

## Electronic Supplementary Information (ESI)

**Journal name:** New journal of chemistry

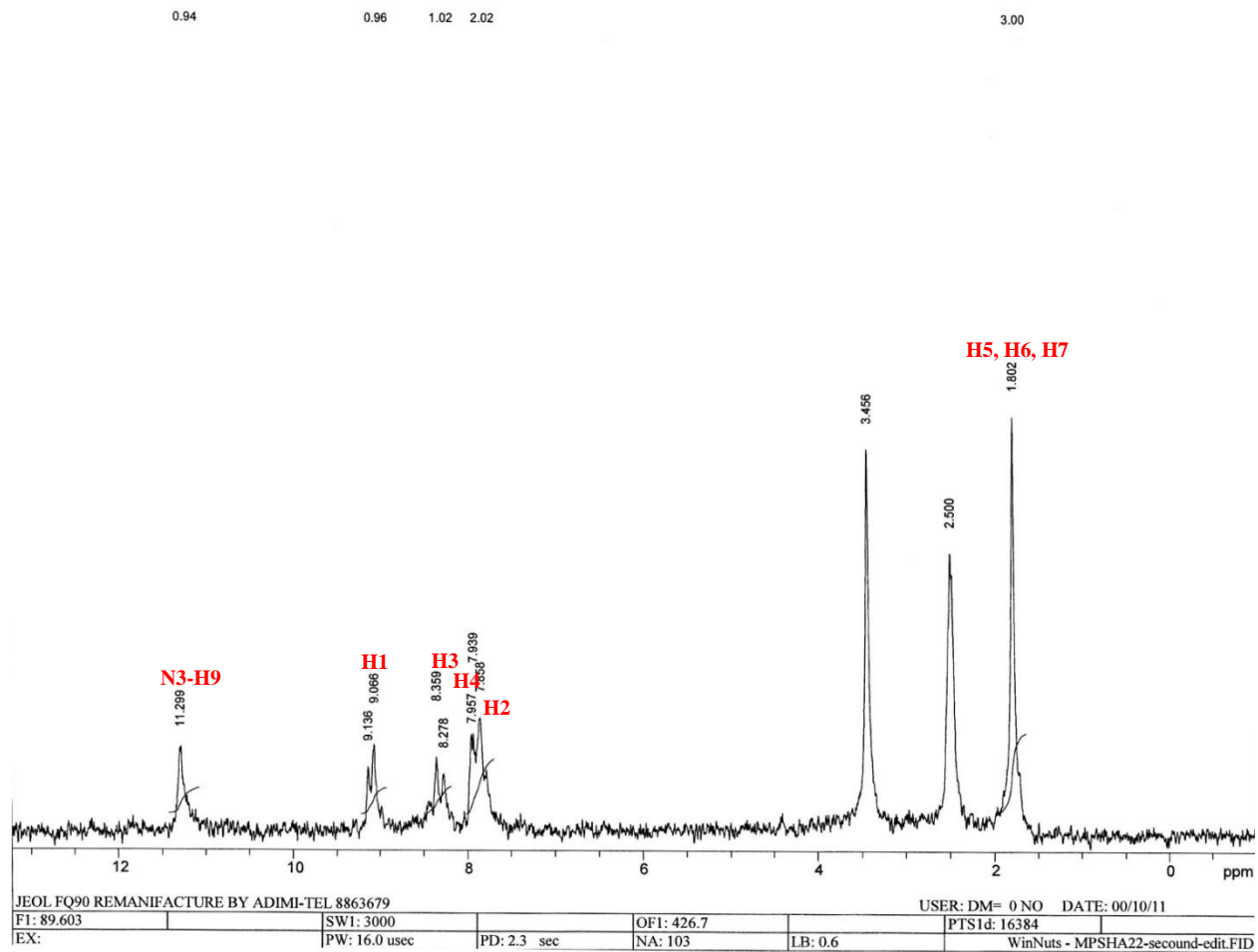
### **Gold(III) complexes of 5-methyl-5-(pyridyl)-2,4-imidazolidenedione: Synthesis, physicochemical, theoretical, antibacterial, and cytotoxicity investigation**

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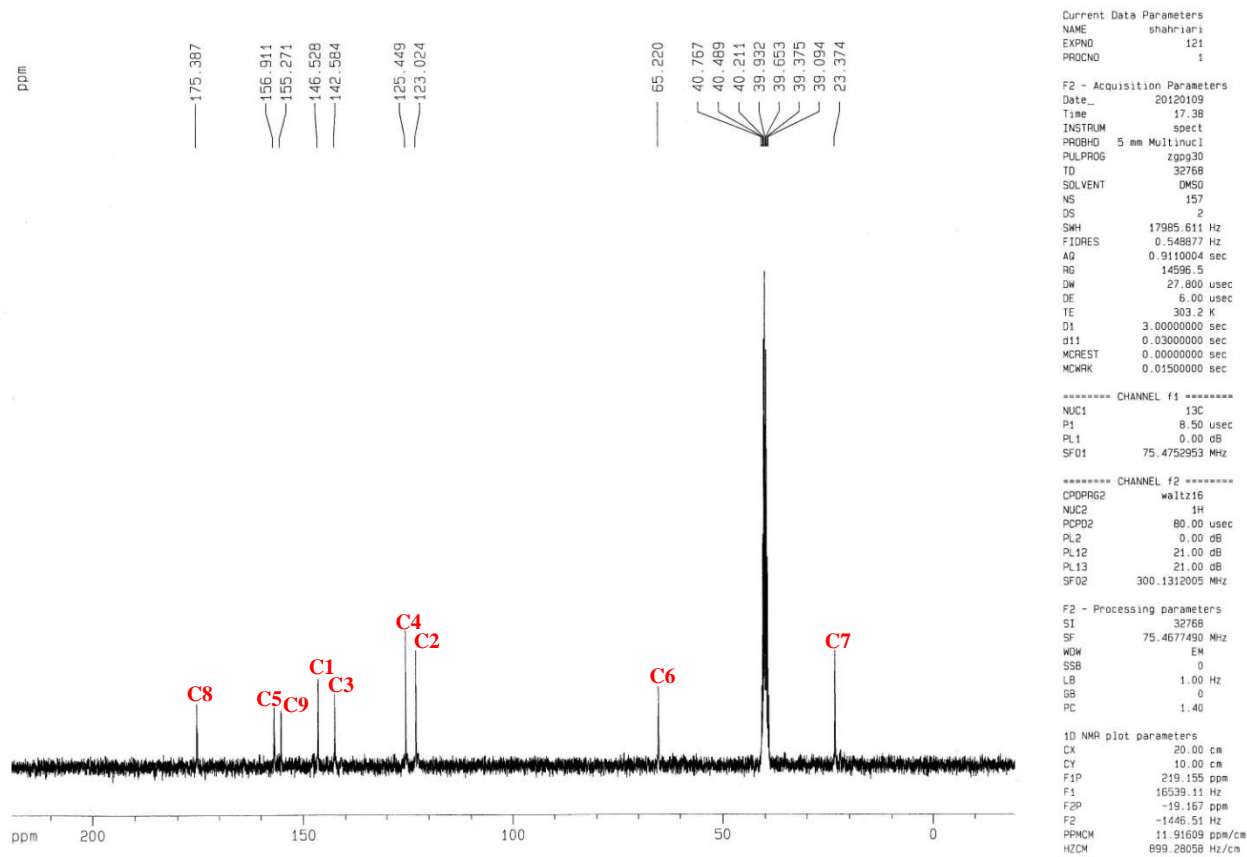
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**Figure A.1.**  $^1\text{H}$ NMR spectrum of **1** with peak assignment according to **Figure 2**



**Figure A.2.**  $^{13}\text{C}$ NMR spectrum of **1** with peak assignment according to **Figure 2**

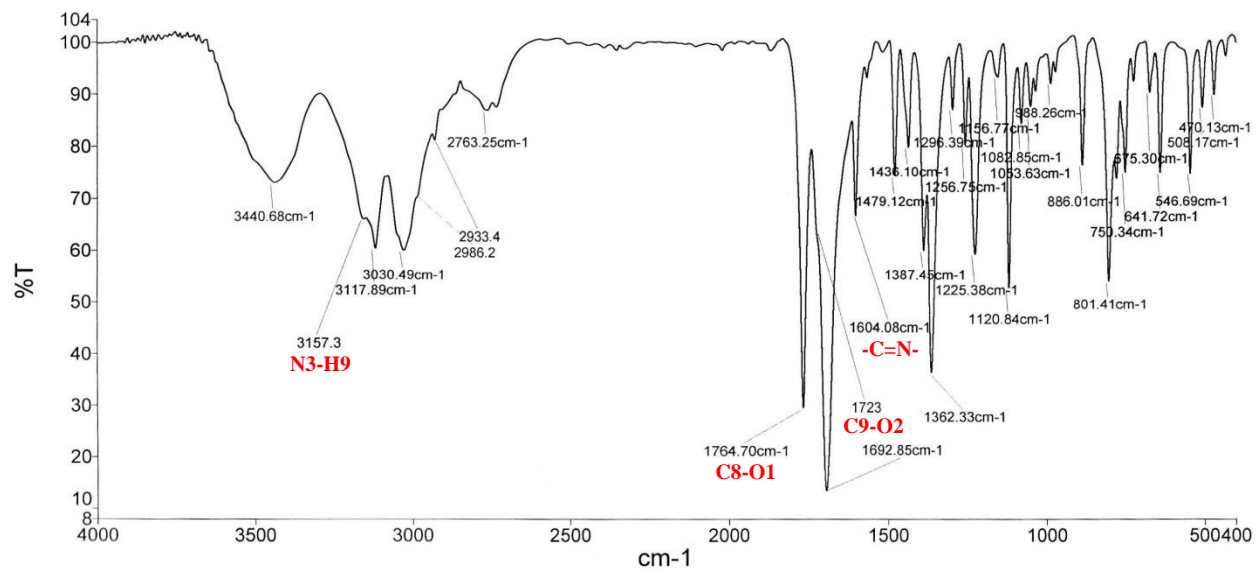
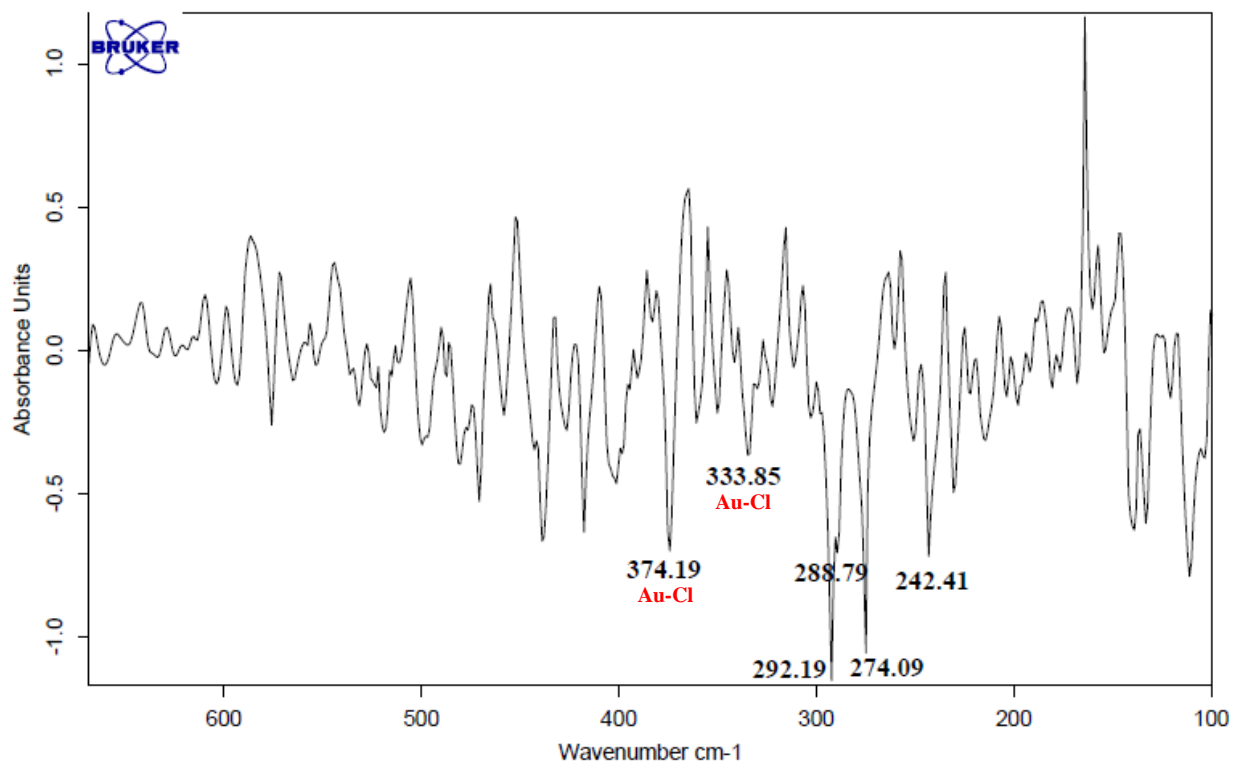


Figure A.3. IR spectrum of 1 with peak assignment according to Figure 2



**Figure A.4.** ATR-IR spectrum of **1**

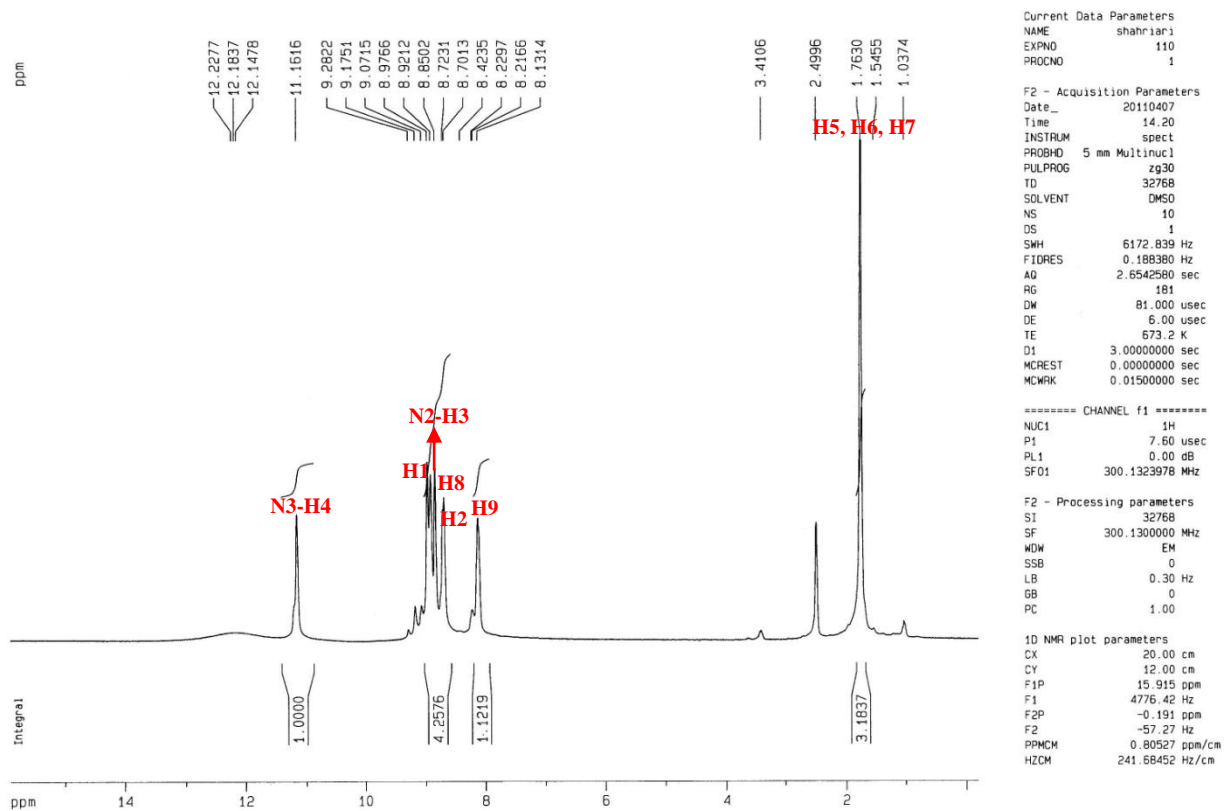


Figure A.5. <sup>1</sup>H NMR spectrum of 2 with peak assignment according to Figure 4

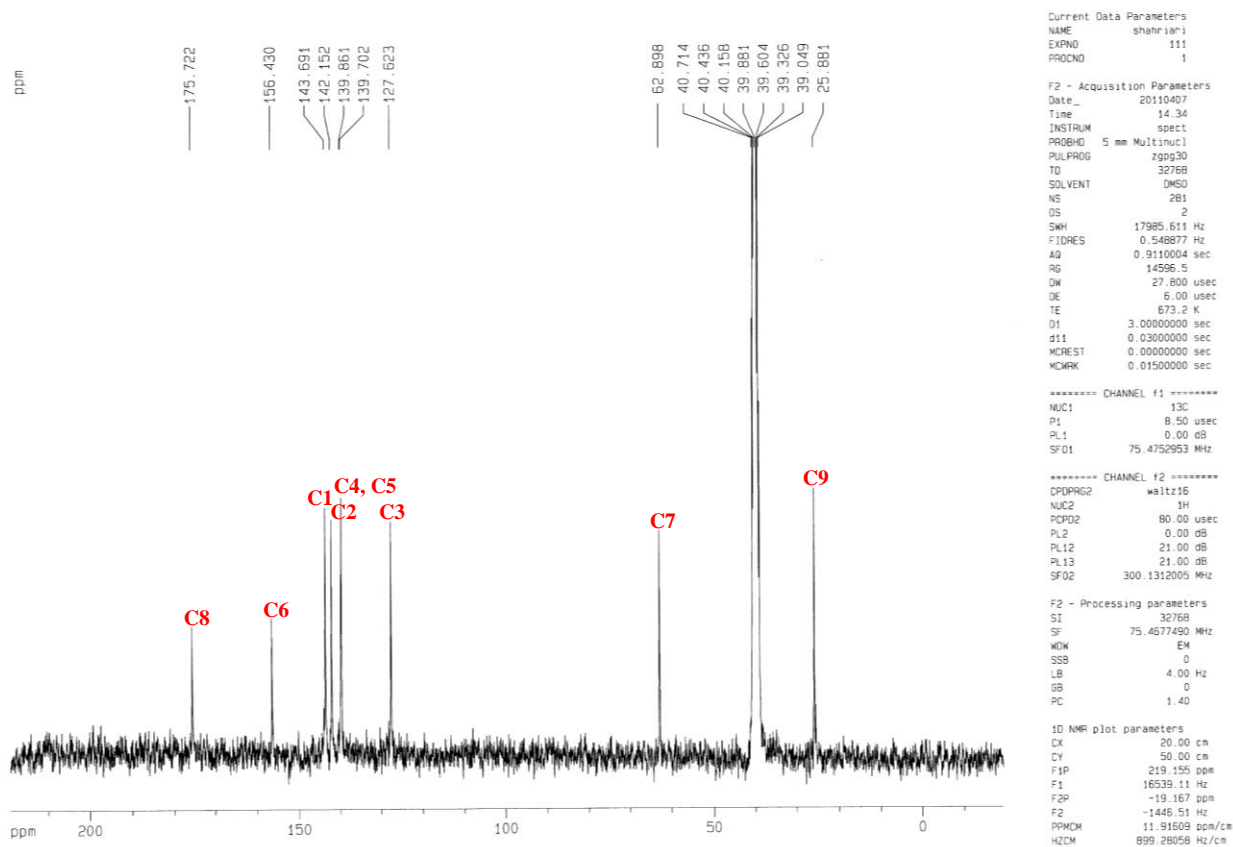


Figure A.6.  $^{13}\text{C}$ NMR spectrum of 2 with peak assignment according to Figure 4

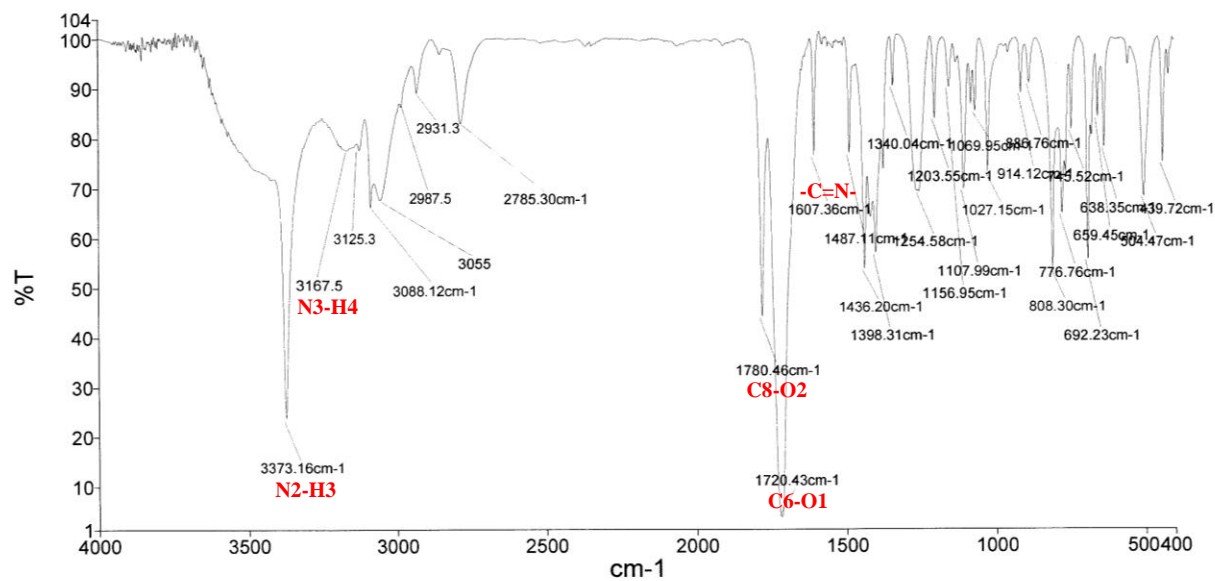
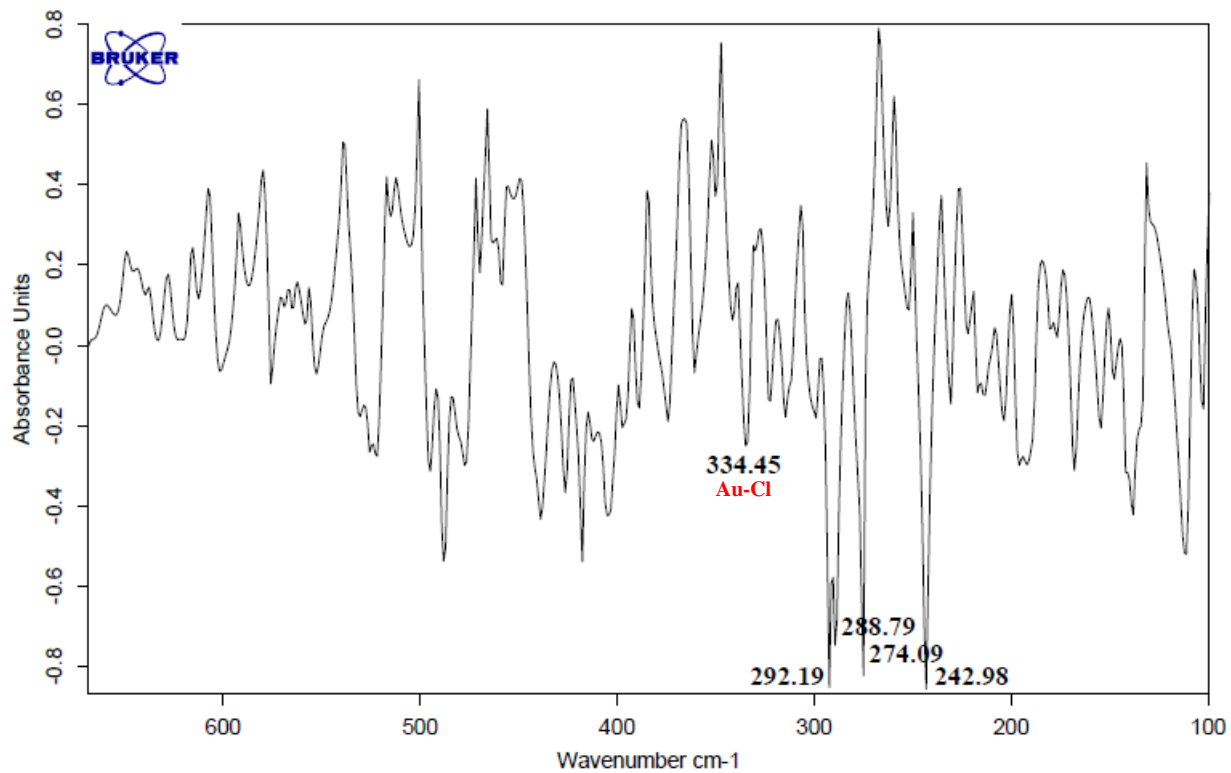


Figure A.7. IR spectrum of **2** with peak assignment according to **Figure 4**





**Figure A.8.** ATR-IR spectrum of **2**

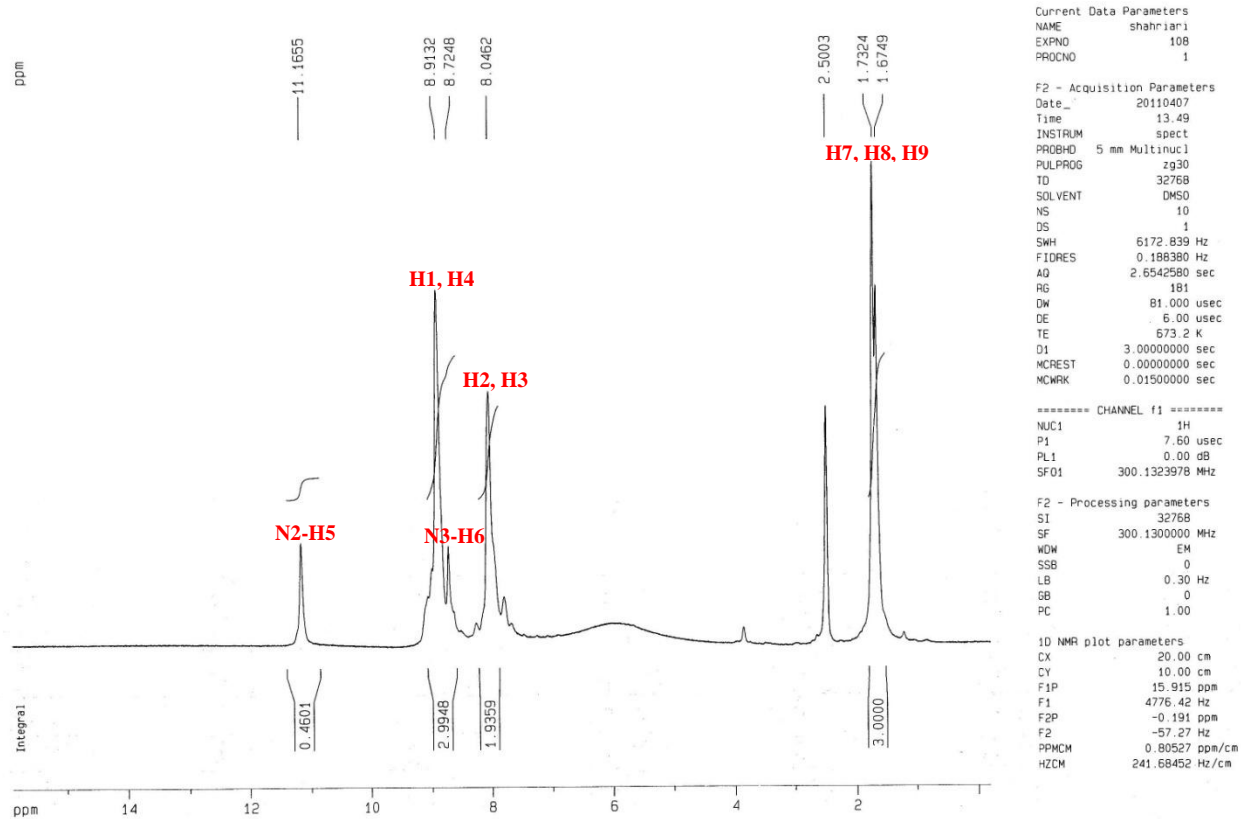


Figure A.9. <sup>1</sup>H NMR spectrum of 3 with peak assignment according to Figure 4

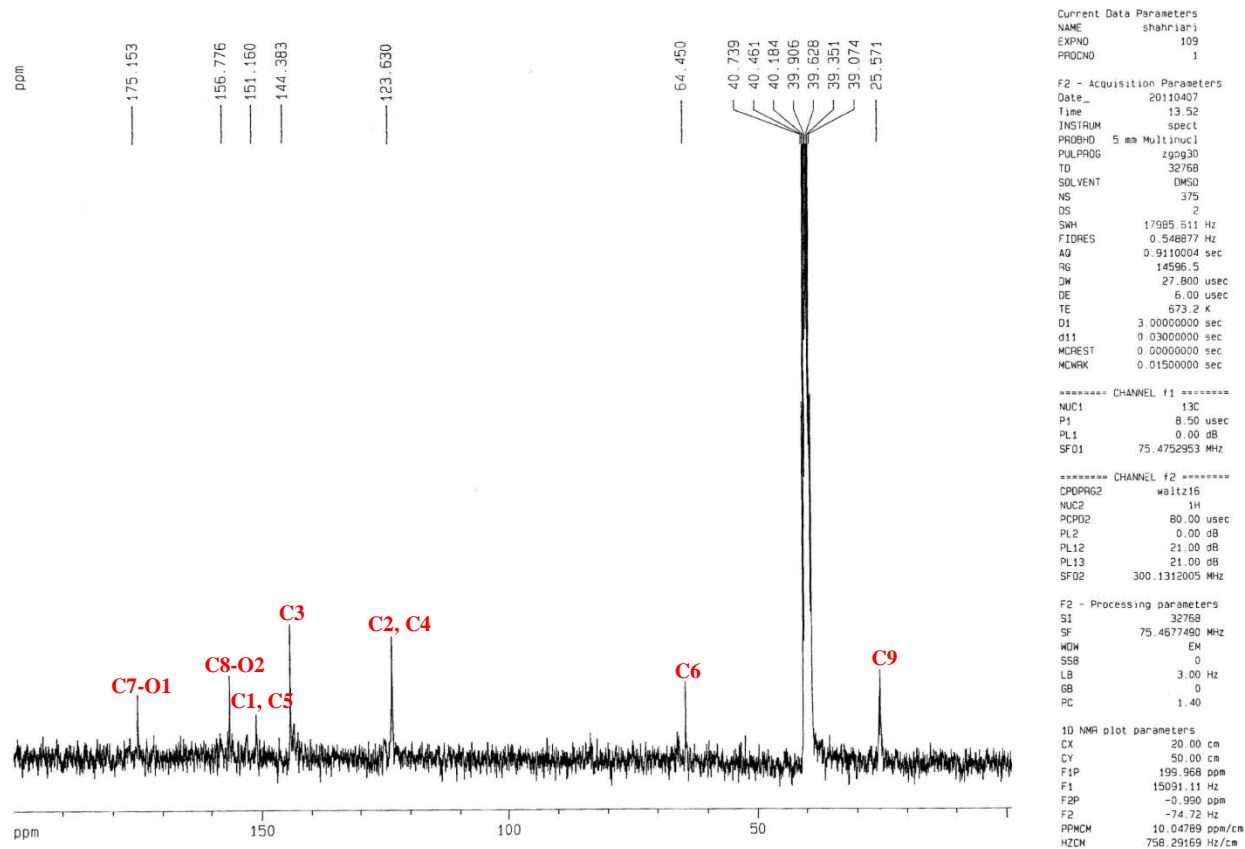


Fig. A.10.  $^{13}\text{C}$ NMR spectrum of 3 with peak assignment according to Figure 4

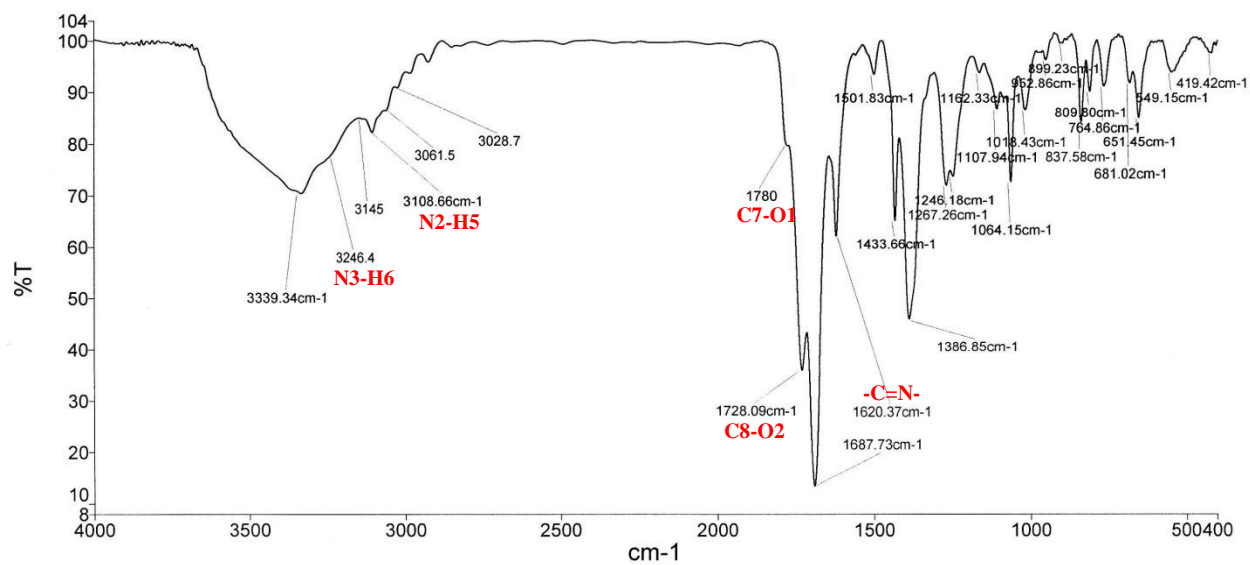
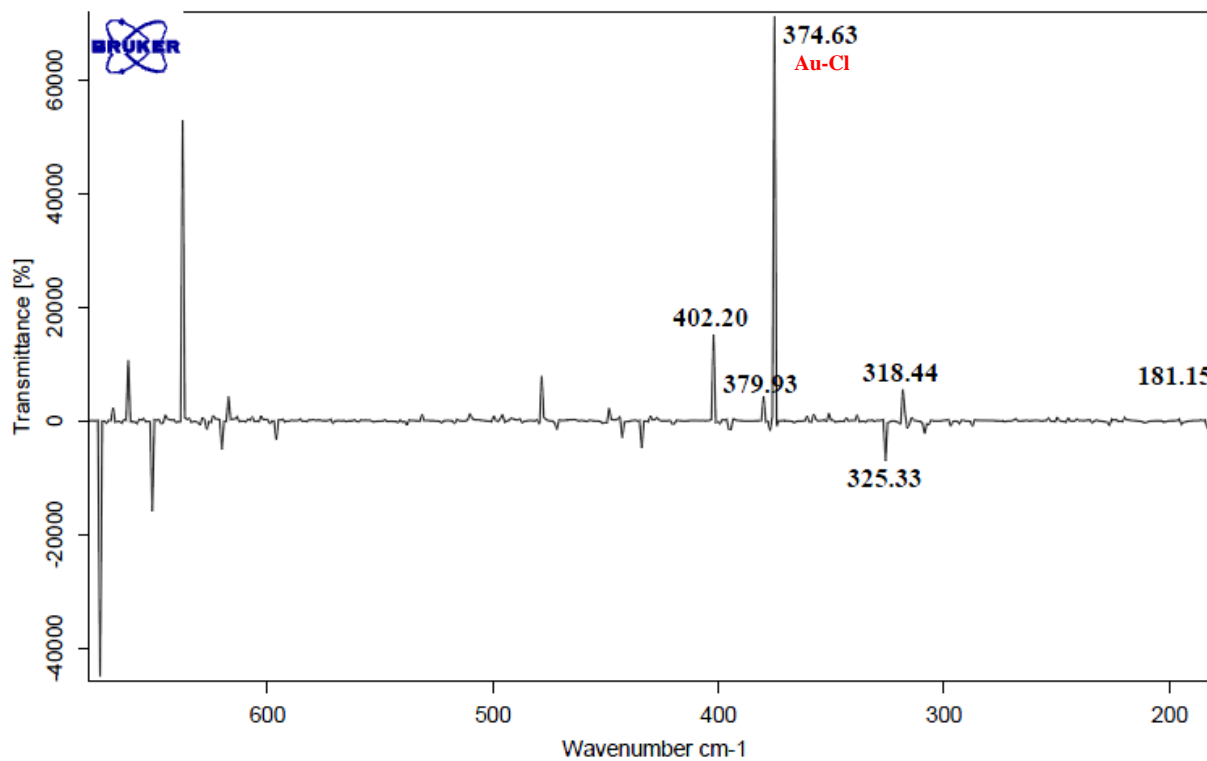


Figure A.11. IR spectrum of 3 with peak assignment according to Figure 4



**Figure A.12.** ATR-IR spectrum of **3**

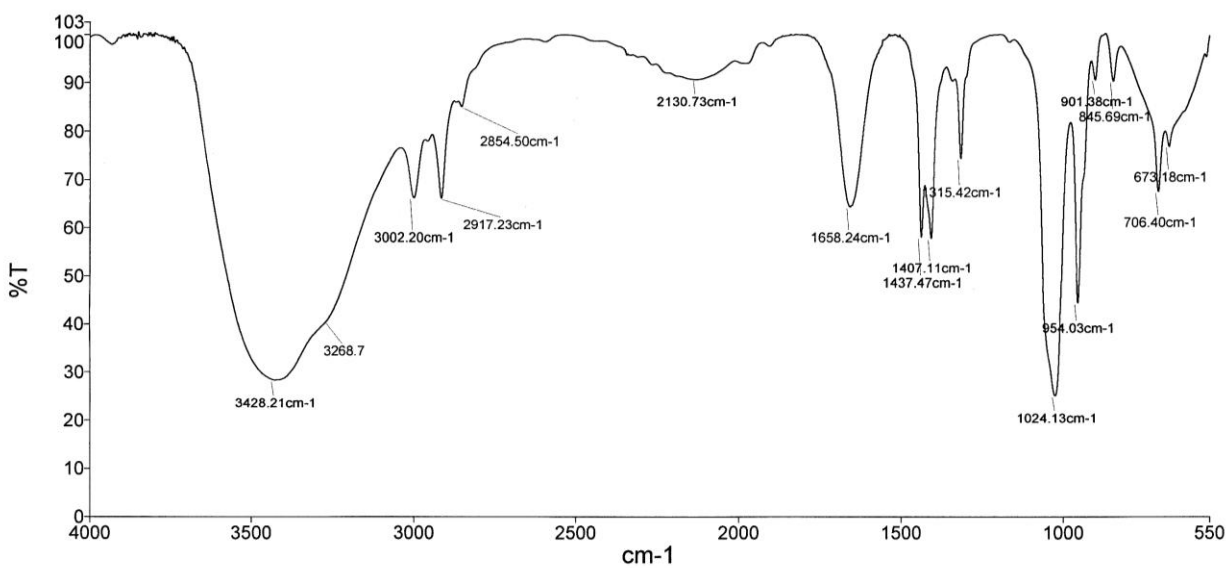


Figure A.13. IR spectrum of DMSO solvent

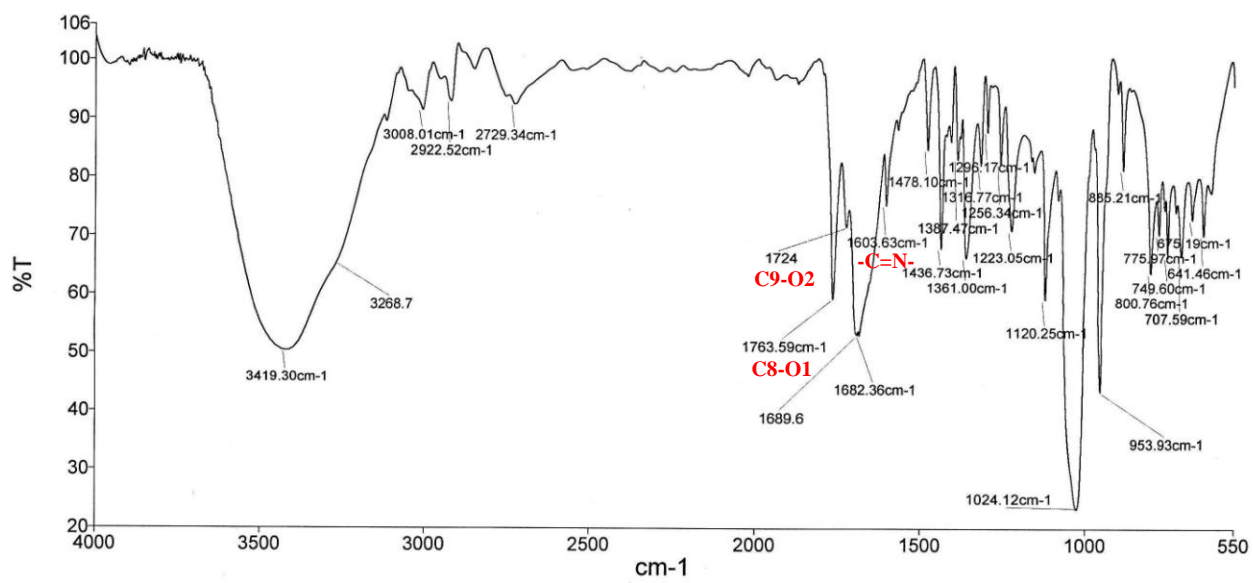


Figure A.14. IR spectrum of DMSO solution of **1**

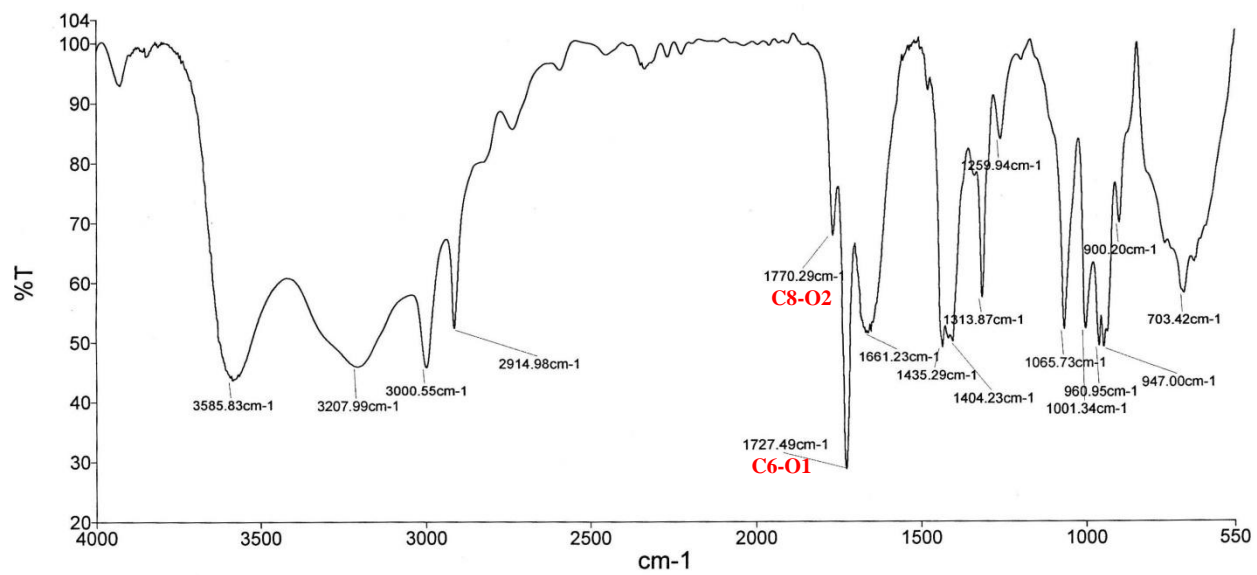


Figure A. 15. IR spectrum of DMSO solution of 2



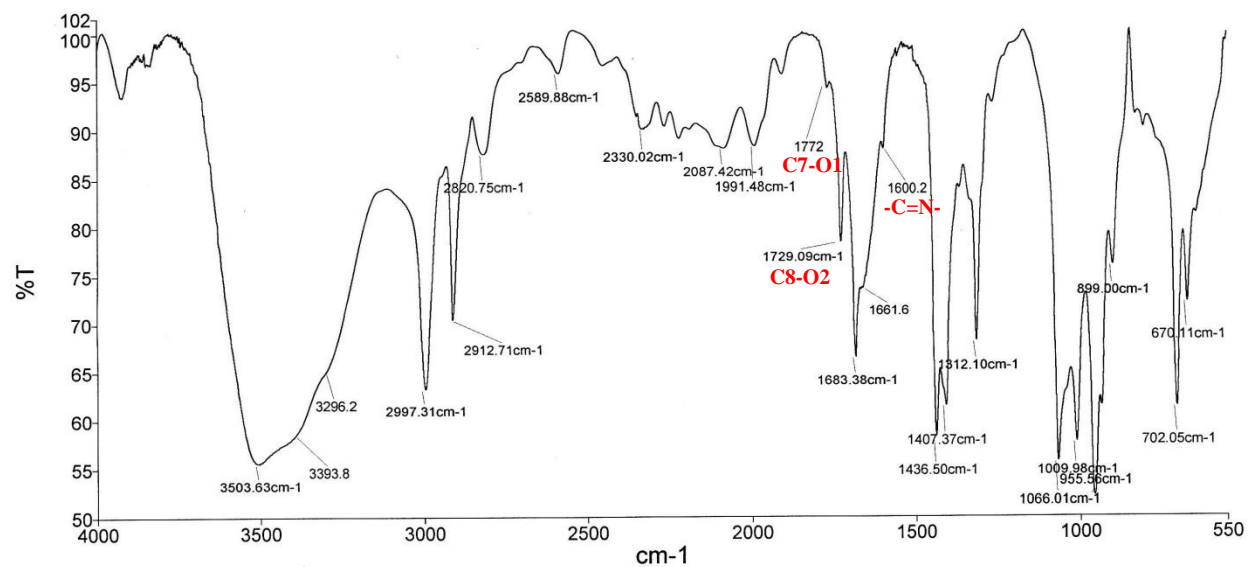


Figure A.16. IR spectrum of DMSO solution of 3

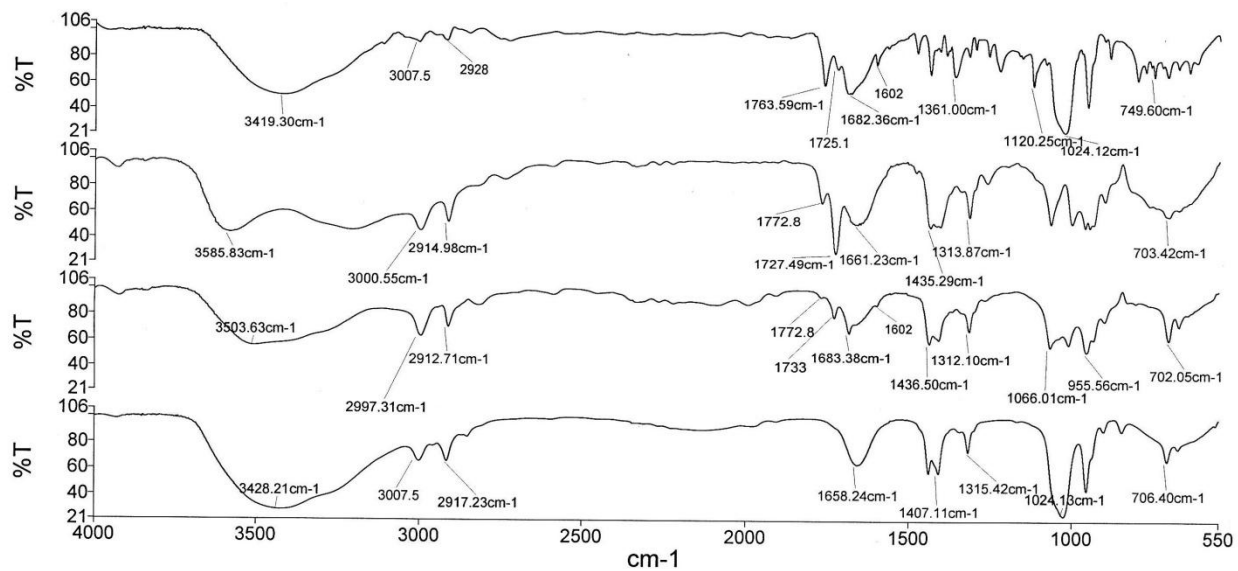
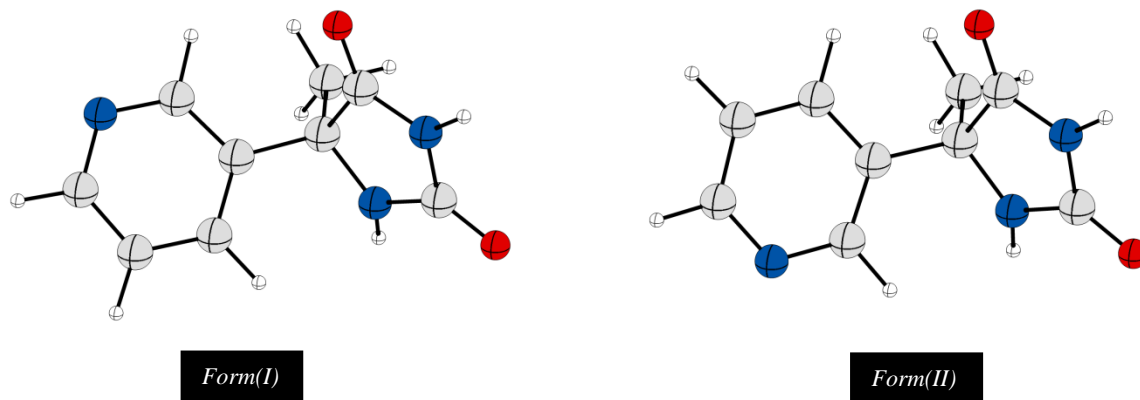
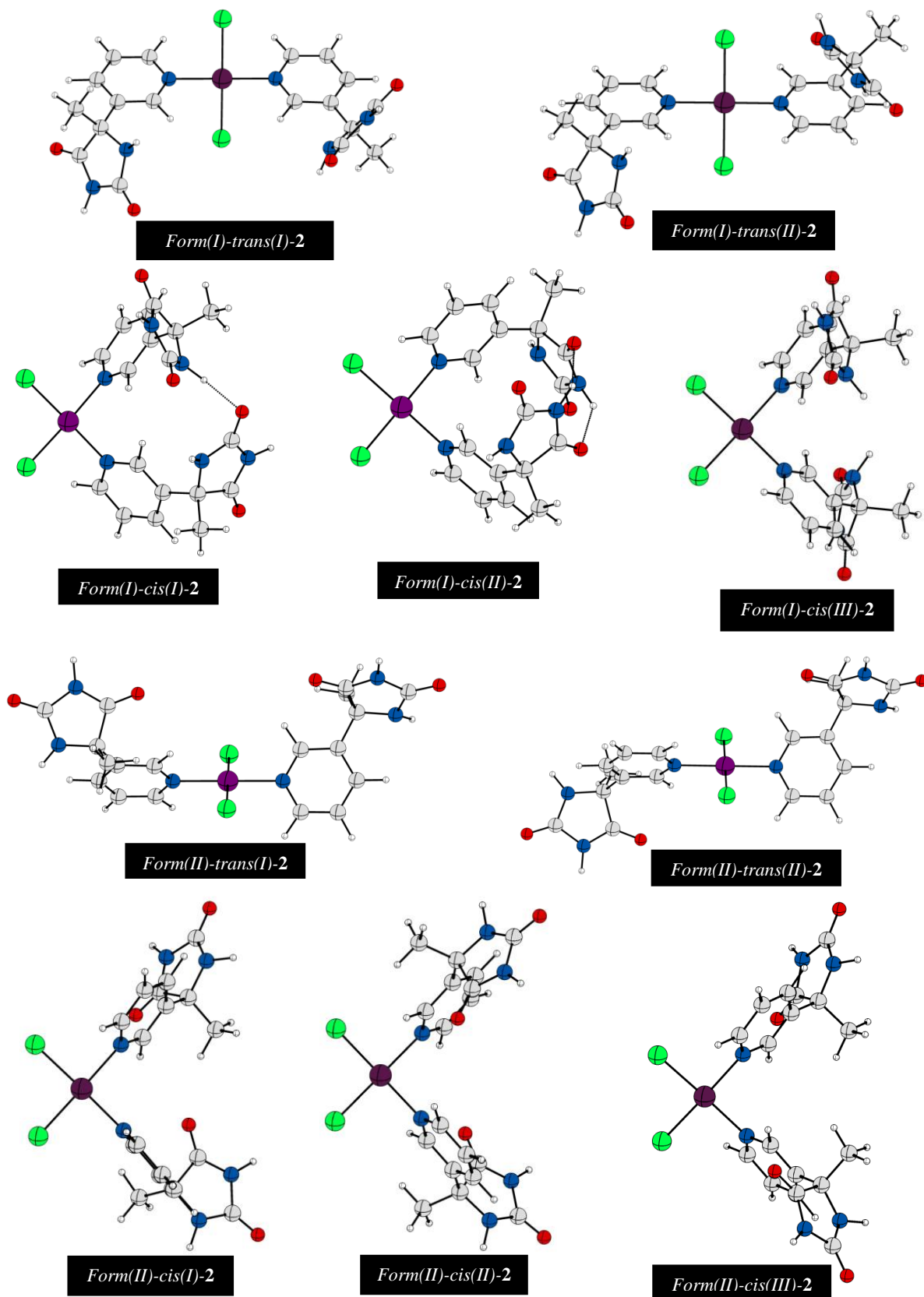


Figure A.17. IR spectrum of DMSO solution of **1**, **2**, **3**, and **DMSO** (up to down) for comparison



**Figure A.18.** Optimized structures of two possible conformers for **L2** at BP86/TZVP level of theory



**Figure A.19.** Optimized structures of all possible conformers for **2** at BP86/TZVP level of theory

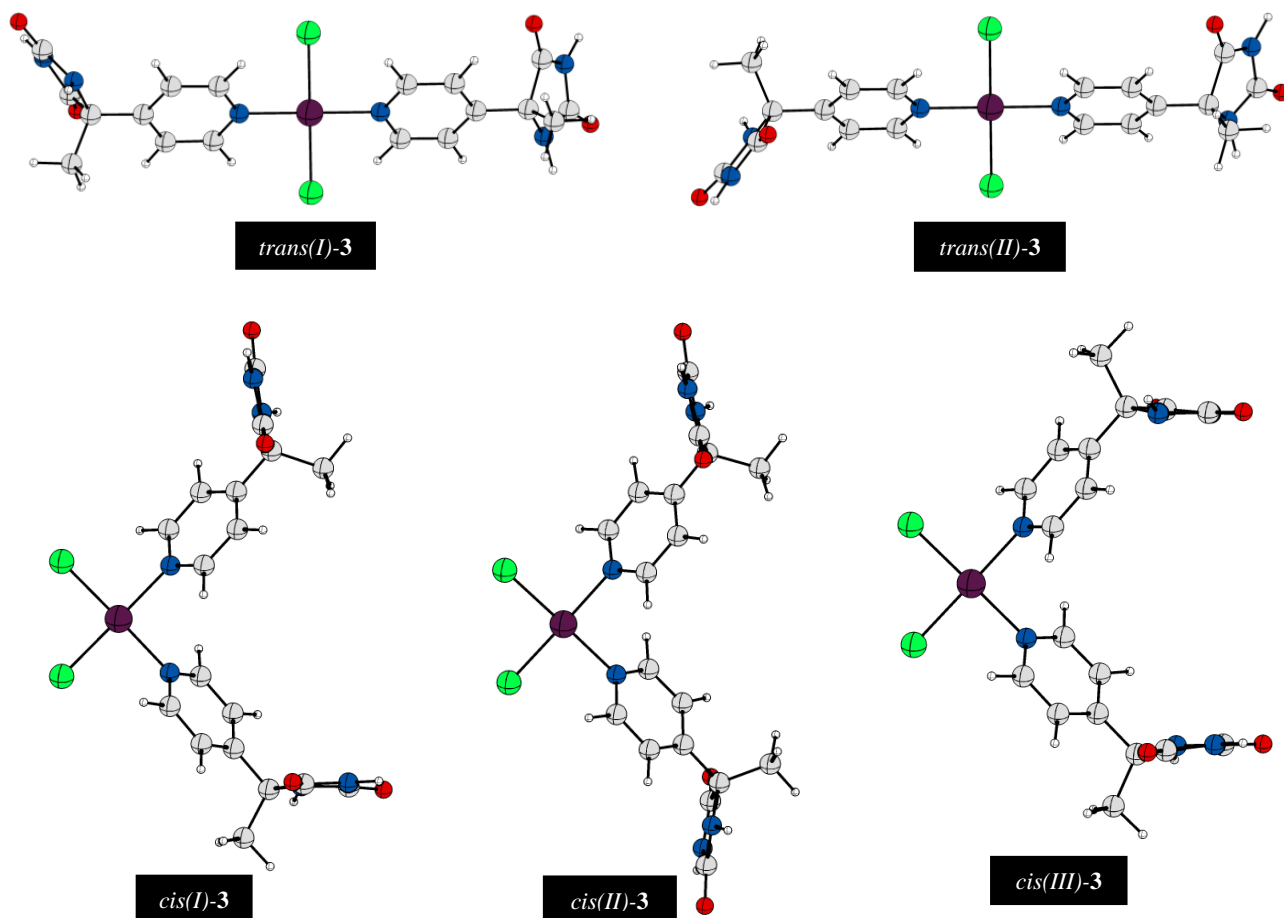
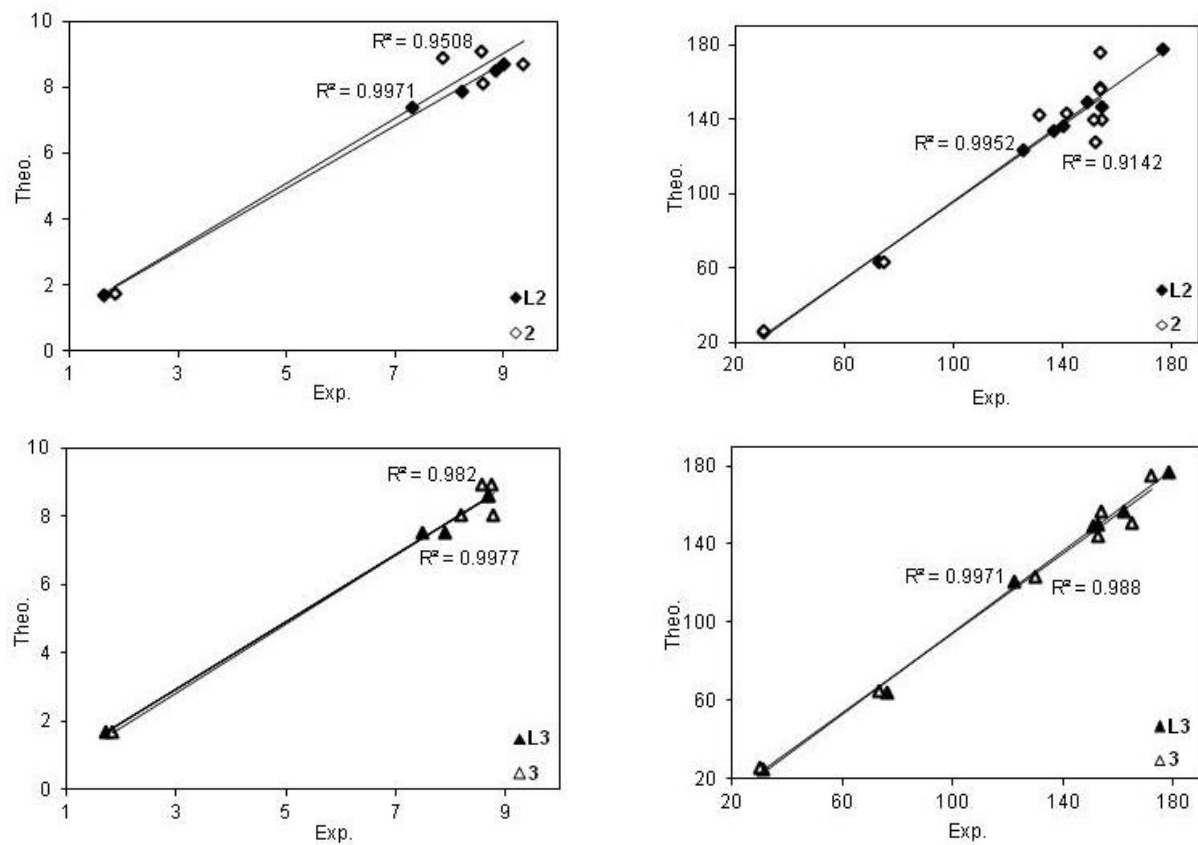


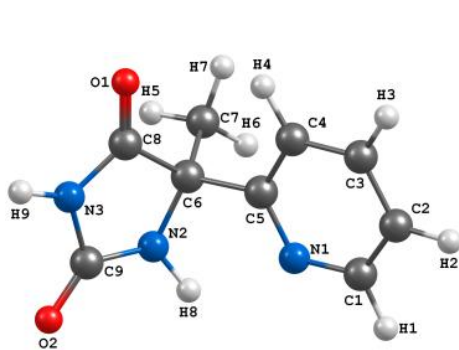
Figure A.20. Optimized structures of all possible conformers for **3** at BP86/TZVP level of theory



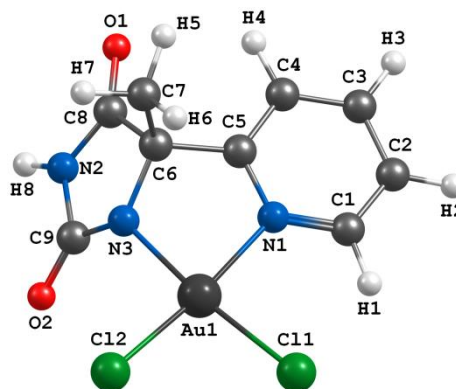
**Figure A.21.** Correlations between theoretical and corresponding experimental values of  $^1\text{H}$  (the left) and  $^{13}\text{C}$  (the right) chemical shifts ( $\delta$ , ppm) for **L2**, **L3**, **2**, and **3**

**Table A.1.** Selected bond lengths (Å) and angles (°) for **L1** and **1**

<b>L1</b>			<b>1</b>		
	BP86/TZVP	Exp. [64]		BP86/TZVP	
Bond lengths			Bond lengths		
C(1)–N(1)	1.342	1.332	Au(1)–Cl(1)	2.317	
C(5)–N(1)	1.342	1.333	Au(1)–Cl(2)	2.276	
C(6)–C(8)	1.553	1.538	Au(1)–N(1)	2.095	
C(8)–O(1)	1.219	1.207	Au(1)–N(3)	2.034	
C(8)–N(3)	1.375	1.361	N(1)–C(1)	1.348	
C(9)–N(3)	1.420	1.383	N(1)–C(5)	1.360	
C(9)–O(2)	1.216	1.233	N(3)–C(6)	1.466	
C(9)–N(2)	1.380	1.331	N(3)–C(9)	1.378	
C(6)–N(2)	1.463	1.461	C(5)–C(6)	1.518	
N(2)–H(2B)	1.020	0.900	Bond angles		
N(3)–H(3B)	1.016	0.850	Cl(1)–Au(1)–Cl(2)	90.81	
Bond angles			Cl(1)–Au(1)–N(3)	173.67	
C(7)–C(6)–C(5)	109.96	114.34	Cl(1)–Au(1)–N(1)	94.31	
C(7)–C(6)–C(8)	109.55	110.39	Cl(2)–Au(1)–N(3)	95.45	
N(2)–C(6)–C(7)	112.00	112.31	Cl(2)–Au(1)–N(1)	174.33	
C(5)–C(6)–C(8)	112.13	107.55	N(3)–Au(1)–N(1)	79.38	
N(2)–C(6)–C(8)	102.04	100.19	Au(1)–N(3)–C(6)	112.59	
N(2)–C(6)–C(5)	110.94	111.05	Au(1)–N(1)–C(5)	114.47	



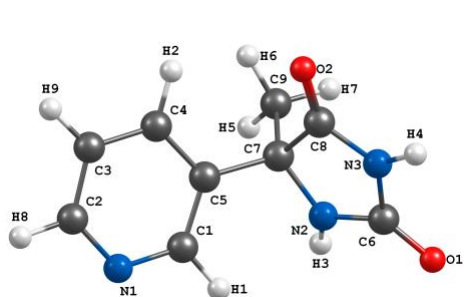
**L1**



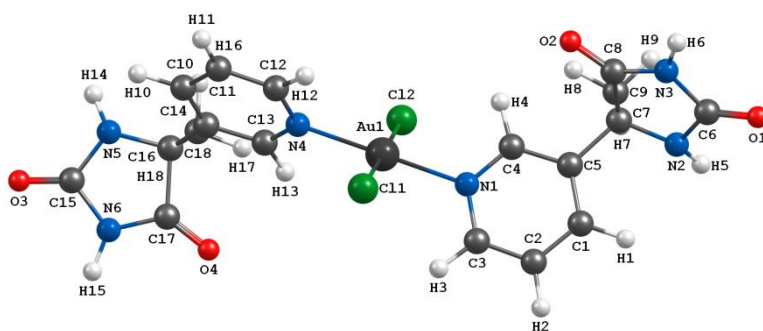
**1**

**Table A.2.** Selected bond lengths (Å) and angles (°) for **L2** and **2**

<b>L2</b>		<i>trans-2</i>	
	BP86/TZVP		BP86/TZVP
Bond lengths		Bond lengths	
C(1)–N(1)	1.342	Au(1)–Cl(1)	2.312
C(2)–N(1)	1.340	Au(1)–Cl(2)	2.316
C(1)–C(5)	1.402	Au(1)–N(1)	2.055
C(5)–O(7)	1.530	Au(1)–N(4)	2.055
C(7)–N(2)	1.462	N(1)–C(3)	1.353
C(6)–N(2)	1.375	N(1)–C(4)	1.349
C(6)–O(1)	1.216	N(4)–C(12)	1.353
C(6)–N(3)	1.417	N(4)–C(13)	1.349
C(8)–N(3)	1.376	C(5)–C(7)	1.529
N(2)–H(3)	1.014	Bond angles	
N(3)–H(4)	1.016	Cl(1)–Au(1)–Cl(2)	179.92
Bond angles		Cl(1)–Au(1)–N(4)	89.88
C(1)–C(5)–C(7)	121.94	Cl(1)–Au(1)–N(1)	89.96
C(1)–C(5)–C(4)	117.34	Cl(2)–Au(1)–N(4)	90.06
C(5)–C(7)–N(2)	113.10	Cl(2)–Au(1)–N(1)	90.08
C(5)–C(7)–C(8)	109.81	N(4)–Au(1)–N(1)	179.74
C(5)–C(7)–C(9)	111.61	Au(1)–N(4)–C(12)	119.72
N(2)–C(6)–N(3)	105.20	Au(1)–N(1)–C(4)	119.30



**L2**

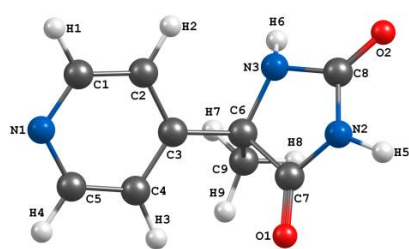


*trans-2*

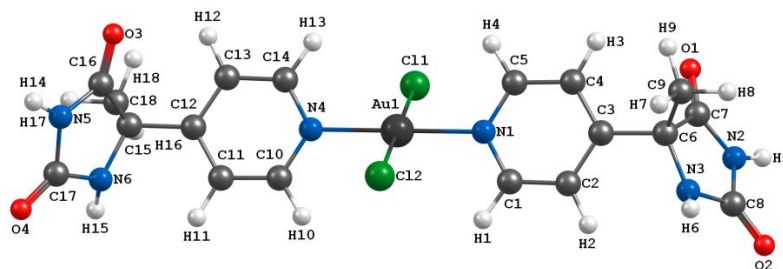


**Table A.3.** Selected bond lengths (Å) and angles (°) for **L3** and **3**

<b>L3</b>		<i>trans-3</i>	
	BP86/TZVP		BP86/TZVP
Bond lengths		Bond lengths	
C(1)–N(1)	1.352	Au(1)–Cl(1)	2.313
C(5)–N(1)	1.354	Au(1)–Cl(2)	2.314
C(6)–C(9)	1.538	Au(1)–N(1)	2.055
C(6)–N(3)	1.488	Au(1)–N(4)	2.056
C(6)–C(7)	1.557	N(1)–C(1)	1.351
C(7)–O(1)	1.216	N(1)–C(5)	1.353
C(7)–N(2)	1.386	N(4)–C(10)	1.352
C(8)–N(2)	1.421	N(4)–C(14)	1.354
C(8)–N(2)	1.407	C(12)–C(15)	1.524
N(2)–H(5)	1.033	C(15)–C(18)	1.543
N(3)–H(6)	1.036	Bond angles	
Bond angles		Cl(1)–Au(1)–Cl(2)	179.75
C(3)–C(6)–C(7)	110.63	Cl(1)–Au(1)–N(4)	90.13
C(3)–C(6)–C(9)	112.26	Cl(1)–Au(1)–N(1)	89.87
C(3)–C(6)–N(3)	111.65	Cl(2)–Au(1)–N(4)	90.07
C(2)–C(3)–C(6)	121.22	Cl(2)–Au(1)–N(1)	89.91
C(4)–C(3)–C(6)	121.22	N(4)–Au(1)–N(1)	179.81
N(2)–C(8)–N(3)	105.79	Au(1)–N(1)–C(1)	120.02



**L3**



*trans-3*

**Table A.4.** Electronic energies (Hartree) of all possible isomers and conformers for **L2**, **2** and **3** at BP86/TZVP level

Compounds	Gas	Solvation		
		Water	Ethanol	Water/Ethanol
<b>2</b>				
<i>form(I)-L2</i>	-663.3823400	-663.4103065	-663.4092305	-663.4097685
<i>form(I)-Trans(I)-2</i>	-2383.0309705	-2383.1363859	-2383.1310676	-2383.1337267
<i>form(I)-Trans(II)-2</i>	-2383.0309112	-2383.1367312	-2383.1312273	-2383.1339792
<i>form(I)-Cis(I)-2</i>	-2383.0218326	-2383.124992	-2383.1151803	-2383.1200861
<i>form(I)-Cis(II)-2</i>	-2383.0226522	-2383.1229134	-2383.1179335	-2383.1204234
<i>form(I)-Cis(III)-2</i>	-2383.014657	-2383.123489	-2383.123489	-2383.123489
<i>form(II)-L2</i>	-663.3828808	-663.4102839	-663.4092584	-663.40977115
<i>form(II)-Trans(I)-2</i>	-2383.0315743	-2383.1357294	-2383.1297376	-2383.1327335
<i>form(II)-Trans(II)-2</i>	-2383.0318944	-2383.1358501	-2383.129662	-2383.1327560
<i>form(II)-Cis(I)-2</i>	-2383.0182727	-2383.1295312	-2383.1233069	-2383.1264190
<i>form(II)-Cis(II)-2</i>	-2383.021099	-2383.1308115	-2383.1250054	-2383.1279084
<i>form(II)-Cis(III)-2</i>	-2383.0157658	-2383.1267385	-2383.120279	-2383.1235087
<b>3</b>				
<i>Trans(I)-3</i>	-2383.0333242	-2383.1393298	-2383.1345057	-2383.1369177
<i>Trans(II)-3</i>	-2383.0333949	-2383.1393462	-2383.1345271	-2383.1369366
<i>Cis(I)-3</i>	-2383.0197641	-2383.1341201	-2383.1306531	-2383.1323866
<i>Cis(II)-3</i>	-2383.0188748	-2383.1339585	-2383.128709	-2383.1313337
<i>Cis(III)-3</i>	-2383.0206418	-2383.134612	-2383.1293758	-2383.1319939

Cartesian coordinate representation of the optimized molecular structures of **L1**, **L2**, **L3** and corresponding Au(III) complexes at BP86/TZVP level of theory

<b>L1</b>			
C	5.621892000	8.306998000	-1.019618000
H	6.181025000	7.534026000	-1.555344000
C	6.223511000	9.520904000	-0.684408000
H	7.263881000	9.713130000	-0.950745000
C	5.460064000	10.470451000	-0.000952000
H	5.893038000	11.430697000	0.286555000
C	4.133466000	10.176021000	0.315054000
H	3.503790000	10.883927000	0.855702000
C	3.622318000	8.925151000	-0.057317000
C	2.158584000	8.535046000	0.207849000
C	1.233964000	9.238473000	-0.806868000
H	0.193473000	8.919484000	-0.654634000
H	1.539029000	8.976485000	-1.829736000
H	1.294671000	10.328065000	-0.682426000
C	1.710490000	8.890177000	1.652638000
C	1.700473000	6.562605000	1.430219000
N	4.349211000	8.006874000	-0.713589000
N	1.992307000	7.081128000	0.185011000
H	2.627207000	6.552994000	-0.415134000
N	1.447434000	7.685995000	2.262793000
H	1.140800000	7.587182000	3.226766000
O	1.590807000	10.004748000	2.132391000
O	1.644004000	5.399611000	1.780624000

<b>1</b>			
C	-0.230953000	2.637180000	-0.568182000
H	0.803828000	2.896545000	-0.801157000
C	-1.289093000	3.534421000	-0.656440000
H	-1.097610000	4.554372000	-0.989295000
C	-2.573475000	3.103806000	-0.314886000
H	-3.422270000	3.786470000	-0.382695000
C	-2.765480000	1.790379000	0.113004000
H	-3.750283000	1.403291000	0.378325000
C	-1.671977000	0.925723000	0.177880000
C	-1.743820000	-0.515228000	0.650625000
C	-1.847802000	-0.572976000	2.189669000
H	-2.777070000	-0.095350000	2.528608000
H	-0.988400000	-0.062347000	2.646561000
H	-1.843833000	-1.622121000	2.514022000
C	-2.956205000	-1.265150000	0.015470000
C	-0.954482000	-2.196095000	-0.792268000
N	-0.431222000	1.366920000	-0.162349000

N	-2.396055000	-2.239613000	-0.752738000
H	-2.920576000	-2.911300000	-1.308373000
N	-0.582666000	-1.249330000	0.137945000
O	-4.137376000	-1.018494000	0.201614000
O	-0.287437000	-2.899848000	-1.520465000
Au	1.075739000	-0.081185000	-0.014369000
Cl	2.806965000	1.450652000	-0.185426000
Cl	2.564163000	-1.781912000	0.256709000

*form(I)-L2*

C	3.062296000	0.877640000	-0.373618000
C	1.834168000	0.214369000	-0.390181000
C	0.665247000	0.972118000	-0.479789000
N	0.661457000	2.313392000	-0.544228000
C	1.847305000	2.937506000	-0.531354000
C	3.086196000	2.274287000	-0.456335000
C	6.402850000	2.412575000	0.668992000
N	5.578854000	2.203762000	-0.415327000
C	4.396787000	3.066526000	-0.439323000
C	4.545065000	3.808693000	0.930307000
N	5.709036000	3.330781000	1.493839000
C	4.467808000	4.099025000	-1.581676000
O	7.493853000	1.926150000	0.898826000
O	3.790603000	4.644582000	1.385914000
H	3.995517000	0.318057000	-0.290486000
H	1.785868000	-0.874457000	-0.330601000
H	1.807566000	4.029516000	-0.564061000
H	5.966659000	1.773080000	-1.249033000
H	6.085362000	3.646572000	2.383699000
H	4.382173000	3.592456000	-2.554128000
H	3.649137000	4.824340000	-1.494398000
H	5.420983000	4.645545000	-1.544631000
H	-0.315384000	0.486371000	-0.496672000

*form(II)-L2*

C	3.001255000	0.914995000	-0.414654000
N	1.858927000	0.209462000	-0.411591000
C	0.708714000	0.897279000	-0.370347000
C	0.652422000	2.293576000	-0.327636000
C	1.845360000	3.013799000	-0.342938000
C	3.062122000	2.316364000	-0.392578000
C	6.383970000	2.412486000	0.716151000
N	5.556203000	2.183074000	-0.358491000
C	4.394365000	3.069579000	-0.418224000
C	4.571855000	3.877694000	0.908317000
N	5.719297000	3.393520000	1.494890000

C	4.476580000	4.038083000	-1.615781000
O	7.458535000	1.904202000	0.973041000
O	3.845768000	4.762298000	1.320513000
H	3.922789000	0.326551000	-0.427543000
H	1.834604000	4.103215000	-0.289187000
H	5.914233000	1.670902000	-1.158185000
H	6.109197000	3.744453000	2.365497000
H	4.379469000	3.479276000	-2.558065000
H	3.667044000	4.777417000	-1.565471000
H	5.437304000	4.572572000	-1.613141000
H	-0.209635000	0.301690000	-0.367070000
H	-0.309495000	2.807216000	-0.280706000

*form(I)-Trans(I)-2*

C	-0.643976000	2.790423000	0.124196000
N	-1.812311000	2.112939000	0.183753000
C	-2.990135000	2.767716000	0.283923000
C	-3.018666000	4.156986000	0.316057000
C	-1.825478000	4.874055000	0.247208000
C	-0.606406000	4.183326000	0.151423000
C	2.750166000	4.305737000	1.189243000
N	1.877903000	4.026071000	0.138058000
C	0.728362000	4.926541000	0.105995000
C	0.900234000	5.705927000	1.458198000
N	2.082462000	5.260157000	1.994741000
C	0.784058000	5.921729000	-1.070924000
O	3.845192000	3.834048000	1.392764000
O	0.127402000	6.527717000	1.906753000
H	0.270293000	2.205087000	0.052180000
H	-3.891376000	2.162200000	0.354160000
H	-3.979366000	4.664600000	0.401397000
H	-1.835960000	5.963026000	0.294354000
H	2.305522000	3.690428000	-0.723027000
H	2.486823000	5.612625000	2.860010000
H	0.687272000	5.387759000	-2.027448000
H	-0.025516000	6.659255000	-0.997583000
H	1.740256000	6.462729000	-1.060670000
Au	-1.785540000	0.055543000	0.116879000
C	-0.564325000	-2.643206000	-0.005385000
N	-1.752102000	-2.001094000	0.051076000
C	-2.914714000	-2.689671000	0.058878000
C	-2.906489000	-4.077788000	-0.007135000
C	-1.691568000	-4.759759000	-0.049746000
C	-0.488647000	-4.034991000	-0.037056000
C	2.797271000	-3.991909000	-1.280405000
N	1.986520000	-3.802827000	-0.161459000

C	0.866168000	-4.738345000	-0.113670000
C	0.971919000	-5.429624000	-1.520138000
N	2.104066000	-4.914960000	-2.101155000
C	1.023941000	-5.799120000	0.993792000
O	3.865304000	-3.477811000	-1.520089000
O	0.193744000	-6.246451000	-1.967957000
H	0.335162000	-2.031776000	-0.050204000
H	-3.834628000	-2.112933000	0.129170000
H	-3.855966000	-4.612796000	-0.019720000
H	-1.676291000	-5.847602000	-0.115691000
H	2.461003000	-3.510726000	0.690766000
H	2.459664000	-5.199214000	-3.011722000
H	0.961444000	-5.329222000	1.986189000
H	0.240217000	-6.563507000	0.917515000
H	1.997339000	-6.299442000	0.898186000
Cl	-0.460237000	0.134046000	-1.780340000
Cl	-3.119693000	-0.031610000	2.005018000

*form(I)-Trans(II)-2*

Au	0.139211000	-0.058072000	0.097635000
C	2.837576000	-6.039048000	0.443237000
C	1.286124000	2.675902000	0.316138000
C	1.283841000	4.057187000	0.469519000
C	0.075378000	4.731475000	0.636331000
C	-1.127581000	4.006795000	0.647173000
C	-4.502178000	4.154012000	-0.324034000
C	2.847412000	-5.384871000	-2.011789000
C	-2.478309000	4.707041000	0.791929000
C	-2.689646000	5.620404000	-0.468001000
C	2.722808000	-4.855355000	-0.537985000
C	-2.539527000	5.569526000	2.068696000
C	4.695495000	-4.026249000	-1.570844000
C	1.379379000	-4.137812000	-0.411457000
C	0.165178000	-4.835755000	-0.516739000
C	-1.039676000	-4.140389000	-0.428449000
C	-1.026638000	-2.765290000	-0.227998000
C	1.325564000	-2.754652000	-0.245498000
C	-1.059003000	2.623854000	0.488138000
Cl	1.473988000	0.164083000	-1.778338000
Cl	-1.192459000	-0.294974000	1.978037000
H	-3.511242000	6.078202000	2.132003000
H	-4.010076000	3.347591000	1.504493000
H	0.062189000	5.817081000	0.732003000
H	-1.754128000	6.336137000	2.060751000
H	-2.408227000	4.940543000	2.961238000
H	2.232401000	4.593540000	0.448260000

H	2.199331000	2.105248000	0.160427000
H	-1.959124000	2.012534000	0.485827000
H	3.805337000	-6.542245000	0.311897000
H	2.045049000	-6.776247000	0.262149000
H	2.758567000	-5.685670000	1.481706000
H	4.375166000	-5.021279000	-3.435141000
H	4.321809000	-3.763989000	0.433903000
H	-4.295404000	5.635176000	-1.851430000
H	0.163994000	-5.911715000	-0.689444000
H	-1.997027000	-4.654773000	-0.510528000
H	-1.938065000	-2.180815000	-0.119695000
H	2.235040000	-2.157284000	-0.214290000
N	3.860801000	-3.943872000	-0.455984000
N	0.147025000	-2.100605000	-0.148645000
N	0.123271000	1.987516000	0.331838000
N	-3.606800000	3.786983000	0.679248000
N	-3.869472000	5.204166000	-1.033354000
N	4.003955000	-4.834532000	-2.505728000
O	-1.943188000	6.503951000	-0.836164000
O	5.780112000	-3.514474000	-1.725938000
O	2.063228000	-6.127471000	-2.565462000
O	-5.589389000	3.679652000	-0.560772000

*form(I)-Cis(I)-2*

Au	-2.657989000	1.761093000	1.572465000
C	1.770812000	-2.910512000	2.558894000
C	-3.251569000	1.794512000	-1.370449000
C	-2.993398000	1.941598000	-2.727941000
C	-1.674982000	2.047461000	-3.174518000
C	-0.620315000	1.984891000	-2.251879000
C	2.590563000	2.665704000	-1.127770000
C	0.766838000	-3.599703000	0.318656000
C	0.849548000	2.142982000	-2.650511000
C	1.166296000	3.683216000	-2.677505000
C	0.929604000	-2.438857000	1.360394000
C	1.168143000	1.536613000	-4.027763000
C	1.855894000	-1.835055000	-0.738910000
C	-0.474999000	-1.991020000	1.780891000
C	-1.374935000	-2.867123000	2.409042000
C	-2.651557000	-2.414480000	2.738885000
C	-3.010908000	-1.098253000	2.464071000
C	-0.909606000	-0.693361000	1.516952000
C	-0.956919000	1.852884000	-0.902438000
Cl	-3.222581000	3.956568000	1.315750000
Cl	-3.147474000	1.860644000	3.800771000
H	2.242314000	1.635739000	-4.233185000

H	2.101889000	0.702046000	-1.609993000
H	-1.473094000	2.186995000	-4.236175000
H	0.625820000	2.065073000	-4.822335000
H	0.905637000	0.469532000	-4.054488000
H	-3.829571000	1.985305000	-3.425866000
H	-4.263118000	1.730517000	-0.972580000
H	-0.173070000	1.852976000	-0.145329000
H	2.760992000	-3.244549000	2.220053000
H	1.279670000	-3.752373000	3.063610000
H	1.897535000	-2.093543000	3.283718000
H	1.362923000	-3.658894000	-1.723122000
H	2.209246000	-0.710005000	0.958434000
H	2.602062000	4.764040000	-1.550003000
H	-1.086145000	-3.898538000	2.614059000
H	-3.375721000	-3.072752000	3.218912000
H	-3.981191000	-0.688935000	2.739610000
H	-0.252568000	0.015721000	1.017581000
N	1.603855000	-1.421662000	0.553602000
N	-2.141882000	-0.261763000	1.856076000
N	-2.233608000	1.751483000	-0.481879000
N	1.746989000	1.670220000	-1.600476000
N	2.164097000	3.866804000	-1.748949000
N	1.316134000	-3.125633000	-0.856933000
O	0.620070000	4.504705000	-3.381983000
O	2.411574000	-1.207773000	-1.628441000
O	0.242620000	-4.673052000	0.516623000
O	3.494444000	2.554978000	-0.326231000

*form(I)-Cis(II)-2*

C	-2.284261000	1.357390000	-0.490654000
N	-1.437452000	1.883409000	0.420487000
C	-0.333631000	2.554261000	0.021542000
C	-0.036467000	2.680461000	-1.330918000
C	-0.888539000	2.117823000	-2.281214000
C	-2.049428000	1.449215000	-1.863563000
C	-4.413379000	-1.047653000	-2.147371000
N	-4.236076000	0.328275000	-2.214868000
C	-2.980012000	0.721463000	-2.844908000
C	-2.314534000	-0.678227000	-3.087526000
N	-3.204157000	-1.610088000	-2.637641000
C	-3.175768000	1.468323000	-4.172998000
O	-5.374076000	-1.659540000	-1.739033000
O	-1.196958000	-0.854006000	-3.548155000
H	-3.170842000	0.847329000	-0.115730000
H	0.288375000	2.989079000	0.802297000
H	0.866749000	3.212924000	-1.628719000



H	-0.643283000	2.195739000	-3.340069000
H	-5.063206000	0.920049000	-2.236690000
H	-2.977968000	-2.605425000	-2.540782000
H	-3.581406000	2.475012000	-3.997345000
H	-2.225744000	1.558255000	-4.714957000
H	-3.873933000	0.911291000	-4.812069000
Au	-1.827561000	1.633762000	2.470742000
C	-1.056267000	-1.148121000	1.621614000
N	-2.029454000	-0.445771000	2.240954000
C	-3.138169000	-1.069622000	2.698335000
C	-3.307732000	-2.436149000	2.505347000
C	-2.322428000	-3.168099000	1.842723000
C	-1.159197000	-2.521966000	1.397129000
C	1.414571000	-2.060165000	-0.853842000
N	1.134597000	-2.441692000	0.452037000
C	-0.079623000	-3.241543000	0.575342000
C	-0.602761000	-3.223540000	-0.903459000
N	0.309539000	-2.510269000	-1.625358000
C	0.187467000	-4.681099000	1.040440000
O	2.375661000	-1.451659000	-1.266250000
O	-1.650739000	-3.722775000	-1.283687000
H	-0.173529000	-0.600384000	1.293722000
H	-3.868048000	-0.455977000	3.223927000
H	-4.216479000	-2.915164000	2.869657000
H	-2.465996000	-4.234388000	1.670079000
H	1.909590000	-2.526874000	1.105461000
H	0.155668000	-2.215796000	-2.595335000
H	0.491565000	-4.698719000	2.096865000
H	-0.707736000	-5.304073000	0.918545000
H	0.988394000	-5.124105000	0.433490000
Cl	-1.594337000	3.886414000	2.742030000
Cl	-2.266729000	1.384080000	4.694964000

*form(I)-Cis(III)-2*

C	-1.098868000	1.632855000	-0.581125000
N	-2.167799000	1.746469000	0.237445000
C	-3.366773000	2.135827000	-0.249171000
C	-3.524350000	2.408813000	-1.603648000
C	-2.430747000	2.294949000	-2.460724000
C	-1.184867000	1.895664000	-1.948409000
C	2.283348000	2.377292000	-2.212755000
N	1.256157000	1.435644000	-2.098598000
C	0.056581000	1.824543000	-2.837401000
C	0.414572000	3.292082000	-3.272852000
N	1.702420000	3.502273000	-2.842675000
C	-0.174475000	0.960895000	-4.092334000

O	3.429576000	2.266619000	-1.844511000
O	-0.321382000	4.052280000	-3.865410000
H	-0.147564000	1.351233000	-0.130719000
H	-4.179435000	2.247232000	0.466938000
H	-4.499119000	2.728822000	-1.971886000
H	-2.535779000	2.545233000	-3.516307000
H	1.556272000	0.462794000	-2.078869000
H	2.228144000	4.358280000	-3.009908000
H	-0.415148000	-0.073830000	-3.806889000
H	-0.999636000	1.358983000	-4.696393000
H	0.729438000	0.954952000	-4.716783000
Au	-1.918559000	1.507254000	2.306370000
C	-2.273918000	-1.405785000	1.663562000
N	-1.373340000	-0.510000000	2.124138000
C	-0.171248000	-0.920195000	2.585269000
C	0.165482000	-2.269461000	2.576801000
C	-0.753020000	-3.205353000	2.103562000
C	-2.003896000	-2.773971000	1.630976000
C	-5.417459000	-3.583201000	1.479055000
N	-4.310801000	-3.116893000	0.762992000
C	-3.067408000	-3.769565000	1.168033000
C	-3.534208000	-4.586863000	2.427198000
N	-4.890515000	-4.386382000	2.516874000
C	-2.530190000	-4.740270000	0.098793000
O	-6.584483000	-3.347272000	1.269093000
O	-2.815240000	-5.246791000	3.147088000
H	-3.241511000	-1.024998000	1.338108000
H	0.495181000	-0.154916000	2.980060000
H	1.137959000	-2.577416000	2.961030000
H	-0.512798000	-4.268139000	2.130237000
H	-4.484276000	-2.902100000	-0.217144000
H	-5.486916000	-4.819715000	3.219462000
H	-2.209233000	-4.186211000	-0.795670000
H	-1.675945000	-5.312737000	0.481941000
H	-3.313933000	-5.454330000	-0.189126000
Cl	-2.552179000	3.684987000	2.554250000
Cl	-1.613754000	1.304175000	4.558313000

*form(II)-Trans(I)-2*

Au	-1.650678000	-1.190227000	0.551076000
C	0.975417000	-3.891062000	2.581909000
C	-0.135616000	-3.196018000	2.125661000
C	-4.741923000	3.478520000	1.766500000
C	1.224128000	-1.868336000	0.735436000
C	2.383549000	-2.522503000	1.169272000
C	5.771371000	-1.892993000	1.851727000

C	-3.530938000	4.103778000	-0.378538000
C	3.742794000	-2.072423000	0.630501000
C	3.986491000	-0.592521000	1.092812000
C	-4.737939000	3.308815000	0.233291000
C	3.806466000	-2.148054000	-0.908871000
C	-5.507533000	5.103353000	-1.118035000
C	-4.601002000	1.842008000	-0.179099000
C	-3.492615000	1.107741000	0.259953000
C	-4.199507000	-0.805564000	-0.916445000
C	-5.325664000	-0.134197000	-1.371062000
C	-5.523538000	1.200070000	-1.011568000
C	2.243797000	-3.546484000	2.111669000
Cl	-1.090368000	-1.709010000	-1.633593000
Cl	-2.226848000	-0.696271000	2.737374000
H	4.786238000	-1.797910000	-1.261581000
H	3.656383000	-3.183873000	-1.246424000
H	1.260815000	-1.054624000	0.015264000
H	-1.143097000	-3.400959000	2.481680000
H	0.839982000	-4.687920000	3.313064000
H	5.228888000	-3.632072000	0.892603000
H	3.033151000	-1.517615000	-1.366473000
H	3.131148000	-4.060451000	2.483932000
H	-4.819555000	4.543219000	2.026008000
H	-3.817327000	3.085430000	2.208616000
H	-5.594587000	2.941935000	2.207437000
H	-3.555096000	5.807068000	-1.638275000
H	-6.792769000	3.976535000	0.029564000
H	5.611321000	0.214037000	2.187411000
H	-2.729736000	1.548013000	0.897372000
H	-3.979137000	-1.835023000	-1.191063000
H	-6.032158000	-0.657672000	-2.015077000
H	-6.386227000	1.752712000	-1.386384000
N	-5.873105000	3.963701000	-0.406573000
N	-3.309886000	-0.175981000	-0.114584000
N	0.008721000	-2.204109000	1.216786000
N	4.853745000	-2.765475000	1.272650000
N	5.167544000	-0.610241000	1.787521000
N	-4.088466000	5.099120000	-1.137665000
O	3.253947000	0.349773000	0.862220000
O	-6.228413000	5.930404000	-1.625600000
O	-2.355190000	3.856523000	-0.193568000
O	6.854508000	-2.152039000	2.321848000
<i>form(II)-Trans(II)-2</i>			
C	4.102800000	-2.441492000	1.040772000
C	2.936330000	-2.873505000	1.674483000

C	1.766186000	-2.141998000	1.528052000
N	1.752722000	-1.027956000	0.759950000
C	2.864519000	-0.605830000	0.121578000
C	4.078328000	-1.292796000	0.243738000
C	7.534555000	-0.682537000	0.396174000
N	6.527656000	-1.491296000	-0.123343000
C	5.320819000	-0.745203000	-0.461299000
C	5.645737000	0.666677000	0.141973000
N	6.930554000	0.583984000	0.610100000
C	5.109415000	-0.619581000	-1.984132000
O	8.683566000	-0.976342000	0.629870000
O	4.886437000	1.616049000	0.170389000
H	5.038817000	-2.985947000	1.173684000
H	2.928362000	-3.768938000	2.295812000
H	0.837115000	-2.415320000	2.023898000
H	2.778530000	0.302095000	-0.470471000
H	6.827397000	-2.293197000	-0.673944000
H	7.439732000	1.358435000	1.031128000
H	4.908804000	-1.607784000	-2.423098000
H	4.261740000	0.039789000	-2.211233000
H	6.007949000	-0.197542000	-2.454768000
Au	0.013117000	0.050022000	0.570138000
C	-4.099457000	2.515372000	0.174128000
C	-3.025786000	3.048410000	0.889985000
C	-1.845435000	2.325670000	0.993508000
N	-1.730502000	1.122055000	0.386078000
C	-2.748437000	0.600070000	-0.329931000
C	-3.969415000	1.273281000	-0.455033000
C	-7.408810000	0.577655000	-0.657902000
N	-6.358587000	1.357889000	-1.134305000
C	-5.106863000	0.616420000	-1.240195000
C	-5.480828000	-0.733608000	-0.533801000
N	-6.815152000	-0.641242000	-0.238027000
C	-4.703850000	0.338837000	-2.703445000
O	-8.582693000	0.859774000	-0.599297000
O	-4.716112000	-1.652754000	-0.311266000
H	-5.046316000	3.053791000	0.113544000
H	-3.100242000	4.017072000	1.384000000
H	-0.989564000	2.677592000	1.565752000
H	-2.584843000	-0.375308000	-0.781878000
H	-6.601831000	2.085083000	-1.803730000
H	-7.359622000	-1.382654000	0.198067000
H	-4.468575000	1.281718000	-3.218294000
H	-3.821470000	-0.312380000	-2.751512000
H	-5.527460000	-0.159148000	-3.233310000
Cl	-0.145840000	0.195914000	2.872457000

Cl 0.171817000 -0.093089000 -1.736149000

*form(II)-Cis(I)-2*

Au	-3.268099000	0.040258000	2.586139000
C	-0.512539000	-3.022423000	3.861764000
C	-1.644015000	-2.304697000	3.499161000
C	-1.976492000	3.825677000	-1.447520000
C	-0.317082000	-0.516784000	2.748546000
C	0.862808000	-1.174969000	3.120597000
C	4.012607000	-0.452254000	4.496774000
C	0.041910000	2.294221000	-1.649702000
C	2.209366000	-0.468719000	2.950552000
C	2.190520000	0.840083000	3.817546000
C	-1.473646000	2.478690000	-2.007973000
C	2.491350000	-0.106379000	1.478500000
C	-0.132083000	2.535005000	-3.965862000
C	-2.230100000	1.281625000	-1.432258000
C	-2.366735000	1.155780000	-0.044510000
C	-3.480402000	-0.898233000	-0.256513000
C	-3.387139000	-0.832708000	-1.640639000
C	-2.751841000	0.260172000	-2.233700000
C	0.747987000	-2.448171000	3.688772000
Cl	-5.157009000	1.272685000	2.226091000
Cl	-3.669222000	-0.011600000	4.829793000
H	3.462595000	0.401732000	1.400076000
H	2.519593000	-1.018606000	0.864023000
H	-0.290423000	0.489135000	2.331422000
H	-2.651963000	-2.681960000	3.663351000
H	-0.627203000	-4.012832000	4.302312000
H	3.844616000	-1.893302000	3.038194000
H	1.723120000	0.567527000	1.076477000
H	1.645925000	-2.974455000	4.015503000
H	-1.400742000	4.651095000	-1.887847000
H	-1.857749000	3.875961000	-0.357607000
H	-3.039725000	3.965567000	-1.690014000
H	1.728806000	2.311837000	-2.930368000
H	-2.156363000	2.912109000	-4.022463000
H	3.526610000	1.451718000	5.343041000
H	-1.993079000	1.916188000	0.638243000
H	-3.976708000	-1.721887000	0.255072000
H	-3.812806000	-1.634423000	-2.244134000
H	-2.654154000	0.324952000	-3.318322000
N	-1.428142000	2.467790000	-3.466657000
N	-2.965498000	0.084909000	0.513963000
N	-1.529510000	-1.074664000	2.947796000
N	3.305683000	-1.209705000	3.565800000

N	3.258095000	0.736673000	4.669912000
N	0.716185000	2.357659000	-2.836715000
O	1.378674000	1.740026000	3.723009000
O	0.227721000	2.695042000	-5.107773000
O	0.487479000	2.122149000	-0.528550000
O	5.047964000	-0.731740000	5.054400000

*form(II)-Cis(II)-2*

Au	-1.241425000	1.627299000	2.509316000
C	2.799285000	0.123723000	2.831067000
C	1.680582000	0.916199000	2.608299000
C	-0.745120000	5.389963000	-1.763884000
C	0.260614000	-0.863608000	3.184240000
C	1.344327000	-1.722524000	3.403405000
C	2.300834000	-5.093116000	3.077943000
C	1.575236000	4.351123000	-1.669443000
C	1.075868000	-3.180970000	3.770405000
C	0.391841000	-3.863137000	2.532881000
C	0.098067000	4.161853000	-2.166285000
C	0.163319000	-3.317704000	5.007211000
C	1.583173000	4.389044000	-4.004544000
C	-0.431994000	2.866120000	-1.554766000
C	-0.599771000	2.785309000	-0.167137000
C	-1.265766000	0.536794000	-0.294941000
C	-1.141461000	0.556462000	-1.678165000
C	-0.710494000	1.723730000	-2.312622000
C	2.631875000	-1.207440000	3.219353000
Cl	-3.055162000	2.982747000	2.225808000
Cl	-1.545973000	1.588954000	4.770508000
H	-0.022994000	-4.379318000	5.219339000
H	0.641589000	-2.858802000	5.884575000
H	-0.767323000	-1.193705000	3.316443000
H	1.757781000	1.957391000	2.296324000
H	3.792233000	0.551884000	2.693784000
H	2.788121000	-4.047560000	4.782573000
H	-0.805384000	-2.828208000	4.844465000
H	3.498084000	-1.853052000	3.372079000
H	-0.314906000	6.299855000	-2.204055000
H	-0.769169000	5.517813000	-0.674135000
H	-1.778003000	5.275650000	-2.123305000
H	3.336192000	4.658793000	-2.805591000
H	-0.457827000	4.309162000	-4.258318000
H	0.960485000	-5.618969000	1.493567000
H	-0.409910000	3.636432000	0.482969000
H	-1.589907000	-0.350838000	0.247653000
H	-1.377178000	-0.342474000	-2.247784000

H	-0.580338000	1.749860000	-3.395597000
N	0.288461000	4.066306000	-3.609650000
N	-0.988694000	1.641952000	0.432423000
N	0.438905000	0.410731000	2.781427000
N	2.300188000	-3.965061000	3.892735000
N	1.168177000	-4.948648000	2.231073000
N	2.333553000	4.482516000	-2.800733000
O	-0.617819000	-3.472162000	1.976197000
O	2.007994000	4.549524000	-5.124259000
O	1.935907000	4.363789000	-0.506712000
O	3.089765000	-6.008204000	3.064186000

*form(II)-Cis(III)-2*

Au	-3.125260000	1.739127000	3.214987000
C	-0.655439000	-1.625781000	4.324360000
C	-1.725811000	-0.784210000	4.050814000
C	-2.029029000	-1.362336000	-1.692220000
C	-0.287038000	0.773995000	3.041493000
C	0.837982000	-0.015230000	3.310849000
C	4.177840000	0.491740000	4.267608000
C	-4.536264000	-1.083711000	-1.418316000
C	2.229971000	0.483720000	2.907880000
C	2.465105000	1.899807000	3.539311000
C	-3.207465000	-0.382518000	-1.868583000
C	2.371734000	0.578961000	1.374617000
C	-4.688227000	-0.651080000	-3.706638000
C	-3.010068000	0.887612000	-1.034241000
C	-2.999556000	0.805127000	0.363769000
C	-2.730354000	3.128370000	0.582241000
C	-2.706066000	3.275945000	-0.798443000
C	-2.867614000	2.153839000	-1.613013000
C	0.636783000	-1.231847000	3.972567000
Cl	-4.842809000	3.232685000	3.054433000
Cl	-3.468225000	1.564240000	5.464064000
H	3.372438000	0.946597000	1.108562000
H	2.222985000	-0.409323000	0.915273000
H	-0.185722000	1.749871000	2.568175000
H	-2.745621000	-1.018180000	4.350954000
H	-0.838414000	-2.570797000	4.835910000
H	3.694441000	-1.114154000	3.073451000
H	1.629983000	1.275418000	0.961404000
H	1.493195000	-1.856110000	4.231069000
H	-2.196203000	-2.267953000	-2.291622000
H	-1.930540000	-1.661723000	-0.640236000
H	-1.088958000	-0.891511000	-2.015394000
H	-6.235203000	-1.599407000	-2.571393000

H	-2.749926000	-0.005112000	-3.959813000
H	4.009820000	2.549265000	4.832978000
H	-3.150049000	-0.147572000	0.870002000
H	-2.662261000	3.975451000	1.262458000
H	-2.588870000	4.271999000	-1.225473000
H	-2.906803000	2.260836000	-2.697899000
N	-3.491605000	-0.089135000	-3.268081000
N	-2.876274000	1.903695000	1.138395000
N	-1.526509000	0.395381000	3.418837000
N	3.298459000	-0.292704000	3.525147000
N	3.586385000	1.781848000	4.314688000
N	-5.315782000	-1.162893000	-2.540211000
O	1.773036000	2.882981000	3.349367000
O	-5.120266000	-0.701936000	-4.833571000
O	-4.784685000	-1.471225000	-0.291615000
O	5.224699000	0.164669000	4.773879000

### L3

N	1.441878000	1.137180000	-0.406724000
C	2.619342000	0.481650000	-0.526081000
C	3.865326000	1.098570000	-0.656071000
C	3.933670000	2.495995000	-0.655344000
C	2.729473000	3.204162000	-0.538925000
C	1.537044000	2.488395000	-0.424066000
C	5.271245000	3.222728000	-0.765920000
C	5.309616000	4.110731000	-2.045444000
N	6.334127000	3.606230000	-2.831262000
C	7.159995000	2.700800000	-2.110616000
N	6.392665000	2.274996000	-1.010741000
C	5.546195000	4.125904000	0.449262000
O	4.596050000	5.063807000	-2.294577000
O	8.286321000	2.356329000	-2.412820000
H	2.547738000	-0.611439000	-0.517040000
H	4.769526000	0.500212000	-0.766994000
H	2.712915000	4.294504000	-0.564229000
H	0.584548000	3.022460000	-0.340182000
H	6.742613000	4.158580000	-3.603265000
H	6.997064000	2.069650000	-0.193894000
H	5.565239000	3.527595000	1.372132000
H	6.512826000	4.637944000	0.328645000
H	4.760625000	4.886445000	0.543178000

### Trans(I)-3

N	2.053669000	-0.234346000	-0.310298000
C	2.778062000	0.794980000	-0.804257000
C	4.165939000	0.767223000	-0.787113000



C	4.841897000	-0.335845000	-0.250552000
C	4.064157000	-1.386659000	0.264686000
C	2.680369000	-1.311329000	0.219477000
C	6.363511000	-0.392018000	-0.186715000
C	6.789671000	-0.394645000	1.329178000
N	7.613648000	0.690540000	1.480263000
C	7.838289000	1.411402000	0.279408000
N	6.995002000	0.833032000	-0.665453000
C	6.919910000	-1.658402000	-0.871730000
O	6.444876000	-1.208808000	2.160806000
O	8.602323000	2.336658000	0.131722000
H	2.223975000	1.647240000	-1.192902000
H	4.718562000	1.621960000	-1.176459000
H	4.525320000	-2.257177000	0.728832000
H	2.048927000	-2.113705000	0.595918000
H	8.085009000	0.933123000	2.349404000
H	7.263568000	0.944069000	-1.640933000
H	6.641103000	-1.671684000	-1.935407000
H	8.015350000	-1.674608000	-0.791462000
H	6.528208000	-2.565622000	-0.394579000
N	-2.054056000	-0.091033000	-0.374023000
C	-2.771133000	-1.118086000	0.135241000
C	-4.159009000	-1.087231000	0.144973000
C	-4.842703000	0.003955000	-0.405751000
C	-4.072650000	1.053254000	-0.935612000
C	-2.688283000	0.986201000	-0.894200000
C	-6.364906000	0.080002000	-0.409122000
C	-6.798999000	1.296344000	0.491197000
N	-7.614821000	0.765122000	1.456666000
C	-7.830769000	-0.630183000	1.320210000
N	-6.987682000	-1.038693000	0.290273000
C	-6.922614000	0.280924000	-1.834586000
O	-6.465619000	2.452183000	0.329781000
O	-8.588366000	-1.305362000	1.977412000
H	-2.211388000	-1.966323000	0.524603000
H	-4.705163000	-1.917926000	0.591273000
H	-4.541321000	1.946224000	-1.346670000
H	-2.062250000	1.798199000	-1.259006000
H	-8.089325000	1.315514000	2.169645000
H	-7.252345000	-1.889620000	-0.201587000
H	-6.637888000	-0.563007000	-2.479581000
H	-8.018560000	0.348051000	-1.800552000
H	-6.536123000	1.207633000	-2.277407000
Au	-0.000009000	-0.161921000	-0.347473000
Cl	0.057451000	1.939352000	0.618796000
Cl	-0.057906000	-2.262215000	-1.319173000

*Trans(II)-3*

N	2.042396000	-0.027482000	0.204266000
C	2.715092000	-1.091332000	-0.289250000
C	4.096519000	-1.178053000	-0.181162000
C	4.815422000	-0.172383000	0.476815000
C	4.090054000	0.918160000	0.986409000
C	2.714061000	0.971618000	0.823613000
C	6.331623000	-0.231358000	0.622115000
C	6.952713000	0.994490000	-0.145768000
N	7.816311000	0.453328000	-1.062778000
C	7.899203000	-0.961429000	-1.006797000
N	6.924682000	-1.356091000	-0.093997000
C	6.760569000	-0.171335000	2.103867000
O	6.701967000	2.163683000	0.063082000
O	8.660205000	-1.659713000	-1.635299000
Au	-0.001618000	0.073859000	0.016909000
Cl	0.192544000	2.187343000	-0.903566000
Cl	-0.187169000	-2.043164000	0.933497000
H	2.124897000	-1.873818000	-0.762349000
H	4.609975000	-2.033845000	-0.618789000
H	4.592444000	1.750790000	1.476902000
H	2.126784000	1.819501000	1.170813000
H	8.404942000	1.002391000	-1.686042000
H	7.068720000	-2.255606000	0.360227000
H	6.348560000	-1.028541000	2.655928000
H	7.856394000	-0.195129000	2.176751000
H	6.404777000	0.753698000	2.574884000
N	-2.047142000	0.177465000	-0.164347000
C	-2.728892000	-0.838855000	-0.739456000
C	-4.110290000	-0.791965000	-0.869937000
C	-4.824747000	0.317386000	-0.400694000
C	-4.091839000	1.355353000	0.199414000
C	-2.712199000	1.261243000	0.300969000
C	-6.343591000	0.396958000	-0.497872000
C	-6.928339000	0.410956000	0.963978000
N	-7.781199000	-0.660552000	1.027822000
C	-7.888402000	-1.381297000	-0.189308000
N	-6.940533000	-0.818838000	-1.039814000
C	-6.803402000	1.670119000	-1.239951000
O	-6.661109000	1.221866000	1.826821000
O	-8.647037000	-2.294924000	-0.416137000
H	-2.148325000	-1.696620000	-1.073433000
H	-4.628621000	-1.636952000	-1.322696000
H	-4.588403000	2.230365000	0.616150000
H	-2.113972000	2.053729000	0.746111000

H	-8.347464000	-0.892194000	1.841507000
H	-7.106157000	-0.927593000	-2.038194000
H	-6.416817000	1.673243000	-2.269474000
H	-7.900820000	1.706674000	-1.272778000
H	-6.445613000	2.572243000	-0.727909000

*Cis(I)-3*

N	1.977991000	2.124129000	0.529276000
C	2.059004000	3.266494000	-0.189616000
C	2.070321000	3.246006000	-1.578923000
C	2.003657000	2.027436000	-2.265937000
C	1.927646000	0.851989000	-1.497429000
C	1.921569000	0.933901000	-0.112783000
C	2.056584000	1.959689000	-3.788253000
C	3.369824000	1.192517000	-4.198419000
N	4.066858000	2.059948000	-4.997922000
C	3.399968000	3.291321000	-5.225826000
N	2.274769000	3.263235000	-4.404793000
C	0.834579000	1.218989000	-4.371542000
O	3.664383000	0.064235000	-3.860876000
O	3.754399000	4.170080000	-5.975792000
H	2.143665000	4.195178000	0.372676000
H	2.160242000	4.185108000	-2.124613000
H	1.917611000	-0.129921000	-1.968667000
H	1.885200000	0.038513000	0.506874000
H	4.948660000	1.833608000	-5.453908000
H	1.494984000	3.853098000	-4.687761000
H	-0.094272000	1.744603000	-4.105821000
H	0.914153000	1.173052000	-5.466201000
H	0.780448000	0.191797000	-3.989100000
N	0.333168000	1.041914000	2.827221000
C	-0.845996000	1.498006000	2.350098000
C	-2.027679000	0.794613000	2.543775000
C	-2.016136000	-0.412024000	3.256166000
C	-0.778005000	-0.869188000	3.738406000
C	0.370326000	-0.122156000	3.517519000
C	-3.286734000	-1.222569000	3.481270000
C	-3.145463000	-2.581828000	2.699798000
N	-4.222893000	-2.631388000	1.852893000
C	-5.089579000	-1.513431000	1.961577000
N	-4.454681000	-0.633003000	2.833751000
C	-3.521404000	-1.519726000	4.978018000
O	-2.255172000	-3.394183000	2.843796000
O	-6.148285000	-1.370956000	1.395397000
H	-0.829166000	2.446136000	1.813277000
H	-2.957937000	1.187166000	2.133516000

H	-0.692929000	-1.813860000	4.273539000
H	1.339969000	-0.434719000	3.902517000
H	-4.438225000	-3.421651000	1.248241000
H	-5.054621000	0.025040000	3.327355000
H	-3.631279000	-0.581748000	5.541288000
H	-4.435583000	-2.116460000	5.099965000
H	-2.683483000	-2.087398000	5.401668000
Au	2.073093000	2.187940000	2.623022000
Cl	2.220405000	2.237074000	4.899644000
Cl	3.953099000	3.468043000	2.450254000

*Cis(II)-3*

N	2.201225000	2.274114000	0.452712000
C	2.439313000	3.384984000	-0.280771000
C	2.440692000	3.347655000	-1.669913000
C	2.198466000	2.142975000	-2.341358000
C	1.962199000	0.999044000	-1.557812000
C	1.975352000	1.096050000	-0.174330000
C	2.224849000	2.044015000	-3.862160000
C	3.398810000	1.076912000	-4.272802000
N	4.208648000	1.812701000	-5.096971000
C	3.736107000	3.128625000	-5.339445000
N	2.632653000	3.287771000	-4.504276000
C	0.896221000	1.489063000	-4.419248000
O	3.520970000	-0.077760000	-3.917646000
O	4.210526000	3.929366000	-6.110012000
Au	2.324828000	2.356087000	2.544150000
Cl	2.515081000	2.431005000	4.816379000
Cl	4.380862000	3.320991000	2.328482000
H	2.655503000	4.299976000	0.268717000
H	2.659293000	4.260115000	-2.224662000
H	1.813210000	0.023617000	-2.018809000
H	1.818317000	0.222866000	0.458056000
H	5.038435000	1.445739000	-5.559122000
H	1.950422000	3.988646000	-4.786011000
H	0.062993000	2.157639000	-4.157828000
H	0.954612000	1.407176000	-5.513123000
H	0.688930000	0.491174000	-4.011996000
N	0.425209000	1.501460000	2.783237000
C	0.265849000	0.427051000	3.588818000
C	-0.990306000	-0.116475000	3.829168000
C	-2.126517000	0.450088000	3.238579000
C	-1.937453000	1.572147000	2.411788000
C	-0.659801000	2.072676000	2.210088000
C	-3.528568000	-0.087770000	3.499905000
C	-4.361188000	1.037357000	4.223041000

N	-4.785252000	0.480170000	5.400408000
C	-4.395912000	-0.874265000	5.566735000
N	-3.550821000	-1.153030000	4.495030000
C	-4.241884000	-0.478099000	2.187503000
O	-4.568294000	2.152697000	3.790086000
O	-4.734277000	-1.612009000	6.461876000
H	1.163257000	0.027574000	4.058887000
H	-1.079214000	-0.968884000	4.502675000
H	-2.784896000	2.086293000	1.960493000
H	-0.485488000	2.953844000	1.593500000
H	-5.384283000	0.953964000	6.073811000
H	-3.468555000	-2.131647000	4.227483000
H	-3.685768000	-1.274968000	1.672393000
H	-5.256184000	-0.838713000	2.406207000
H	-4.323380000	0.386089000	1.515833000

*Cis(III)-3*

N	2.132094000	1.862897000	0.492429000
C	2.034147000	0.684866000	-0.162574000
C	1.943634000	0.630036000	-1.547259000
C	1.960714000	1.813737000	-2.297282000
C	2.064947000	3.026568000	-1.594838000
C	2.155647000	3.019684000	-0.210091000
C	1.835734000	1.805899000	-3.816249000
C	0.470137000	2.492782000	-4.194698000
N	-0.213443000	1.564525000	-4.936878000
C	0.497748000	0.353294000	-5.136726000
N	1.649636000	0.465446000	-4.362471000
C	2.993326000	2.570059000	-4.493947000
O	0.128182000	3.613853000	-3.878792000
O	0.150596000	-0.574114000	-5.830239000
H	2.032695000	-0.220396000	0.443900000
H	1.851918000	-0.337452000	-2.040472000
H	2.056899000	3.982921000	-2.115303000
H	2.263960000	3.939459000	0.362837000
H	-1.117926000	1.734707000	-5.372175000
H	2.444454000	-0.102271000	-4.649612000
H	3.956907000	2.100304000	-4.248970000
H	2.859567000	2.557729000	-5.584190000
H	3.019072000	3.616423000	-4.164879000
N	0.551843000	0.854703000	2.855355000
C	-0.609575000	1.354761000	2.378460000
C	-1.820185000	0.709470000	2.594274000
C	-1.856200000	-0.484068000	3.327858000
C	-0.636560000	-0.984176000	3.815322000
C	0.542420000	-0.294110000	3.571162000

C	-3.156181000	-1.242948000	3.566804000
C	-3.064860000	-2.615874000	2.800889000
N	-4.145718000	-2.637451000	1.957651000
C	-4.971565000	-1.487891000	2.054091000
N	-4.303698000	-0.620420000	2.914522000
C	-3.398213000	-1.513802000	5.067233000
O	-2.202866000	-3.457021000	2.952446000
O	-6.025832000	-1.314856000	1.488282000
H	-0.554389000	2.288674000	1.819823000
H	-2.735181000	1.134982000	2.182661000
H	-0.591383000	-1.920247000	4.369660000
H	1.500468000	-0.639791000	3.956670000
H	-4.389577000	-3.425824000	1.361382000
H	-4.877887000	0.066226000	3.399611000
H	-3.473965000	-0.566016000	5.619625000
H	-4.332646000	-2.076325000	5.197910000
H	-2.580290000	-2.105948000	5.496413000
Au	2.345936000	1.899047000	2.575833000
Cl	2.620199000	1.920147000	4.840669000
Cl	4.284966000	3.069077000	2.299515000