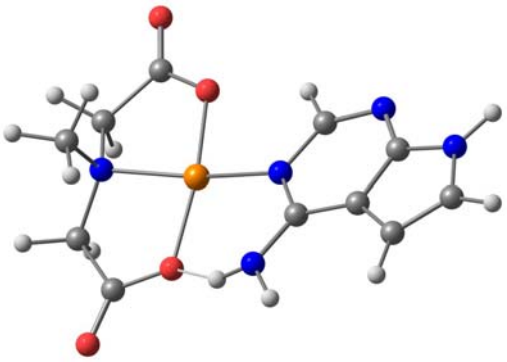


UM06l/6-31G* Free Energy: -2641.652404

IVa-1p3

Cu	0.906151200935	-0.060712406837	-0.131172515439
O	1.167730108330	-1.934260913110	-0.170714730600
O	2.747953845014	-3.533980683119	-0.210054013826
O	1.086120415126	1.817959702666	-0.328123506317
O	2.570141991304	3.508604565614	-0.287611061327
N	2.857718472980	0.003261160053	0.353653936519
C	-2.013917142478	0.850601703482	0.121759044886
N	-5.125369389705	-0.951608696746	-0.040565158123
C	-4.594785702759	1.287645077675	0.290650257677
C	-1.565136955071	-1.423161809123	-0.241216907968
H	-0.837464225615	-2.218192576715	-0.370914658862
N	-1.106693571779	-0.182487170761	-0.062581648964
C	-3.383593913340	0.568270258394	0.139119005690
C	-3.818221830415	-0.773831749108	-0.055423238569
N	-2.860351568099	-1.740420745365	-0.242831595282
C	-5.589613098522	0.326859877479	0.175150578346
H	-6.661381304099	0.492158390452	0.239068497906
C	3.456929598560	-1.250094136746	-0.130350378123
H	4.324387115952	-1.550359394414	0.472835554262
H	3.810811070910	-1.091056929625	-1.156235305350
C	2.403518567703	-2.369286641745	-0.160317889651
C	3.398846713893	1.260035896087	-0.183313262982
H	3.758208182595	1.074368489138	-1.202901822722
H	4.250637043847	1.626912670450	0.404740150230
C	2.295975688183	2.326130330773	-0.257189574276
C	2.789990793140	0.031699755270	1.820943527328
H	2.234583203564	0.918316106636	2.145050183308
H	3.797275819477	0.062374858208	2.262072994005
H	2.271520915650	-0.864066736939	2.178058317509
H	-4.728985837672	2.349346943140	0.465552185289
N	-1.527829398005	2.086539888670	0.317971458733
H	-0.553105261348	2.303846985159	0.089113556388
H	-2.191412498396	2.845163832689	0.331094282805
H	-3.147967049531	-2.703089900624	-0.381842263044



UM06l/6-31G* Free Energy: -2641.673688

IVa-1p9

Cu	0.913519252883	-0.105508433844	-0.260210197734
O	1.224621429162	-1.971884540896	-0.206125170679
O	2.847088980826	-3.531093014108	-0.230951143306
O	1.055798948724	1.778206726998	-0.538303652315
O	2.503558586942	3.500687523635	-0.573727501822
N	2.881790857654	0.027354178677	0.157930803722
C	-1.940408425843	0.784287842550	0.143821546050
N	-5.044896833406	-0.903711143004	0.008555378165
C	-4.516769290676	1.228004807685	0.469058213959
C	-1.597232681430	-1.474145245964	-0.392927976303
H	-0.852412501848	-2.237004349152	-0.602043418878
N	-1.080439973870	-0.233652538879	-0.144852290410
C	-3.320285526577	0.497613790037	0.204084776910
C	-3.686903234006	-0.827157869416	-0.078414789855
N	-2.861492929722	-1.839385052828	-0.383798416200
C	-5.549995705511	0.337607649761	0.341662461434
H	-6.615282318900	0.480105208793	0.462451730272
C	3.495750326434	-1.231378788174	-0.289178647787
H	4.392959201432	-1.481187075454	0.293540839231
H	3.806097068192	-1.112026410471	-1.334466373888
C	2.468382995640	-2.374833102432	-0.224165328778
C	3.379920328932	1.270611060606	-0.444166833122
H	3.702999650084	1.052445994462	-1.469601886723
H	4.246993019562	1.674019546221	0.096328242251
C	2.254636518650	2.312570235857	-0.511942104747
C	2.853009117546	0.115136845325	1.623438258839
H	2.284073767516	1.000953940645	1.926456364085
H	3.870750735979	0.188432408992	2.035458755069
H	2.366061368718	-0.777103974465	2.030099528711
H	-4.621922299293	2.273843600583	0.730610788979
N	-1.459603258179	2.014115602144	0.405169038981
H	-0.513122037706	2.250739461771	0.087360215485
H	-2.128896120457	2.766721837739	0.450620107312
H	-5.576540017352	-1.747487722639	-0.146467317648

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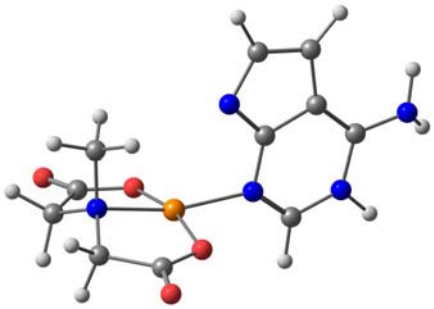

UM06l/6-31G* Free Energy: -2641.631779

IVa-3p1

Cu	0.822043565632	0.300483319734	-0.797850573903
O	0.579921386078	-1.164119124769	-1.967394801832
O	1.667921691085	-2.945786044732	-2.810536596206
O	1.459009431046	1.840875367363	0.089880760220
O	3.316496332086	2.686009733478	1.041081987355
N	2.524965952055	-0.576866542506	-0.245049683863
C	-3.863768999396	1.303533968136	-0.648357047663
N	-1.182013282305	-0.405677664592	0.964325492599
C	-3.450840553921	-0.238221032924	1.419030043947
C	-1.765297490487	1.675065091178	-1.796015278239
H	-1.295041275577	2.167277206140	-2.639566140859
N	-3.119484781398	1.863265203662	-1.658546664466
H	-3.572595055033	2.491587877802	-2.309713972213
C	-3.172037131429	0.531928022764	0.265451642535
C	-1.755780551245	0.372914679365	0.060349805075
N	-1.077247153671	0.946485337893	-0.972002648287
C	-2.221139255528	-0.765682545395	1.786127635835
H	-2.025910732174	-1.413313408726	2.635773750361
C	2.870239235909	-1.498894277147	-1.339866130607
H	3.432864583651	-2.369416772510	-0.975847506594
H	3.516510272800	-0.966236021478	-2.048276874599
C	1.610389059225	-1.951074473049	-2.107553462592
C	3.461944019717	0.522010792104	0.043017485005
H	4.019294650395	0.749418981946	-0.874081775367
H	4.196237508578	0.239617972919	0.809688110773
C	2.708866041253	1.802613507095	0.460602571645
C	2.152370635793	-1.303437064247	0.975288878278
H	1.773012208484	-0.595847311732	1.718755804934
H	3.020588269647	-1.841143507205	1.386553270637
H	1.353840861517	-2.015329574904	0.745446775079
H	-4.400202596528	-0.382622587949	1.922490736687
N	-5.193718323345	1.607799153016	-0.603964866600
H	-5.733665632715	1.053288564453	0.045336074862
H	-5.677169888394	1.773812175580	-1.476396802654

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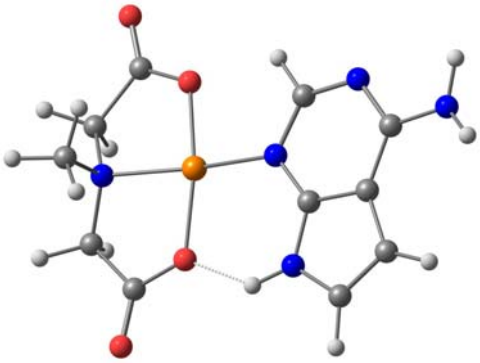

UM06l/6-31G* Free Energy: -2641.678203

IVa-3p9

Cu	0.833912408452	-0.154441044683	-0.127879635145
O	1.274721922523	-1.986919578065	-0.275091193012
O	3.014977247809	-3.392340136106	-0.525358525387
O	0.787532116569	1.759307112023	-0.111028312689
O	2.088677831105	3.593624142911	-0.172316854498
N	2.795814979596	0.103559550245	0.203262439033
C	-3.828114952646	-1.068926780852	0.154867069883
N	-1.873643951182	1.873715537151	0.057226910354
C	-4.097093895459	1.558787352546	0.181561495847
C	-1.621632579327	-1.684828388719	0.010487621806
H	-0.881839069173	-2.479990306573	-0.048457044865
N	-2.896263924384	-2.039088851987	0.089684029392
C	-3.452433484043	0.287114397378	0.138744407633
C	-2.067451447331	0.531885580060	0.059469582072
N	-1.117469057544	-0.433915617102	-0.001250539252
C	-3.100207519803	2.497324860352	0.128744848437
H	-3.155452748475	3.577582358672	0.133174291896
C	3.470177647465	-1.046773389284	-0.417467267669
H	4.427866561476	-1.274653935072	0.070111138370
H	3.684774155752	-0.797165843986	-1.463985430292
C	2.543773605008	-2.277870457778	-0.397504174303
C	3.145501231533	1.443795230824	-0.285380021286
H	3.413743865347	1.366373990311	-1.346330825473
H	4.012825662125	1.863713074113	0.242180075899
C	1.938293733993	2.387099007541	-0.168691781122
C	2.861755931180	0.033534478435	1.668512356237
H	2.246740209946	0.830364092047	2.099875937028
H	3.896937415380	0.149044040669	2.023071844605
H	2.475961115029	-0.935002395890	2.002682525919
H	-5.158644342525	1.766220942097	0.233693526582
N	-5.119736570563	-1.474824049732	0.200954183646
H	-5.282320109390	-2.458284032447	0.360655397620
H	-5.843618890280	-0.831916951956	0.478714255908
H	-0.938827098053	2.292724012361	-0.001645332818

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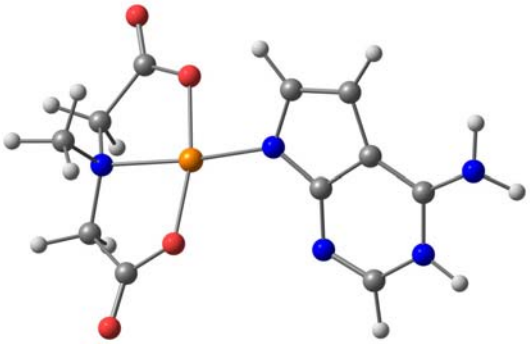

UM06l/6-31G* Free Energy: -2641.638751

IVa-9p1

Cu	0.485830092122	-1.992274974924	-2.809192427859
O	-0.144799925889	-1.188688438853	-4.425012539284
O	0.169675526881	-1.223900044954	-6.656230315949
O	1.164536687164	-3.113927340411	-1.426823230654
O	2.663243021862	-4.759094097939	-1.070133595890
N	1.162309345575	-3.427980280760	-4.026634312880
C	-0.950668711353	1.292885358387	1.215515035981
N	-0.406899962557	-0.678798817411	-1.686317143757
C	-2.123035214317	0.693905012414	-1.028863164370
C	1.187812127905	0.179260815301	1.315003596570
H	2.078976758109	0.055196995906	1.924383384332
N	0.219995743813	1.006015133739	1.859896093973
C	-1.132748070700	0.686535421184	-0.016293041831
C	-0.083940044209	-0.179413677938	-0.487245535282
N	1.077070896504	-0.409446873355	0.170419460671
C	-1.630307220209	-0.140193672413	-2.009889210243
H	-2.066784316378	-0.385471269994	-2.971560601782
C	1.411787832377	-2.769542405813	-5.314925740140
H	1.385670375810	-3.478278558444	-6.154821292041
H	2.416946650109	-2.329520123995	-5.286816546548
C	0.387382133765	-1.634795725642	-5.528771998552
C	2.297222730113	-4.037040307013	-3.321162180136
H	3.194971187414	-3.443985273389	-3.537648858635
H	2.491213279040	-5.065084846648	-3.658695175365
C	2.040406957202	-4.002992980652	-1.798017288701
C	0.028969852547	-4.354523862382	-4.110929767162
H	-0.211910828604	-4.721909369659	-3.108345196912
H	0.267017061274	-5.209728526178	-4.761908360265
H	-0.840643810342	-3.827501378424	-4.516921209837
H	-3.067449152853	1.225120198693	-1.049086012007
N	-1.857604828599	2.089931805527	1.850968916463
H	-2.620077143595	2.416645155750	1.274704050064
H	-1.516163631171	2.790932353208	2.494056080725
H	0.374229600882	1.374245598000	2.790276126590

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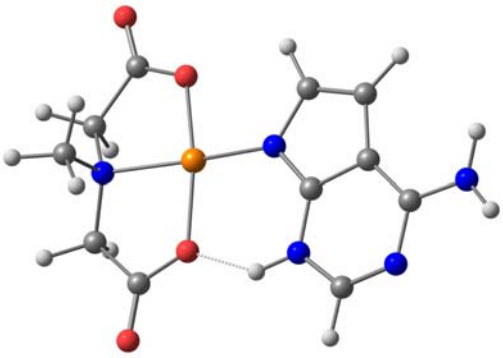

UM06l/6-31G* Free Energy: -2641.672949

IVa-9p3

Cu	0.945721020859	-0.203114055071	-0.066880565470
O	1.721962662739	-1.930117984933	-0.124129550574
O	3.702023054063	-2.973093052465	-0.375748110292
O	0.517941503692	1.676892352692	-0.110586694473
O	1.442284439066	3.718805766892	-0.317248862421
N	2.814437474499	0.446256541591	0.213004207903
C	-4.411717527899	-0.197459451059	0.022503291210
N	-0.893356185107	-0.793869651769	0.014418500958
C	-2.697246809702	-2.208905979483	0.063435645016
C	-3.353402427627	1.836786733291	-0.056374594419
H	-3.395630995295	2.922246222793	-0.093777277885
N	-4.477528102734	1.158983389218	-0.019762068068
C	-3.179014542374	-0.870750671167	0.029020126704
C	-2.017651171561	-0.065370110442	-0.004146274223
N	-2.122734101345	1.293901095609	-0.047901022338
C	-1.324812324561	-2.109355884219	0.048938614970
H	-0.575583582808	-2.892410493456	0.057959936330
C	3.687325208919	-0.582953946172	-0.374368517424
H	4.679751547574	-0.597829461845	0.096572547894
H	3.830442235948	-0.347447246709	-1.436312419696
C	3.018472589332	-1.970315499047	-0.275483368056
C	2.888364543962	1.804445525346	-0.342823385537
H	3.149266759535	1.729307194259	-1.405854983722
H	3.666863563189	2.409125306347	0.142491415782
C	1.525042204217	2.508025528028	-0.240072461977
C	2.917968725471	0.460446973267	1.677486838933
H	2.166007560497	1.141663494533	2.089529231091
H	3.916507551035	0.791835355098	1.999965736061
H	2.734046493044	-0.547601196449	2.062664116058
H	-3.273351076501	-3.126148358400	0.086079837487
N	-5.600989948191	-0.839707893323	0.029839067488
H	-5.648722095796	-1.823696125206	0.238512140525
H	-6.434064760046	-0.285016068135	0.156909933384
H	-1.244240485856	1.843502650518	-0.080126031183

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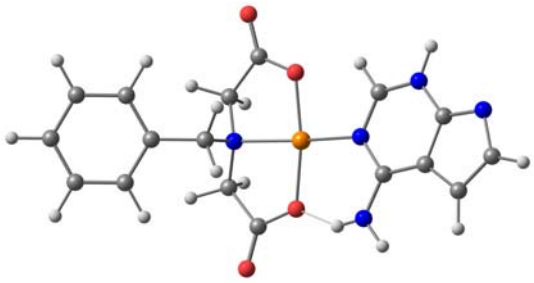
UM06l/6-31G* Free Energy: -2872.601125



IVb-1p3

Cu	0.822431281481	-0.764314489912	0.180426854785
O	0.529230653250	-2.161089142594	1.431384296613
O	1.584378740312	-3.688436759341	2.702421760247
O	1.524754535554	0.440834402504	-1.115085300962
O	3.444045011129	1.304656916557	-1.913432407627
N	2.755929530087	-1.020990141046	0.670054535069
C	-1.685795375838	0.842772412929	-0.585115011683
N	-5.184212378342	0.298619071012	0.067191875145
C	-4.013311783962	1.948845173149	-1.077574231668
C	-1.934663914362	-1.114998433168	0.683403441623
H	-1.476537906990	-1.951131572206	1.202487880682
N	-1.128825189934	-0.249878057404	0.063959907866
C	-3.073660329176	1.019062798052	-0.567389040773
C	-3.886337646038	0.064164191877	0.106721469403
N	-3.261849815206	-0.992951761228	0.722965015225
C	-5.246299488407	1.463116603655	-0.664972128139
H	-6.217566286792	1.907730938263	-0.862710467952
C	2.883651243699	-2.402650720593	1.149276351885
H	3.755347298250	-2.544157442412	1.800286386025
H	3.019694797328	-3.051821540902	0.274882658820
C	1.584330169793	-2.813662733408	1.857028864559
C	3.551875164805	-0.638048455653	-0.501095724539
H	3.615164460926	-1.508150082076	-1.166834074121
H	4.577221237226	-0.349810731982	-0.238085591658
C	2.832228338094	0.490481878886	-1.250608228393
C	2.852589506400	-0.019249679757	1.779189727693
H	2.563192180562	0.946699252964	1.342921855296
H	2.079632554448	-0.299453601026	2.507227894540
H	-3.825319815279	2.845898303117	-1.657092696805
N	-0.855836303563	1.713297154802	-1.178285405067
H	0.129221769850	1.478634574030	-1.335878388253
H	-1.269875892162	2.444721761674	-1.734184175265
H	-3.821419112925	-1.681673812643	1.214082743760
C	4.197150077427	0.072018336919	2.433309231988
C	4.508578944100	-0.740647138363	3.528868980276
C	5.165372953871	0.958259237760	1.948953554830
C	5.766196647416	-0.677194098181	4.120935113265
C	6.423299909552	1.022816777595	2.540664918030
C	6.725569458143	0.203204404009	3.625758808669
H	3.752425340883	-1.422019225072	3.922783813131
H	4.923494576664	1.607656707867	1.105655535698
H	5.994809831959	-1.312170422244	4.974585431730
H	7.166472505032	1.718983602106	2.156953312677
H	7.707977676589	0.256103157547	4.091128219776

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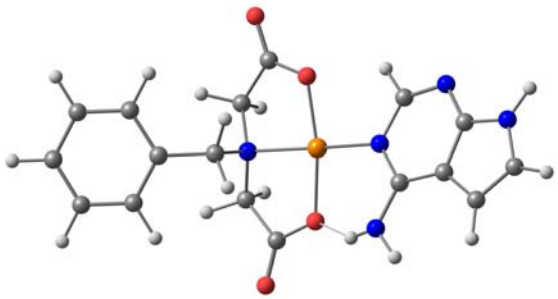

UM06l/6-31G* Free Energy: -2872.623114

IVb-1p9

Cu	0.342325301563	-0.695576454022	1.352975865297
O	-0.047599331602	0.645288138671	2.640137948530
O	0.643283611133	1.503913120493	4.603346205082
O	1.034898282112	-2.183474906842	0.361966597766
O	2.794845305835	-3.582041170383	0.228213996553
N	2.042260785502	-0.907339844853	2.409551148814
C	-1.284796039012	-0.555016312099	-1.181756887533
N	-4.412636385084	0.897306557310	-1.965426973068
C	-2.927878207766	-0.228727118570	-3.215485756846
C	-2.186956448671	0.473841093741	0.724484264581
H	-2.018441013546	0.715858701412	1.770139468823
N	-1.174110758014	-0.228785355383	0.136993039710
C	-2.430320643945	-0.122895286313	-1.882711981621
C	-3.380750309644	0.585580231825	-1.131337627744
N	-3.301134581431	0.901423037390	0.169970517969
C	-4.140765206957	0.407987102658	-3.227837153554
H	-4.843302070525	0.559510809089	-4.036081247220
C	1.735761950326	-0.460738376687	3.773212898016
H	2.632394251495	-0.163747905919	4.331761693206
H	1.279851449918	-1.303277854073	4.309007181066
C	0.711809382153	0.684164434134	3.705486379745
C	2.486546542743	-2.293789666178	2.236855633773
H	1.936839696410	-2.915758825604	2.955096447625
H	3.557408727652	-2.424149696052	2.438247786822
C	2.126288271173	-2.755027210271	0.818822600557
C	2.907950524483	0.065503687328	1.672374314515
H	2.919842475360	-0.268478816432	0.625633196367
H	2.379273655784	1.027116215888	1.707570012856
H	-2.461861370694	-0.701956133669	-4.071169764929
N	-0.293234968157	-1.233744491701	-1.788112501603
H	0.367886721925	-1.762824827793	-1.208145536050
H	-0.482225535429	-1.593512656968	-2.710787925030
H	-5.233712444103	1.412277405417	-1.683871049655
C	4.302071255803	0.199343024347	2.204816657212
C	5.326671351842	-0.628633999003	1.733646253492
C	4.593617793360	1.142588517576	3.196097042435
C	6.614718037725	-0.522922302217	2.250387016317
C	5.881445265853	1.249248864852	3.713225898704
C	6.892585306826	0.415016416650	3.241995153299
H	5.109363123687	-1.356587954765	0.949986750592
H	3.801965965638	1.800429694848	3.558493205820
H	7.403662914719	-1.170801454020	1.873305297577
H	6.095741424333	1.989042818266	4.481900969779
H	7.900660090760	0.500539356751	3.643821947267

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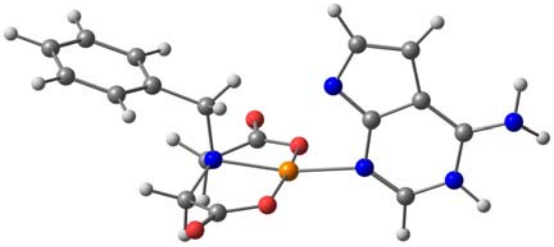

UM06l/6-31G* Free Energy: -2872.579894

IVb-3p1

Cu	0.471215452637	-0.950007139591	0.265454476460
O	0.377786114735	-1.494742964566	-1.547182795309
O	-1.114019780654	-2.060368977100	-3.137556196267
O	0.292906858195	-0.680383208340	2.130577084425
O	-1.276515506588	-0.522034695912	3.739086897022
N	-1.521054576170	-0.911205554486	0.209306360722
C	4.980483921690	0.625607728041	-0.191642915727
N	1.535457182493	1.538683379553	-0.289424648065
C	3.495961276200	2.726162671615	-0.646826084927
C	3.554123246225	-1.259745557050	0.328479927519
H	3.541603942121	-2.313470885229	0.583333892363
N	4.792314399316	-0.694135154489	0.141966936318
H	5.602713728919	-1.275507499778	0.313781722253
C	3.838979937609	1.393186713248	-0.319232449767
C	2.573406133462	0.736351402636	-0.114124439276
N	2.453866273479	-0.582991354997	0.203725034347
C	2.109052559286	2.744571953208	-0.607015052406
H	1.470276257343	3.601534864989	-0.799578493371
C	-1.898649653188	-1.810989562885	-0.888579720087
H	-2.890116990578	-1.580310435578	-1.298204793366
H	-1.943341376569	-2.830926019908	-0.485232611924
C	-0.817521846843	-1.782551070782	-1.987090000966
C	-1.953924925416	-1.269164092820	1.566722749928
H	-1.983221307418	-2.364677716528	1.629997164957
H	-2.962435078263	-0.903024493746	1.796287406582
C	-0.924360118056	-0.762253467457	2.595981546162
C	-1.760666546424	0.529209065538	-0.114690715890
H	-1.249802962756	1.107782725050	0.665696091410
H	-1.224536790701	0.724191483192	-1.052332867299
H	4.154197465315	3.559100588233	-0.867332998615
N	6.267287583667	1.068179575689	-0.304285621886
H	6.363030143607	1.989986764352	-0.706801939359
H	6.968888604898	0.420100760334	-0.636583286391
C	-3.205637691660	0.912532778242	-0.220888567613
C	-3.877102237361	0.827729490512	-1.445636577482
C	-3.909942635710	1.349271607668	0.906639958324
C	-5.225681354480	1.159117271033	-1.538909916990
C	-5.258460149267	1.681106373385	0.815160355455
C	-5.918857946194	1.583805554926	-0.407632093533
H	-3.329270462192	0.505448757132	-2.332903007147
H	-3.388145567790	1.434133119176	1.861530372634
H	-5.734771910091	1.090566186307	-2.498642619261
H	-5.793228583780	2.021409206426	1.700090109352
H	-6.972966083011	1.845980830744	-0.480446673467

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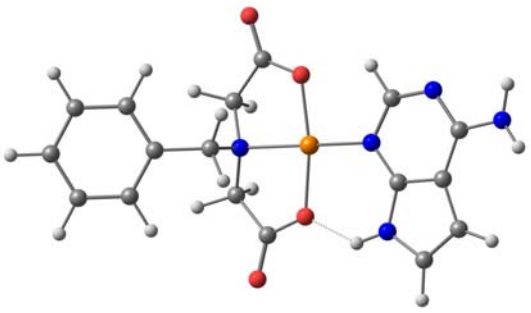

UM06l/6-31G* Free Energy: -2872.626739

IVb-3p9

Cu	0.687177378130	0.523239336303	0.144584006831
O	1.453627661770	-0.684834250113	-1.100680580124
O	3.406306952404	-1.236417616146	-2.077399807919
O	0.288061822336	1.914505196016	1.405394931325
O	1.224616595929	3.576287178277	2.599277684430
N	2.587211474491	1.049176520604	0.507347186333
C	-3.628884534585	-1.444440708916	-0.259321816056
N	-2.272876195067	1.210872006832	1.637837276341
C	-4.355158763077	0.368982973667	1.519015735252
C	-1.398968607610	-1.268387266893	-0.774150504432
H	-0.545700439448	-1.632871671494	-1.341634243990
N	-2.560911438540	-1.880131527660	-0.954349150826
C	-3.509365087600	-0.365253789740	0.635793254729
C	-2.221288163655	0.195543174289	0.741015224684
N	-1.136181448077	-0.234704477205	0.051006637030
C	-3.563295024520	1.319333994072	2.108262836937
H	-3.808907319978	2.081847450264	2.835111335449
C	3.331035079224	0.738432087607	-0.719736293644
H	4.406917064886	0.616555285445	-0.541846420806
H	3.205891536375	1.581558424819	-1.411358009890
C	2.723748657770	-0.518224341219	-1.368776451800
C	2.563805982755	2.445633132582	0.954457654560
H	2.546054780207	3.085769139324	0.063000911224
H	3.453253739385	2.719290639770	1.536016266046
C	1.279613875942	2.701506157821	1.755673603632
C	2.899160525836	0.098567764165	1.619980812333
H	2.154654372814	0.293676932255	2.403772426642
H	2.706068138214	-0.906321752248	1.221697173010
H	-5.414222106318	0.229539518867	1.696848902361
N	-4.803845893048	-2.075802425666	-0.498943324964
H	-4.757672142635	-2.931628554549	-1.032579756998
H	-5.573619684461	-1.969978860448	0.142026868026
H	-1.450415589601	1.779231276655	1.870556419116
C	4.289730523060	0.202214287704	2.167782692277
C	4.571447122424	1.070344750345	3.228158879892
C	5.329728892891	-0.553824260882	1.615905444198
C	5.867513987735	1.188652691788	3.720627725438
C	6.626346929041	-0.436182725148	2.107511777756
C	6.896925047153	0.436555331593	3.159057565648
H	3.761971431653	1.651919318420	3.673184830173
H	5.114364863359	-1.244273398305	0.798621763019
H	6.072457837196	1.865080088601	4.548185019217
H	7.425925663141	-1.032144495607	1.671680483351
H	7.910276662915	0.525586947942	3.546196133617

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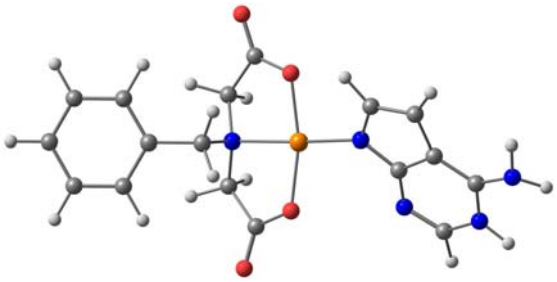
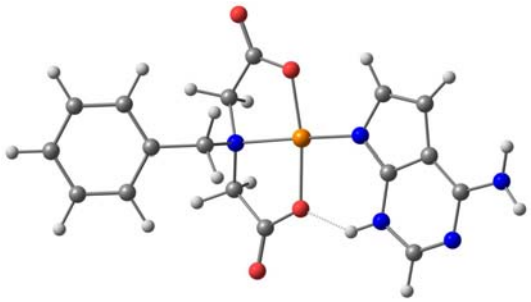


UM06l/6-31G* Free Energy: -2872.587362

IVb-9p1

Cu	0.284461196453	-1.633691365761	-3.339370392299
O	-1.103668018854	-1.263634593033	-4.610300594049
O	-1.723541495057	-1.728077346905	-6.727471310879
O	1.668387665259	-2.396807519564	-2.266726821181
O	3.462719542249	-3.754103136735	-2.404754456339
N	0.833455681859	-3.025922411596	-4.662489770291
C	-0.361600502848	1.748163421672	0.806116575403
N	-0.433828275278	-0.389833613402	-2.027132227439
C	-2.078294163146	0.647072743549	-0.809966563004
C	1.872270366283	1.146191425580	0.120268273700
H	2.924291941307	1.292207912318	0.350157999908
N	0.994590577193	1.800851633360	0.967606888808
C	-0.820345569103	0.976389797045	-0.248416794540
C	0.166383286451	0.308190193221	-1.055444576029
N	1.504721343493	0.416166874098	-0.880287507125
C	-1.784059090118	-0.172889083249	-1.878717393019
H	-2.462090525492	-0.623865485561	-2.594753764284
C	0.419113066269	-2.497788103462	-5.966495009775
H	0.367243624027	-3.272585043360	-6.742535817613
H	1.170741456392	-1.762779992729	-6.283961275086
C	-0.936005821794	-1.781732534096	-5.796419456574
C	2.263020746846	-3.244421209095	-4.417553736611
H	2.816365989205	-2.439404123100	-4.919046719820
H	2.623295904216	-4.196656403758	-4.828491061758
C	2.519758217868	-3.154773870675	-2.898106941365
C	0.000015931166	-4.186987763929	-4.229202174468
H	0.257687300673	-4.370269302335	-3.178187887116
H	-1.042085415857	-3.842756269070	-4.260765315244
H	-3.065979845615	0.953954926737	-0.486225835842
N	-1.144319361168	2.397028522100	1.715966840215
H	-2.119366951246	2.476320514344	1.464710992979
H	-0.778975884349	3.227473845074	2.161353040698
H	1.378031132808	2.299433291587	1.760950239585
C	0.180147790561	-5.426485759142	-5.051725054697
C	1.153611870551	-6.370818911523	-4.708160011860
C	-0.606617498272	-5.646199491375	-6.187749652642
C	1.342265857775	-7.507788351040	-5.488277190187
C	-0.418758402730	-6.782972612211	-6.968431322749
C	0.556719866541	-7.714674373096	-6.620085378245
H	1.763795110796	-6.208327950086	-3.817845648167
H	-1.372567605956	-4.916053788487	-6.455499993194
H	2.101566517514	-8.235971739323	-5.208824051581
H	-1.038900801000	-6.943397767957	-7.848544670999
H	0.701552355154	-8.605614605817	-7.228742896835



UM06l/6-31G* Free Energy: -2872.621307

IVb-9p3

Cu	-0.278589000000	0.501137000000	0.503570000000
O	0.270548000000	2.315606000000	0.365761000000
O	2.082864000000	3.631039000000	0.613725000000
O	-0.467154000000	-1.406872000000	0.756730000000
O	0.686888000000	-3.256240000000	1.320889000000
N	1.665071000000	0.116085000000	0.743277000000
C	-5.425730000000	-0.356326000000	-0.711253000000
N	-2.113329000000	0.787234000000	-0.038549000000
C	-4.022309000000	1.883456000000	-0.680345000000
C	-4.160785000000	-2.175145000000	-0.114074000000
H	-4.069660000000	-3.242678000000	0.068896000000
N	-5.323690000000	-1.692524000000	-0.487548000000
C	-4.323126000000	0.498864000000	-0.551710000000
C	-3.107570000000	-0.103265000000	-0.153711000000
N	-3.042882000000	-1.448372000000	0.062967000000
C	-2.689329000000	2.004549000000	-0.360331000000
H	-2.063522000000	2.888971000000	-0.332379000000
C	2.233611000000	1.343610000000	1.316614000000
H	3.319206000000	1.413596000000	1.173468000000
H	2.043589000000	1.326707000000	2.397727000000
C	1.507047000000	2.561072000000	0.710969000000
C	1.765038000000	-1.117138000000	1.531092000000
H	1.679371000000	-0.848864000000	2.592020000000
H	2.728432000000	-1.626364000000	1.400557000000
C	0.597584000000	-2.051256000000	1.177653000000
C	2.068453000000	-0.085875000000	-0.683346000000
H	1.455978000000	-0.917184000000	-1.057956000000
H	1.756506000000	0.821794000000	-1.216677000000
H	-4.689906000000	2.689012000000	-0.961679000000
N	-6.653640000000	0.084478000000	-1.065970000000
H	-6.775356000000	1.017096000000	-1.425986000000
H	-7.352582000000	-0.606935000000	-1.292679000000
H	-2.131039000000	-1.845170000000	0.358084000000
C	3.526904000000	-0.356191000000	-0.894200000000
C	4.423016000000	0.703366000000	-1.074593000000
C	4.016928000000	-1.666488000000	-0.895953000000
C	5.782139000000	0.457762000000	-1.243570000000
C	5.376141000000	-1.913250000000	-1.065338000000
C	6.260398000000	-0.850789000000	-1.237640000000
H	4.045190000000	1.727244000000	-1.085236000000
H	3.321022000000	-2.498239000000	-0.771599000000
H	6.468369000000	1.290432000000	-1.385449000000
H	5.744109000000	-2.937514000000	-1.068410000000
H	7.323038000000	-1.043166000000	-1.373871000000

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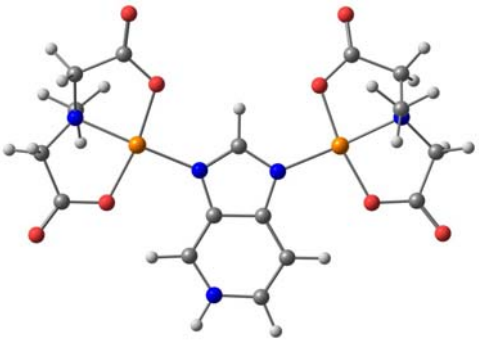

UM06l/6-31G* Free Energy: -4776.859005

Va-p1

Cu	-2.937067752350	-0.204864786636	-0.096911112157
O	-3.825715798174	1.474894583987	0.055945079044
O	-5.868396361746	2.413033440311	0.066988600463
O	-2.371623969836	-1.970353568609	-0.434576922561
O	-3.175733178680	-4.020701959914	-0.906811369984
N	-4.741790769438	-0.994638736832	0.214383545054
C	-1.424681835290	3.020985077105	0.024908732108
N	1.145780787454	0.568474771637	-0.005108558302
N	-1.125160194045	0.533382307928	0.013973238098
C	0.662282324266	4.221061815302	0.000334112313
H	1.089999739022	5.216886872289	-0.005812247834
N	-0.703887250961	4.164530645143	0.018945476437
C	-0.707944977056	1.842879040421	0.010660766495
C	0.715752246803	1.859159257640	-0.000663130986
C	1.416060046454	3.074027266438	-0.009981203626
C	0.011755903286	-0.169801484447	0.004056511697
H	0.028928180306	-1.255491167670	0.005020383445
C	-5.723025577552	0.032664272270	-0.166502866982
H	-6.662036016657	-0.066486778443	0.394737779287
H	-5.964060405808	-0.096127530740	-1.228871734670
C	-5.133960065246	1.443082544893	0.015509343299
C	-4.750475150241	-2.264651436386	-0.530936800412
H	-5.103837787052	-2.063290342960	-1.549693633946
H	-5.435998009009	-2.997305991060	-0.084206218119
C	-3.324330465626	-2.846619969111	-0.627869492714
C	-4.736728936954	-1.224436053104	1.664504221609
H	-3.911604911102	-1.896126668430	1.922643663517
H	-5.683565775932	-1.676713477316	1.995375189391
H	-4.597373947431	-0.270672412426	2.184400198537
H	-2.512777870251	3.065864983178	0.044222943434
H	2.504062424823	3.093244641726	-0.029826279304
Cu	2.958036545532	-0.178058925394	0.103697388873
O	3.877603467328	1.477587552012	-0.069640821039
O	5.941363842653	2.371434649937	-0.093054506263
O	2.358719673909	-1.934096280955	0.450060883224
O	3.120676810725	-3.997140965493	0.936881272003
N	4.744120570877	-1.010918577209	-0.209342682827
C	5.746805972249	-0.001130282352	0.161701353374
H	6.682381537878	-0.123987199350	-0.400698506360
H	5.986849954077	-0.126785967757	1.224676590118
C	5.184405864397	1.419639205348	-0.031383213123
C	4.730147445778	-2.276362903530	0.542383740822
H	5.092356000685	-2.077005884071	1.558446836501
H	5.398516031980	-3.025571860150	0.096847800729
C	3.293280605153	-2.828448060152	0.648357937421
C	4.727379239808	-1.246982192954	-1.658077371587
H	3.887193018653	-1.902472410989	-1.909422852005
H	5.663107029857	-1.720273057284	-1.991403425642
H	4.605464663467	-0.292533848897	-2.181025460489
H	-1.216169920985	5.038317853054	0.029116823639

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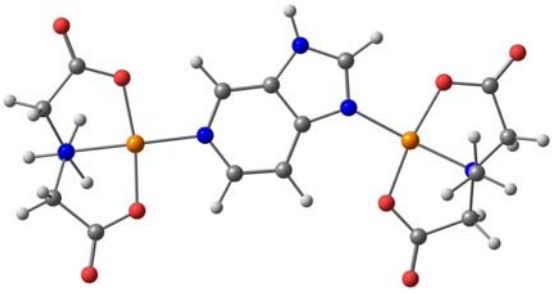

UM06l/6-31G* Free Energy: -4776.857016

Va-p7

Cu	-0.850065006818	-3.451316772820	-6.363966062160
O	-0.665387350031	-4.982824562023	-5.277177736418
O	0.188826945172	-7.066008939708	-5.284852230395
O	-0.951551044919	-2.127007372985	-7.716506216087
O	-0.351925445066	-1.716039751428	-9.846398881407
N	0.541404975916	-4.289975732113	-7.519357958332
C	-2.370109077791	-1.204993690437	-5.413526461546
N	-4.163695256245	-0.064539752613	-2.528399823247
N	-3.730456227086	0.756695293555	-4.545033784057
H	-3.732837118514	1.403664200806	-5.321605516093
C	-2.171473750354	-2.913282241922	-3.816297718300
H	-1.752683549098	-3.900367684859	-3.636392701544
N	-1.906408197685	-2.409955878499	-5.050635444144
C	-3.118126953969	-0.483562097364	-4.500058568822
C	-3.397876080747	-0.989390943070	-3.217254692683
C	-2.910765597100	-2.245158444091	-2.855625113943
C	-4.332238208834	0.956998202237	-3.352843762648
H	-4.891232076266	1.846797990128	-3.084469869879
C	0.460551109892	-5.735170752545	-7.254285349810
H	1.417623910617	-6.241620485074	-7.438471317760
H	-0.278226465833	-6.170113025884	-7.938866470262
C	-0.017358802516	-5.988678607857	-5.809768633486
C	0.271307340709	-3.819584047656	-8.886849182505
H	-0.439103833520	-4.511948909953	-9.355473067995
H	1.178154415200	-3.811406598685	-9.506654552299
C	-0.375147730129	-2.421034317998	-8.855047563695
C	1.784069971508	-3.716208141624	-6.989180709468
H	1.750296660411	-2.625687709326	-7.082863426709
H	2.658969685862	-4.095419315514	-7.537971186214
H	1.884750285572	-3.981529672624	-5.931656114687
H	-2.118329142719	-0.872793269403	-6.419382746140
H	-3.103391410065	-2.661931856208	-1.869958793360
Cu	-4.884904261089	-0.039496555699	-0.695252491205
O	-4.178366210803	-1.699281083817	-0.137076131476
O	-4.012198082383	-3.023922570916	1.674599608340
O	-5.627587743318	1.687196840755	-0.941289287701
O	-6.722847816532	3.311179269231	0.167183306648
N	-5.954683861184	-0.094436632685	0.979861506625
C	-5.200161692986	-0.958429680260	1.902171924094
H	-5.853817449534	-1.440136044577	2.641532194422
H	-4.485407172092	-0.334395033812	2.452772420457
C	-4.403150189457	-2.018340995892	1.114256839952
C	-6.169097894269	1.310825889196	1.361572270143
H	-5.323252522729	1.632335661843	1.981908866777
H	-7.081535297877	1.439844016594	1.959130689125
C	-6.211874949686	2.209152731827	0.109196290115
C	-7.205622572035	-0.731599760589	0.549716460501
H	-7.671172758398	-0.126408047725	-0.235129185687
H	-7.907689227048	-0.827707567140	1.391020714620
H	-6.988217274137	-1.728179549014	0.151829660471

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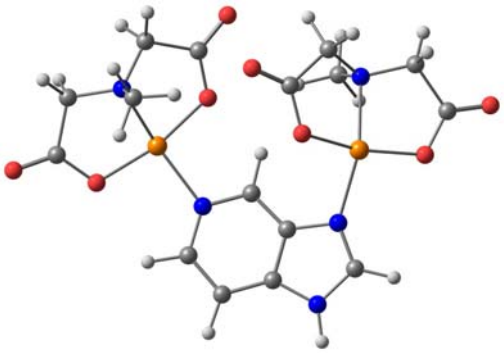

UM06l/6-31G* Free Energy: -4776.856860

Va-p9

Cu	-2.768471687365	0.209645348338	0.375946257410
O	-1.256455970908	-0.221929203256	1.436243128889
O	0.064442399303	-1.942135551738	2.013279772364
O	-4.505299256773	0.336122885597	-0.319065529156
O	-6.234765869562	-0.967099735661	-0.927636028077
N	-2.812995300048	-1.717940260678	-0.125763413305
C	0.058527139602	1.349931579294	-0.473270213125
N	-1.670059256474	4.272959428675	0.409441371014
N	-2.218027129451	2.128169878733	0.172363850967
C	1.718699384203	2.984650254351	-0.417866409592
H	2.787470366378	3.160498283098	-0.513742168749
N	1.340555700599	1.693474618848	-0.602997214617
C	-0.875512967703	2.297822420243	-0.104886987656
C	-0.499125008897	3.635000508041	0.056931342301
C	0.836004877102	4.009217589852	-0.110291557994
C	-2.657860775459	3.327746243028	0.470229028314
H	-3.679705884858	3.565865426064	0.736175896157
C	-1.956699132816	-2.440895364968	0.838696223617
H	-1.429486500242	-3.274723375032	0.359653664025
H	-2.589261636703	-2.844767113993	1.638589510903
C	-0.937598169728	-1.487839043222	1.478154161955
C	-4.249862274262	-2.047078126733	-0.142658291108
H	-4.545354151891	-2.353359375795	0.868834821707
H	-4.466052990391	-2.885661608337	-0.817948260881
C	-5.097382296790	-0.815456103570	-0.523275808891
C	-2.238877018125	-1.774391832093	-1.482580292318
H	-2.787407772008	-1.089242810349	-2.138338609819
H	-2.310836420081	-2.795210181545	-1.884452291633
H	-1.174267889195	-1.513911605910	-1.453251356498
H	-0.195779418381	0.309807187791	-0.646123787239
H	1.192178980993	5.027915024458	0.011735434253
Cu	2.536894054389	0.104977480702	-0.565801682483
O	1.203981015089	-1.161360481186	-1.044592234876
O	0.687874632428	-3.339140750268	-0.904871929210
O	4.138596983764	1.074320332079	-0.358847460537
O	6.327435388598	0.746449910746	0.049879101319
N	3.470336830686	-1.401171626455	0.330026490617
C	2.856932594758	-2.653538609475	-0.151693295240
H	2.804993887009	-3.407385754760	0.643874605722
H	3.479239837770	-3.065504292948	-0.955535014084
C	1.453169101693	-2.405108391077	-0.725494509477
C	4.894296835791	-1.171798776023	0.032509256154
H	5.125465370427	-1.633577566405	-0.936064604274
H	5.549119257888	-1.632665593466	0.784820765937
C	5.188055412304	0.339845885348	-0.079938267331
C	3.181955489788	-1.168461263471	1.757181779690
H	3.541452885838	-0.171912866594	2.034974137070
H	3.698504276613	-1.917305050506	2.376393009426
H	2.102257551417	-1.239171091811	1.937192934132
H	-1.789916476285	5.255574122089	0.613046674347

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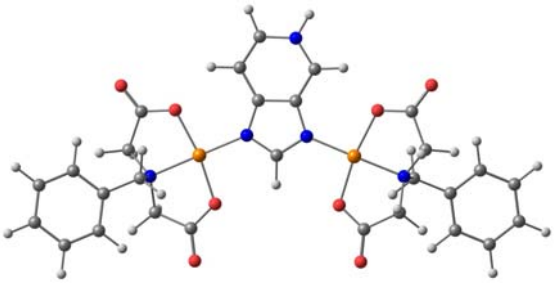

UM06l/6-31G* Free Energy: -5238.754959

Vb-p1

Cu	2.862676234144	0.269554358075	0.697276852339
O	3.730560125113	1.965368976875	0.879069689237
O	5.723586705935	2.900240896467	1.337769820342
O	2.308430870770	-1.536291361636	0.612463531471
O	3.104616801749	-3.632380728838	0.841169767292
N	4.707178353208	-0.471806471413	0.835472430507
C	1.398575706153	3.495335529919	0.315231523772
N	-1.118961344148	1.048248192541	-0.230515978405
N	1.101421690437	1.008122319041	0.246298077496
C	-0.639529221750	4.700078593408	-0.120444204555
H	-1.056237973475	5.696847155158	-0.207268763245
N	0.696310979991	4.640468468124	0.165706973373
C	0.695131707169	2.318633619259	0.164078982028
C	-0.695907266238	2.338097948388	-0.138595193566
C	-1.378450863513	3.554768849553	-0.281620503507
C	-0.011399567024	0.306895651478	0.005807225046
H	-0.031172605450	-0.779124395490	-0.001322378401
C	5.496958732299	0.519475315974	1.575167087384
H	6.573984697324	0.427962693391	1.386285767422
H	5.338373534635	0.345865342147	2.647318327356
C	4.991333032723	1.931619589251	1.236094168695
C	4.538422279308	-1.804751700275	1.430147824282
H	4.459771059794	-1.678858578775	2.517792660295
H	5.392978548240	-2.464737127534	1.236023261436
C	3.224217336650	-2.423596357142	0.913395121800
C	5.078887700675	-0.535124081259	-0.612234352986
H	4.303336845804	-1.142528874069	-1.097440266544
H	4.986144617863	0.490478436792	-0.994683047368
H	2.462875782356	3.536666506954	0.544071409692
H	-2.442384668512	3.576003706882	-0.510007875320
Cu	-2.880753357928	0.307902125951	-0.689537312641
O	-3.776325984147	1.984489344978	-0.864304914180
O	-5.790281008507	2.880431657100	-1.316138263185
O	-2.293503000923	-1.491295822388	-0.613873011632
O	-3.047615908839	-3.601883274716	-0.851704860442
N	-4.710340573306	-0.470757991913	-0.831117618703
C	-5.514281794046	0.508695506007	-1.571267626821
H	-6.590455805636	0.396261866017	-1.389129636756
H	-5.345414336933	0.342249551949	-2.643005653909
C	-5.035514594426	1.928518204308	-1.221455116889
C	-4.519553240805	-1.799858148779	-1.426263266584
H	-4.448431378735	-1.672784521281	-2.514281605567
H	-5.360971601496	-2.475673072900	-1.228706316374
C	-3.192177024458	-2.395282492887	-0.916689822426
C	-5.081865670592	-0.540041944499	0.615953310038
H	-4.300148763719	-1.139860155329	1.100818580080
H	-5.000355974559	0.486057107472	0.999508478167
H	1.199212333528	5.512958565309	0.274573597502
C	-6.441211957383	-1.107063335135	0.890273828196
C	-7.561291805443	-0.270571166226	0.946649537911
C	-6.612576733991	-2.483284702197	1.075483872500
C	-8.828479868535	-0.799418170876	1.172709578457
C	-7.879387994082	-3.013161264275	1.301516045026
C	-8.988923161334	-2.172020350502	1.348206126667
H	-7.432168338069	0.805673097095	0.818218113716

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H	-5.741298965667	-3.139837400158	1.047893747148
H	-9.691205063063	-0.137444214536	1.217425497993
H	-7.998844780246	-4.085030741829	1.446944002123
H	-9.979232591153	-2.586100693706	1.528612476160
C	6.443785864438	-1.087802438450	-0.887683930615
C	6.628416594635	-2.462624785604	-1.070993260717
C	7.555292829478	-0.240258103864	-0.946996729608
C	7.900134189324	-2.980070848485	-1.297923050666
C	8.827436320416	-0.756729028583	-1.174017619967
C	9.001165766201	-2.127959051452	-1.347491714019
H	5.763788467019	-3.127779449415	-1.040654833487
H	7.415522639547	0.834989925992	-0.820892484795
H	8.030068773811	-4.050878756693	-1.441886020113
H	9.683495150394	-0.086350985267	-1.221283906353
H	9.995256517004	-2.532421513477	-1.528737152542

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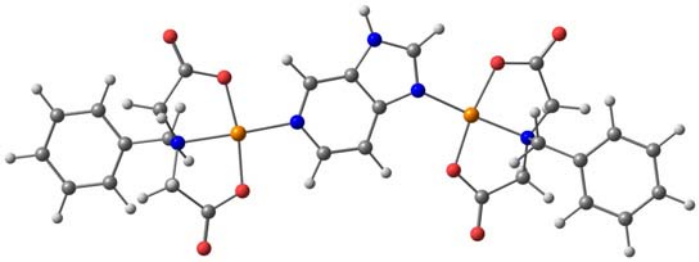
UM06l/6-31G* Free Energy: -5238.753962



Vb-p7

Cu	-3.764349502	-0.001702379	-0.791616696
O	-3.625360891	1.875552885	-0.589795768
O	-4.875276871	3.749325042	-0.609605854
O	-4.223818668	-1.824654038	-1.074012278
O	-5.982414543	-3.156057737	-1.524920099
N	-5.731422281	0.311394711	-0.796896710
C	-1.427365505	-1.646396479	-0.483827600
N	2.077803772	-1.415571531	0.224086482
N	0.660813337	-3.068181911	-0.210969415
H	0.327151455	-4.009327345	-0.367455366
C	-0.982200295	0.637468897	-0.174713488
H	-1.436316560	1.625257413	-0.167070463
N	-1.849623425	-0.374445413	-0.439978598
C	-0.089133367	-1.905490393	-0.245247822
C	0.820621717	-0.868920115	0.033919395
C	0.366682837	0.449252289	0.071573669
C	1.935229126	-2.722519459	0.072997396
H	2.759165181	-3.421391875	0.170222802
C	-5.907656917	1.689059105	-1.274563581
H	-6.872613664	2.118541970	-0.977565067
H	-5.880538711	1.670484645	-2.371729334
C	-4.733320266	2.551687389	-0.773283668
C	-6.307101084	-0.778938858	-1.594356700
H	-6.237711072	-0.494868203	-2.652354229
H	-7.367499708	-0.951337918	-1.371135658
C	-5.476936348	-2.057776282	-1.380201154
C	-6.025446777	0.170219545	0.662775765
H	-5.669793744	-0.829060951	0.948353924
H	-5.391144896	0.907785020	1.172638498
H	-2.182299181	-2.399110002	-0.705276579
H	1.044525152	1.272480534	0.284345634
Cu	3.816768428	-0.616219536	0.697024735
O	3.243881158	1.186677532	0.775074233
O	4.027706625	3.263900378	1.148278927
O	4.665456620	-2.317116664	0.718211056
O	6.675999096	-3.275261892	1.048543364
N	5.654716470	0.122001937	0.843146130
C	5.501828956	1.410274808	1.532917345
H	6.344573516	2.088304936	1.350152662
H	5.468111688	1.212570233	2.612035015
C	4.166207554	2.055518072	1.115511215
C	6.447355769	-0.928058795	1.497108434
H	6.295272626	-0.838884495	2.580510535
H	7.522879945	-0.822829168	1.308188541
C	5.935066699	-2.309698306	1.047834754
C	6.001823527	0.285087607	-0.603273325
H	5.890018684	-0.709470586	-1.055839386
H	5.225637924	0.934545722	-1.029948985
C	-7.465000005	0.352446456	1.035194841
C	-7.960707554	1.621134184	1.354998339
C	-8.337876526	-0.740801605	1.051139159
C	-9.304120250	1.794852639	1.673905667
C	-9.681412462	-0.568165238	1.369944714
C	-10.166229613	0.700592995	1.679591841
H	-7.281768283	2.475629826	1.359593067

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H	-7.954089480	-1.735578811	0.817658986
H	-9.676704769	2.786306805	1.923946660
H	-10.349454405	-1.427202578	1.381954524
H	-11.216173223	0.835704298	1.932661369
C	7.368136527	0.841751241	-0.862600057
C	8.469771738	-0.010976530	-0.992591953
C	7.564261832	2.223629873	-0.960178266
C	9.743627402	0.507693118	-1.204218168
C	8.837720445	2.743199442	-1.171867562
C	9.929003897	1.885606569	-1.291656399
H	8.321282153	-1.090745436	-0.934191544
H	6.706670257	2.893537437	-0.876055534
H	10.591985164	-0.166169412	-1.306801583
H	8.976608759	3.819741311	-1.249136911
H	10.924557813	2.291538076	-1.460868878

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S4. Additional Crystal data and Structural information concerning [Cu(TEBIDA)(H7azain)(H_2O)]·3H_2O (**1**)

Table S4.1. Crystal data and structure refinement for [Cu(TEBIDA)(H7azain)(H_2O)]·3H_2O

Identification code	09jnac551	
Empirical formula	C15 H27 Cu N3 O8	
Formula weight	440.94	
Temperature	110(2) K	
Wavelength	0.71073 A	
Crystal system, space group	Orthorhombic, P c c n	
Unit cell dimensions	a = 34.292(18) Å b = 9.563(5) Å c = 11.407(6) Å	alpha = 90 deg. beta = 90 deg. gamma = 90 deg.
Volume	3741(3) A^3	
Z, Calculated density	8, 1.566 Mg/m^3	
Absorption coefficient	1.216 mm^-1	
F(000)	1848	
Crystal size	0.23 x 0.22 x 0.04 mm	
Theta range for data collection	1.19 to 26.02 deg.	
Limiting indices	0<=h<=42, 0<=k<=11, 0<=l<=14	
Reflections collected / unique	18037 / 3676 [R(int) = 0.0564]	
Completeness to theta = 26.02	99.8 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.9530 and 0.7672	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	3676 / 6 / 244	
Goodness-of-fit on F^2	1.389	
Final R indices [I>2sigma(I)]	R1 = 0.0761, wR2 = 0.2011	
R indices (all data)	R1 = 0.0934, wR2 = 0.2125	
Largest diff. peak and hole	0.592 and -1.377 e.A^-3	

Table S4.2. Selected bond lengths [Å] and angles [deg] for [Cu(TEBIDA)(H7azain)(H_2O)]·3H_2O

Cu(1)-O(21)	1.921(4)
Cu(1)-O(11)	1.927(4)
Cu(1)-N(3)	1.971(5)
Cu(1)-N(10)	2.026(5)
Cu(1)-O(1)	2.302(5)
O(21)-Cu(1)-O(11)	170.12(18)
O(21)-Cu(1)-N(3)	93.80(18)
O(11)-Cu(1)-N(3)	95.31(18)
O(21)-Cu(1)-N(10)	85.88(18)
O(11)-Cu(1)-N(10)	87.20(18)
N(3)-Cu(1)-N(10)	157.3(2)
O(21)-Cu(1)-O(1)	87.38(17)
O(11)-Cu(1)-O(1)	86.83(17)
N(3)-Cu(1)-O(1)	103.09(18)
N(10)-Cu(1)-O(1)	99.56(18)

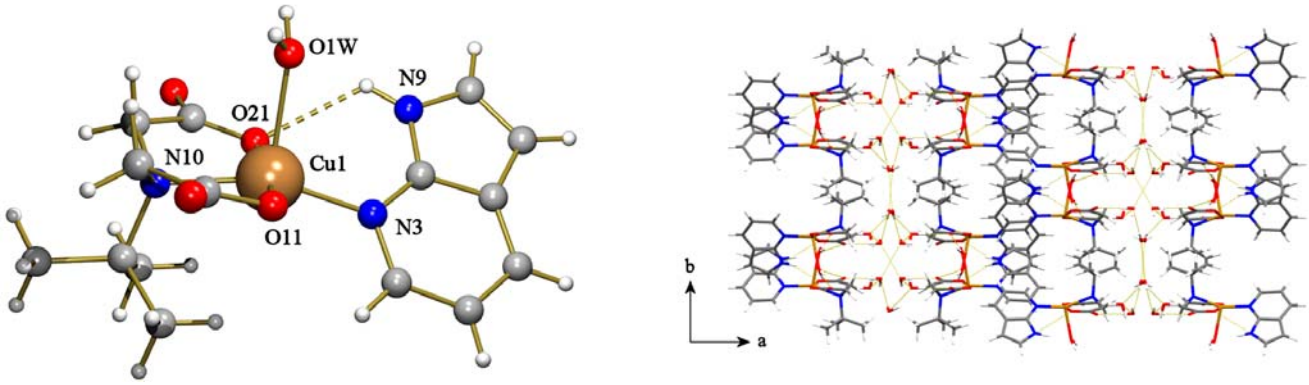
Table S4.3. Hydrogen bonds for [Cu(TEBIDA)(H7azain)(H_2O)]·3H_2O [Å and deg.]

D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)
O(1)-H(1A)...O(12)#1	0.97	1.86	2.799(6)	162.4
O(1)-H(1B)...O(22)#2	0.83	2.03	2.828(6)	159.2
N(9)-H(9A)...O(21)	0.90	2.29	2.883(7)	123.2
O(2)-H(2A)...O(22)#2	0.83	1.89	2.718(6)	171.4
O(2)-H(2B)...O(4)	0.83	1.95	2.710(7)	150.2
O(3)-H(3A)...O(2)	0.85	2.06	2.840(7)	151.3
O(3)-H(3B)...O(4)#3	0.85	1.83	2.680(8)	172.4

Symmetry transformations used to generate equivalent atoms:

#1 x,-y+1/2,z+1/2 #2 x,-y+1/2,z-1/2 #3 -x+1/2,y,z-1/2

Figure and comments S4.4. Complex molecule of [Cu(TEBIDA)(H7azain)(H_2O)]·3H_2O (left) and view of the 3D network in the ba plane (right).



In the crystal (orthorhombic, Pccn), apical aqua ligands use their H atoms to build intermolecular H-bonds, giving rise to chains that run along the c axis. These former chains are further connected by pi,pi-stacking interactions between adjacent H7azain ligands, involving both aromatic moieties, to build layers. Thereby, each H7azain ligand stacks its six-membered ring with the five- and six-membered rings of one adjacent H7azain ligand (see Table S14.1). Finally, the 3D architecture is accomplished by H-bonding interactions that involve the non-coordinated water molecules (see Table S4.3).

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S4. Additional Crystal data and Structural information concerning {[Cu(FBIDA)(H7azain)]·2H_2O}$_n$ (**2**).

Table S5.1. Crystal data and structure refinement for {[Cu(FBIDA)(H7azain)]·2H_2O}$_n$

Identification code	c554	
Empirical formula	C36 H36 Cu2 F2 N6 O10	
Formula weight	877.79	
Temperature	100(2) K	
Wavelength	0.73780 Å	
Crystal system	Monoclinic	
Space group	C2/c	
Unit cell dimensions	a = 37.308(8) Å b = 8.0550(16) Å c = 25.933(5) Å	α= 90 deg. β= 111.42(3) deg. γ = 90° deg.
Volume	7255(3) Å^3	
Z	8	
Density (calculated)	1.607 Mg/m^3	
Absorption coefficient	1.251 mm^{-1}	
F(000)	3600	
Theta range for data collection	2.43 to 28.14°.	
Index ranges	0<=h<=46, 0<=k<=9, -32<=l<=30	
Reflections collected	7249 / 7249 [R(int) = 0.0000]	
Completeness to theta = 28.14°	97.9 %	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	7249 / 0 / 505	
Goodness-of-fit on F^2	1.078	
Final R indices [I>2sigma(I)]	R1 = 0.0414, wR2 = 0.1152	
R indices (all data)	R1 = 0.0518, wR2 = 0.1198	
Largest diff. peak and hole	1.040 and -1.193 e.Å^{-3}	

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Table S5.2. Selected bond lengths [Å] and angles [deg] for {[Cu(FBIDA)(H7azain)]·2H_2O}$_n$

Cu(1)-O(21)	1.9341(17)
Cu(1)-O(11)	1.9341(18)
Cu(1)-N(3)	1.996(2)
Cu(1)-N(10)	2.014(2)
Cu(1)-O(12A)#1	2.3764(19)
Cu(2)-O(21A)	1.9314(17)
Cu(2)-O(11A)	1.9322(17)
Cu(2)-N(3A)	1.988(2)
Cu(2)-N(10A)	2.010(2)
Cu(2)-O(12)	2.374(2)
O(4)-Cu(1)-O(8)	169.87(7)
O(21)-Cu(1)-O(11)	169.84(7)
O(21)-Cu(1)-N(3)	95.76(8)
O(11)-Cu(1)-N(3)	94.38(8)
O(21)-Cu(1)-N(10)	85.71(8)
O(11)-Cu(1)-N(10)	84.36(8)
N(3)-Cu(1)-N(10)	163.89(9)
O(21)-Cu(1)-O(12A)#1	91.17(7)
O(11)-Cu(1)-O(12A)#1	86.05(7)
N(3)-Cu(1)-O(12A)#1	109.60(7)
N(10)-Cu(1)-O(12A)#1	86.37(8)
O(21A)-Cu(2)-O(11A)	170.12(7)
O(21A)-Cu(2)-N(3A)	95.86(8)
O(11A)-Cu(2)-N(3A)	94.02(8)
O(21A)-Cu(2)-N(10A)	85.87(8)
O(11A)-Cu(2)-N(10A)	84.74(8)
N(3A)-Cu(2)-N(10A)	163.18(8)
O(21A)-Cu(2)-O(12)	90.16(7)
O(11A)-Cu(2)-O(12)	86.06(7)
N(3A)-Cu(2)-O(12)	111.21(8)
N(10A)-Cu(2)-O(12)	85.48(8)

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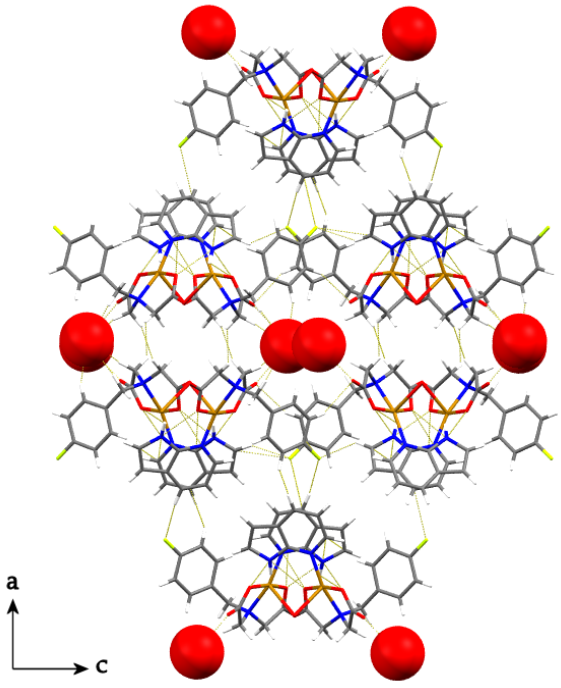
Table S5.3. Hydrogen bonds for {[Cu(FBIDA)(H7azain)]·2H_2O}$_n$ [Å and deg.]

D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)
N(9A)-H(9A)...O(21)#1	0.92	2.28	2.933(3)	127.4
N(9A)-H(9A)...O(11A)	0.92	2.19	2.876(3)	130.9
N(9)-H(9)...O(11)	0.91	2.30	2.928(3)	126.7
N(9)-H(9)...O(21A)	0.91	2.18	2.900(3)	136.2
Non-classical H-bonds				
C(9) --H(9) ..F(35)#2	0.95	2.34	3.138(3)	141.0
C(6A) --H(6A) ..F(35A)#3	0.95	2.38	3.318(4)	169.5
C(8A) --H(8A) ..F(35A)#4	0.95	2.41	3.178(4)	137.4

Symmetry transformations used to generate equivalent atoms:
#1 x,1+y,z #2 x,1-y,1/2+z #3 3/2-x,3/2-y,2-z #4 x,2-y,-1/2+z

Figure and comments S5.4. View of the 3D network in the ac plane.



Compound 2 crystallizes in the monoclinic system (space group C2/c). In the crystal, the polymeric chains extend throughout the b axis connecting to each other by means of non-coordinated water molecules. Hence, the resulting 2D layer presents a honeycomb-like topology

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where the non-coordinated molecules are hosted into channels that extend along b axis. Weak non-classical intermolecular H-bonding interactions, that involve the fluoro atoms, also contribute to the crystal structure associating layers in the 3D network (see Table S5.3). Despite the presence of aromatic moieties in the both FBIDA and H7azain ligands, no pi,pi-stacking interactions are observed in this crystal.

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S6. Additional Crystal data and Structural information concerning $\{[Cu(CBIDA)(H4abim)]\cdot 2H_2O\}_n$ (**3**)

Table S6.1. Crystal data and structure refinement for $\{[Cu(CBIDA)(H4abim)]\cdot 2H_2O\}_n$

Identification code	c482
Empirical formula	C17 H19 Cl Cu N4 O6
Formula weight	474.35
Temperature	100(2) K
Wavelength	0.71073 A
Crystal system, space group	Monoclinic, P 21/c
Unit cell dimensions	a = 13.418(4) Å α = 90 deg. b = 7.707(2) Å β = 106.648(13) deg. c = 19.083(5) Å γ = 90º deg.
Volume	1890.7(9) A^3
Z, Calculated density	4, 1.666 Mg/m^3
Absorption coefficient	1.341 mm^-1
F(000)	972
Crystal size	0.34 x 0.04 x 0.01 mm
Theta range for data collection	1.58 to 27.26 deg.
Limiting indices	-17<=h<=16, 0<=k<=9, 0<=l<=24
Reflections collected / unique	20471 / 4314 [R(int) = 0.0981]
Completeness to theta = 27.26	99.7 %
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.9867 and 0.6585
Data / restraints / parameters	4314 / 0 / 263
Goodness-of-fit on F^2	1.037
Final R indices [I>2sigma(I)]	R1 = 0.0722, wR2 = 0.1945
R indices (all data)	R1 = 0.0896, wR2 = 0.2107
Extinction coefficient	0.0021(13)
Largest diff. peak and hole	1.536 and -1.771 e.A^-3

Table S6.2. Selected bond lengths [Å] and angles [deg] for {[Cu(CBIDA)(H4abim)]·2H_2O}$_n$

Cu(1)-O(11)	1.949(3)
Cu(1)-N(7)	1.945(4)
Cu(1)-O(21)	1.957(3)
Cu(1)-N(10)	1.984(4)
Cu(1)-O(22)#1	2.261(4)
O(11)-Cu(1)-N(7)	93.21(16)
O(11)-Cu(1)-O(21)	168.58(17)
N(7)-Cu(1)-O(21)	97.06(16)
O(11)-Cu(1)-N(10)	85.13(16)
N(7)-Cu(1)-N(10)	168.15(17)
O(21)-Cu(1)-N(10)	83.80(16)
O(11)-Cu(1)-O(22)#1	95.24(14)
N(7)-Cu(1)-O(22)#1	103.83(16)
O(21)-Cu(1)-O(22)#1	87.15(14)
N(10)-Cu(1)-O(22)#1	88.01(16)

Symmetry transformations used to generate equivalent atoms:

#1 -x,y+1/2,-z+1/2

Table S6.3. Hydrogen bonds for {[Cu(CBIDA)(H4abim)]·2H_2O}$_n$ [Å and deg.]

D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)
N(9)-H(9A)...O(12)#3	0.88	1.86	2.739(7)	173.6
O(1)-H(1A)...N(3)#4	0.85	2.08	2.880(8)	156.6
O(1)-H(1B)...O(2)	0.85	1.86	2.707(8)	170.9
O(2)-H(2A)...O(1)#5	0.85	1.89	2.691(8)	155.7
O(2)-H(2B)...O(12)	0.86	2.10	2.7489(7)	132.7

Symmetry transformations used to generate equivalent atoms:

#1 -x,y+1/2,-z+1/2 #2 -x,y-1/2,-z+1/2 #3 -x,-y+1,-z #4 x+1,-y+1/2,z+1/2 #5 -x+1,y+1/2,-z+1/2

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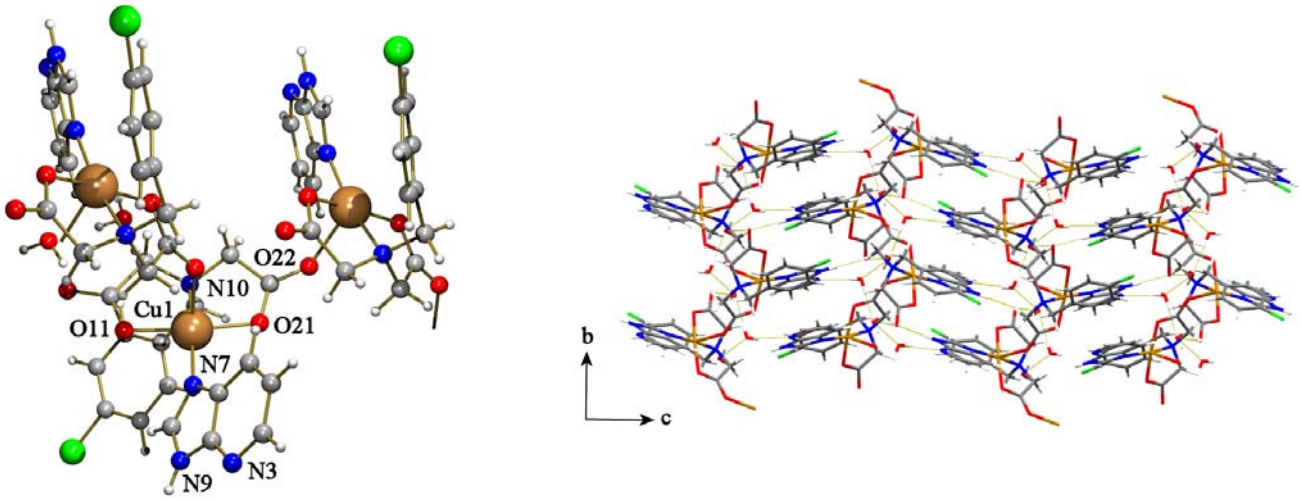
Figure and comments S6.4. Fragment of the polymer $\{[Cu(CBIDA)(H4abim)]\cdot 2H_2O\}_n$ (left) and view of the 3D network in the bc plane (right).



In the crystal (monoclinic, $P2_1/c$), the water molecules build helical motifs running along the 2_1 screw axes addressing the same direction than the polymeric chains. These latter chains associate each other through inter-molecular H-bonds that involve the N9-H groups of H4abim. Finally, the 3D network is reached thanks to H-bonding interactions that comprises the non-coordinated water molecules (see Table S6.3).

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S7. Additional Crystal data and Structural information concerning [Cu(H_2EDTA)(H4abim)]·0.5H_2O (**4**)

Table S7.1. Crystal data and structure refinement for [Cu(H_2EDTA)(H4abim)]·0.5H_2O

Identification code	c555	
Empirical formula	C32 H40 Cu2 N10 O17	
Formula weight	963.82	
Temperature	100(2) K	
Wavelength	0.7380 Å	
Crystal system	Triclinic	
Space group	P-1	
Unit cell dimensions	a = 7.270(5) Å b = 8.502(5) Å c = 14.780(5) Å	α = 90.628(5) deg. β = 92.540(5) deg. γ = 97.828(5) deg.
Volume	903.9(3) $Å^3$	
Z; Density (calculated)	1; 1.770 Mg/m^3	
Absorption coefficient	1.272 mm^{-1}	
F(000)	496	
Theta range for data collection	3.84 to 27.46°.	
Index ranges	0<=h<=8, -10<=k<=10, -17<=l<=17	
Reflections collected	3381	
Independent reflections	3381 [R(int) = 0.0000]	
Completeness to theta = 26.25°	91.6 %	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	3381 / 0 / 284	
Goodness-of-fit on F^2	1.041	
Final R indices [I>2sigma(I)]	R1 = 0.0326, wR2 = 0.0859	
R indices (all data)	R1 = 0.0329, wR2 = 0.0860	
Largest diff. peak and hole	0.442 and -1.004 $e.Å^{-3}$	

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Table S7.2. Selected bond lengths [Å] and angles [deg] for [Cu(H_2EDTA)(H4abim)]·0.5H_2O

Cu(1)-O(21)	1.9599(17)
Cu(1)-O(11)	1.9612(17)
Cu(1)-N(9)	1.9751(18)
Cu(1)-N(10)	2.0793(18)
Cu(1)-N(20)	2.3609(17)
Cu(1)-O(16)	2.583(2)
O(21)-Cu(1)-O(11)	173.25(6)
O(21)-Cu(1)-N(9)	89.40(8)
O(11)-Cu(1)-N(9)	96.81(8)
O(21)-Cu(1)-N(10)	89.99(7)
O(11)-Cu(1)-N(10)	85.03(7)
N(9)-Cu(1)-N(10)	160.61(7)
O(21)-Cu(1)-N(20)	79.08(6)
O(11)-Cu(1)-N(20)	95.71(7)
N(9)-Cu(1)-N(20)	116.50(7)
N(10)-Cu(1)-N(20)	82.36(6)

Table S7.3. Hydrogen bonds for [Cu(H_2EDTA)(H4abim)]·0.5H_2O [Å and deg.]

D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)
O(17)-H(17)...O(12)#1	0.84	1.70	2.535(2)	173.4
O(26)-H(26)...O(22)#2	0.84	1.73	2.561(2)	170.7
N(7)-H(7)...O(22)#3	0.88	2.17	2.946(2)	147.5
O(1)-H(1A)...O(25)#5	0.87	2.29	2.948(5)	132.9
O(1)-H(1B)...O(26)	0.86	2.29	2.941(5)	132.6

Symmetry transformations used to generate equivalent atoms:

#1 x+1,y,z #2 x-1,y,z #3 -x+1,-y,-z #4 -x+1,-y+1,-z #5 -x,-y-1,-z+1

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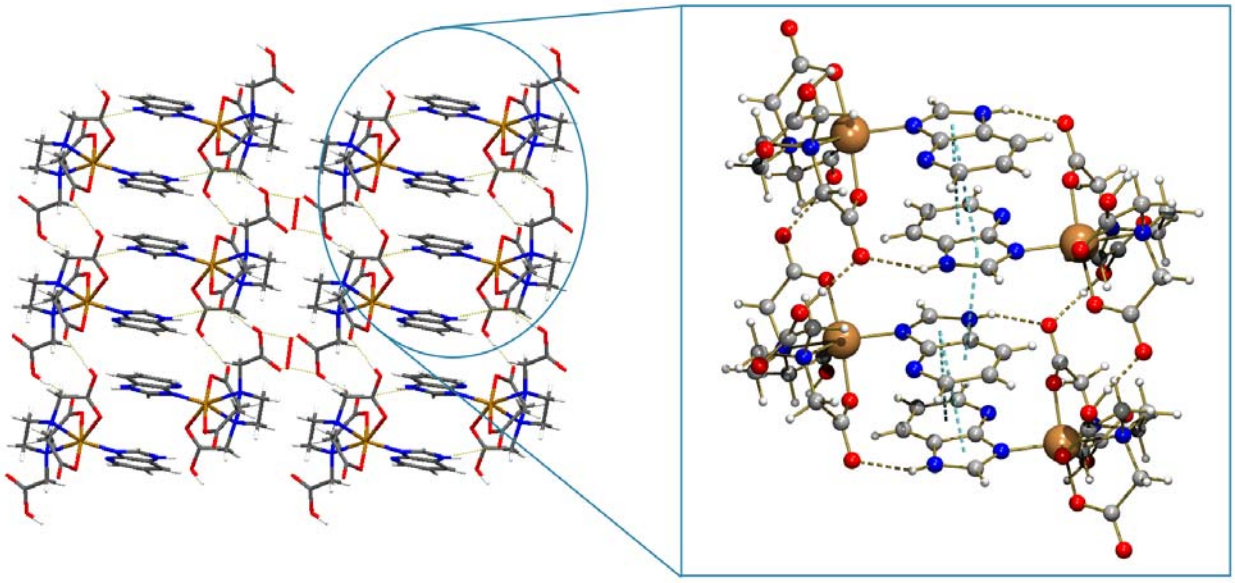
Figure and comments S7.4. 2D layers in the crystal of compound **4** and detail of pi,pi-stacking interactions between anti-parallel H4abim ligands.



Compound 4 crystallizes in the triclinic P-1 space group. In the crystal, pi,pi-stacking interactions among anti-parallel H4abim ligands build 1D ribbons along the a axis (see Table S13.2), which are further intra-stabilized by inter-molecular H-bonds involving the N7-H group of H4abim and the free carboxylic groups (see Table S7.3). The referred ribbons connect to each other by means of non-coordinated water molecules leading to corrugated layers that are further connected by hydrophobic interactions giving rise to the 3D array.

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S8. Additional Crystal data and Structural information concerning {[Cu_2(IDA)$_2$(μ_2-N7,N9-H5abim)]·H_2O}$_n$ (**5**)

Table S8.1. Crystal data and structure refinement for {[Cu_2(IDA)$_2$(μ_2-N7,N9-H5abim)]·H_2O}$_n$

Identification code	c607	
Empirical formula	C14 H17 Cu2 N5 O9	
Formula weight	526.41	
Temperature	100(2) K	
Wavelength	0.73800 Å	
Crystal system	Orthorhombic	
Space group	Cmc21	
Unit cell dimensions	a = 15.401(3) Å b = 14.480(3) Å c = 8.1120(16) Å	α = 90 deg. β = 90 deg. γ = 90 deg.
Volume	1809.0(6) Å^3	
Z; Density (calculated)	4; 1.933 Mg/m^3	
Absorption coefficient	2.415 mm^{-1}	
F(000)	1064	
Crystal size	0.08 x 0.02 x 0.02 mm^3	
Theta range for data collection	4.60 to 28.21°.	
Index ranges	0<=h<=19, 0<=k<=18, -9<=l<=0	
Reflections collected	1048	
Independent reflections	1048 [R(int) = 0.0000]	
Completeness to theta = 28.21°	94.7 %	
Data / restraints / parameters	1048 / 4 / 140	
Goodness-of-fit on F^2	1.037	
Final R indices [I>2sigma(I)]	R1 = 0.0460, wR2 = 0.1278	
R indices (all data)	R1 = 0.0463, wR2 = 0.1286	
Extinction coefficient	0.033(4)	
Largest diff. peak and hole	0.682 and -0.673 e.Å^{-3}	

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Table S8.2. Selected bond lengths [Å] and angles [deg] for {[Cu_2(IDA)$_2$(μ_2-N7,N9-H5abim)]·H_2O}$_n$

Cu(1)-O(8)	1.947(5)
Cu(1)-N(1)	1.969(6)
Cu(1)-N(11)	1.977(5)
Cu(1)-O(4)	1.985(5)
Cu(1)-O(5)#1	2.507(4)
Cu(1)-O(9)#2	2.524(5)
O(8)-Cu(1)-N(1)	84.7(3)
O(8)-Cu(1)-N(11)	98.9(2)
N(1)-Cu(1)-N(11)	176.3(3)
O(8)-Cu(1)-O(4)	166.85(17)
N(1)-Cu(1)-O(4)	83.1(3)
N(11)-Cu(1)-O(4)	93.3(2)
O(8)-Cu(1)-O(5)#1	84.62(18)
N(1)-Cu(1)-O(5)#1	95.8(2)
N(11)-Cu(1)-O(5)#1	85.67(18)
O(4)-Cu(1)-O(5)#1	101.44(18)
O(8)-Cu(1)-O(9)#2	85.55(18)
N(1)-Cu(1)-O(9)#2	81.18(19)
N(11)-Cu(1)-O(9)#2	97.89(17)
O(4)-Cu(1)-O(9)#2	87.78(18)
O(5)#1-Cu(1)-O(9)#2	170.0(2)

Symmetry transformations used to generate equivalent atoms:
#1 -x+1/2,-y+1/2,z+1/2 #2 x,-y,z-1/2

Table S8.3. Hydrogen bonds for {[Cu_2(IDA)$_2$(μ_2-N7,N9-H5abim)]·H_2O}$_n$ [Å and deg.]

D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)
O(1)-H(1A)...O(12)	0.86	2.03	2.885(7)	170.1
N(1)-H(1)...O(21)#4	0.85	2.09	2.910(8)	163.9

Symmetry transformations used to generate equivalent atoms:
#1 -x+1/2,-y+1/2,z+1/2 #2 x,-y,z-1/2 #3 -x+1,y,z #4 x,y,z-1

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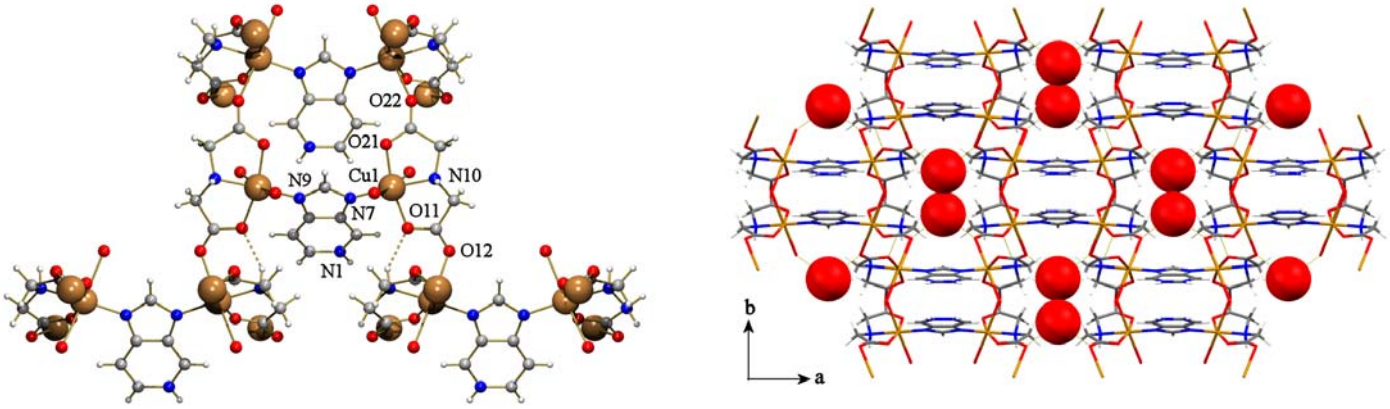
Figure and comments S8.4. Fragment of the polymer $\{[Cu_2(IDA)_2(\mu_2\text{-N7,N9-H5abim})]\cdot H_2O\}_n$ (left) and view of the 3D network in the ba plane (right).



Compound 5 crystallizes in the orthorhombic $Cmc2_1$ space group. In the crystal, the dinuclear units extend leading to 3D network which is reinforced by H-bonding interactions that involve the N1-H group of H5abim, the non-coordinated water molecule and the N-H group of the IDA moiety (see Table S8.3), contributing massively to the stability of the 3D network.

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S9. Additional Crystal data and Structural information concerning $[Cu_2(NBzIDA)_2(\mu_2\text{-}N7,N9\text{-}H5abim)(H_2O)_2]\cdot H_2O$ (**6**).

Table S9.1. Crystal data and structure refinement for $[Cu_2(NBzIDA)_2(\mu_2\text{-}N7,N9\text{-}H5abim)(H_2O)_2]\cdot H_2O$

Identification code	c484	
Empirical formula	C28 H33 Cu2 N5 O11	
Formula weight	742.680	
Temperature	293(2) K	
Wavelength	1.54178 Å	
Crystal system	Monoclinic	
Space group	C2/c	
Unit cell dimensions	a = 17.6777(11) Å b = 10.0875(6) Å c = 20.9883(13) Å	α = 90 deg. β = 110.719(2) deg. γ = 90 deg.
Volume	3500.7(4) $Å^3$	
Z; Density (calculated)	4; 1.443 Mg/m3	
Absorption coefficient	2.056 mm-1	
F(000)	1568	
Crystal size	0.12 x 0.10 x 0.10 mm3	
Theta range for data collection	5.65 to 66.49∞.	
Index ranges	-20<=h<=20, -11<=k<=11, -24<=l<=24	
Reflections collected	19804 / 2912 [R(int) = 0.0530]	
Completeness to theta = 66.49∞	94.9 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.8208 and 0.7905	
Data / restraints / parameters	2912 / 199 / 278	
Goodness-of-fit on F2	1.076	
Final R indices [I>2sigma(I)]	R1 = 0.0463, wR2 = 0.1285	
R indices (all data)	R1 = 0.0482, wR2 = 0.1304	
Largest diff. peak and hole	0.426 and -0.323 e. $Å^{-3}$	

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Table S9.2. Selected bond lengths [Å] and angles [deg] for $[Cu_2(NBzIDA)_2(\mu_2\text{-}N7,N9\text{-}H5abim)(H_2O)_2]\cdot H_2O$

Cu(1)-O(21)	1.9797(19)
Cu(1)-O(11)	1.969(2)
Cu(1)-N(10)	2.014(2)
Cu(1)-O(1)	2.273(2)
Cu(1)-N(9)	1.960(2)
O(21)-Cu(1)-N(10)	82.64(8)
O(21)-Cu(1)-O(1)	92.68(9)
O(11)-Cu(1)-O(21)	165.78(9)
O(11)-Cu(1)-N(10)	83.51(8)
O(11)-Cu(1)-O(1)	92.08(9)
N(10)-Cu(1)-O(1)	96.45(9)
N(9)-Cu(1)-O(21)	94.30(8)
N(9)-Cu(1)-O(11)	98.31(8)
N(9)-Cu(1)-N(10)	165.50(10)
N(9)-Cu(1)-O(1)	97.86(10)

Table S9.3. Hydrogen bonds for $[Cu_2(NBzIDA)_2(\mu_2\text{-}N7,N9\text{-}H5abim)(H_2O)_2]\cdot H_2O$ [Å and deg.]

D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)
O(1)-H(1a)...O(22)#2	0.87	1.93	2.774(3)	162.6
O(1)-H(1b)...O(12)#3	0.87	1.96	2.734(3)	147.8
C(1)-H(1c)...O(22)#4	0.93	2.08	2.886(4)	144.5
N(1)-H(1d)...O(22)#4	0.86	2.14	2.886(4)	145.6
O(2)-H(2a)...O(2A)	0.85	2.09	2.877(12)	153.1
Non-classical H-bonds				
C(8) --H(8)···O(21)	0.93	2.50	2.997(3)	113.3

Symmetry transformations used to generate equivalent atoms:

#1 -x+1,y,-z+3/2 #2 -x+3/2,y-1/2,-z+3/2 #3 -x+3/2,y+1/2,-z+3/2 #4 x,y-1,z

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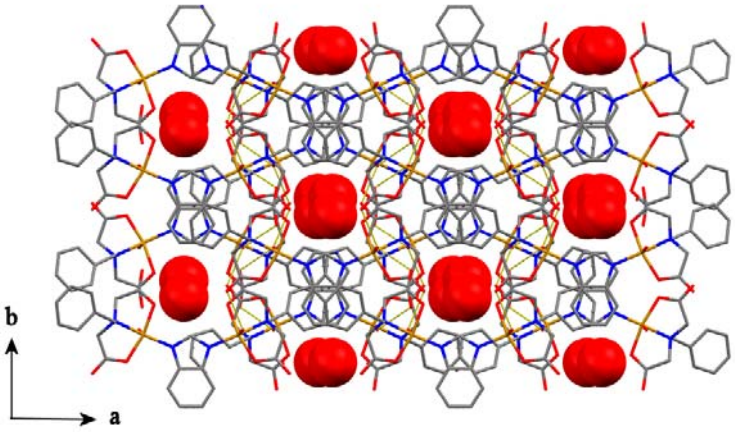
Figure and comments S9.4. View in the ba plane of the 3D architecture showing the channels that host solvent molecules.



In the crystal (monoclinic, C2/c), the dinuclear units build ribbons connected through intermolecular H-bonding interactions along the b axis that involve the N1-H group of H5abim ligand (see Table S9.3). Note that N1-H is delocalised in two positions, thereby the O22-acceptor of each NBzIDA moiety is involved 50% of the time in this interaction. These ribbons are further connected by symmetry related H-bonding interaction that involve the apical aqua ligands of both moieties, leading to 2D layers. Finally, adjacent layers connect each other by very weak, but massive, pi,pi-stacking interactions among the NBzIDA moieties of both disordered positions (see Table S14.3), accomplishing the 3D array. Moreover, channels are built in the honeycomb-like structure that extends throughout the c axis, in which the non-coordinated water molecules are hosted.

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S10. Additional Crystal data and Structural information concerning [Cu(IDA)(H7deaA)(H_2O)]·$2H_2O$ (**7**)

Table S10.1. Crystal data and structure refinement for [Cu(IDA)(H7deaA)(H_2O)]·$2H_2O$

Identification code	c606	
Empirical formula	C10 H17 Cu N5 O7	
Formula weight	382.83	
Temperature	120(2) K	
Wavelength	1.54178 Å	
Crystal system, Space group	Triclinic, P-1	
Unit cell dimensions	a = 6.7944(11) Å b = 7.8048(12) Å c = 14.257(2) Å	α = 90.174(8)°. β = 92.347(8)°. γ = 110.213(7)°.
Volume	708.75(19) Å3	
Z; Density (calculated)	2; 1.794 Mg/m3	
Absorption coefficient	2.645 mm-1	
F(000)	394	
Crystal size	0.10 x 0.08 x 0.04 mm3	
Theta range for data collection	3.10 to 66.49°.	
Index ranges	-8<=h<=8, -9<=k<=9, -16<=l<=16	
Reflections collected	9355 / 2344 [R(int) = 0.0595]	
Completeness to theta = 66.49°	94.2 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.9016 and 0.7779	
Refinement method	Full-matrix least-squares on F2	
Data / restraints / parameters	2344 / 0 / 208	
Goodness-of-fit on F2	1.070	
Final R indices [I>2sigma(I)]	R1 = 0.0428, wR2 = 0.1131	
R indices (all data)	R1 = 0.0491, wR2 = 0.1180	
Largest diff. peak and hole	0.898 and -0.413 e.Å-3	

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Table S10.2. Selected bond lengths [Å] and angles [deg] for [Cu(IDA)(H7deaA)(H_2O)]·2H_2O

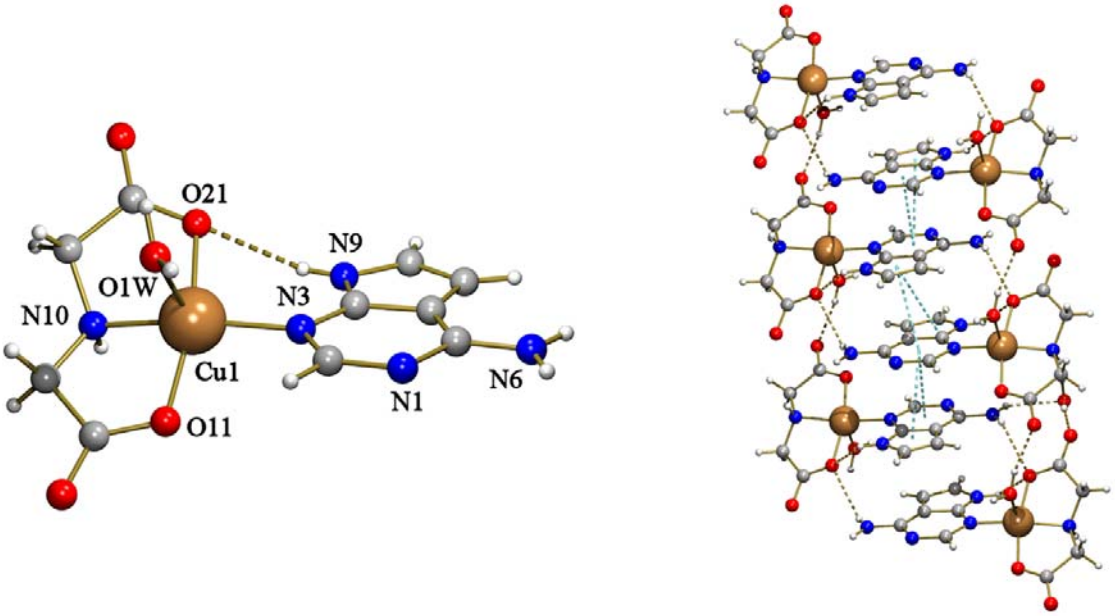
Cu(1)-N(3)	1.964(3)
Cu(1)-O(11)	1.973(2)
Cu(1)-N(10)	1.978(3)
Cu(1)-O(21)	1.984(2)
Cu(1)-O(1)	2.273(2)
N(3)-Cu(1)-O(11)	95.52(10)
N(3)-Cu(1)-N(10)	165.48(11)
O(11)-Cu(1)-N(10)	83.99(10)
N(3)-Cu(1)-O(21)	96.63(10)
O(11)-Cu(1)-O(21)	167.68(9)
N(10)-Cu(1)-O(21)	83.73(11)
N(3)-Cu(1)-O(1)	98.65(10)
O(11)-Cu(1)-O(1)	92.13(9)
N(10)-Cu(1)-O(1)	95.87(11)
O(21)-Cu(1)-O(1)	88.11(9)

Table S10.3. Hydrogen bonds for [Cu(IDA)(H7deaA)(H_2O)]·2H_2O [Å and deg.]

D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)
N(9)-H(9)...O(21)	0.88	2.46	3.011(3)	121.2
N(9)-H(9)...O(12)#1	0.88	2.58	3.179(4)	126.4
N(6)-H(6A)...O(3)#2	0.88	2.35	3.053(4)	136.5
N(6)-H(6B)...O(21)#3	0.88	2.41	3.057(3)	130.2
O(1)-H(1A)...O(12)#4	0.87	1.99	2.838(3)	166.7
O(1)-H(1B)...N(1)#2	0.87	1.91	2.778(3)	172.0
O(2)-H(2C)...O(12)#4	0.83	2.03	2.839(4)	162.6
O(2)-H(2D)...O(22)#5	0.84	1.95	2.774(4)	163.7
O(3)-H(3A)...O(22)#6	0.85	1.92	2.748(4)	164.8
O(3)-H(3B)...O(2)	0.86	1.90	2.729(4)	163.5

Symmetry transformations used to generate equivalent atoms:
#1 x+1,y+1,z #2 -x+1,-y+1,-z+1 #3 -x+2,-y+2,-z+1 #4 x+1,y,z #5 -x+2,-y+1,-z+2 #6 x-1,y-1,z

Figure and comments S10.4. Complex molecule of [Cu(IDA)(H7deaA)(H_2O)]·2H_2O (left) and detail of pi,pi-stacking interactions within the 1D chains (right)



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In the crystal (triclinic P-1), pi,pi-stacking interaction between anti-parallel H7deaA ligands connect the complex molecules leading to multi-stacked chains that extend along the a axis (see Table S14.4). Aside, symmetry related inter-molecular H-bonds contribute to the stability of such chains that are futher connected by inter-molecular H-bonds building layers. Additional H-bonds that involve the non-coordinated water molecules build the 3D architecture (see Table S10.3).

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S11. Additional Crystal data and Structural information concerning $[Cu_2(MIDA)_2(\mu_2\text{-N1-N3-H7deaA})(H_2O)_2]\cdot 5H_2O$ (**8**)

Table S11.1. Crystal data and structure refinement for $[Cu_2(MIDA)_2(\mu_2\text{-N1-N3 H7deaA})(H_2O)_2]\cdot 5H_2O$

Identification code	c618	
Empirical formula	C16 H34 Cu2 N6 O15	
Formula weight	677.57	
Temperature	100(2) K	
Wavelength	0.73780 Å	
Crystal system	Triclinic	
Space group	P-1	
Unit cell dimensions	a = 6.9590(14) Å b = 13.536(3) Å c = 14.250(3) Å	α= 93.62(3) deg. β= 102.40(3) deg. γ = 95.27(3) deg.
Volume	1300.7(4) $Å^3$	
Z; Density (calculated)	2; 1.730 Mg/m^3	
Absorption coefficient	1.718 mm^{-1}	
F(000)	700	
Theta range for data collection	1.57 to 26.20°.	
Index ranges	0<=h<=8, -16<=k<=16, -17<=l<=17	
Reflections collected	19103 / 4975 [R(int) = 0.0777]	
Completeness to theta = 26.20°	93.4 %	
Data / restraints / parameters	4975 / 3 / 371	
Goodness-of-fit on F^2	1.039	
Final R indices [I>2sigma(I)]	R1 = 0.0647, wR2 = 0.1802	
R indices (all data)	R1 = 0.0731, wR2 = 0.1881	
Extinction coefficient	0.0109(19)	
Largest diff. peak and hole	0.921 and -1.237 $e.Å^{-3}$	

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Table S11.2. Selected bond lengths [Å] and angles [deg] for $[Cu_2(MIDA)_2(\mu_2\text{-N1-N3-H7deaA})(H_2O)_2]\cdot 5H_2O$

Cu(1)-O(11)	1.968(3)
Cu(1)-O(21)	1.985(3)
Cu(1)-N(10)	1.988(4)
Cu(1)-N(1)	1.990(4)
Cu(1)-O(1)	2.225(4)
Cu(2)-O(41)	1.955(3)
Cu(2)-O(31)	1.966(3)
Cu(2)-N(3)	1.984(4)
Cu(2)-N(30)	2.010(4)
Cu(2)-O(2)	2.267(4)
O(11)-Cu(1)-O(21)	165.80(14)
O(11)-Cu(1)-N(10)	83.23(16)
O(21)-Cu(1)-N(10)	83.08(15)
O(11)-Cu(1)-N(1)	95.78(15)
O(21)-Cu(1)-N(1)	96.39(14)
N(10)-Cu(1)-N(1)	164.33(18)
O(11)-Cu(1)-O(1)	97.33(15)
O(21)-Cu(1)-O(1)	88.15(14)
N(10)-Cu(1)-O(1)	97.49(18)
N(1)-Cu(1)-O(1)	98.15(15)
O(41)-Cu(2)-O(31)	167.18(13)
O(41)-Cu(2)-N(3)	94.83(14)
O(31)-Cu(2)-N(3)	95.50(14)
O(41)-Cu(2)-N(30)	84.02(15)
O(31)-Cu(2)-N(30)	84.18(15)
N(3)-Cu(2)-N(30)	166.66(17)
O(41)-Cu(2)-O(2)	93.29(14)
O(31)-Cu(2)-O(2)	92.98(15)
N(3)-Cu(2)-O(2)	96.92(15)
N(30)-Cu(2)-O(2)	96.41(17)

Table S11.3. Hydrogen bonds for $[Cu_2(MIDA)_2(\mu_2\text{-N1-N3-H7deaA})(H_2O)_2]\cdot 5H_2O$ [Å and deg.]

D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)
N(6)-H(6A)...O(41)#1	0.89	2.14	3.019(5)	169.5
N(6)-H(6B)...O(11)	0.89	2.06	2.859(6)	149.4
N(9)-H(9)...O(5)#2	0.96	1.81	2.745(5)	164.0

Symmetry transformations used to generate equivalent atoms:
#1 -x+1,-y+1,-z #2 x-1,y,z #3 x,y-1,z #4 –z,-y,-z

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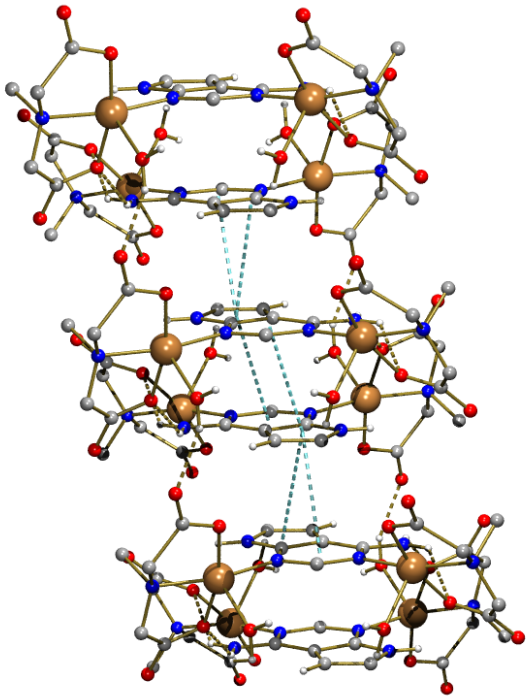
Figure and comments S11.4. Detail of multi-stacked chains in the crystal of compound **8**.



Compound 8 crystallizes in the triclinic P-1 space group. In the crystal, pairs of complex molecules are associated by means of pi,pi-stacking interactions between anti-parallel H7deaA ligands as well as weak intermolecular H-bonds. The referred pairs of molecules are further associated by pi,pi-stacking interactions (see Table S14.5). Additional inter-molecular H-bonding interactions contribute to stabilise the 1D chains (see Table S11.3). The former chains build layers involving the apical aqua ligands into inter-molecular H-bonds. The 3D array is accomplished by additional H-bonding interactions that involve the non-coordinated water molecules (see Table S11.3).

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S12. Additional Crystal data and Structural information concerning $[Cu(NBzIDA)(H7deaA)]_n$ (**9**)

Table S12.1. Crystal data and structure refinement for $[Cu(NBzIDA)(H7deaA)]_n$

Identification code	c616	
Empirical formula	C17 H17 Cu N5 O4	
Formula weight	418.90	
Temperature	100(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	P2(1)/c	
Unit cell dimensions	a = 8.7865(18) Å b = 21.951(5) Å c = 9.1750(19) Å	α = 90 deg. β = 107.828(3) deg. γ = 90 deg.
Volume	1684.7(6) $Å^3$	
Z; Density (calculated)	4; 1.652 Mg/m^3	
Absorption coefficient	1.333 mm^{-1}	
F(000)	860	
Crystal size	0.10 x 0.08 x 0.06 mm^3	
Theta range for data collection	1.86 to 25.00°.	
Index ranges	-10<=h<=9, 0<=k<=26, 0<=l<=10	
Reflections collected	3372 / 3465 [R(int) = 0.0000]	
Completeness to theta = 25.00°	98.1 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.7456 and 0.5110	
Data / restraints / parameters	3465 / 0 / 245	
Goodness-of-fit on F^2	1.051	
Final R indices [I>2sigma(I)]	R1 = 0.0499, wR2 = 0.1262	
R indices (all data)	R1 = 0.0622, wR2 = 0.1342	
Largest diff. peak and hole	0.786 and -0.405 $e.Å^{-3}$	

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Table S12.2. Selected bond lengths [Å] and angles [deg] for $[Cu(NBzIDA)(H7deaA)]_n$

Cu(1)-O(11)	1.957(3)
Cu(1)-O(21)	1.957(3)
Cu(1)-N(3)	1.971(3)
Cu(1)-N(10)	2.012(3)
Cu(1)-O(22)#1	2.244(3)
O(11)-Cu(1)-O(21)	165.63(12)
O(11)-Cu(1)-N(3)	98.65(13)
O(21)-Cu(1)-N(3)	94.49(13)
O(11)-Cu(1)-N(10)	82.67(13)
O(21)-Cu(1)-N(10)	83.06(12)
N(3)-Cu(1)-N(10)	162.50(14)
O(11)-Cu(1)-O(22)#1	91.00(12)
O(21)-Cu(1)-O(22)#1	93.34(11)
N(3)-Cu(1)-O(22)#1	96.25(12)
N(1)-Cu(1)-O(22)#1	101.19(12)

Symmetry transformations used to generate equivalent atoms:
#1 x,-y+1/2,z-1/2

Table S12.3. Hydrogen bonds for $[Cu(NBzIDA)(H7deaA)]_n$ [Å and deg.]

D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)
N(6)-H(6A)...O(22)#3	0.88	2.02	2.890(4)	171.9
N(6)-H(6B)...O(12)#4	0.88	2.25	2.996(4)	142.9
N(9)-H(9)...O(21)	0.88	2.24	2.847(4)	126.0
N(9)-H(9)...O(11)#2	0.88	2.32	2.882(4)	122.1

Symmetry transformations used to generate equivalent atoms:
#1 x,-y+1/2,z-1/2 #2 x,-y+1/2,z+1/2 #3 x+1,-y+1/2,z-1/2 #4 x+1,-y+1/2,z+1/2

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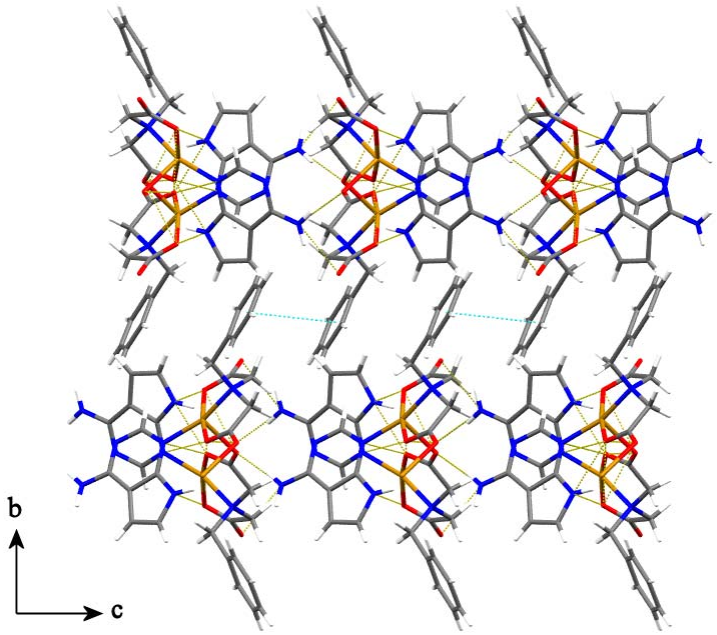
Figure and comments S12.4. View in the bc plane of the 3D architecture showing a detail of pi,pi-stacking interactions between adjacent NBzIDA ligands.



Compound 9 and 10 have similar structures and crystallize in the monoclinic $P2_1/c$ space group. The polymeric chains are connected by means of inter-molecular H-bonds, involving the exocyclic amino group of H7deaA (see Table S12.3), generating a layer structure. In **9**, these layers connect to each other by weak pi,pi-stacking interactions between the benzyl-moieties of the NBzIDA ligand as well as weak C-H/pi interaction (see Table S14.6) leading to the 3D arrangement.

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S13. Additional Crystal data and Structural information concerning $[Cu(MEBIDA)(H7deaA)]_n$ (**10**)

Table S13.1. Crystal data and structure refinement for $[Cu(MEBIDA)(H7deaA)]_n$

Identification code	c613	
Empirical formula	C18 H19 Cu N5 O4	
Formula weight	432.92	
Temperature	100(2) K	
Wavelength	0.71073 A	
Crystal system, space group	Monoclinic, P 21/c	
Unit cell dimensions	a = 8.8187(3) Å b = 24.1440(10) Å c = 8.9808(3) Å	α = 90 deg. β = 110.342(2) deg. γ = 90 deg.
Volume	1792.93(11) A^3	
Z, Calculated density	4, 1.604 Mg/m^3	
Absorption coefficient	1.255 mm^-1	
F(000)	892	
Crystal size	0.79 x 0.04 x 0.03 mm	
Theta range for data collection	1.69 to 26.37 deg.	
Limiting indices	-11<=h<=10, 0<=k<=30, 0<=l<=11	
Reflections collected / unique	31679 / 3659 [R(int) = 0.0597]	
Completeness to theta = 26.37	100.0 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.9633 and 0.4371	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	3659 / 0 / 253	
Goodness-of-fit on F^2	1.181	
Final R indices [I>2sigma(I)]	R1 = 0.0501, wR2 = 0.0906	
R indices (all data)	R1 = 0.0711, wR2 = 0.0979	
Largest diff. peak and hole	0.779 and -0.571 e.A^-3	

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Table S13.2. Selected bond lengths [Å] and angles [deg] for $[Cu(MEBIDA)(H7deaA)]_n$

Cu(1)-O(11)	1.946(2)
Cu(1)-O(21)	1.949(2)
Cu(1)-N(3)	1.987(3)
Cu(1)-N(10)	2.022(3)
Cu(1)-O(22)#1	2.309(2)
O(11)-Cu(1)-O(21)	167.48(10)
O(11)-Cu(1)-N(3)	97.51(11)
O(21)-Cu(1)-N(3)	95.01(10)
O(11)-Cu(1)-N(10)	84.50(10)
O(21)-Cu(1)-N(10)	83.40(10)
N(3)-Cu(1)-N(10)	162.96(12)
O(11)-Cu(1)-O(22)#1	88.16(9)
O(21)-Cu(1)-O(22)#1	91.23(9)
N(3)-Cu(1)-O(22)#1	94.87(10)
N(10)-Cu(1)-O(22)#1	102.12(10)

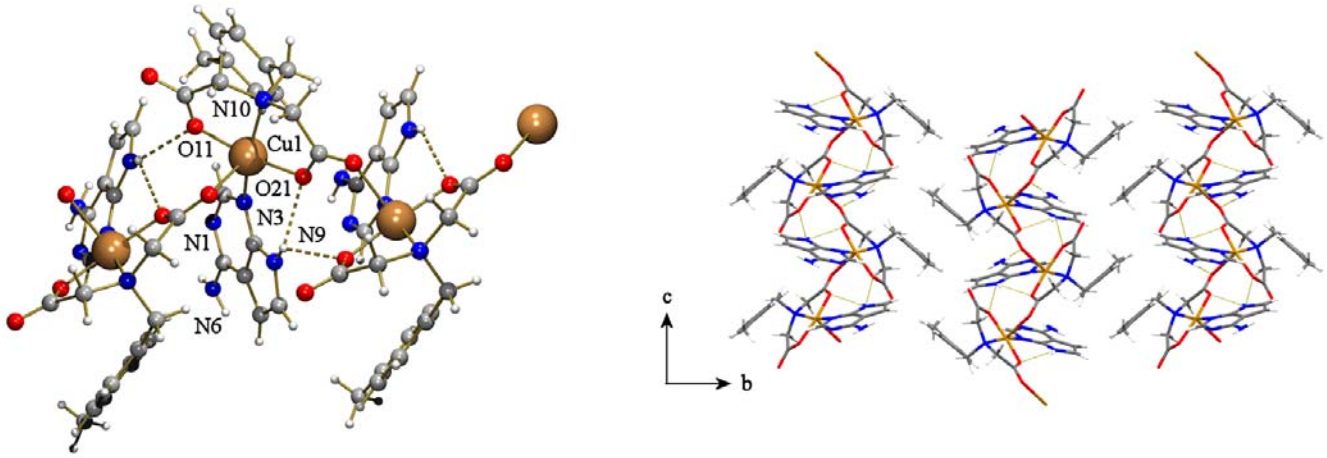
Symmetry transformations used to generate equivalent atoms:
#1 x,-y+1/2,z+1/2

Table S13.3. Hydrogen bonds for $[Cu(MEBIDA)(H7deaA)]_n$ [Å and deg.]

D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)
N(6)-H(6A)...O(22)#3	0.87	2.06	2.916(4)	168.8
N(6)-H(6B)...O(12)#4	0.88	2.15	2.938(4)	150.1
N(9)-H(9)...O(11)#2	0.88	2.21	2.835(4)	127.5
N(9)-H(9)...O(21)	0.88	2.27	2.899(4)	128.0

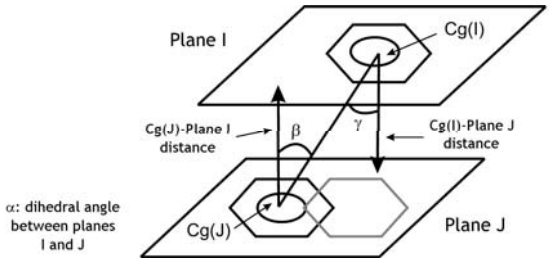
Symmetry transformations used to generate equivalent atoms:
#1 x,-y+1/2,z+1/2 #2 x,-y+1/2,z-1/2 #3 x-1,-y+1/2,z+1/2 #4 x-1,-y+1/2,z-1/2

Plot S13.4. Fragment of the polymer $[Cu(MEBIDA)(H7deaA)]_n$ (left) and view of the 3D network in the cb plane (right)



Compound **9** and **10** have similar structures and crystallize in the monoclinic $P2_1/c$ space group. The polymeric chains are connected by means of inter-molecular H-bonds, involving the exocyclic amino group of H7deaA (see Table S13.3), generating a layer structure. In **10**, despite the presence of the N-benzyl moiety in MEBIDA, no relevant pi,pi-stacking interactions were observed, therefore the 3D structure is ruled by hydrophobic interactions.

S14. PI,PI-Stacking interactions analyses of compounds 1, 4, 6, 7, 8 and 9



Parameters for π,π-stacking interactions (illustrated for two six-membered aromatic rings).

Note that those interactions considered in this paper are highlighted in red within each analysis.

S14.1. Analysis of compound **1** [Cu(TEBIDA)(H7azain)(H_2O)]·3H_2O

Ring 3 is the five-membered ring in the purine moiety of H7azain
Ring 4 is the six-membered ring in the purine moiety of H7azain

==========

Analysis of Short Ring-Interactions with Cg-Cg Distances < 6.0 Angstrom and Beta < 60.0Deg.

==========

Cg(I) Res(I)	Cg(J)	[ARU(J)]	Cg-Cg	Transformed J-Plane P, Q, R, S				Alpha	Beta	Gamma	CgI_Perp	CgJ_Perp	Slippage
Cg(3)	[1] -> Cg(4)	[5556.01]	3.5645	-0.1010	0.6139	-0.7829	-6.1688	1.896	16.89	18.51	3.3802	3.4107	
Cg(4)	[1] -> Cg(3)	[5556.01]	3.5645	-0.0762	0.6322	-0.7710	-6.1146	1.896	18.51	16.89	3.4107	3.3802	
Cg(4)	[1] -> Cg(4)	[5556.01]	3.5654	-0.1010	0.6139	-0.7829	-6.1688	0	17.15	17.15	3.4068	3.4068	1.051
		----------		----------									
		Min or Max	3.564		0.03	4.25	78.47	-4.519	-4.827				

[5556] = -X,-Y,1-Z

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S14.2. Analysis of compound **4** $[Cu(H_2EDTA)(H4abim)]\cdot 0.5H_2O$

Ring 5 is the five-membered ring in the purine moiety of H4abim
Ring 6 is the six-membered ring in the purine moiety of H4abim

==========

Analysis of Short Ring-Interactions with Cg-Cg Distances < 6.0 Angstrom and Beta < 60.0Deg.

==========

Cg(I)	Res(I)	Cg(J)	[ARU(J)]	Cg-Cg	Transformed J-Plane P, Q, R, S				Alpha	Beta	Gamma	CgI_Perp	CgJ_Perp	Slippage	
Cg(2)	[1] ->	Cg(6)	[1565.01]	5.567(4)	0.9924	-0.0428	-0.1152	0.1711	63.75(12)		36.15	80.18	0.9497(10)	-4.4949(11)	
Cg(5)	[1] ->	Cg(5)	[2555.01]	3.873(3)	-0.9945	0.0574	0.0873	1.7003	0		28.59	28.59	-3.4006(12)	-3.4005(12)	1.853
Cg(5)	[1] ->	Cg(5)	[2655.01]	4.032(3)	-0.9945	0.0574	0.0873	-5.5299	0		18.24	18.24	3.8296(12)	3.8297(12)	1.262
Cg(5)	[1] ->	Cg(6)	[2555.01]	3.566(3)	-0.9924	0.0428	0.1152	1.6808	1.81(15)		16.74	18.54	-3.3811(12)	-3.4150(12)	
Cg(5)	[1] ->	Cg(6)	[2655.01]	3.917(3)	-0.9924	0.0428	0.1152	-5.5342	1.81(15)		13.06	11.79	3.8338(12)	3.8152(12)	
Cg(6)	[1] ->	Cg(5)	[2555.01]	3.566(3)	-0.9945	0.0574	0.0873	1.7003	1.81(15)		18.54	16.74	-3.4150(12)	-3.3810(12)	
Cg(6)	[1] ->	Cg(5)	[2655.01]	3.917(3)	-0.9945	0.0574	0.0873	-5.5299	1.81(15)		11.79	13.06	3.8152(12)	3.8339(12)	
Cg(6)	[1] ->	Cg(6)	[2555.01]	4.375(3)	-0.9924	0.0428	0.1152	1.6808	0		39.79	39.79	-3.3615(12)	-3.3615(12)	2.800
Cg(6)	[1] ->	Cg(6)	[2655.01]	4.808(4)	-0.9924	0.0428	0.1152	-5.5342	0		36.73	36.73	3.8534(12)	3.8534(12)	2.876
			----------		----------										
		Min or Max	3.566		0.00				11.79	80.18		-3.415	-4.495		

[1565] = X,1+Y,Z
[2555] = -X,-Y,-Z
[2655] = 1-X,-Y,-Z

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S14.3. Analysis of compound **6** $[Cu_2(NBzIDA)_2(\mu_2\text{-N7,N9-H5abim})(H_2O)_2]\cdot H_2O$

Ring 4 is the six-membered ring of the benzyl-group of the chelating ligand NBzBIDA in one disordered position
Ring 5 is the six-membered ring of the benzyl-group of the chelating ligand NBzBIDA in the other disordered position (A)

==========

Analysis of Short Ring-Interactions with Cg-Cg Distances < 6.0 Angstrom and Beta < 60.0Deg.

==========

Cg(I)	Res(I)	Cg(J)	[ARU(J)]	Cg-Cg	Transformed J-Plane P, Q, R, S				Alpha	Beta	Gamma	CgI_Perp	CgJ_Perp	Slippage
Cg(3)	[1] ->	Cg(4)	[7667.01]	4.160(7)	0.6638	0.1975	-0.7214	-10.4373	20.5(7)	23.17	39.89	3.1927(11)	3.825(7)	
Cg(3)	[1] ->	Cg(4)	[8464.01]	4.160(7)	-0.6638	0.1975	0.7214	6.4629	20.5(7)	23.17	39.89	3.1928(11)	-3.825(7)	
Cg(3)	[1] ->	Cg(5)	[7667.01]	4.067(8)	0.6799	0.2025	-0.7047	-9.9546	21.7(8)	21.29	41.69	3.0379(11)	3.790(8)	
Cg(3)	[1] ->	Cg(5)	[8464.01]	4.067(8)	-0.6799	0.2025	0.7047	6.3507	21.7(8)	21.29	41.69	3.0379(11)	-3.790(8)	
Cg(4)	[1] ->	Cg(3)	[7667.01]	4.161(7)	0.4307	0.0000	-0.9025	-18.5290	20.5(7)	39.89	23.17	3.825(7)	3.1928(11)	
Cg(4)	[1] ->	Cg(3)	[8565.01]	4.161(7)	-0.4307	0.0000	0.9025	18.5290	20.5(7)	39.89	23.17	-3.825(7)	3.1928(11)	
Cg(4)	[1] ->	Cg(4)	[3777.01]	3.908(13)	0.6638	0.1975	-0.7214	-3.5738	0	23.65	23.65	-3.578(8)	-3.579(8)	1.568
Cg(4)	[1] ->	Cg(5)	[3777.01]	4.061(14)	0.6799	0.2025	-0.7047	-2.9232	1.4(10)	25.32	24.17	-3.704(8)	-3.670(9)	
Cg(5)	[1] ->	Cg(3)	[7667.01]	4.068(8)	0.4307	0.0000	-0.9025	-18.5290	21.7(8)	41.69	21.29	3.790(8)	3.0379(11)	
Cg(5)	[1] ->	Cg(3)	[8565.01]	4.068(8)	-0.4307	0.0000	0.9025	18.5290	21.7(8)	41.69	21.29	-3.790(8)	3.0379(11)	
Cg(5)	[1] ->	Cg(4)	[3777.01]	4.061(14)	0.6638	0.1975	-0.7214	-3.5738	1.4(10)	24.17	25.32	-3.670(9)	-3.705(8)	
Cg(5)	[1] ->	Cg(5)	[3777.01]	4.268(15)	0.6799	0.2025	-0.7047	-2.9232	0	27.20	27.20	-3.795(9)	-3.795(9)	1.951
			----------		----------									
			Min or Max	3.908					0.00	21.29	41.69	-3.825	-3.825	

[7667] = 3/2-X,3/2-Y,2-Z
[8464] = -1/2+X,3/2-Y,-1/2+Z
[8565] = 1/2+X,3/2-Y,1/2+Z
[3777] = 2-X,2-Y,2-Z

S14.4. Analysis of compound **7** [Cu(IDA)(H7deaA)(H_2O)]·2H_2O

Ring 3 is the five-membered ring in the purine moiety of H7deaA
Ring 4 is the six-membered ring in the purine moiety of H7deaA

Analysis of Short Ring-Interactions with Cg-Cg Distances < 6.0 Angstrom and Beta < 60.0Deg.

Cg(I)	Res(I)	Cg(J)	[ARU(J)]	Cg-Cg	Transformed J-Plane P, Q, R, S				Alpha	Beta	Gamma	CgI_Perp	CgJ_Perp	Slippage
Cg(3)	[1] ->	Cg(3)	[2676.01]	4.784(2)	-0.9404	0.3369	0.0452	3.9609	0	48.04	48.04	-3.1985(14)	-3.1984(14)	3.558
Cg(3)	[1] ->	Cg(3)	[2776.01]	3.495(2)	-0.9404	0.3369	0.0452	-2.4288	0	24.07	24.07	3.1912(14)	3.1914(14)	1.425
Cg(3)	[1] ->	Cg(4)	[2676.01]	3.500(2)	-0.9326	0.3581	0.0449	4.1024	1.29(17)	24.74	25.85	-3.1499(14)	-3.1790(13)	
Cg(3)	[1] ->	Cg(4)	[2776.01]	3.397(2)	-0.9326	0.3581	0.0449	-2.2342	1.29(17)	19.08	20.28	3.1868(14)	3.2107(13)	
Cg(4)	[1] ->	Cg(3)	[2676.01]	3.500(2)	-0.9404	0.3369	0.0452	3.9609	1.29(17)	25.85	24.74	-3.1790(13)	-3.1497(14)	
Cg(4)	[1] ->	Cg(3)	[2776.01]	3.398(2)	-0.9404	0.3369	0.0452	-2.4288	1.29(17)	20.28	19.08	3.2107(13)	3.1869(14)	
Cg(4)	[1] ->	Cg(4)	[2676.01]	3.2589(18)	-0.9326	0.3581	0.0449	4.1024	0	12.93	12.93	-3.1763(13)	-3.1763(13)	0.729
Cg(4)	[1] ->	Cg(4)	[2776.01]	4.4579(19)	-0.9326	0.3581	0.0449	-2.2342	0	44.85	44.85	3.1603(13)	3.1603(13)	3.144
			Min or Max	3.259					0.00	12.93	48.04	-3.198	-3.198	

[2676] = 1-X,2-Y,1-Z
[2776] = 2-X,2-Y,1-Z

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S14.5. Analysis of compound **8** $[Cu_2(MIDA)_2(\mu_2\text{-N1-N3-H7deaA})(H_2O)_2]\cdot 5H_2O$

Ring 7 is the five-membered ring in the purine moiety of H7deaA
Ring 8 is the six-membered ring in the purine moiety of H7deaA

Analysis of Short Ring-Interactions with Cg-Cg Distances < 6.0 Angstrom and Beta < 60.0Deg.

Cg(I)	Res(I)	Cg(J)	[ARU(J)]	Cg-Cg	Transformed J-Plane P, Q, R, S				Alpha	Beta	Gamma	CgI_Perp	CgJ_Perp	Slippage
Cg(7)	[1] ->	Cg(7)	[2555.01]	3.938(3)	-0.9815	-0.0075	0.1914	1.6915	0	30.77	30.77	-3.383(2)	-3.383(2)	2.015
Cg(7)	[1] ->	Cg(7)	[2655.01]	3.666(3)	-0.9815	-0.0075	0.1914	-5.1386	0	19.94	19.94	3.447(2)	3.447(2)	1.250
Cg(7)	[1] ->	Cg(8)	[2555.01]	3.640(3)	-0.9814	0.0039	0.1918	1.6774	0.7(3)	21.53	21.94	-3.376(2)	-3.386(2)	
Cg(7)	[1] ->	Cg(8)	[2655.01]	3.552(3)	-0.9814	0.0039	0.1918	-5.1523	0.7(3)	14.14	13.52	3.454(2)	3.445(2)	
Cg(8)	[1] ->	Cg(7)	[2555.01]	3.640(3)	-0.9815	-0.0075	0.1914	1.6915	0.7(3)	21.94	21.53	-3.386(2)	-3.376(2)	
Cg(8)	[1] ->	Cg(7)	[2655.01]	3.552(3)	-0.9815	-0.0075	0.1914	-5.1386	0.7(3)	13.52	14.14	3.445(2)	3.454(2)	
Cg(8)	[1] ->	Cg(8)	[2555.01]	4.465(3)	-0.9814	0.0039	0.1918	1.6774	0	41.29	41.29	-3.355(2)	-3.355(2)	2.946
Cg(8)	[1] ->	Cg(8)	[2655.01]	4.554(3)	-0.9814	0.0039	0.1918	-5.1523	0	40.27	40.27	3.475(2)	3.475(2)	2.943
			Min or Max		3.552					0.00	13.52	41.29	-3.386	-3.386

[2555] = -X,-Y,-Z
[2655] = 1-X,-Y,-Z

S14.6. Analysis of compound **9** $[Cu(NBzIDA)(H7deaA)]_n$

Ring 5 is the six-membered ring of the benzyl-group of the chelating ligand NBzBIDA

Analysis of Short Ring-Interactions with Cg-Cg Distances < 6.0 Angstrom and Beta < 60.0Deg.

Cg(I)	Res(I)	Cg(J)	[ARU(J)]	Cg-Cg	Transformed J-Plane P, Q, R, S				Alpha	Beta	Gamma	CgI_Perp	CgJ_Perp	Slippage
Cg(3)	[1] ->	Cg(4)	[4555.01]	4.486(3)	0.2495	-0.3045	0.9193	10.6094	35.1(2)	27.80	58.62	-2.3355(18)	3.9681(15)	
Cg(3)	[1] ->	Cg(5)	[2746.01]	5.528(3)	-0.7787	0.4485	-0.4388	-9.2987	62.8(2)	38.88	78.95	1.0603(19)	-4.3033(19)	
Cg(3)	[1] ->	Cg(5)	[2747.01]	5.562(3)	-0.7787	0.4485	-0.4388	-10.9439	62.8(2)	56.16	60.90	2.7055(19)	3.0976(19)	
Cg(3)	[1] ->	Cg(5)	[4554.01]	5.563(3)	0.7787	-0.4485	0.4388	6.0299	62.8(2)	35.94	66.61	2.2086(19)	-4.5040(19)	
Cg(4)	[1] ->	Cg(3)	[4554.01]	4.486(3)	0.2386	-0.2987	0.9240	3.2216	35.1(2)	58.62	27.80	3.9680(15)	-2.3355(18)	
Cg(4)	[1] ->	Cg(4)	[4554.01]	4.677(2)	0.2495	-0.3045	0.9193	3.2811	35	43.61	32.57	3.9418(15)	-3.3865(15)	
Cg(4)	[1] ->	Cg(4)	[4555.01]	4.677(2)	0.2495	-0.3045	0.9193	10.6094	35	32.57	43.61	-3.3866(15)	3.9419(15)	
Cg(4)	[1] ->	Cg(5)	[2746.01]	5.976(3)	-0.7787	0.4485	-0.4388	-9.2987	62.6(2)	44.00	75.32	1.5144(17)	-4.2989(19)	
Cg(5)	[1] ->	Cg(5)	[3667.01]	3.870(3)	-0.7787	-0.4485	-0.4388	-8.2023	0	22.59	22.59	-3.573(2)	-3.573(2)	1.486
Cg(5)	[1] ->	Cg(5)	[3767.01]	5.316(3)	-0.7787	-0.4485	-0.4388	-15.0440	0	52.07	52.07	3.269(2)	3.268(2)	4.193
			Min or Max	3.870					0.02	22.59	78.95	-3.573	-4.504	

[4555] = X,1/2-Y,1/2+Z
[2746] = 2-X,-1/2+Y,3/2-Z
[2747] = 2-X,-1/2+Y,5/2-Z
[4554] = X,1/2-Y,-1/2+Z
[3667] = 1-X,1-Y,2-Z
[3767] = 2-X,1-Y,2-Z

Analysis of X-H...Cg(Pi-Ring) Interactions (H..Cg < 3.0 Ang. - Gamma < 30.0 Deg)

X--H(I)	Res(I)	Cg(J)	[ARU(J)]	H..Cg	Transformed J-Plane P, Q, R, S				H-Perp	Gamma	X-H..Cg	X..Cg	X-H,Pi
C(31) -H(31A)	[1] ->	Cg(5)	[3767.01]	3.00	-0.7787	-0.4485	-0.4388	-15.0440	2.77	22.80	144	3.844(5)	31
			Min or Max	3.000					2.765	22.80	144.00	3.844	31.00

[3767] = 2-X,1-Y,2-Z

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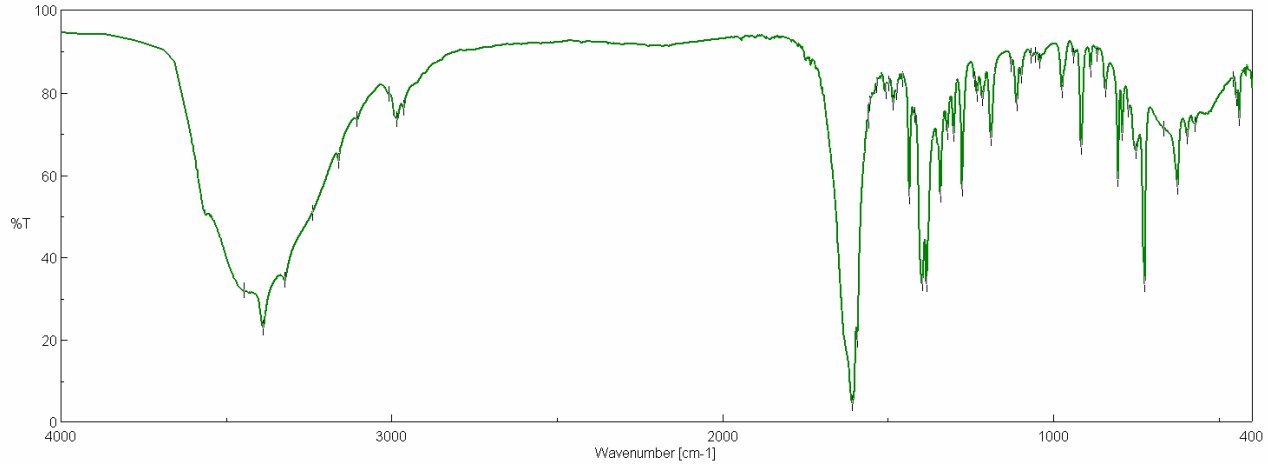
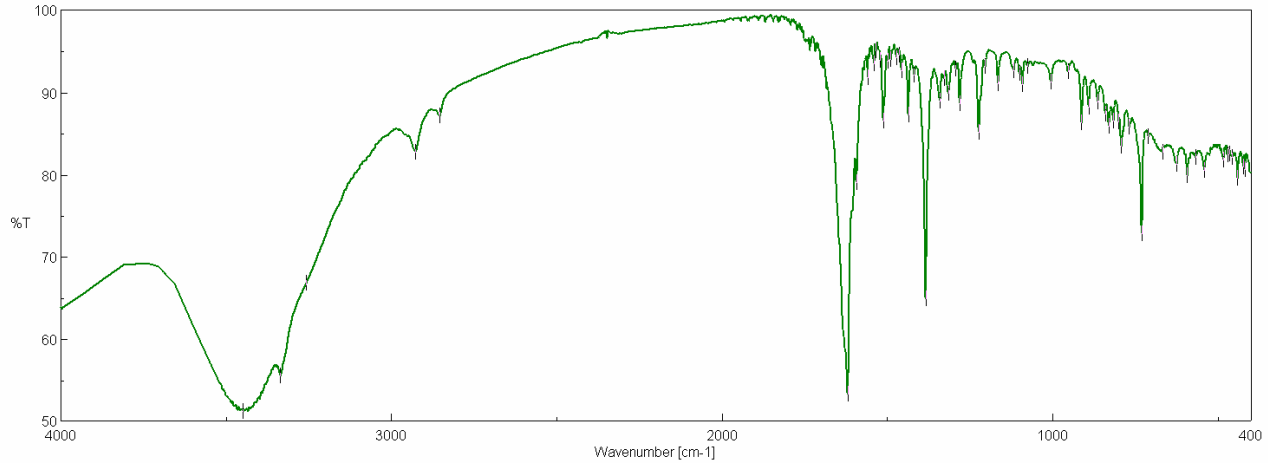
S15. FT-IR spectra

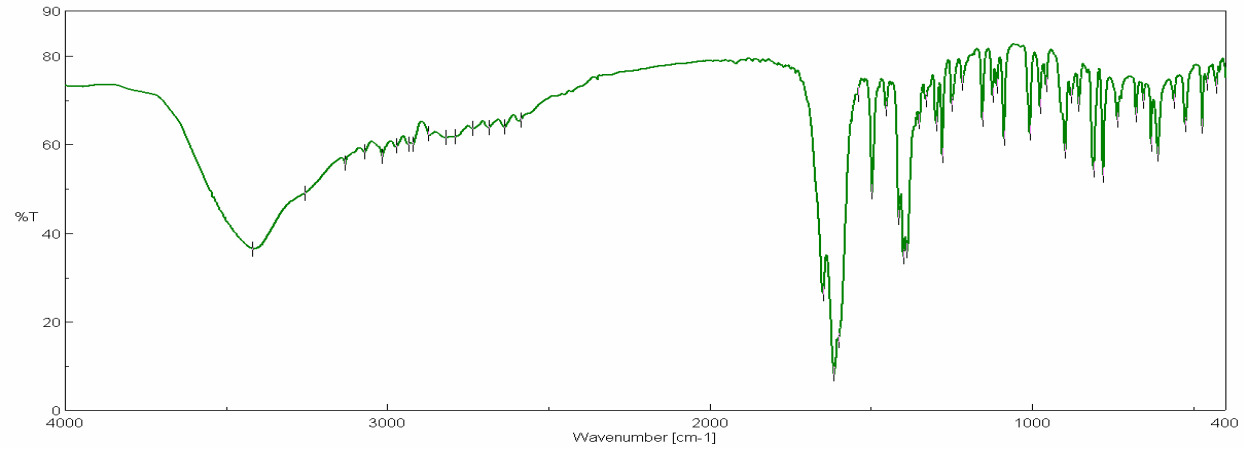
S15.1. FT-IR Spectra of [Cu(TEBIDA)(H7azain)(H_2O)]·3H_2O



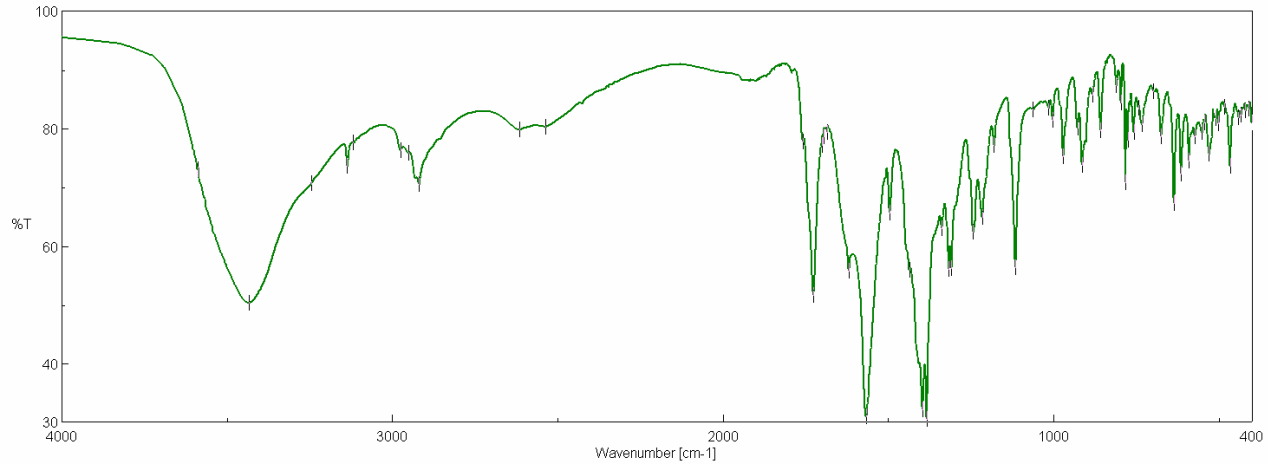
S15.2. FT-IR Spectra of {[Cu(FBIDA)(H7azain)]·H_2O}$_n$



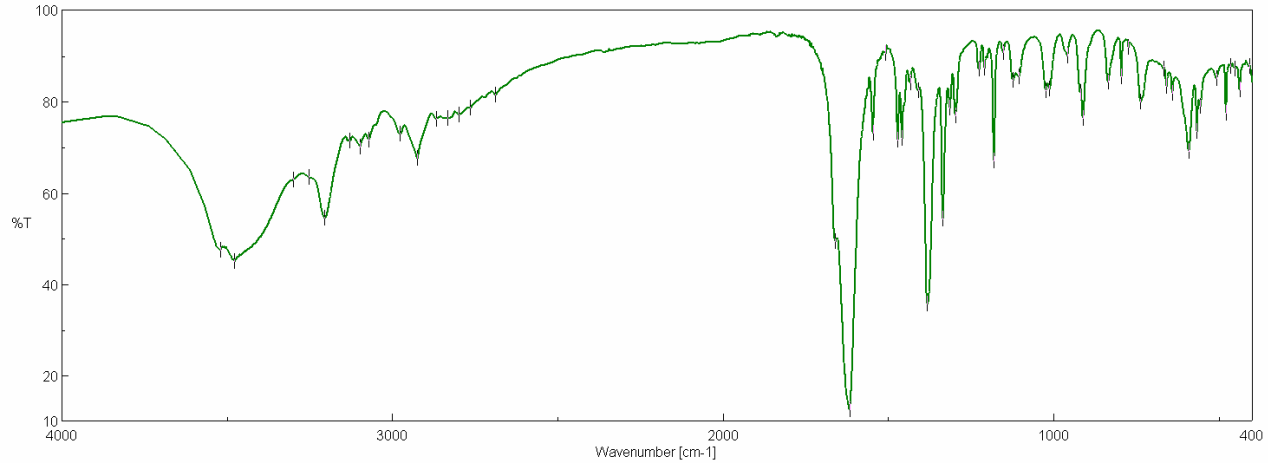
S15.3. FT-IR Spectra of {[Cu(CBIDA)(H4abim)]·2H_2O}$_n$



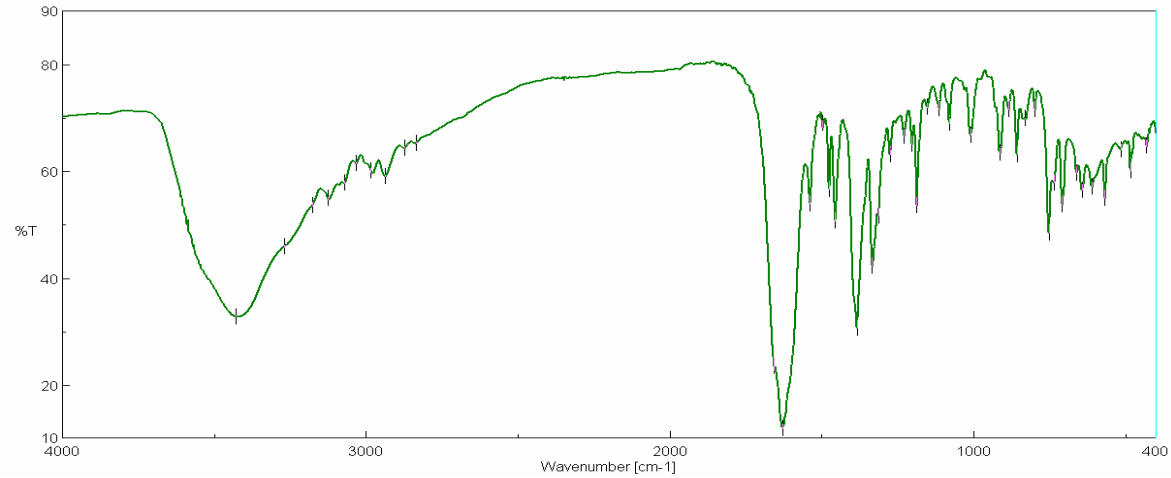
S15.4. FT-IR Spectra of [Cu(H_2EDTA)(H4abim)]·0.5H_2O



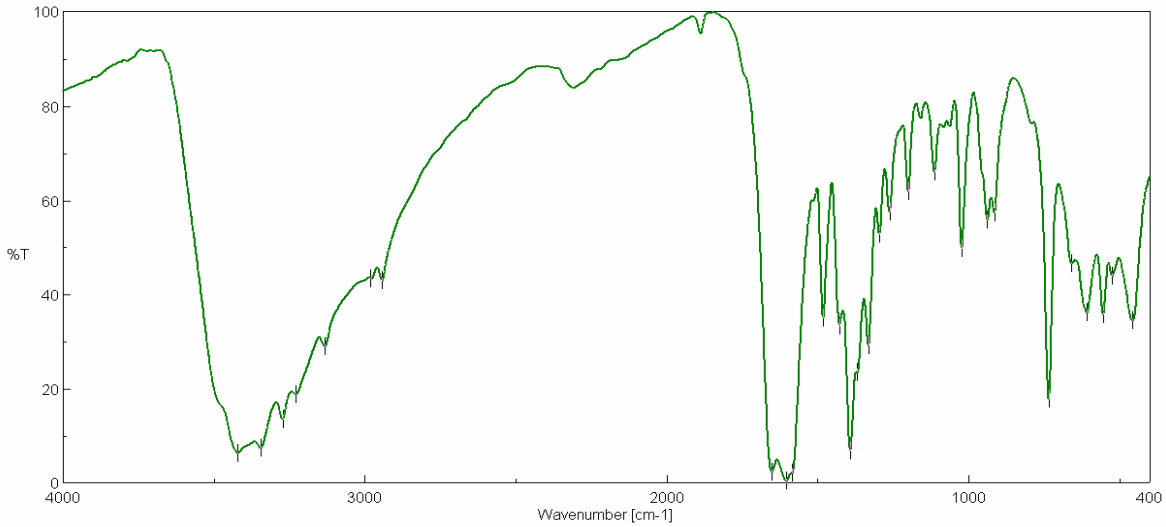
S15.5. FT-IR Spectra of {[Cu_2(IDA)$_2$(μ_2-N7,N9-H5abim)]·H_2O}$_n$



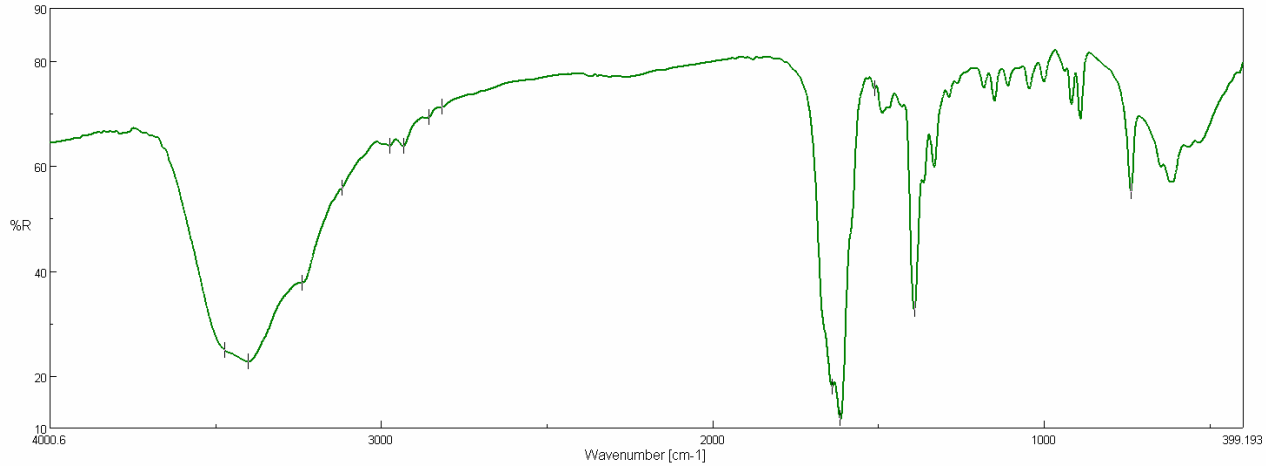
S15.6. FT-IR Spectra of [Cu_2(NBzIDA)$_2$(μ_2-N7,N9-H5abim)(H_2O)$_2$]·H_2O



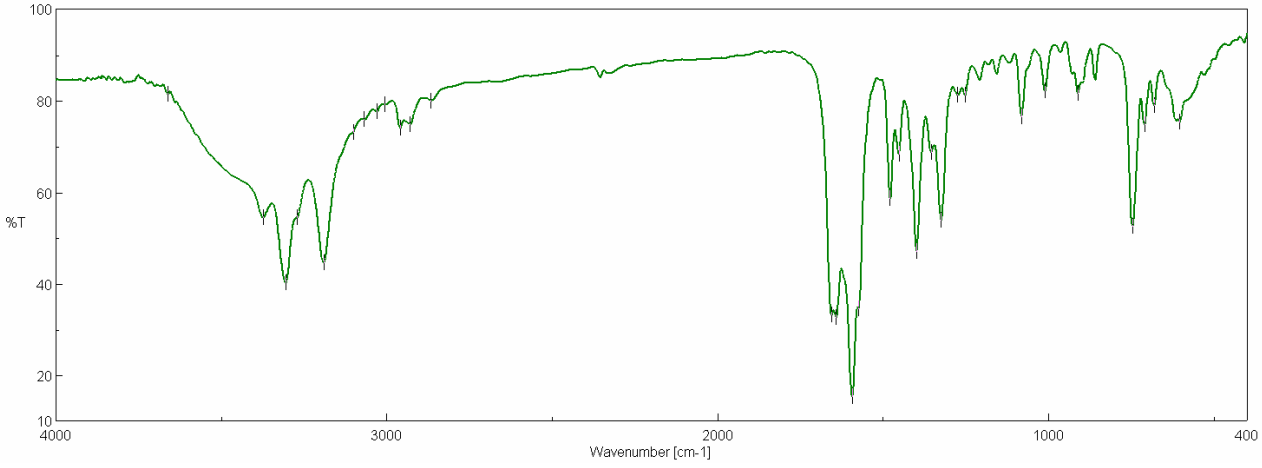
S15.7. FT-IR Spectra of $[Cu(IDA)(H7deaA)(H_2O)]\cdot 2H_2O$



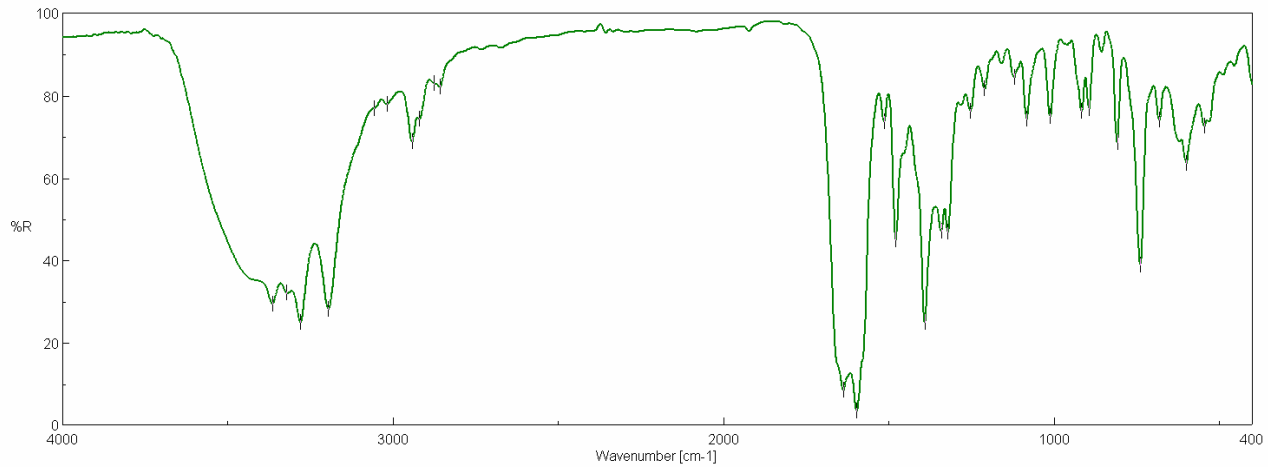
S15.8. FT-IR Spectra of $[Cu_2(MIDA)_2(\mu_2\text{-}N1,N3\text{-}H7deaA)(H_2O)_2]\cdot 5H_2O$



S15.9. FT-IR Spectra of $[Cu(NBzIDA)(H7deaA)]_n$



S15.10. FT-IR Spectra of $[Cu(MEBIDA)(H7deaA)]_n$



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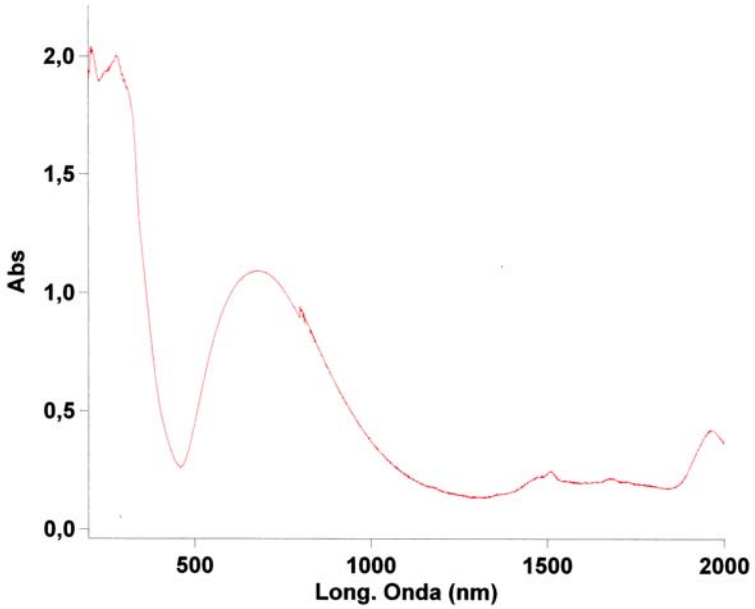
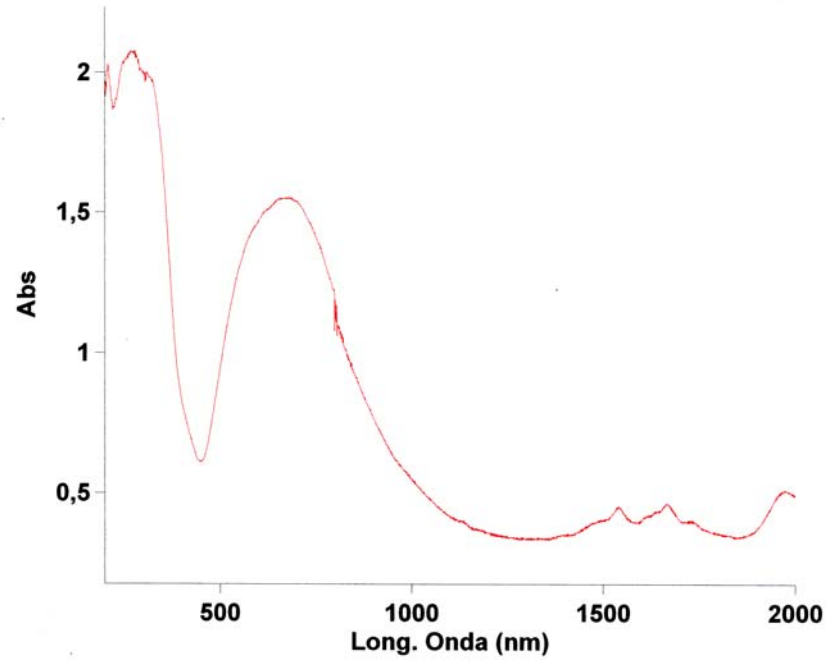
S16. Electronic spectra

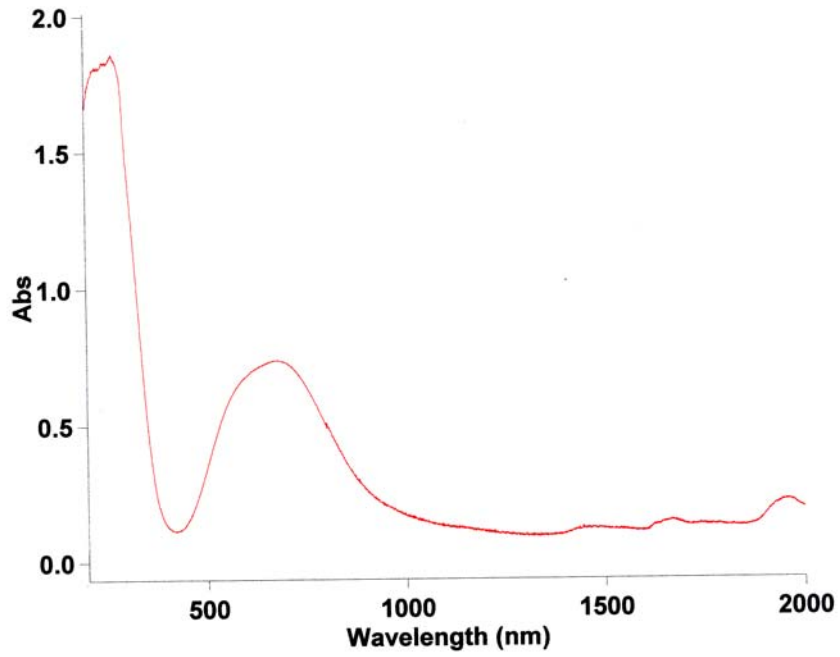
S.16.1. Electronic spectra of [Cu(TEBIDA)(H7azain)(H_2O)]·3H_2O



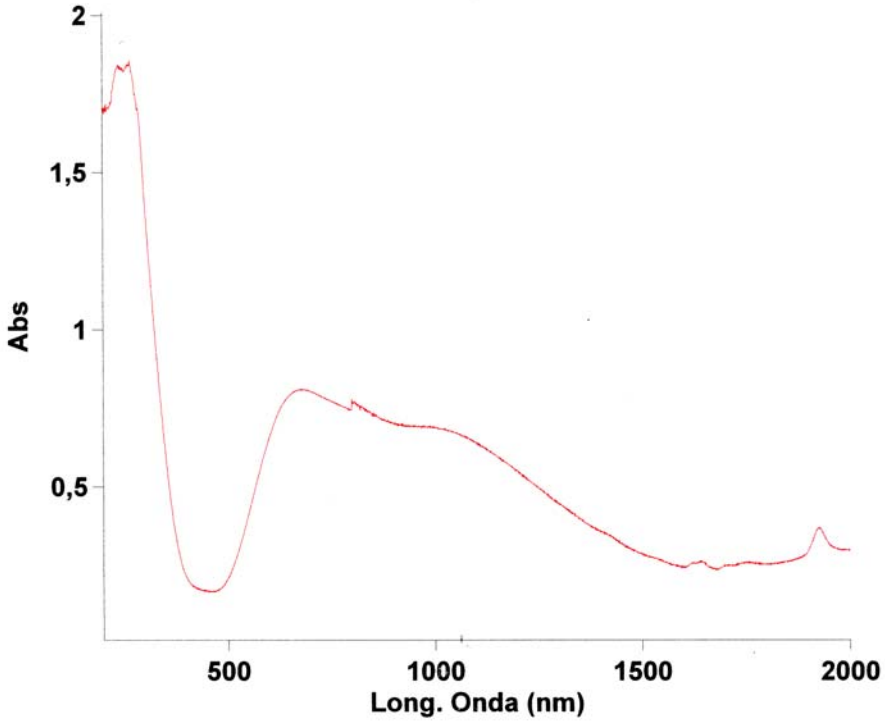
S16.2. Electronic spectra of {[Cu(FBIDA)(H7azain)]·H_2O}$_n$



S16.3. Electronic spectra of $\{[Cu(CBIDA)(H4abim)]\cdot 2H_2O\}_n$



S16.4. Electronic spectra of $[Cu(H_2EDTA)(H4abim)]\cdot 0.5H_2O$



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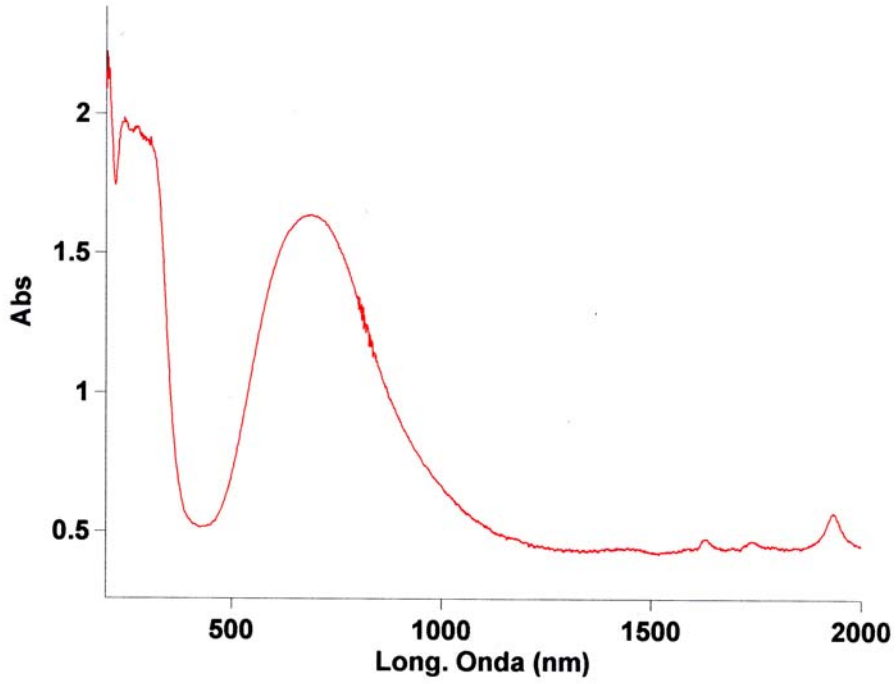
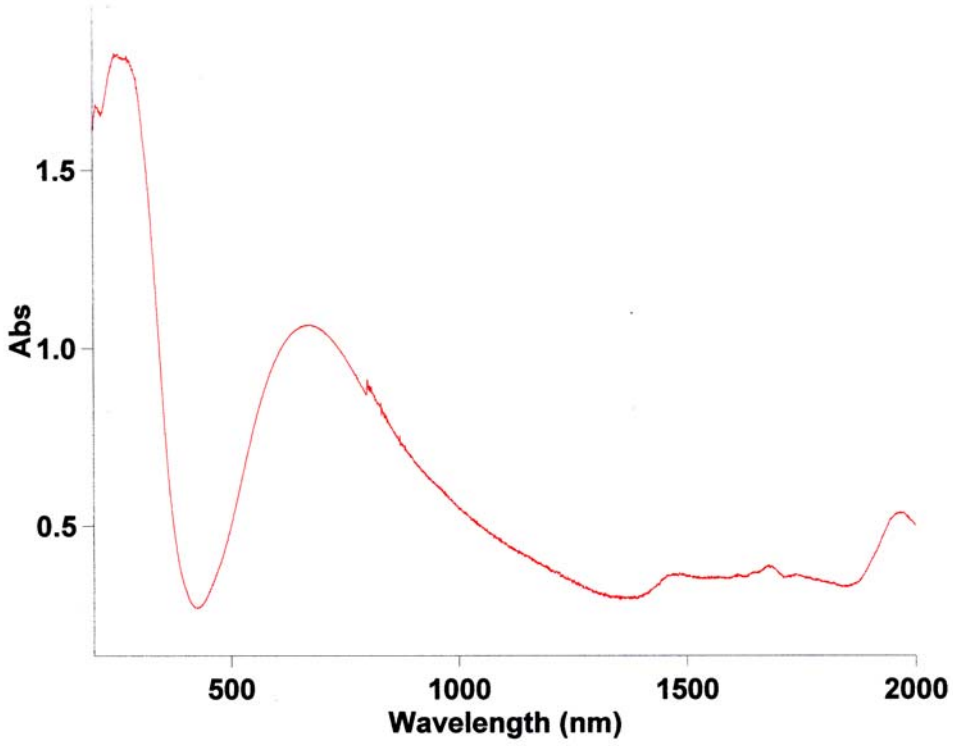
S16.5. Electronic spectra of $\{[Cu_2(IDA)_2(\mu_2\text{-}N7,N9\text{-}H5abim)]\cdot H_2O\}_n$



S16.6. Electronic spectra of $[Cu_2(NBzIDA)_2(\mu_2\text{-}N7,N9\text{-}H5abim)(H_2O)_2]\cdot H_2O$



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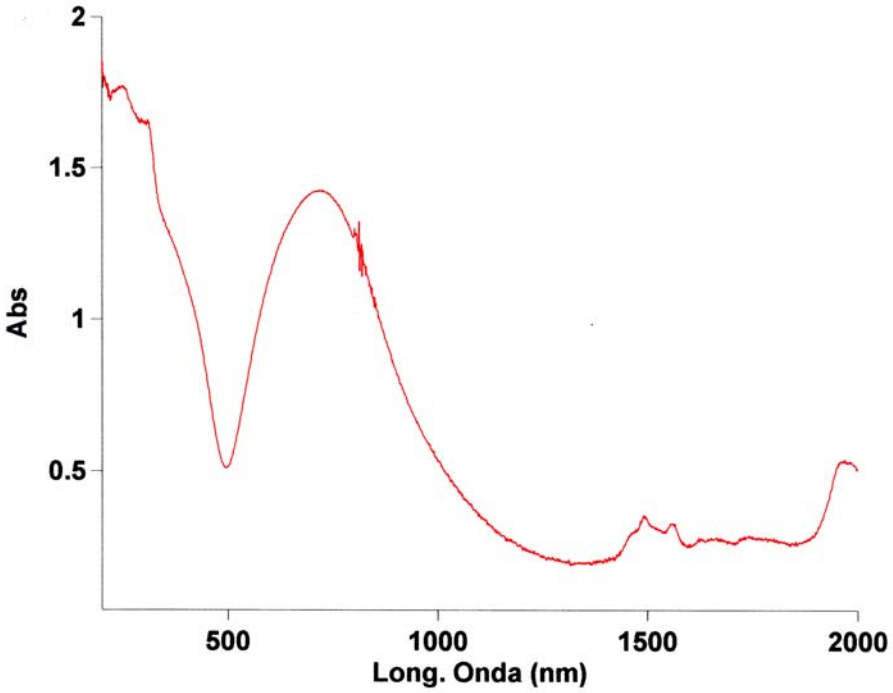
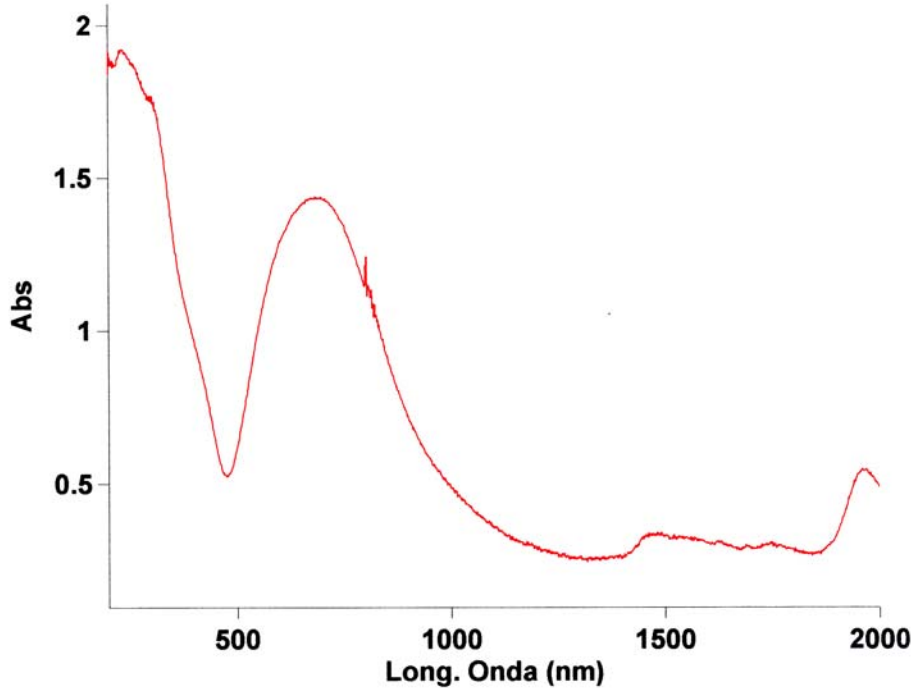
S16.7. Electronic spectra of $[Cu(IDA)(H7deaA)(H_2O)]\cdot 2H_2O$



S16.8. Electronic spectra of $[Cu_2(MIDA)_2(\mu_2\text{-N1-N3-H7deaA})(H_2O)_2]\cdot 5H_2O$



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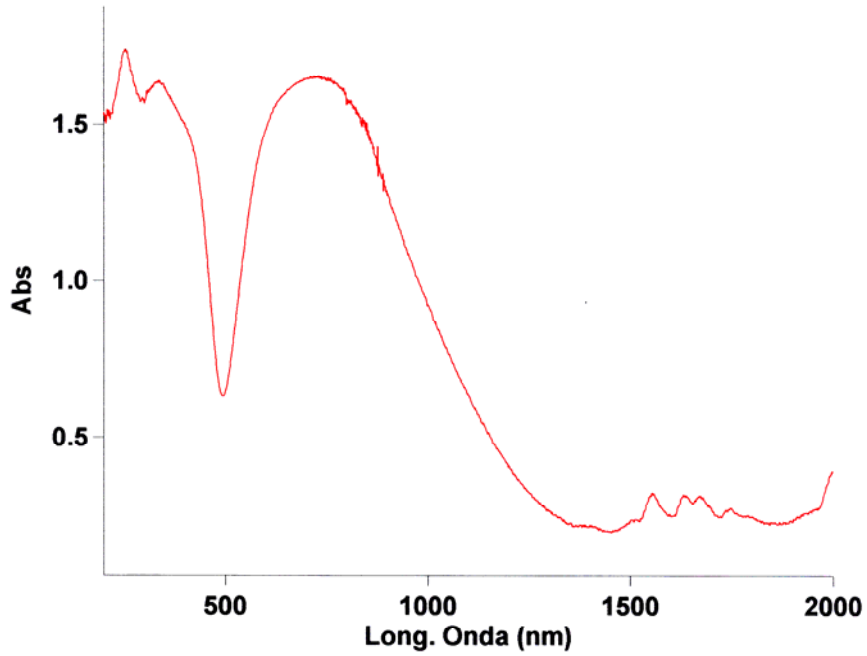
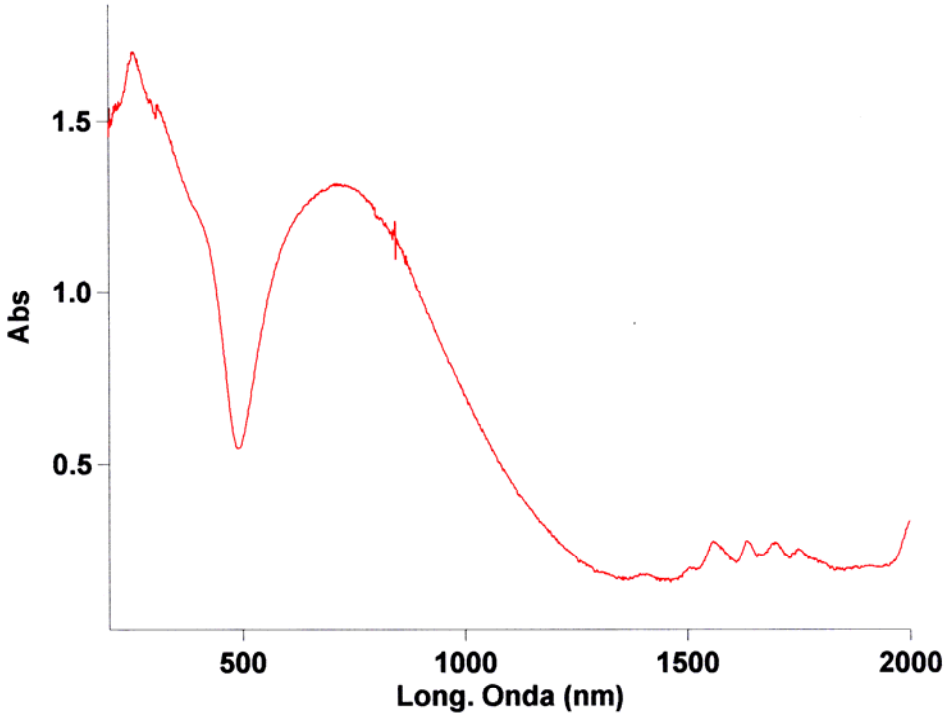
S16.9. Electronic spectra of $[Cu(NBzIDA)(H7deaA)]_n$



S16.10. Electronic spectra of $[Cu(MEBIDA)(H7deaA)]_n$



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S17. EPR spectra

X- and Q-band EPR measurements all the compounds were carried out on powdered samples at room temperature. In all cases, the spin Hamiltonian parameters were estimated by comparison of the experimental spectra with those obtained by a computer simulation program working at the second order of the perturbation theory. The obtained g-values are:

X-band

Muestra	**Frec. (GHz)**	**g_1**	**g_2**	**g_3**	**<g>**
M1	9.4944	2.264	2.101	2.044	2.136
M2*	9.4910	2.131 (2.175)	2.131 (2.140)	2.131 (2.090)	2.131 (2.135)
M3	9.4936	2.240	2.077	2.066	2.128
M4	9.4942	2.312	2.094	2.050	2.152
M5	9.4950	2.236	2.096	2.065	2.132
M6	9.4937	2.244	2.083	2.055	2.127
M7	9.4936	2.273	2.061	2.061	2.132
M8	9.4932	2.242	2.090	2.062	2.131
M9**	9.4933	2.209	2.142	2.067	2.139
M10***	9.4947	2.217	2.102	2.072	2.130

* Broad signal. Anisotropic values are needed to fit the spectrum. However, the obtained values can not be defined as accurate.
** Similar to the previous case but with more reliable g values.
*** Mixthure of phases. The spectrum corresponds to the major phase but more contributions can be observed.

Q-band

Muestra	**Frec. (GHz)**	**g_1**	**g_2**	**g_3**	**<g>**
M1	34.074	2.266	2.101	2.044	2.137
M2*	34.104	*	*	*	*
M3	34.101	2.246	2.077	2.065	2.129
M4	34.102	2.315	2.094	2.048	2.152
M5**	34.102	2.235/2.242	2.099/2.099	2.066/2.062	2.133/2.134
M6	34.074	2.249	2.088	2.057	2.131
M7	34.082	2.280	2.066	2.062	2.136
M8***	34.076	2.245	2.093	2.059	2.132
M9****	34.069	2.208	2.142	2.066	2.138
M10*****	34.069	*****	*****	*****	*****

This band is much more sensitive, fitting values are more reliable but, in constrast, impurities or preferential orientations can be also observed in the spectrum.

* Broad signal, bad resolution. A good fitting is not posible.
** Signal with two extra-peaks not observed in the X-band. The average g value is nearly the same as the X-band what could be attributted to modifications in part of the simple.
*** Signal with clear preferential orientations
**** Very broad signal. It can be fitted very good although the resulting g values are not that reliable.
***** At least two overlapping signals.

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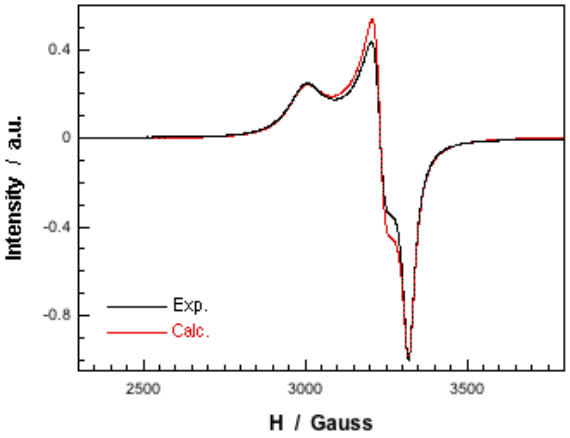
The X-band EPR spectra exhibit near axial symmetries for the *g* tensor but an appreciable extent of rhombicity can be detected operating at Q band. In all cases, the minor *g* value is higher than 2.04 as expected for mainly d*x*2-*y*2 ground states derived from square pyramidal or axially elongated octahedral geometries in Cu(II) ions. No “half-field” transitions or hyperfine lines could be observed in any case.

Experimental and Calculated X-band EPR spectra:

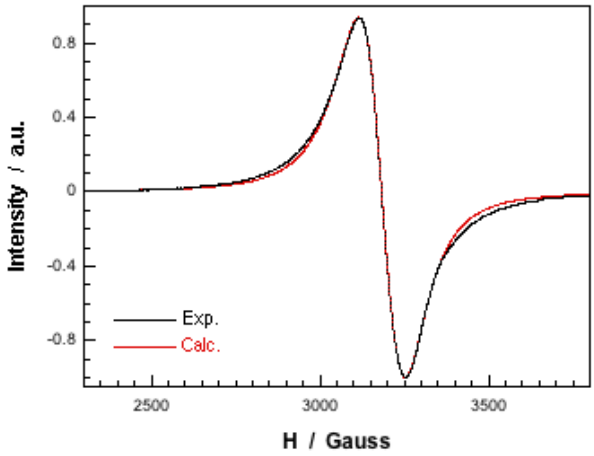
Compound (1)

$[Cu(TEBIDA)(H7azain)(H_2O)]\cdot 3H_2O$



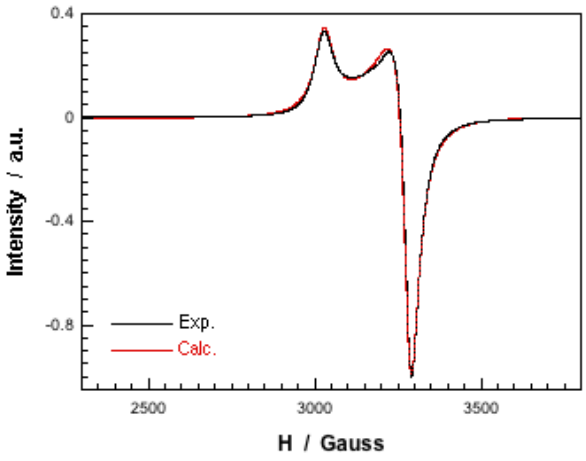
Compound (2)

$\{[Cu(FBIDA)(H7azain)]\cdot H_2O\}_n$



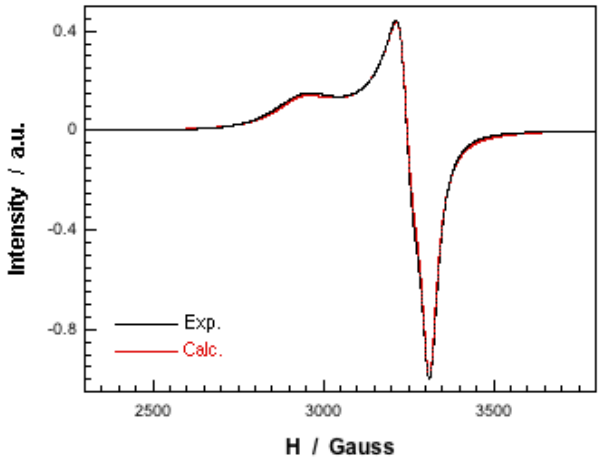
Compound (3)

$\{[Cu(CBIDA)(H4abim)]\cdot 2H_2O\}_n$



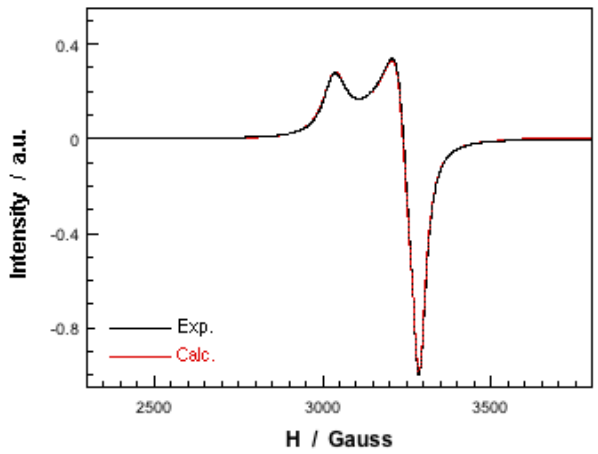
Compound (4)

$[Cu(H_2EDTA)(H4abim)]\cdot 0.5H_2O$



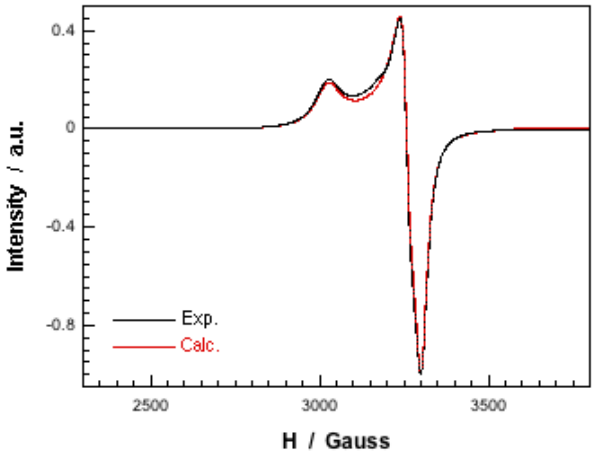
Compound (5)

$\{[Cu_2(IDA)_2(\mu_2\text{-N7,N9-H5abim})]\cdot H_2O\}_n$



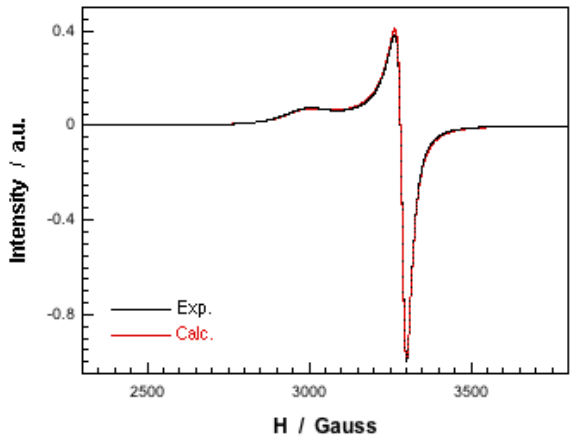
Compound (6)

$[Cu_2(NBzIDA)_2(\mu_2\text{-N7,N9-H5abim})(H_2O)_2]\cdot H_2O$



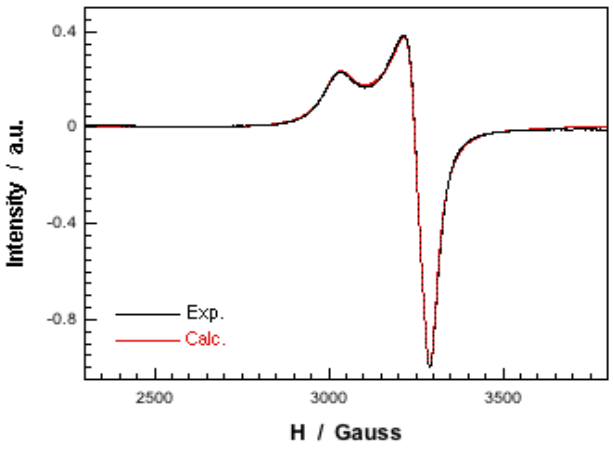
Compound (7)

$[Cu(IDA)(H7deaA)(H_2O)]\cdot 2H_2O$



Compound (8)

$[Cu_2(MIDA)_2(\mu_2\text{-N1,N3-H7deaA})(H_2O)_2]\cdot 5H_2O$



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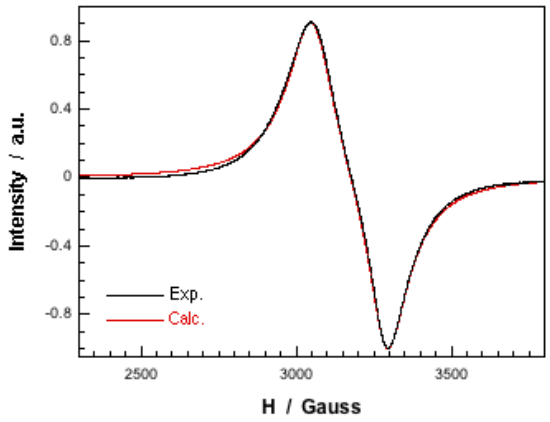
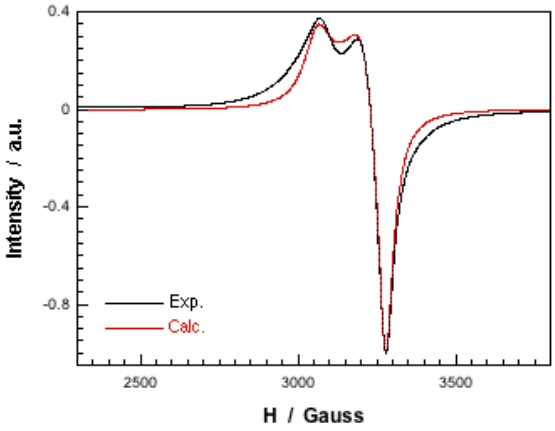
Compound (9)

$[Cu(NBzIDA)(H7deaA)]_n$



Compound (10)

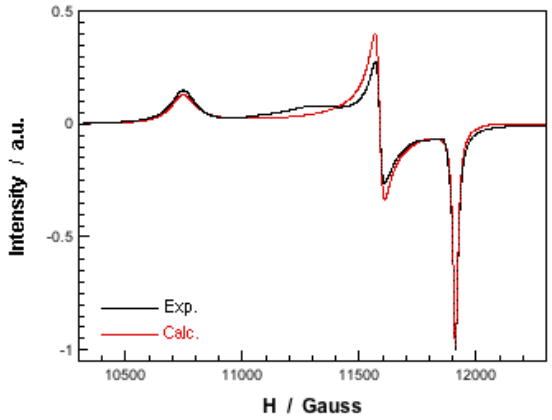
$[Cu(MEBIDA)(H7deaA)]_n$



Experimental and Calculated Q-band EPR spectra:

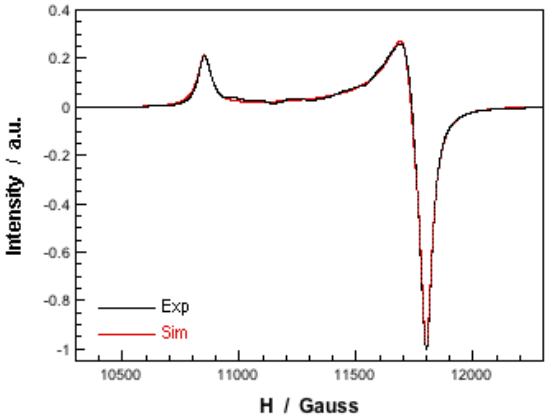
Compound (1)

$[Cu(TEBIDA)(H7azain)(H_2O)]\cdot 3H_2O$



Compound (3)

$\{[Cu(CBIDA)(H4abim)]\cdot 2H_2O\}_n$



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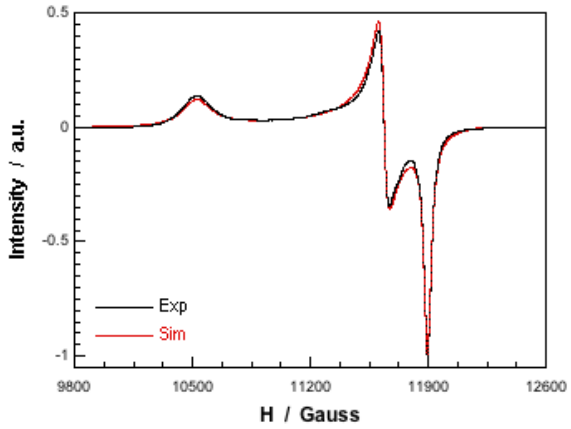
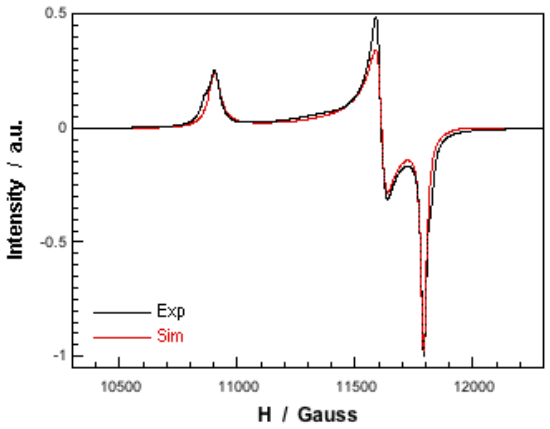
Compound (4)

$[Cu(H_2EDTA)(H4abim)]\cdot 0.5H_2O$



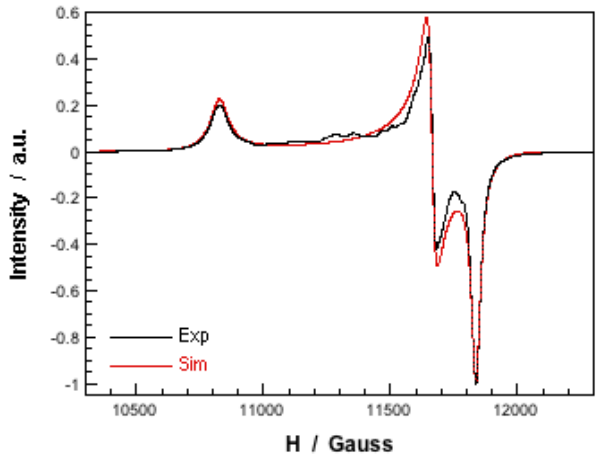
Compound (5)

$\{[Cu_2(IDA)_2(\mu_2\text{-}N7,N9\text{-}H5abim)]\cdot H_2O\}_n$



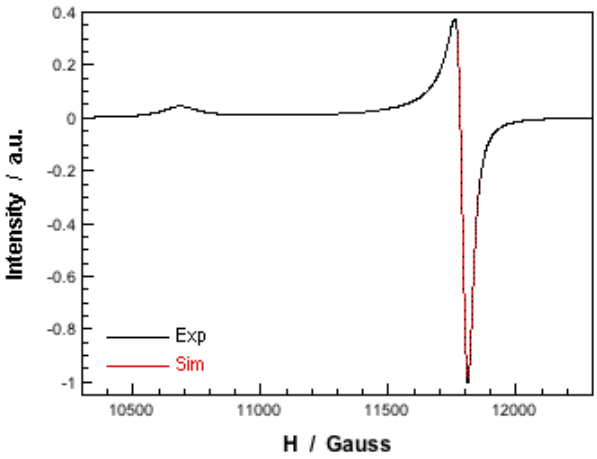
Compound (6)

$[Cu_2(NBzIDA)_2(\mu_2\text{-}N7,N9\text{-}H5abim)(H_2O)_2]\cdot H_2O$



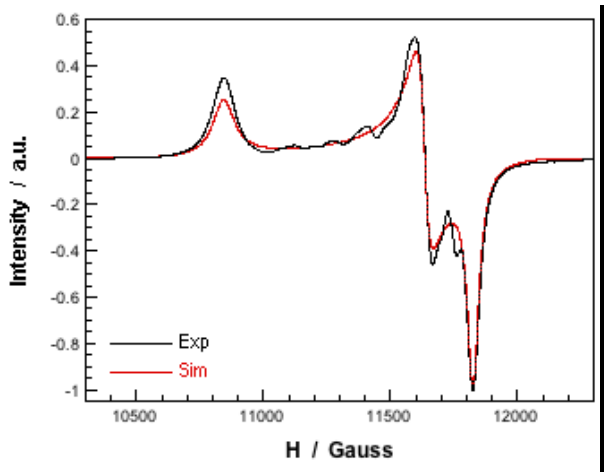
Compound (7)

$[Cu(IDA)(H7deaA)(H_2O)]\cdot 2H_2O$



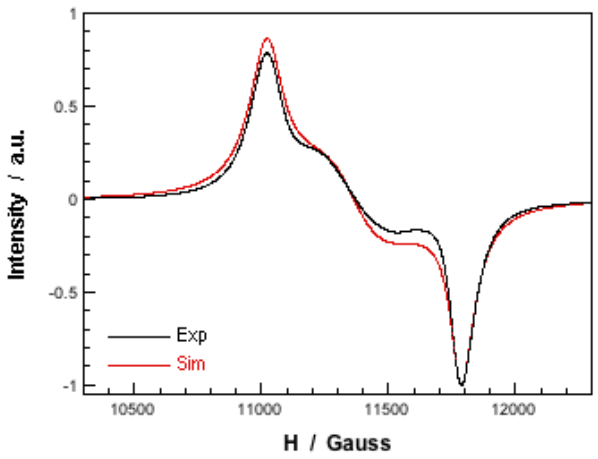
Compound (8)

$[Cu_2(MIDA)_2(\mu_2\text{-}N1,N3\text{-}H7deaA)(H_2O)_2]\cdot 5H_2O$



Compound (9)

$[Cu(NBzIDA)(H7deaA)]_n$



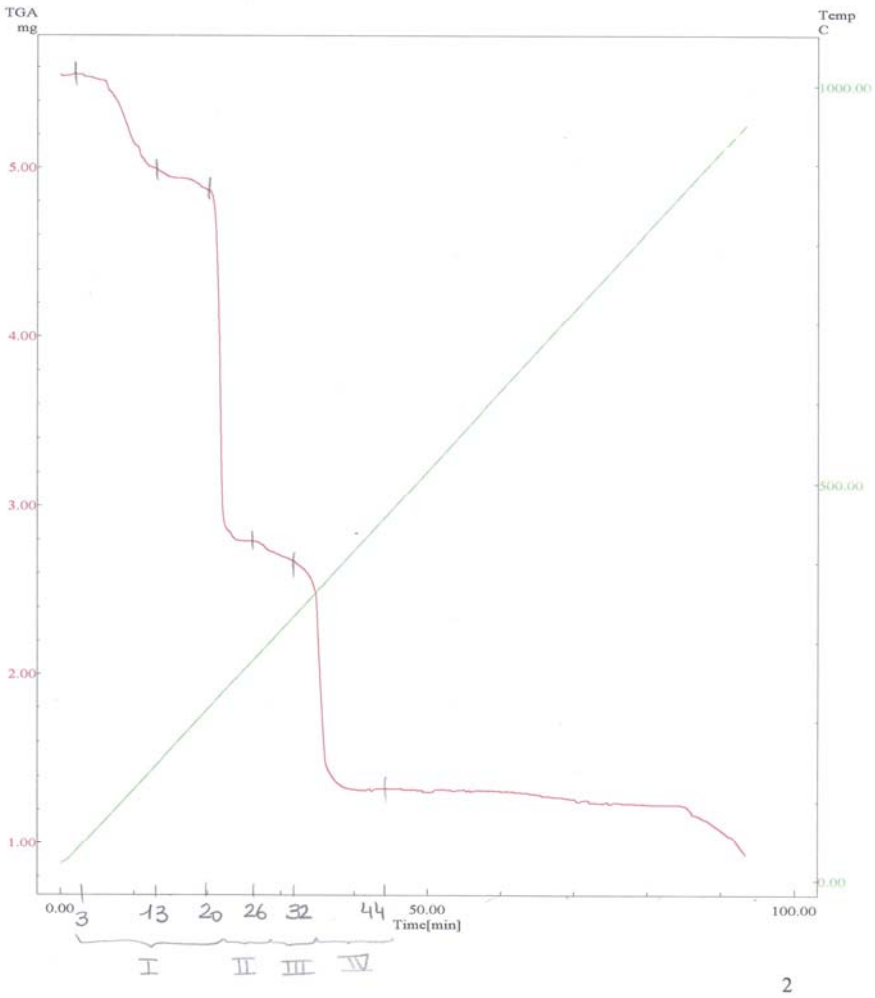
S18. Thermogravimetric analysis of compound $[Cu_2(MIDA)_2(\mu_2\text{-N1-N3-H7deaA})(H_2O)_2]\cdot 5H_2O$ (**8**)

TG-study of compound $[Cu_2(MIDA)_2(\mu_2\text{-N1-N3-H7deaA})(H_2O)_2]\cdot 5H_2O$ with identification by FT-IR spectroscopy of the evolved gasses during pyrolisis.

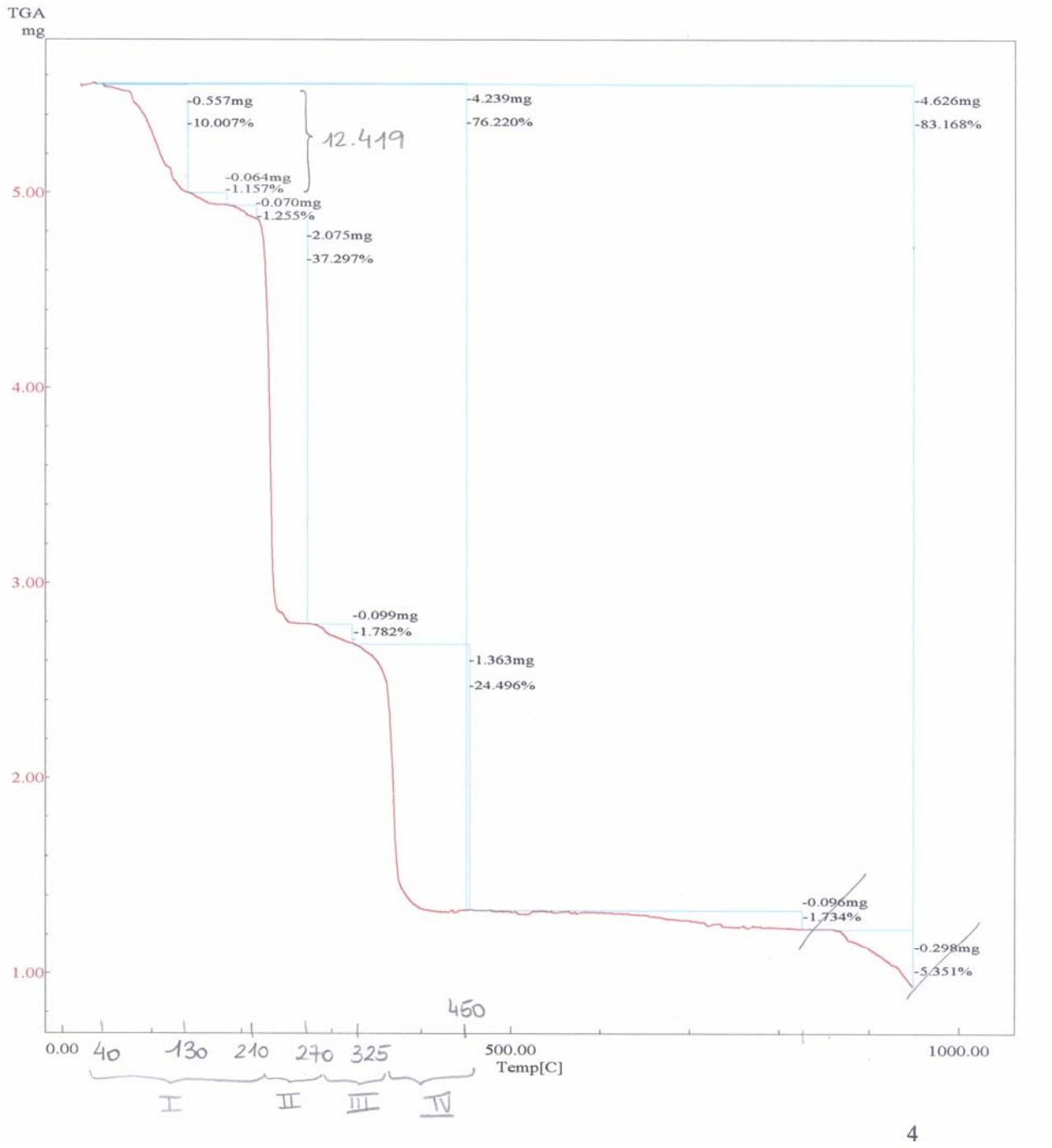
Sample C-616: 5.562 mg.
Air-dry flow: 100.0 mL/minute.
Increasing rate of temperature: 10 ºC/minute.

Note: the experimental weight loss after 450 ºC is not considered within the experiment since does not correspond t the pyrolisis of the compound. Thus, small amounts of particles can be held within the CuO residue, what explains the presence of trace amounts of CO_2 in the FT-IR after minute 44 and the small error in the calculation of %CuO residue. The final drop of the TG curve at 870 ºC is because part of the sample fell down from the thermo-balance at the end of the experiment due to mini-blast of the CuO residue because of such high temperatures.

a) The TG plot of compound **8** as a function of the time (bottom axis) and temperature (right axis). Weight sample in the left axis.



b) The TG-plot of compound **8** with weight loss as a function of the temperature (bottom axis)



c) The four sheets below show a time-spaced sequential series of twenty six FT-IR spectra, recorded at increasing times (minutes) which enable the identification of the evolved gasses. These pictures are followed by the Table-TG, where the results and interpretation are summarized. The spectra 1 to 6 correspond to the first step (water loss), whereas spectra 7 to 22 revealed gases evolved during the different pyrolitic steps that yield a residue of 2CuO. Spectra 23 to 26 are considered the tail of the experiment.

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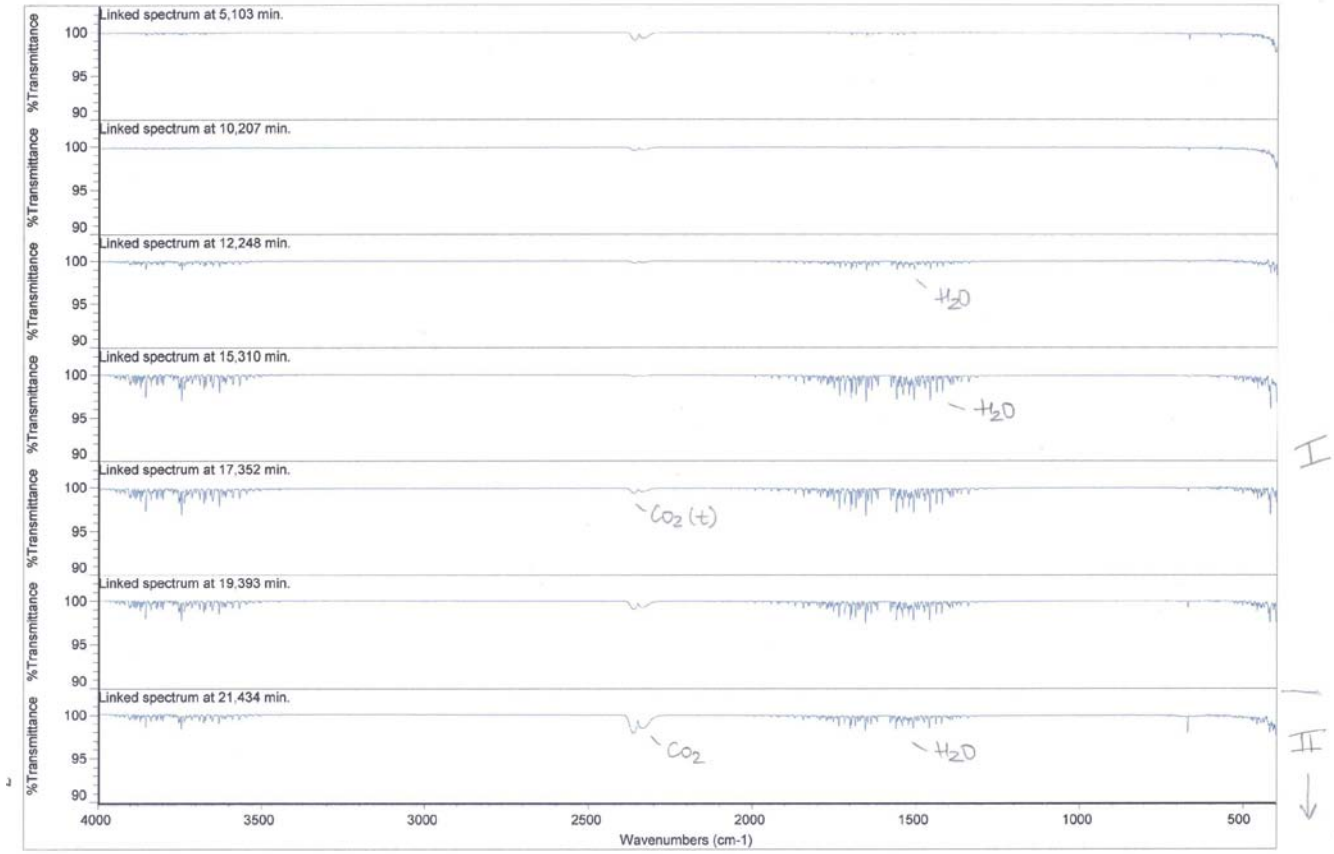
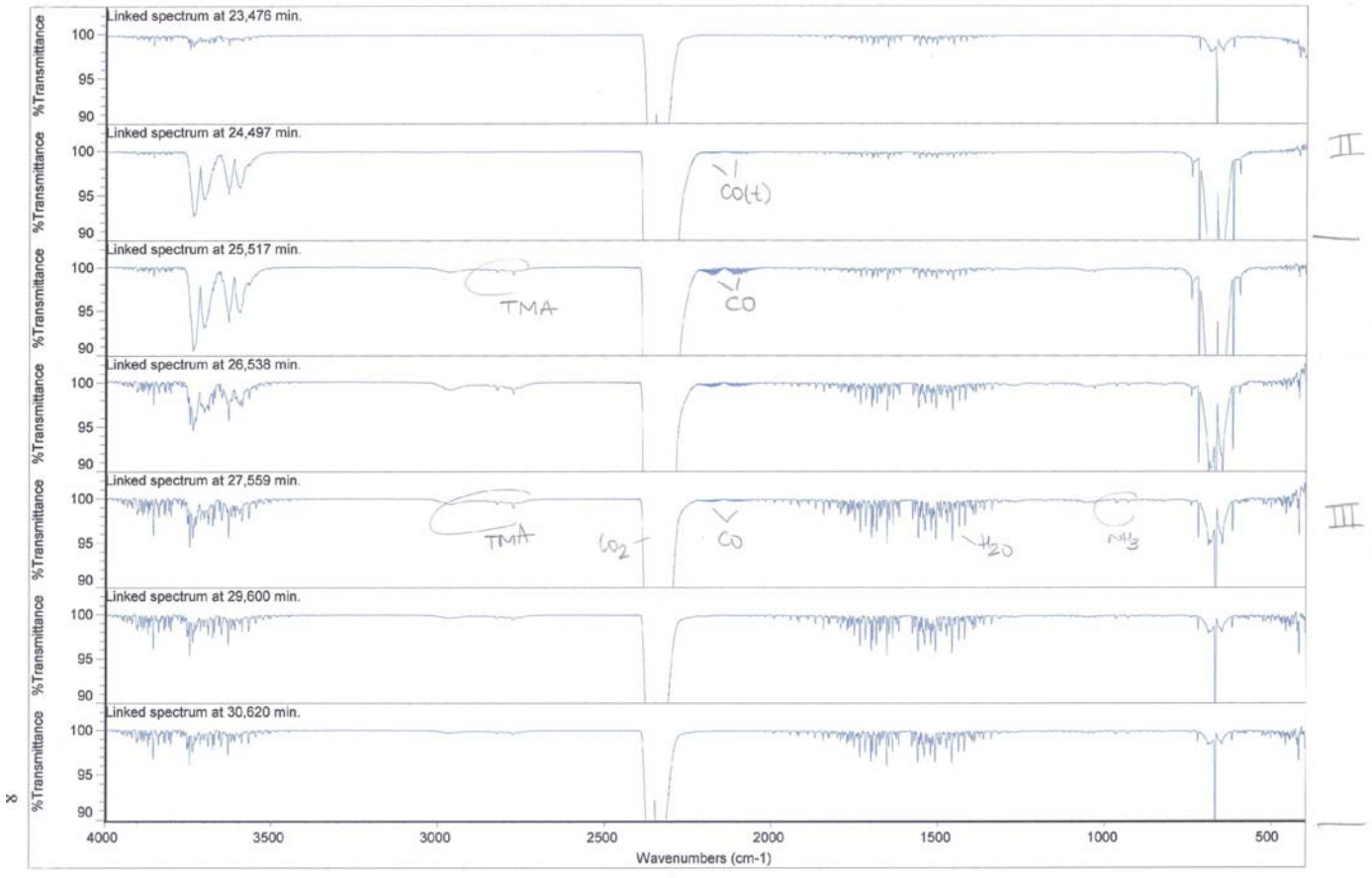
Sheet 1:



Sheet 2:



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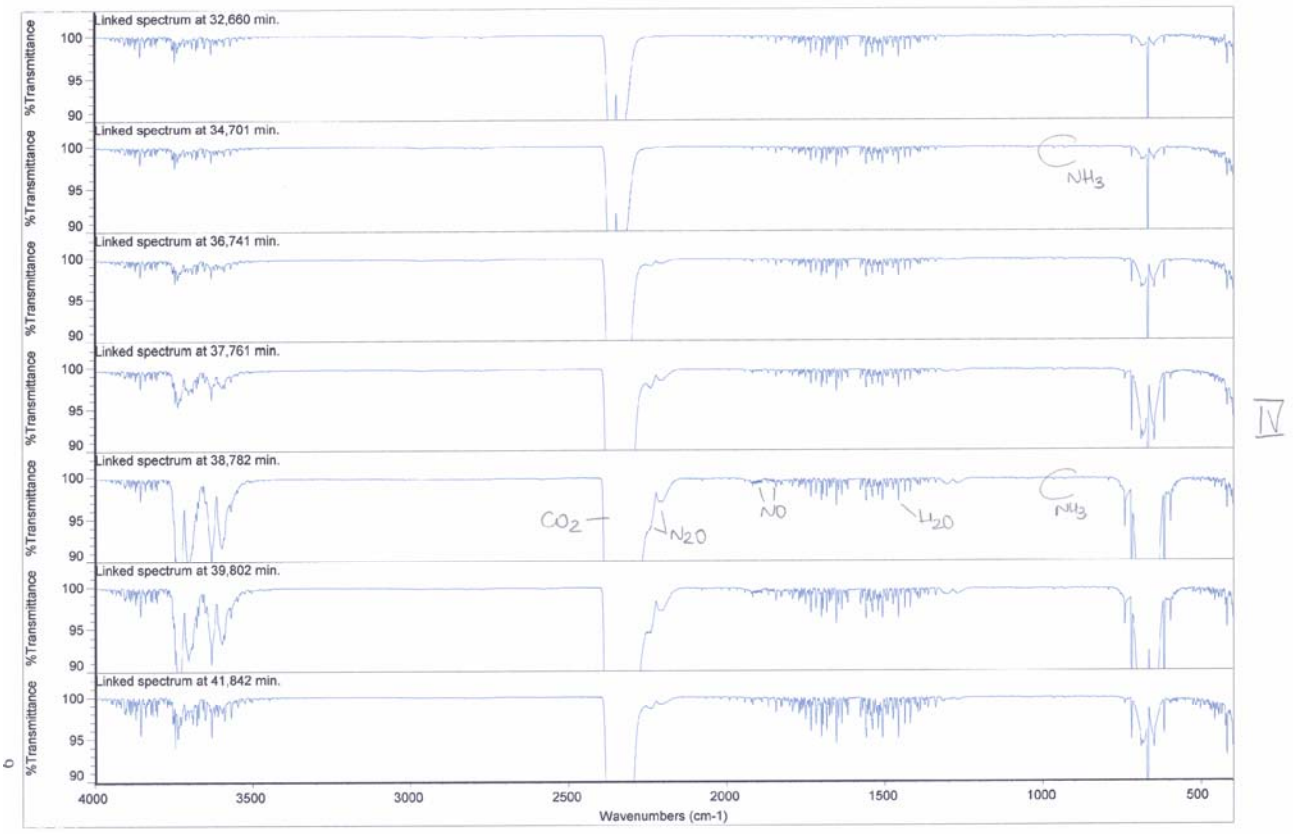
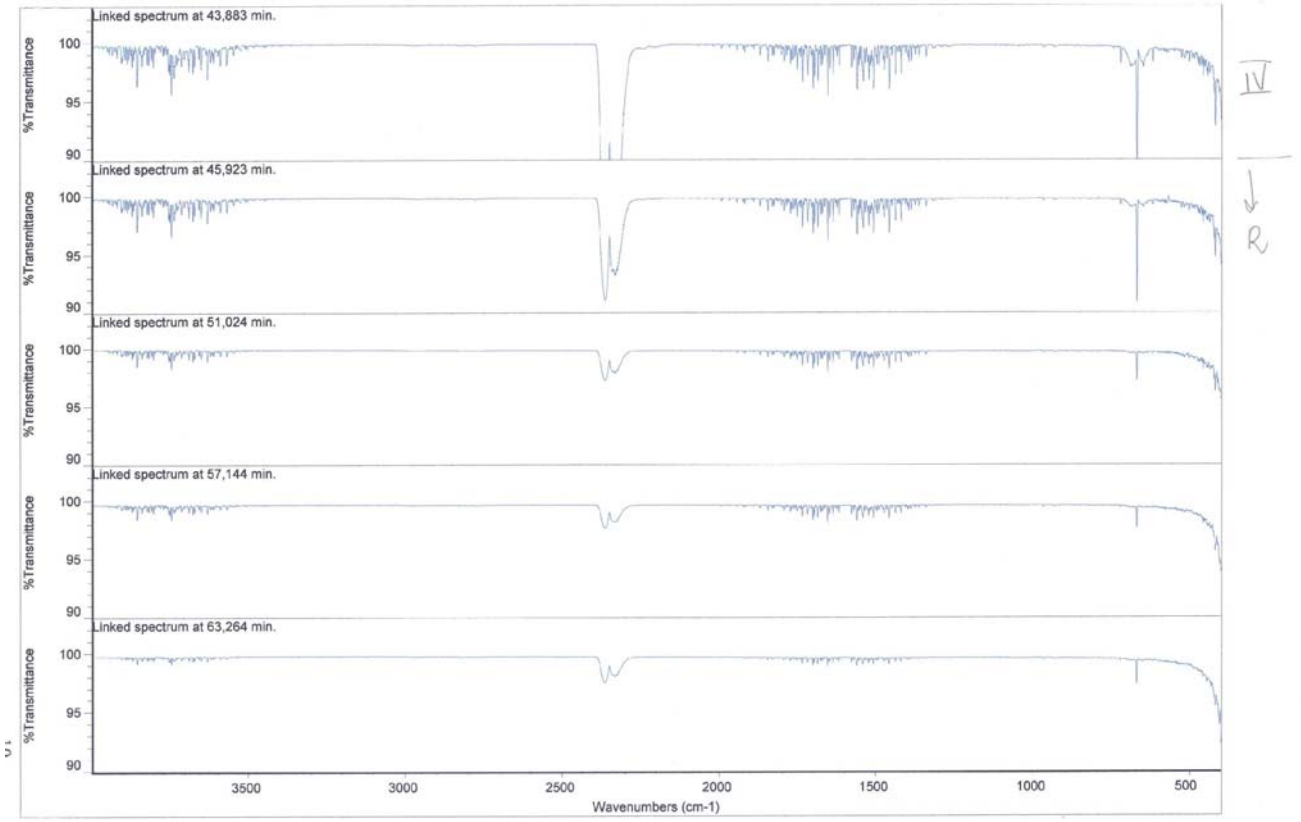
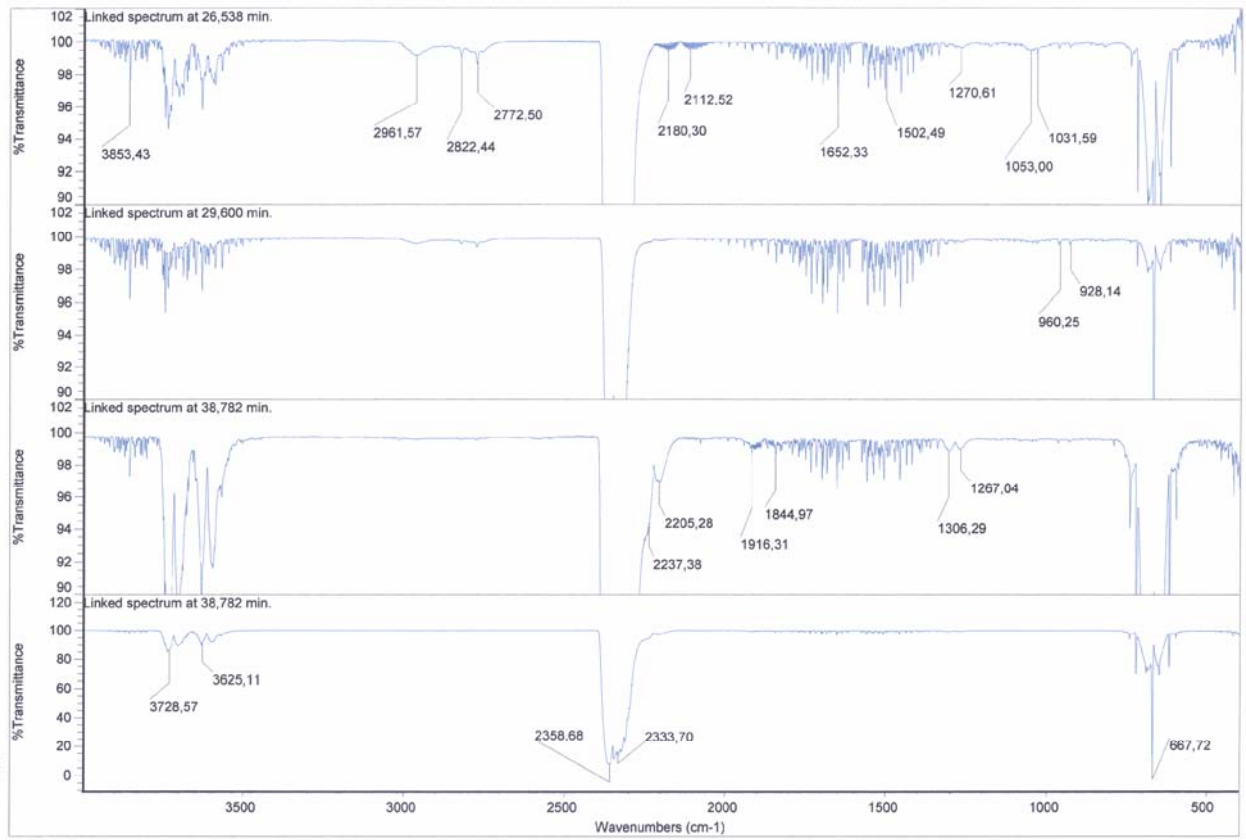
Sheet 3:



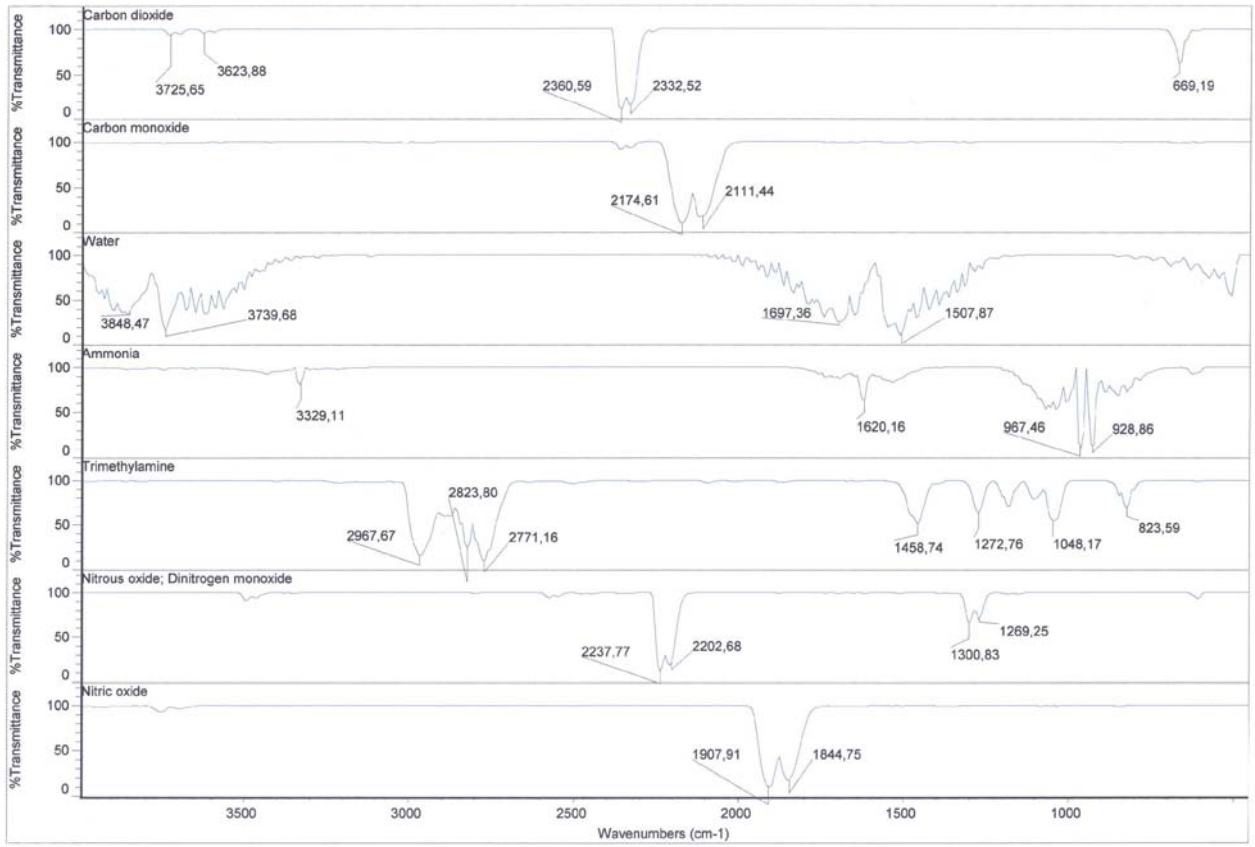
Sheet 4:



d) Sheet with selected FT-IR spectra.



e) Sheet with FT-IR spectra from pure samples of the evolved gases, for identification purposes.



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f) Summary the TG-data and interpretation of results.

Step/ Residue	Temperature (ºC)	Time (minutes)	No. of FT-IR spectra	Weight loss (exp.) %	Weight loss (calc.) %	Gases or residue
1	40-210	3-20	6	12.419	12.317	4.3 H_2O, CO_2(t)
2	210-270	20-26	3	37.297	-	H_2O, CO_2, CO(t)
3	270-325	26-32	5	1.7982	-	H_2O, CO_2, CO, TMA, NH_3(t)
4	325-450	32-44	8	24.496	-	H_2O, CO_2, NH_3, N_2O, NO
Residue	~450	44	-	23.780	25.296	2CuO

(t) = Trace amounts.
TMA = trimethylamine [$N(CH_3)_3$]. This gas is typically observed due to the pyrolysis of MIDA chelating ligand.