

# Structure and Synthesis of Copper Based Schiff base and Reduced Schiff base Complex: A Combined Experimental and Theoretical Investigation of Biomimetic Catalytic Activity

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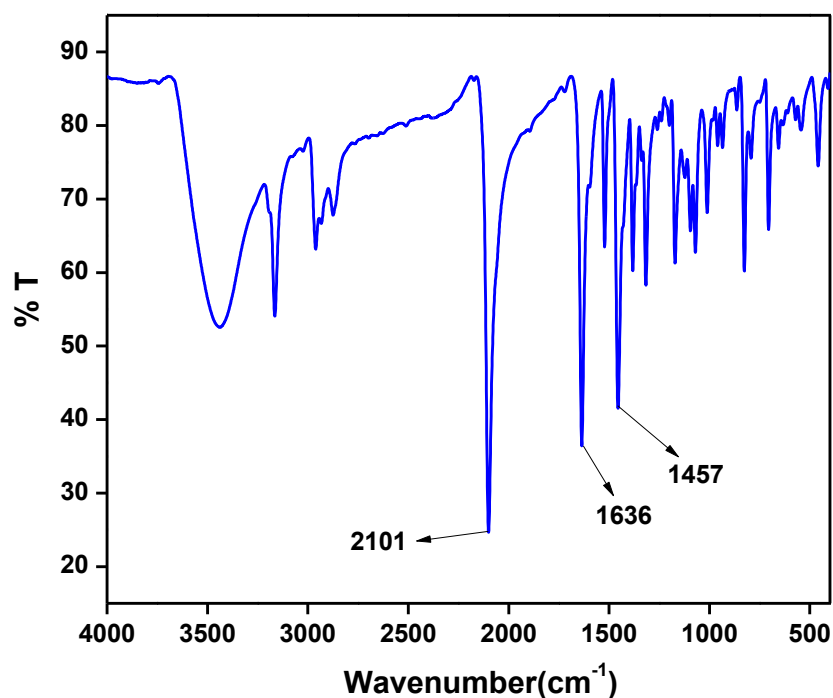
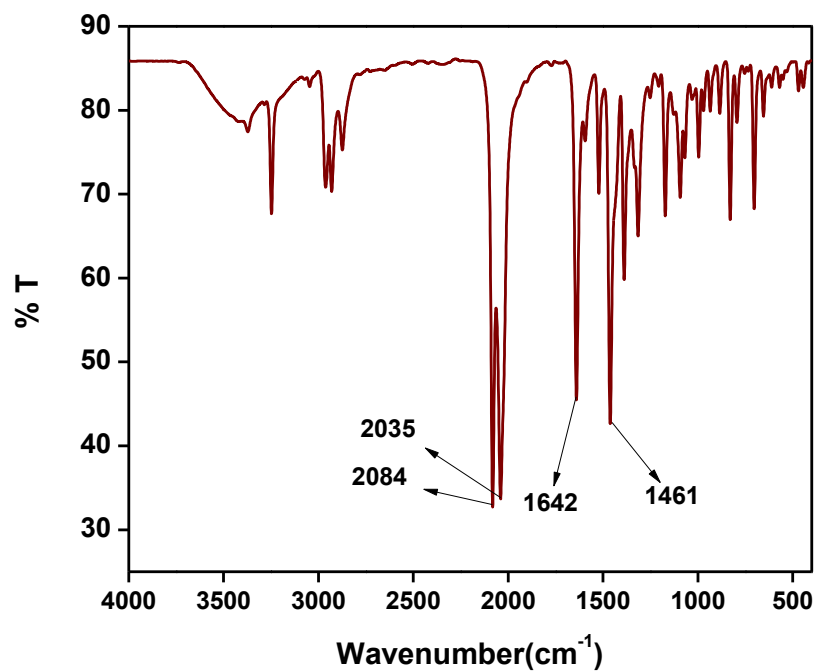
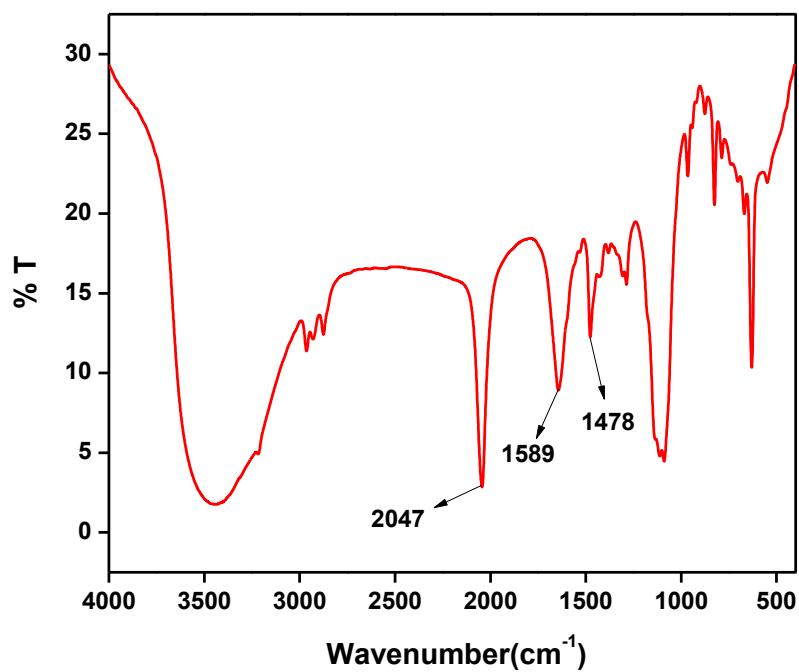


Fig. S1 FTIR spectrum of complex 1.



**Fig. S2** FTIR spectrum of complex 2.



**Fig. S3** FTIR spectrum of complex 3.

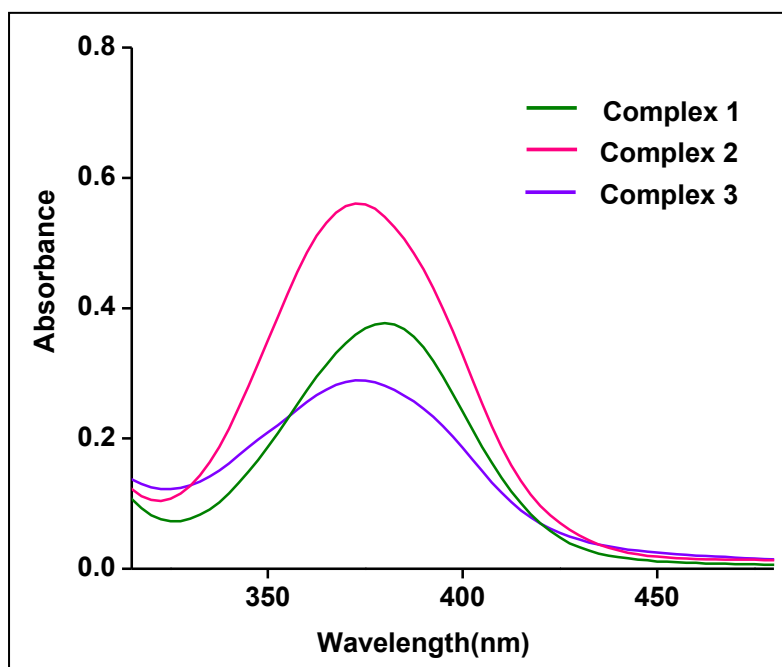


Fig. S4 UV spectra of the complexes 1-3 at room temperature.

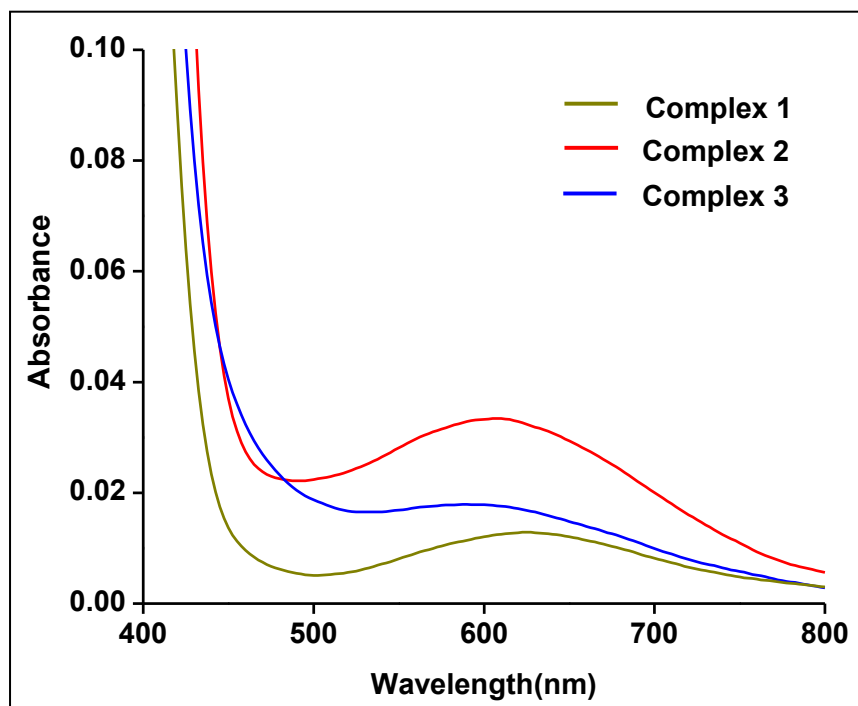


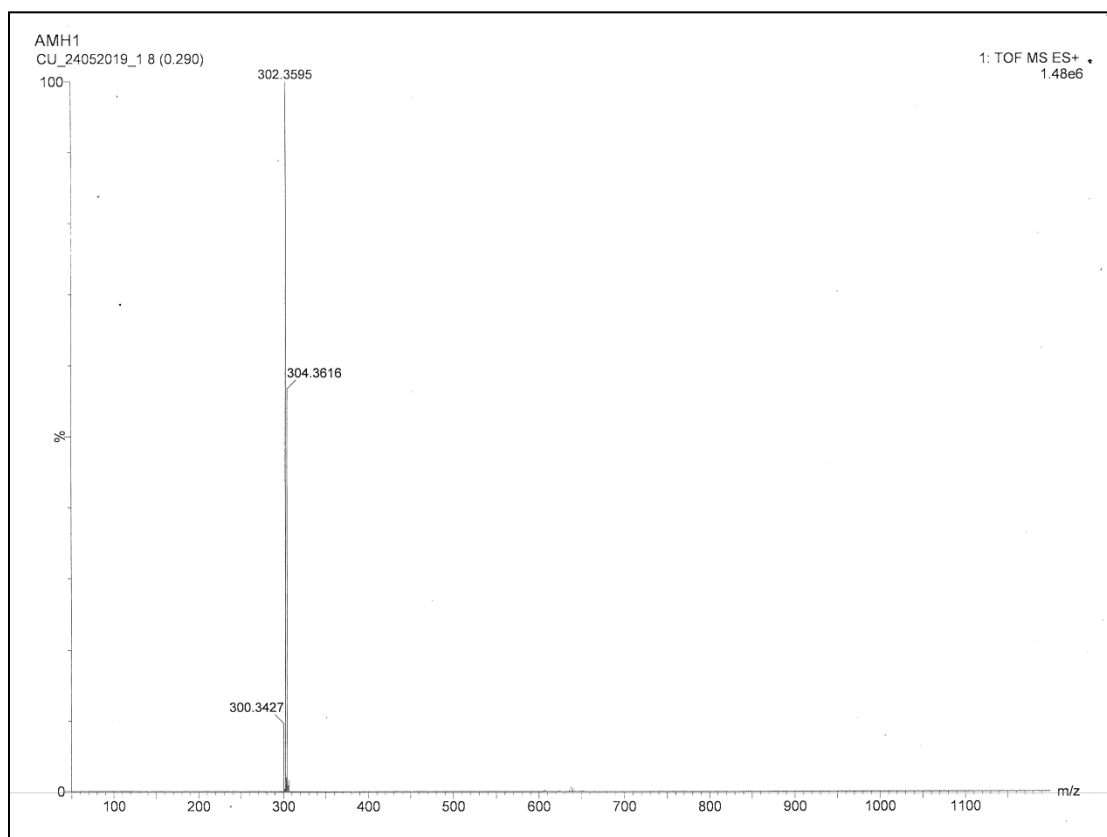
Fig. S5 d-d band of the complexes 1-3.

**Table S1** Crystallographic data and details of refinement for complex **1**, **2** & **3**

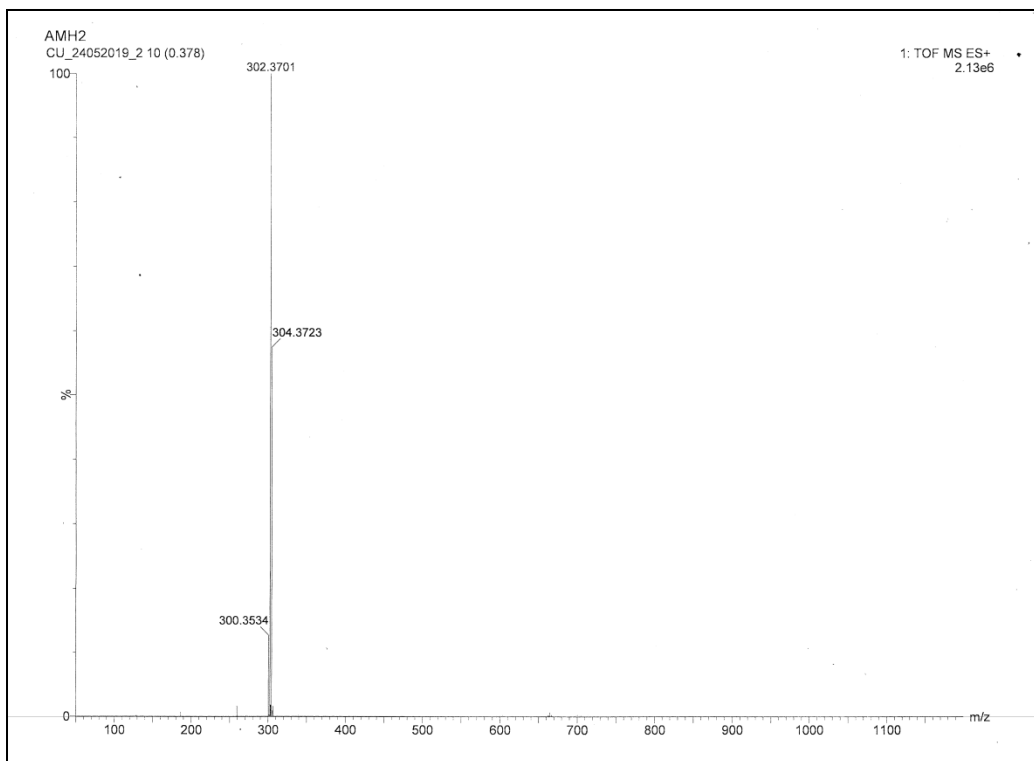
	<b>1</b>	<b>2</b>	<b>3</b>
CCDC Number	2020943	2020944	2020946
Empirical formula	C <sub>13</sub> H <sub>16</sub> ClCuN <sub>3</sub> OS	C <sub>12</sub> H <sub>16</sub> ClCuN <sub>5</sub> O	C <sub>12</sub> H <sub>18</sub> ClCuN <sub>5</sub> O
Formula weight	361.35	344.28	347.18
Crystal system	monoclinic	monoclinic	monoclinic
Space group	P2 <sub>1</sub> /n	P2 <sub>1</sub> /c	P2 <sub>1</sub> /c
<i>a</i> /Å	5.93020(10)	13.10(2)	20.7663(17)
<i>b</i> /Å	20.8486(4)	8.630(14)	9.4400(7)
<i>c</i> /Å	12.2568(3)	13.62(2)	7.5810(7)
$\alpha$ /°	90	90	90
$\beta$ /°	93.582(2)	97.62(4)	98.352(6)
$\gamma$ /°	90	90	90
Volume/Å <sup>3</sup>	1512.43(5)	1526(4)	1470.4(2)
Density(g/cm <sup>3</sup> )	1.587	1.498	1.568
<i>Z</i>	4	4	4
<i>F</i> (000)	740.0	704.0	718.1
$\mu$ /mm <sup>-1</sup>	1.756	1.608	1.670
Mo K $\alpha$ radiation	$\lambda$ =0.71073Å	$\lambda$ =0.71073Å	$\lambda$ =0.71073Å
Temperature/K	293(2)	290(2)	293(2)
<i>R</i> <sub>int</sub>	0.0593	0.0962	0.1448
$\theta$ <sub>min/max</sub> /°	3.331/30.661	2.801/29.654	1.890/24.887
Reflections collected/ unique $[I > 2\sigma(I)]$ <sup>[a]</sup>	23109/3314	34951/2486	20502/1688
GOF on <i>F</i> <sup>2</sup>	1.056	1.007	1.175

$R_{\text{indices}}[I > 2\sigma(I)]$	$RI = 0.0389$ $wR2 = 0.0730$	$RI = 0.0516$ $wR2 = 0.1100$	$RI = 0.1216$ $wR2 = 0.3293$
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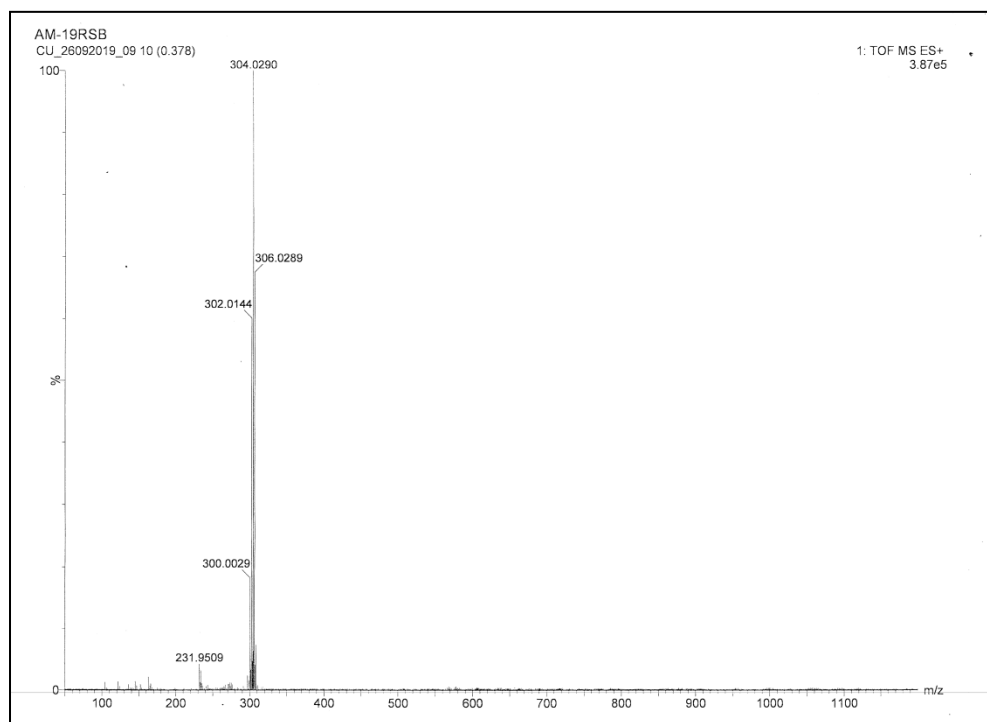
$$[a] R1 = \frac{\sum |Fo| - |Fc|}{\sum |Fo|}, wR2 = \left[ \frac{\sum w (Fo^2 - Fc^2)^2}{\sum w (Fo^2)^2} \right]^{1/2}$$



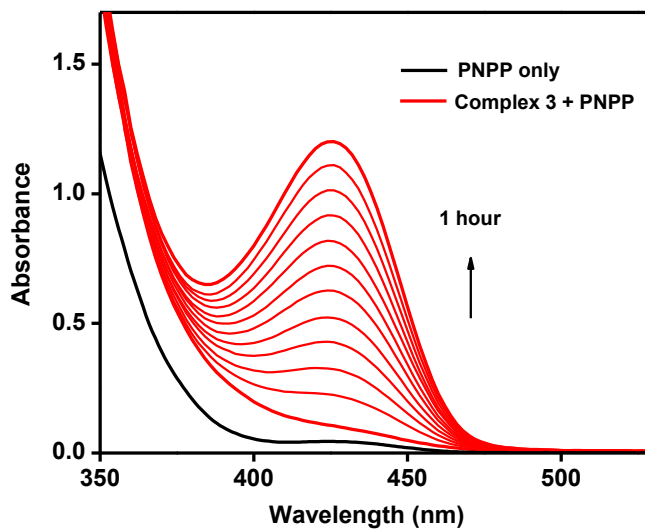
**Fig. S6** ESI-MS spectrum of complex **1**.



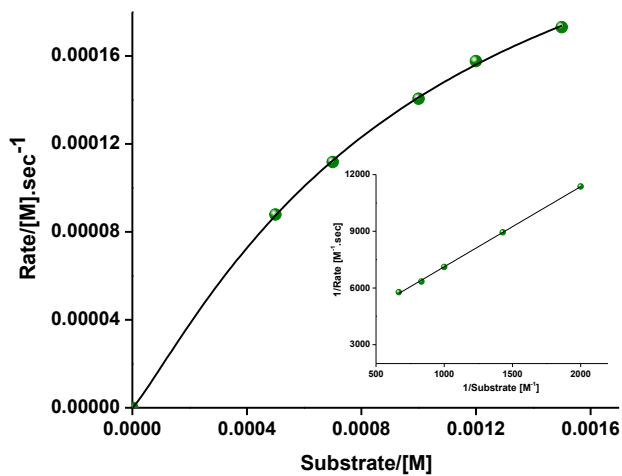
**Fig. S7** ESI-MS spectrum of complex 2



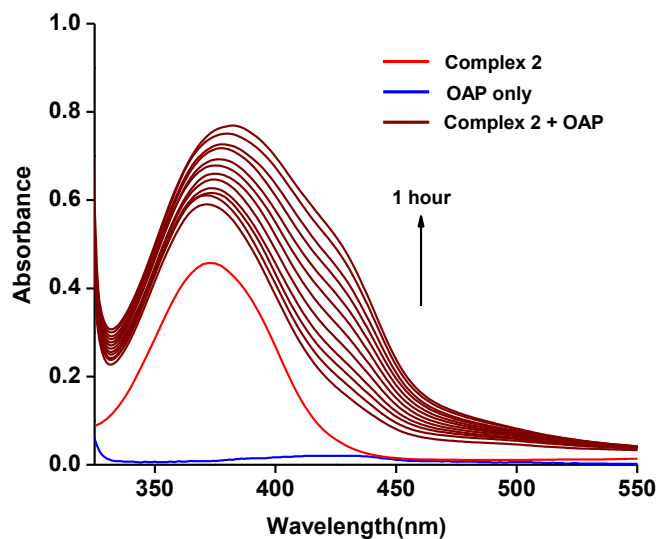
**Fig. S8** ESI-MS spectrum of complex 3



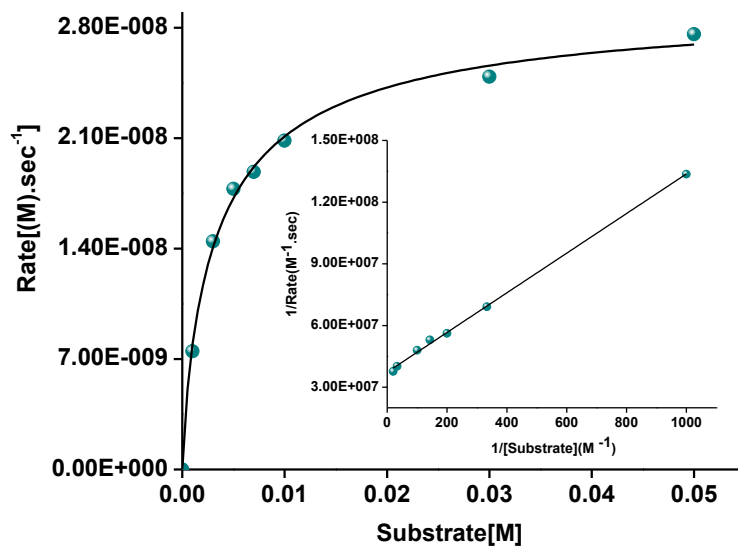
**Fig. S9** Wavelength scan for the hydrolysis of 4-NPP in the presence of complex **3** in 97.5% DMF recorded at 25 °C at intervals of 5 min for 1 h.



**Fig. S10** Kinetics plot for the hydrolysis of 4-NPP of complex **3** (insets: Lineweaver Burk plot)

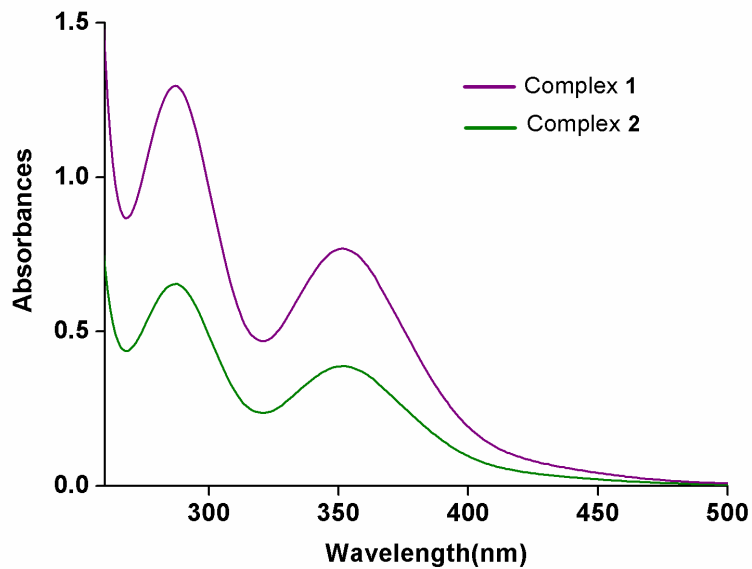


**Fig. S11** UV-Vis spectral scans showing an increase of the APX band at 420 nm after addition of o-aminophenol to a solution of complex **2** in DMF at 25 °C. The spectra were recorded at 5 min interval.

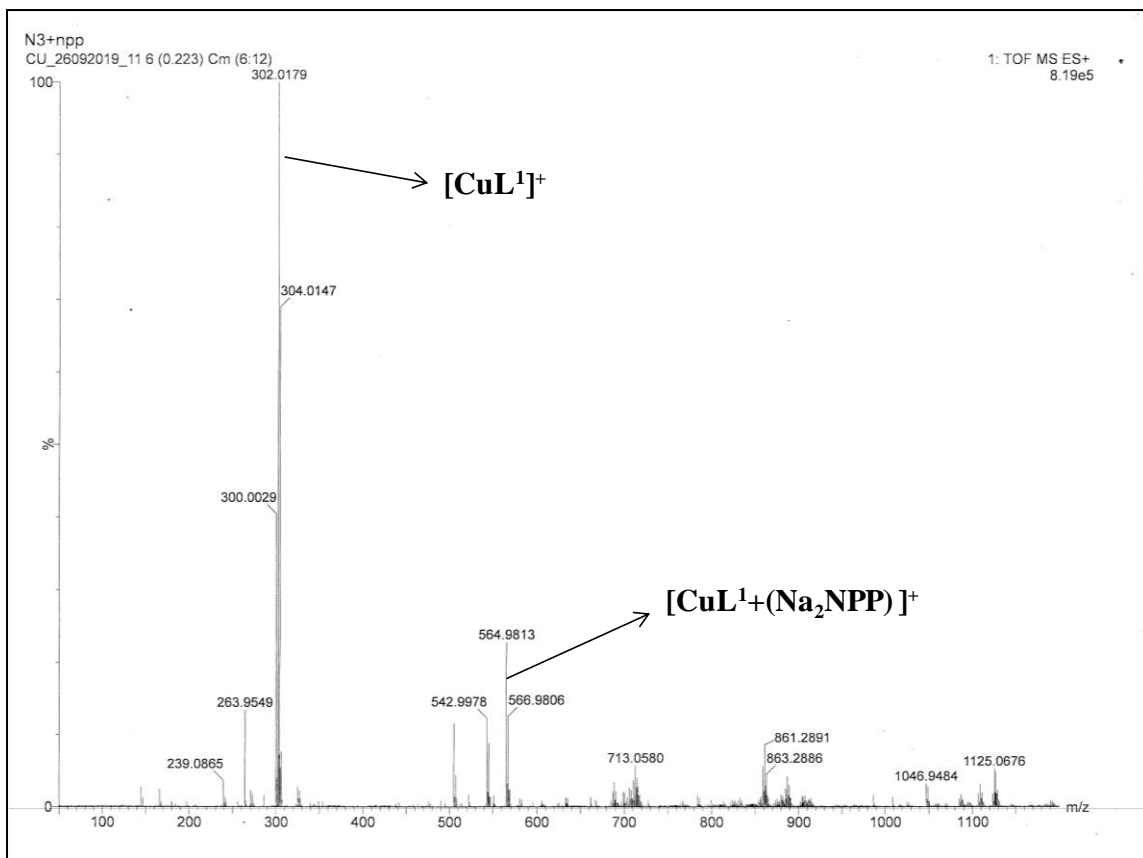


**Fig. S12** Kinetic plot of OAP oxidation by complex **2** (insets: Lineweaver Burk plot)

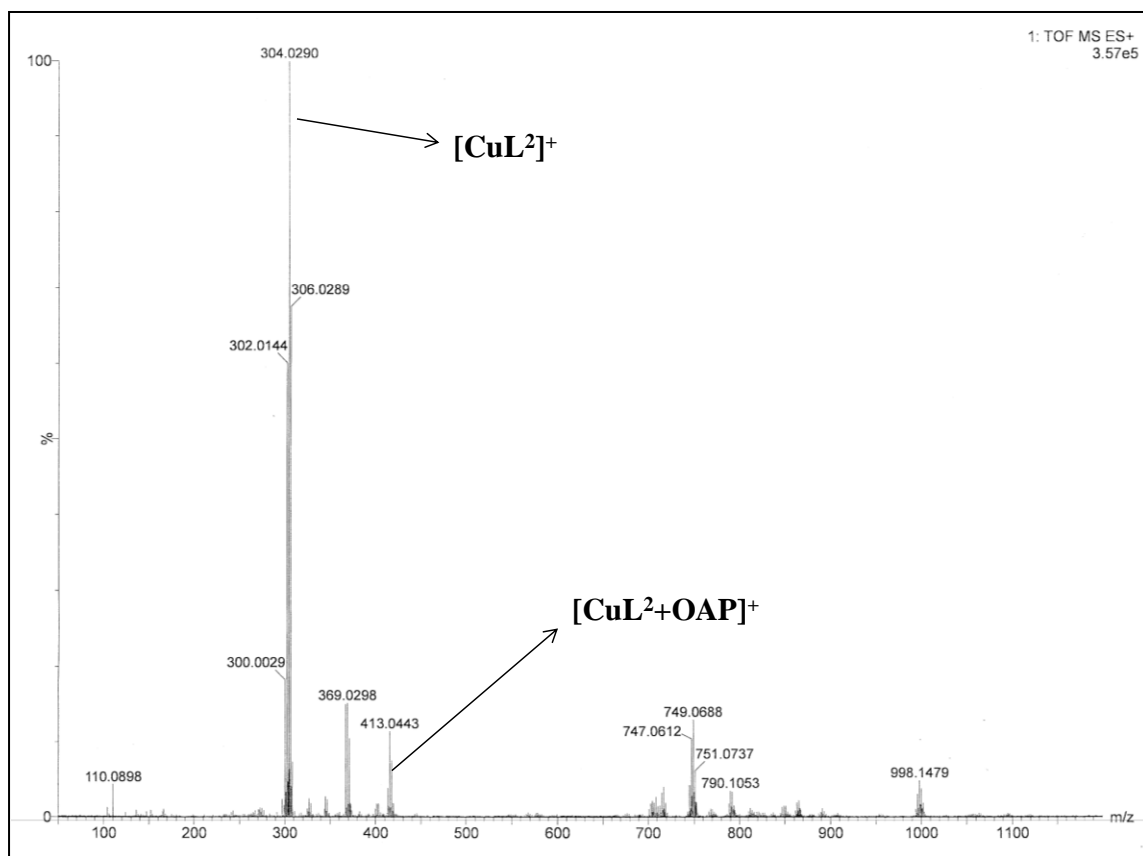




**Fig. S13** Detection of  $\text{H}_2\text{O}_2$  formation during oxidation of OAP observed in UV-Vis spectra.



**Fig. S14** ESI-MS spectrum of intermediate species for the reaction mixture of complex **2** and 4-NPP recorded at room temperature.



**Fig. S15** ESI-MS spectrum of intermediate species for the reaction mixture of complex **3** and OAP recorded at room temperature.

## XYZ Coordinates of the Optimized Structure

### Int1

#### Charge 0, multiplicity 2

C	-1.895800	-0.590800	0.135400
C	-3.089000	-1.359000	0.105800
C	-4.334400	-0.774800	-0.015500
C	-4.471400	0.618900	-0.113600
C	-3.329100	1.393800	-0.082700
C	-2.043000	0.829900	0.039500
H	-2.981600	-2.437100	0.180700
H	-5.218500	-1.406200	-0.034200
H	-5.450000	1.075700	-0.209600
H	-3.407600	2.476800	-0.151800
C	-0.929900	1.762400	0.085800
H	-1.195700	2.826500	0.041900
O	-0.752600	-1.215700	0.241100
N	0.302600	1.435900	0.186100
C	1.380500	2.414200	0.290700
H	1.133800	3.344100	-0.235400
H	1.526200	2.640400	1.354400
C	2.641500	1.744000	-0.252800
H	2.552600	1.678200	-1.359400
H	3.511200	2.394400	-0.054600
C	3.900800	-0.271100	-0.217300
H	4.861300	0.237100	-0.021900
H	3.973500	-1.278300	0.208300
H	3.823200	-0.381500	-1.318300
N	2.788100	0.442500	0.367400
Cu	1.063800	-0.433400	0.225000
O	0.925300	-1.290400	-1.951400
H	0.040000	-1.577800	-1.660200
H	0.759200	-0.560200	-2.567400
O	1.568700	-2.382800	0.823900
H	2.014800	-2.403000	1.685600
H	0.661100	-2.702900	0.981300

### Int2

#### Charge -1, multiplicity 2

C	0.929000	-0.418400	1.510800
C	1.825800	0.376100	2.284100
C	3.165200	0.072200	2.399500
C	3.711300	-1.057500	1.763600
C	2.864300	-1.874800	1.042500
C	1.490100	-1.592900	0.905000
H	1.409400	1.261400	2.756500
H	3.809400	0.722400	2.986400
H	4.768200	-1.285700	1.847100
H	3.255700	-2.764100	0.552000
C	0.702000	-2.535000	0.140400
H	1.242300	-3.410000	-0.247100
O	-0.304600	-0.043600	1.407700
N	-0.553300	-2.430100	-0.090600
C	-1.295600	-3.465100	-0.799800
H	-0.666600	-3.979300	-1.537500
H	-1.639600	-4.201300	-0.061800
C	-2.511900	-2.792900	-1.429900
H	-2.167200	-2.193100	-2.303100
H	-3.179600	-3.570100	-1.844100
C	-4.302500	-1.307200	-1.015900
H	-5.085300	-2.018000	-1.337600
H	-4.766600	-0.625600	-0.291900

H	-4.041200	-0.697600	-1.902900
N	-3.172200	-1.985400	-0.428200
Cu	-1.787400	-0.871500	0.405500
O	-2.227000	0.920000	-0.714300
P	-2.006200	2.280900	-0.112500
O	-0.522200	2.856000	-0.566100
O	-2.918300	3.333700	-0.937700
O	-2.196200	2.492900	1.360900
C	0.595200	2.101200	-0.765300
C	1.791300	2.616000	-0.259700
C	0.586100	0.915100	-1.511000
C	2.979400	1.927500	-0.448900
H	1.767300	3.546500	0.296200
C	1.769800	0.218900	-1.688000
H	-0.346000	0.540500	-1.913300
C	2.948400	0.727000	-1.147100
H	3.913200	2.295000	-0.042100
H	1.787400	-0.715200	-2.236200
N	4.177300	-0.034900	-1.297800
O	4.120500	-1.111600	-1.872800
O	5.208600	0.432400	-0.840000
H	-3.189700	4.067000	-0.363100
O	-3.029200	-0.021400	2.012100
H	-3.935400	-0.003000	1.668900
H	-2.711200	0.915500	1.938900

### Int3

#### Charge 0, multiplicity 2

C	-1.957700	-0.893500	0.262900
C	-2.488600	-2.179100	0.135700
C	-3.816800	-2.352100	-0.232400
C	-4.639400	-1.249500	-0.470100
C	-4.109400	0.025100	-0.346000
C	-2.767100	0.231500	0.008500
H	-1.845300	-3.031700	0.331400
H	-4.213900	-3.357600	-0.328000
H	-5.677700	-1.386700	-0.749600
H	-4.733700	0.894700	-0.533300
C	-2.298400	1.614400	0.079900
H	-3.077400	2.379100	-0.019200
O	-0.673400	-0.736400	0.663000
N	-1.084500	1.978500	0.228500
C	-0.719000	3.391500	0.290700
H	-1.492400	4.027200	-0.154700
H	-0.607400	3.655500	1.348900
C	0.631700	3.532500	-0.402100
H	0.491300	3.404500	-1.493600
H	1.011800	4.556400	-0.254500
C	2.809400	2.573900	-0.553800
H	3.314400	3.544200	-0.418400
H	3.467300	1.790500	-0.171300
H	2.696600	2.424000	-1.643800
N	1.548700	2.557200	0.157700
Cu	0.616600	0.849900	0.231100
O	2.136100	-0.386100	-0.072800
P	2.161600	-1.903300	-0.046300
O	0.910800	-2.633800	0.382300
O	2.543800	-2.471800	-1.505800
O	3.411200	-2.280800	0.899600
H	3.293900	-1.994700	-1.898000

H 3.449100 -3.233000 1.089500  
H -0.125000 -1.617300 0.613300

### TS

#### Charge -1, multiplicity 2

C -3.015900 1.642600 -0.183500  
C -2.978800 2.949600 -0.732100  
C -3.292700 4.067300 0.018000  
C -3.672700 3.949700 1.363200  
C -3.720000 2.688100 1.924100  
C -3.394700 1.531200 1.190300  
H -2.690900 3.045100 -1.775300  
H -3.245000 5.048700 -0.446100  
H -3.923500 4.827200 1.948500  
H -4.012900 2.568000 2.965000  
C -3.484600 0.263500 1.894800  
H -3.881900 0.309500 2.917100  
O -2.725800 0.623300 -0.953200  
N -3.137300 -0.869000 1.414000  
C -3.264200 -2.113500 2.161300  
H -3.276900 -1.935200 3.243500  
H -4.211600 -2.584400 1.870600  
C -2.109400 -3.011800 1.722400  
H -1.171100 -2.615500 2.168900  
H -2.251700 -4.017000 2.157200  
C -0.945000 -3.843100 -0.164600  
H -0.969200 -4.858500 0.268600  
H -0.963100 -3.976800 -1.253900  
H 0.041300 -3.411100 0.103300  
N -2.069300 -3.050900 0.275100  
Cu -2.153900 -1.183600 -0.323900  
O 0.122300 -0.413700 -0.101900  
P 0.295300 -0.162300 -1.581800  
O 1.698200 0.940100 -1.486500  
O 1.172600 -1.145300 -2.552900  
O -0.479600 1.053000 -2.291800  
C 2.792000 0.709700 -0.762700  
C 3.711200 1.774900 -0.658100  
C 3.096500 -0.518000 -0.138100  
C 4.893200 1.629200 0.039800  
H 3.463900 2.712300 -1.143900  
C 4.281800 -0.664800 0.563200  
H 2.397800 -1.342800 -0.189100  
C 5.169300 0.404100 0.647100  
H 5.601500 2.444500 0.121600  
H 4.525600 -1.602700 1.047400  
N 6.407800 0.240500 1.382300  
O 6.632100 -0.840500 1.908500  
O 7.174900 1.191200 1.443100  
H 2.067200 -0.795300 -2.685400  
H -1.441500 0.942100 -2.051100  
O -1.104600 -1.263600 -2.058700  
H -0.747000 -2.151900 -2.208900

### 1-INT1

#### Charge 0, multiplicity 2

C 1.904100000 -0.597300000 -0.152500000  
C 3.098900000 -1.365500000 -0.111300000  
C 4.343000000 -0.780200000 0.036600000  
C 4.476100000 0.614100000 0.151300000  
C 3.331300000 1.388500000 0.108400000

C 2.047100000 0.823800000 -0.040800000  
H 2.997200000 -2.443700000 -0.199400000  
H 5.227900000 -1.411100000 0.063200000  
H 5.452500000 1.072100000 0.267600000  
H 3.408300000 2.471300000 0.188600000  
C 0.932100000 1.756100000 -0.098100000  
H 1.194600000 2.820700000 -0.041400000  
O 0.763400000 -1.220900000 -0.282500000  
N -0.298100000 1.427600000 -0.221400000  
C -1.375300000 2.407200000 -0.329400000  
H -1.120800000 3.343500000 0.182100000  
H -1.529000000 2.617600000 -1.395500000  
C -2.633100000 1.749900000 0.235600000  
H -2.536000000 1.698000000 1.342300000  
H -3.503900000 2.398500000 0.033400000  
C -3.896300000 -0.264400000 0.254600000  
H -3.986600000 -1.275200000 -0.159200000  
H -3.793100000 -0.363300000 1.354400000  
N -2.791100000 0.437200000 -0.360100000  
Cu -1.054500000 -0.438500000 -0.246500000  
O -0.969700000 -1.205200000 1.963100000  
H -0.044200000 -1.483700000 1.852000000  
H -0.957700000 -0.519000000 2.647500000  
O -1.582800000 -2.404500000 -0.775500000  
H -2.102500000 -2.496400000 -1.589500000  
H -0.698800000 -2.766200000 -0.969200000  
C -5.234700000 0.454300000 0.002000000  
H -5.359800000 1.237900000 0.719800000  
H -5.235700000 0.870200000 -0.983900000  
C -6.391600000 -0.553400000 0.135100000  
H -7.325400000 -0.034900000 0.070600000  
H -6.328900000 -1.274600000 -0.652800000  
H -6.324400000 -1.050700000 1.080100000

### 1-INT4

#### Charge -1, multiplicity 2

C 3.542200000 0.471474000 0.259472000  
C 3.018584000 -0.635203000 -0.482475000  
C 3.969677000 -1.560979000 -0.999706000  
C 5.328408000 -1.399796000 -0.805622000  
C 5.833164000 -0.306213000 -0.078441000  
C 4.934217000 0.606135000 0.442491000  
H 3.583327000 -2.407278000 -1.561453000  
H 6.015879000 -2.131934000 -1.222280000  
H 6.900570000 -0.183751000 0.072376000  
H 5.295757000 1.459132000 1.014496000  
C 2.693839000 1.474807000 0.871532000  
H 3.209033000 2.248146000 1.456973000  
C 0.641926000 2.535857000 1.484504000  
H 0.276520000 2.093249000 2.420334000  
H 1.258250000 3.411105000 1.726378000  
C -0.553209000 2.883438000 0.604293000  
H -1.239488000 3.521712000 1.188361000  
H -0.198858000 3.508653000 -0.243967000  
N -1.174614000 1.655269000 0.156720000  
Cu 0.186958000 0.325850000 -0.315893000  
O 1.754152000 -0.842107000 -0.703353000  
N 1.416014000 1.513165000 0.789087000  
C -2.282376000 1.899240000 -0.739667000  
H -2.068345000 2.748727000 -1.425381000  
H -2.421010000 1.015863000 -1.374323000  
C -3.615113000 2.184763000 -0.034925000

H	-3.860621000	1.313886000	0.587297000
H	-3.502129000	3.041540000	0.643500000
C	-4.745595000	2.451715000	-1.026925000
H	-4.881401000	1.594048000	-1.697878000
H	-5.699491000	2.634006000	-0.521034000
H	-4.523614000	3.326492000	-1.649847000
O	-0.972098000	-1.002257000	-1.241305000
C	-1.939770000	-1.539629000	-0.513430000
C	-1.615097000	-2.299925000	0.651825000
C	-3.300003000	-1.415791000	-0.845485000
C	-2.630080000	-2.825447000	1.450420000
C	-4.310396000	-1.956143000	-0.043681000
H	-3.552940000	-0.861558000	-1.746431000
C	-3.978875000	-2.647269000	1.119676000
H	-2.356387000	-3.397383000	2.335602000
H	-5.351798000	-1.824836000	-0.327709000
H	-4.752431000	-3.063118000	1.759164000
N	-0.261756000	-2.555677000	0.931150000
H	0.395956000	-2.040261000	0.349510000
H	-0.011525000	-2.516678000	1.912639000

### 1-INT5

#### Charge -2, multiplicity 2

C	-3.007520000	-0.952814000	0.658984000
C	-2.355601000	-1.698667000	-0.390272000
C	-3.142715000	-2.736086000	-0.989764000
C	-4.442340000	-3.011413000	-0.606267000
C	-5.071689000	-2.256146000	0.397408000
C	-4.344344000	-1.235698000	0.994007000
H	-2.666827000	-3.311514000	-1.780632000
H	-4.983961000	-3.816672000	-1.098696000
H	-6.097013000	-2.457323000	0.691388000
H	-4.814419000	-0.625197000	1.765223000
C	-2.387103000	0.173610000	1.365207000
H	-3.107883000	0.911382000	1.760880000
C	-0.716667000	1.626749000	2.126074000
H	-1.560833000	2.331654000	2.200728000
H	-0.352544000	1.437756000	3.146988000
C	0.457765000	2.235253000	1.292719000
H	0.570806000	3.283695000	1.650126000
H	1.365404000	1.697260000	1.618342000
N	0.386597000	2.156769000	-0.142661000
Cu	0.120271000	0.126440000	-0.431333000
O	-1.160933000	-1.484374000	-0.819652000
N	-1.137078000	0.367437000	1.535402000
C	-0.495612000	3.132488000	-0.731662000
H	-0.365612000	4.126529000	-0.242356000
H	-0.202621000	3.280088000	-1.787510000
C	-2.012572000	2.848673000	-0.756187000
H	-2.170730000	1.850783000	-1.190101000
H	-2.404951000	2.807283000	0.267248000
C	-2.782569000	3.899805000	-1.555304000
H	-2.429499000	3.935941000	-2.593396000
H	-3.858234000	3.694102000	-1.575629000
H	-2.642616000	4.899232000	-1.125034000
O	1.880395000	-1.194524000	-0.253600000
C	3.087287000	-0.802088000	-0.148731000
C	4.194178000	-1.781632000	-0.029581000
C	3.429339000	0.591029000	-0.143333000
C	5.532787000	-1.257152000	0.086294000
C	4.733921000	1.023006000	-0.030742000
H	2.599456000	1.295183000	-0.232688000

C	5.800193000	0.089961000	0.085613000
H	6.345563000	-1.977455000	0.175518000
H	4.953386000	2.088355000	-0.030815000
H	6.823739000	0.444814000	0.173938000
N	3.909096000	-3.076272000	-0.035660000
H	4.785102000	-3.600298000	0.054801000

### 1-INT6

#### Charge -1, multiplicity 1

C	-2.257400000	0.953762000	0.344392000
C	-2.365157000	-0.222287000	-0.463992000
C	-3.654400000	-0.528695000	-0.970026000
C	-4.757683000	0.275808000	-0.727297000
C	-4.630824000	1.451939000	0.022237000
C	-3.379427000	1.775461000	0.531545000
H	-3.746153000	-1.426107000	-1.576933000
H	-5.724272000	-0.006121000	-1.138147000
H	-5.485384000	2.096734000	0.200891000
H	-3.255751000	2.687078000	1.114800000
C	-0.996751000	1.393311000	0.974646000
H	-0.812516000	2.480783000	0.977403000
C	1.109407000	1.114283000	2.001908000
H	1.319573000	2.110470000	1.585305000
H	1.031678000	1.209940000	3.094183000
C	2.240231000	0.105350000	1.681586000
H	3.189204000	0.544984000	2.040802000
H	2.039162000	-0.771996000	2.319820000
N	2.356355000	-0.339111000	0.303636000
Cu	0.528287000	-0.610088000	-0.406140000
O	-1.358300000	-1.000262000	-0.794646000
N	-0.153686000	0.591936000	1.496405000
C	3.326295000	0.401744000	-0.474727000
H	4.303395000	0.436207000	0.051965000
H	3.505124000	-0.148169000	-1.412680000
C	2.963613000	1.847929000	-0.848448000
H	1.967828000	1.845179000	-1.316523000
H	2.881212000	2.451082000	0.065304000
C	3.990841000	2.480898000	-1.785777000
H	4.064317000	1.915729000	-2.722589000
H	3.731860000	3.514514000	-2.037266000
H	4.986150000	2.489163000	-1.325243000
O	2.366364000	-3.052155000	0.353752000
H	1.405500000	-3.213440000	0.292962000
O	-0.553537000	-3.424751000	0.142245000
H	-0.769253000	-4.125747000	-0.489419000
H	2.457701000	-2.037163000	0.322274000
H	-0.997076000	-2.610015000	-0.196225000

### 3-INT1

#### Charge = -1 Multiplicity = 2

C	3.508297000	0.253987000	0.048273000
C	2.736766000	-0.823011000	-0.471905000
C	3.209263000	-2.132842000	-0.209957000
C	4.371402000	-2.349838000	0.515488000
C	5.120361000	-1.282691000	1.016751000
C	4.669670000	0.012766000	0.776103000
H	2.621268000	-2.961439000	-0.595034000
H	4.699956000	-3.370954000	0.697415000
H	6.029067000	-1.457285000	1.584354000
H	5.232802000	0.864006000	1.158454000
C	3.010456000	1.643611000	-0.211630000
H	3.698604000	2.389904000	0.216785000

C	1.124402000	3.172847000	0.292918000	H	-1.953069000	3.359365000	-0.703713000
H	1.675607000	3.841276000	0.973107000	H	-2.350496000	1.771006000	-0.022668000
H	1.249096000	3.533264000	-0.734291000	C	-1.169072000	3.012731000	1.256710000
C	-0.361540000	3.091541000	0.611158000	H	-0.712966000	2.186534000	1.818626000
H	-0.459263000	2.842958000	1.694217000	H	-0.408720000	3.803019000	1.175847000
H	-0.810239000	4.099097000	0.503377000	C	-2.391969000	3.550573000	1.997860000
N	-0.944148000	2.145778000	-0.293506000	H	-3.140501000	2.759373000	2.120414000
Cu	0.179085000	0.607135000	-0.689024000	H	-2.145434000	3.938175000	2.994224000
O	1.651038000	-0.628578000	-1.170429000	H	-2.864381000	4.363459000	1.430313000
N	1.654855000	1.805444000	0.337418000	O	-1.595880000	-1.087237000	0.709717000
C	-2.379652000	2.083186000	-0.225956000	C	-2.719067000	-1.216484000	0.150950000
H	-2.812546000	3.094648000	-0.386035000	C	-3.806153000	-2.008657000	0.793699000
H	-2.730094000	1.454479000	-1.052251000	C	-3.014752000	-1.067945000	-1.119807000
C	-2.969754000	1.528792000	1.080650000	C	-5.046767000	-2.121200000	0.069485000
H	-2.620416000	0.495939000	1.208896000	C	-4.232943000	-0.753599000	-1.744866000
H	-2.592873000	2.109246000	1.934750000	H	-2.224723000	0.006232000	-1.554407000
C	-4.495550000	1.561607000	1.076690000	C	-5.262420000	-1.523637000	-1.149390000
H	-4.881575000	0.982688000	0.231137000	H	-5.838082000	-2.710702000	0.537355000
H	-4.916158000	1.130712000	1.991437000	H	-4.408843000	-0.267624000	-2.702895000
H	-4.866806000	2.590190000	0.982514000	H	-6.221004000	-1.637630000	-1.653394000
O	-1.152830000	-0.567380000	-1.511325000	N	-3.586089000	-2.559264000	1.973995000
C	-2.014953000	-1.254898000	-0.795639000	H	-4.449949000	-3.054689000	2.234950000
C	-1.567266000	-2.163140000	0.215317000	H	3.811895000	1.758725000	0.968836000
C	-3.404030000	-1.156277000	-0.995220000	H	2.040832000	0.934516000	-1.182630000
C	-2.489795000	-2.822924000	1.020580000				
C	-4.317288000	-1.833259000	-0.186100000				
H	-3.746322000	-0.497160000	-1.789412000				
C	-3.866097000	-2.649437000	0.844883000				
H	-2.114285000	-3.505035000	1.781794000				
H	-5.384136000	-1.706539000	-0.358068000				
H	-4.567676000	-3.171461000	1.489769000				
N	-0.187340000	-2.407139000	0.325582000				
H	0.357405000	-1.896269000	-0.369422000				
H	0.201176000	-2.304214000	1.255564000				
H	2.930340000	1.835017000	-1.289926000				
H	1.656213000	1.478965000	1.305710000				

### 3-INT4

Charge = -2 Multiplicity = 2

C	3.721534000	-0.281462000	0.320709000
C	2.886129000	-1.369717000	-0.115589000
C	3.540636000	-2.632525000	-0.256905000
C	4.893059000	-2.800819000	-0.003449000
C	5.688403000	-1.729934000	0.411691000
C	5.073443000	-0.483892000	0.563439000
H	2.921398000	-3.467753000	-0.574824000
H	5.339011000	-3.788203000	-0.129685000
H	6.749526000	-1.858597000	0.610241000
H	5.668382000	0.372749000	0.884842000
C	3.087326000	1.068503000	0.510603000
H	2.240455000	0.973144000	1.220914000
C	1.811962000	2.850984000	-0.565080000
H	1.536905000	2.971818000	0.495298000
H	2.400102000	3.741877000	-0.853102000
C	0.505997000	2.773113000	-1.385084000
H	0.096182000	3.805095000	-1.456901000
H	0.823364000	2.507883000	-2.414600000
N	-0.482813000	1.848071000	-0.906807000
Cu	0.019927000	0.010821000	-0.193884000
O	1.636753000	-1.240450000	-0.373741000
N	2.629133000	1.649718000	-0.752659000
C	-1.521406000	2.485672000	-0.153298000