

Electronic Supplementary Information (ESI†)

NIR-Emissive, Singlet-Oxygen–Sensitizing Gold Tetra(thiocyano)corroles

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- Fig. S1** ORTEP diagram of **2**. Hydrogen atoms are omitted for clarity. Ellipsoids are drawn at 50% probability.
- Fig. S2** (a) Electronic absorption spectra of compounds **1** and **1a** (β -unsubstituted corrolato-Au(III) analogue of compound **1**), and (b) Electronic absorption spectra of compounds **2** and **2a** (β -unsubstituted corrolato-Au(III) analogue of compound **2**) in dichloromethane.
- Fig. S3** Excitation (dashed line) and absorption spectra (solid line) of compound **1** (a) and **2** (b) in toluene solution ($\lambda_{em}=900$ nm).
- Fig. S4** Time-resolved PL decay of **2** (black line) and **1** (red line) recorded in deaerated toluene with $\lambda_{exc} = 365$ nm.
- Fig. S5** FT-IR spectrum of **1** as a KBr pellet.
- Fig. S6** FT-IR spectrum of **2** as a KBr pellet.
- Fig. S7** ESI- MS spectrum of **1** in CH₃CN shows the measured spectrum with an isotopic distribution pattern
- Fig. S8** ESI- MS spectrum of **2** in CH₃CN shows the measured spectrum with an isotopic distribution pattern
- Fig. S9** ¹H NMR (400 MHz) spectrum of **1** in CDCl₃.
- Fig. S10** ¹H NMR (400 MHz) spectrum of **2** in CDCl₃.

Optimized Cartesian coordinates (Å)

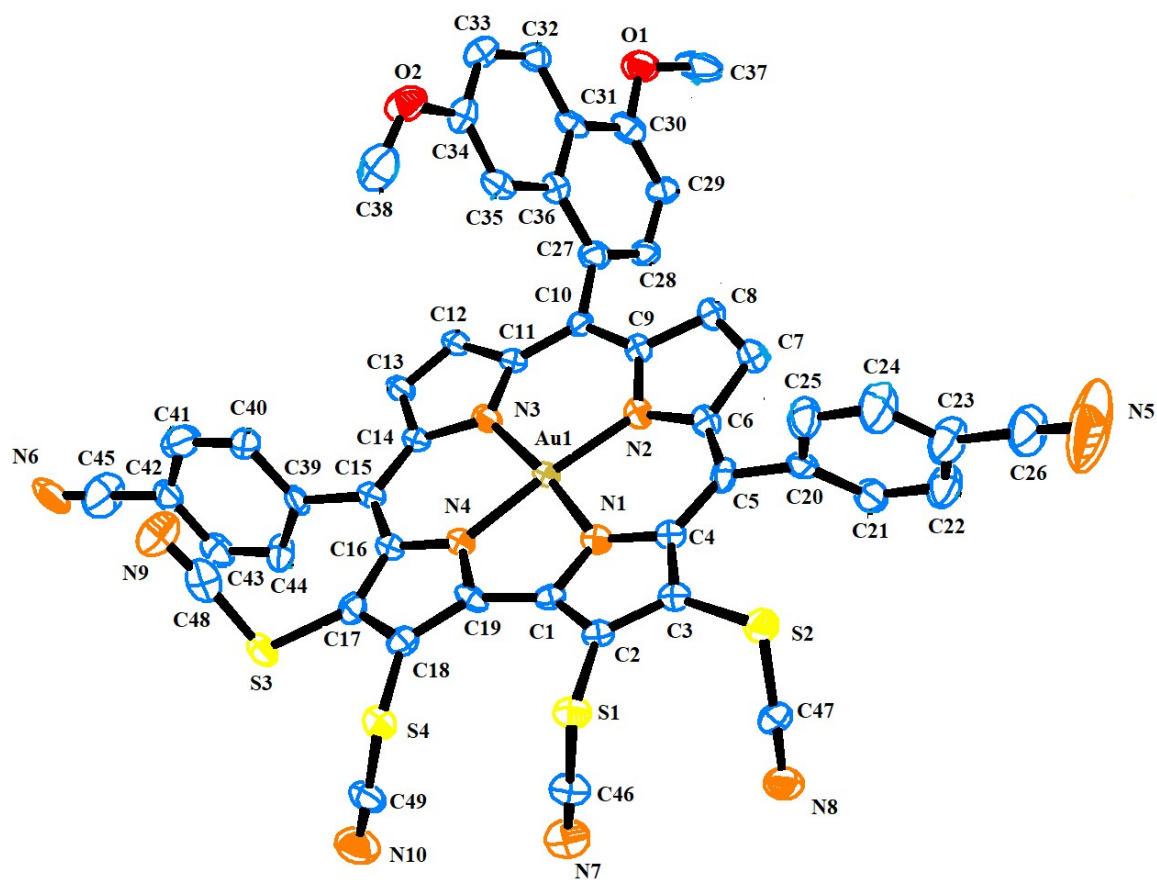


Fig. S1 ORTEP diagram of **2**. Hydrogen atoms are omitted for clarity. Ellipsoids are drawn at 50% probability.

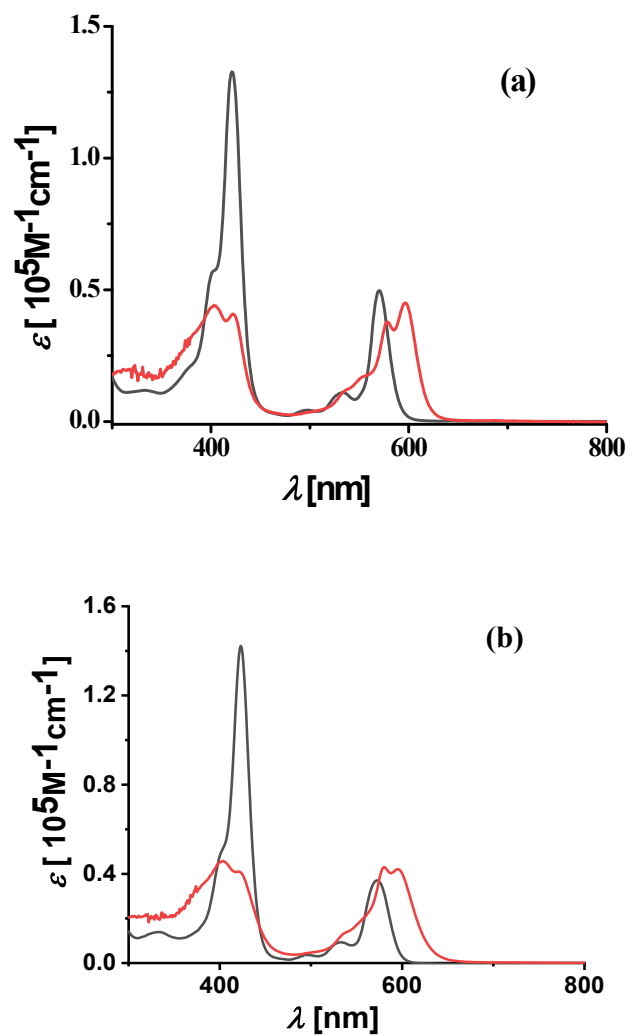


Fig. S2 (a) Electronic absorption spectra of compounds **1** (red solid line) and **1a** (black solid line; β -unsubstituted corrolato-Au(III) analogue of compound **1**), and (b) Electronic absorption spectra of compounds **2** (red solid line) and **2a** (black solid line; β -unsubstituted corrolato-Au(III) analogue of compound **2**) in dichloromethane.

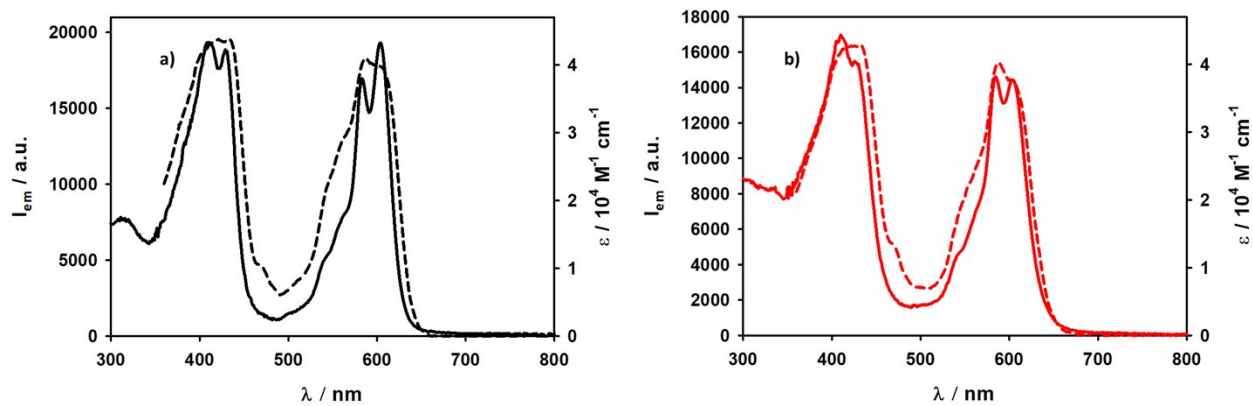


Fig. S3 Excitation (dashed line) and absorption spectra (solid line) of compound **1** (a) and **2** (b) in deaerated toluene solution ($\lambda_{em}=900 \text{ nm}$).

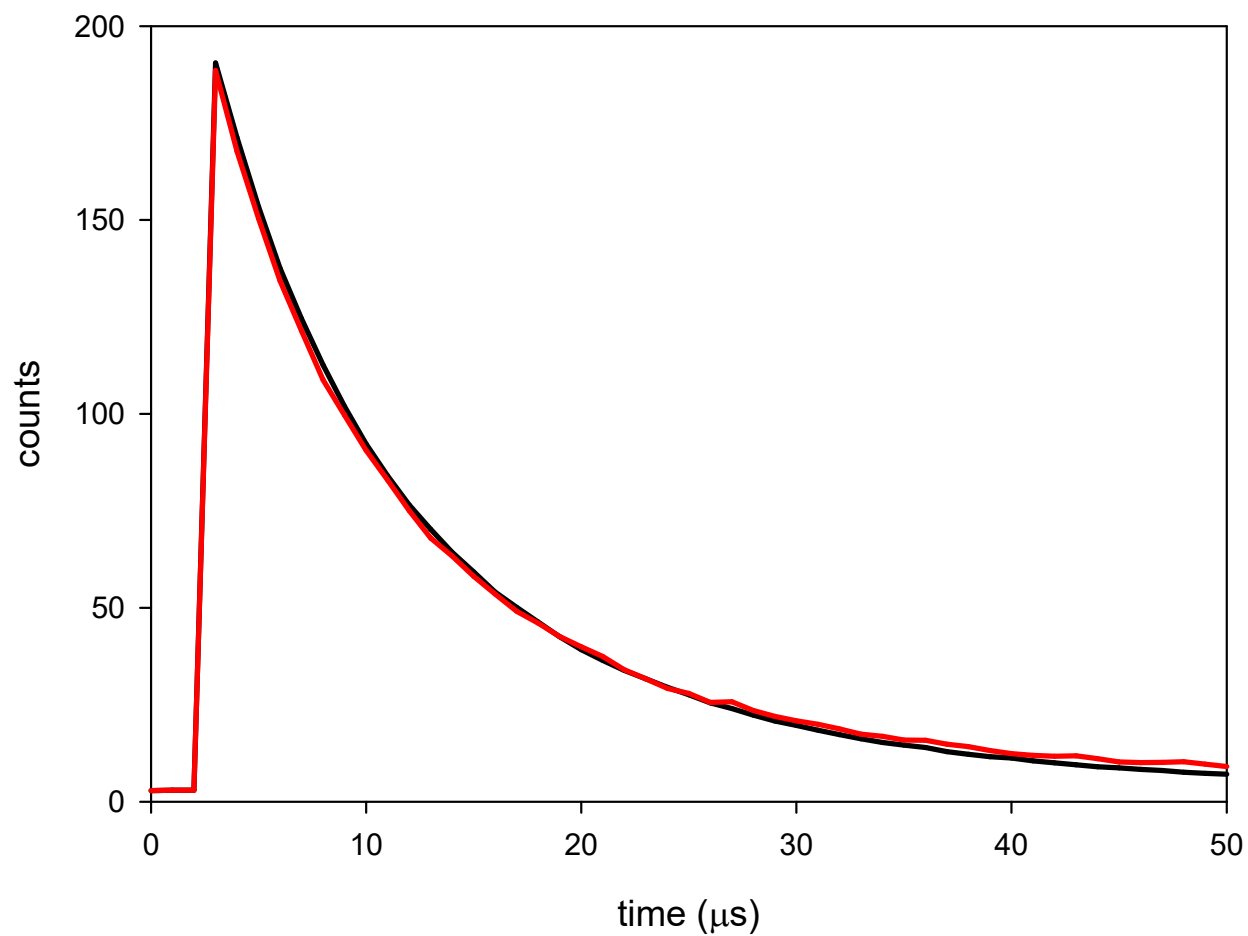


Fig. S4 Time resolved PL decay of **2** (black line) and **1** (red line) recorded in deaerated toluene with $\lambda_{\text{exc}} = 365$ nm.

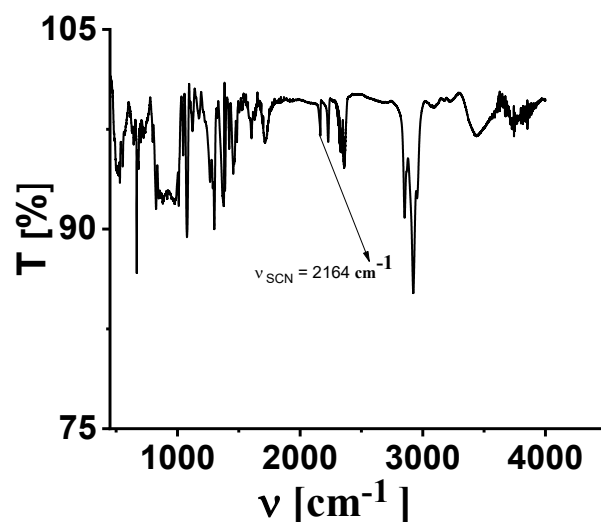


Fig. S5 FT-IR spectrum of **1** as a KBr pellet.

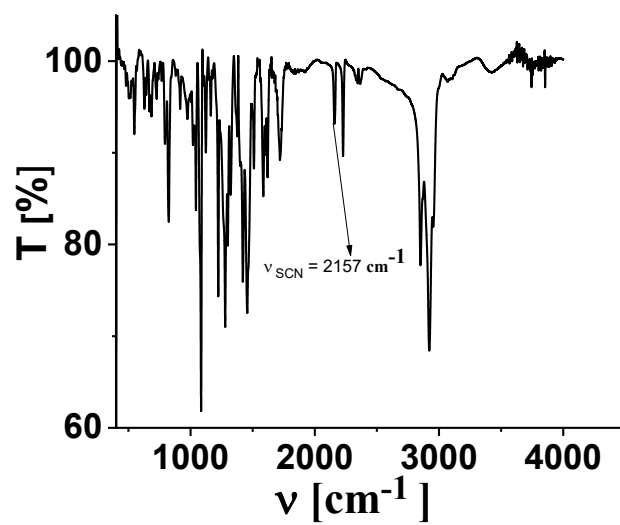


Fig. S6 FT-IR spectrum of **2** as a KBr pellet.

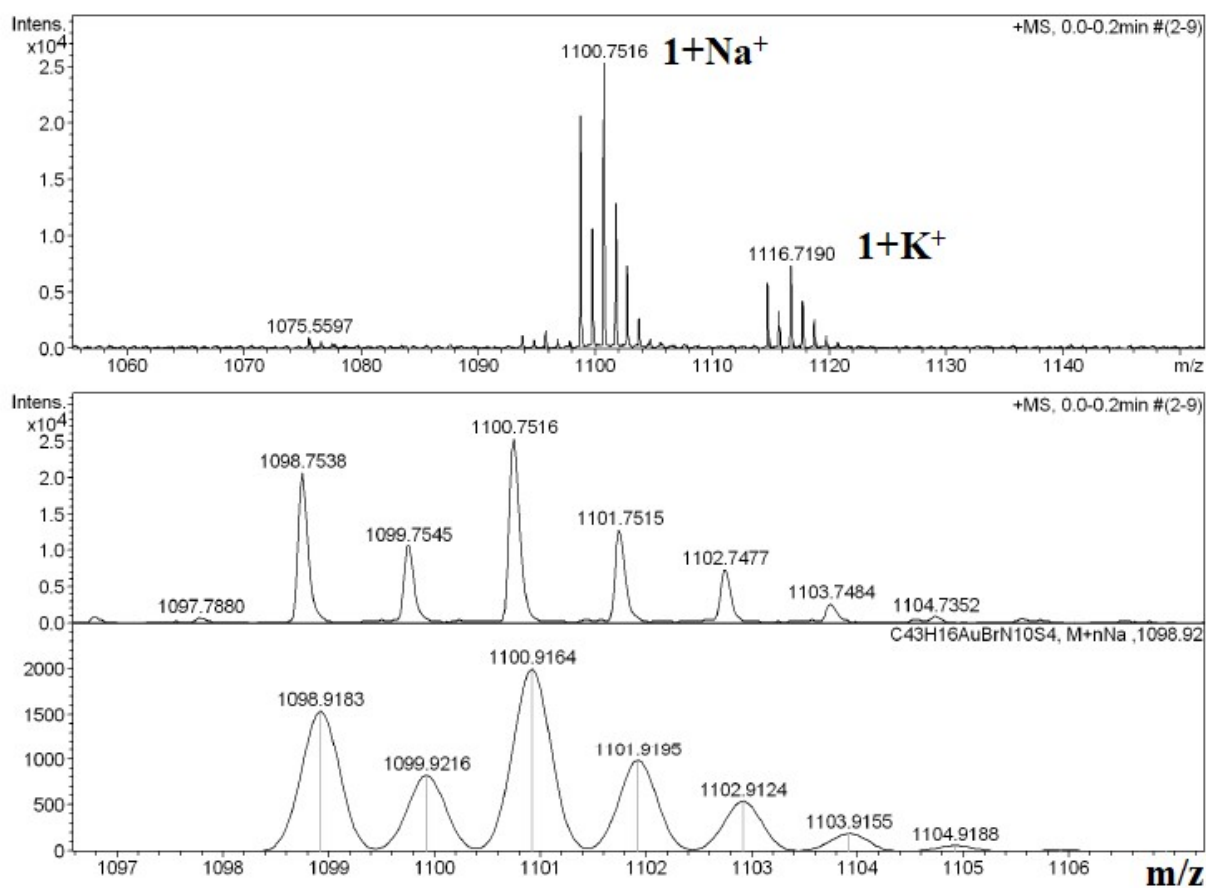


Fig. S7 ESI- MS spectrum of **1** in CH_3CN shows the measured spectrum with isotopic distribution pattern

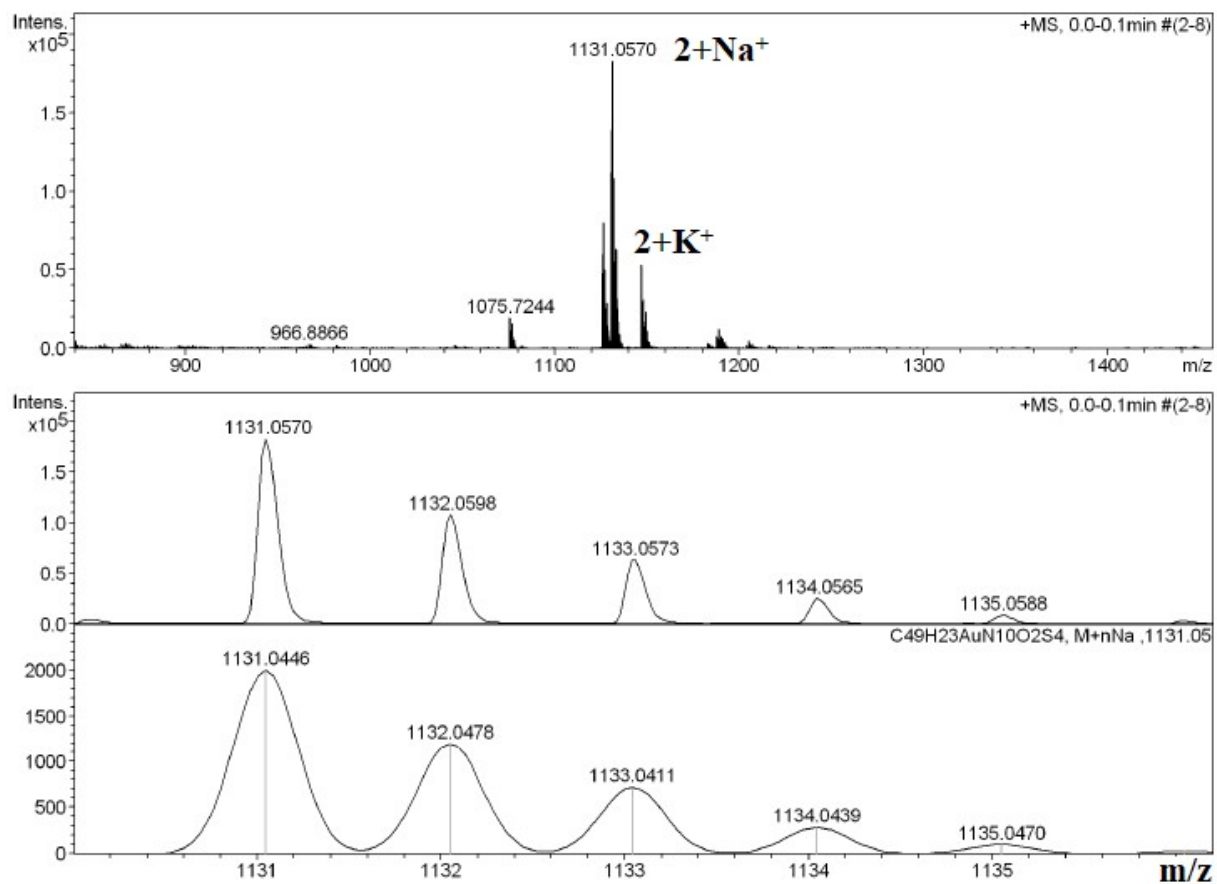


Fig. S8 ESI- MS spectrum of **2** in CH_3CN shows the measured spectrum with isotopic distribution pattern

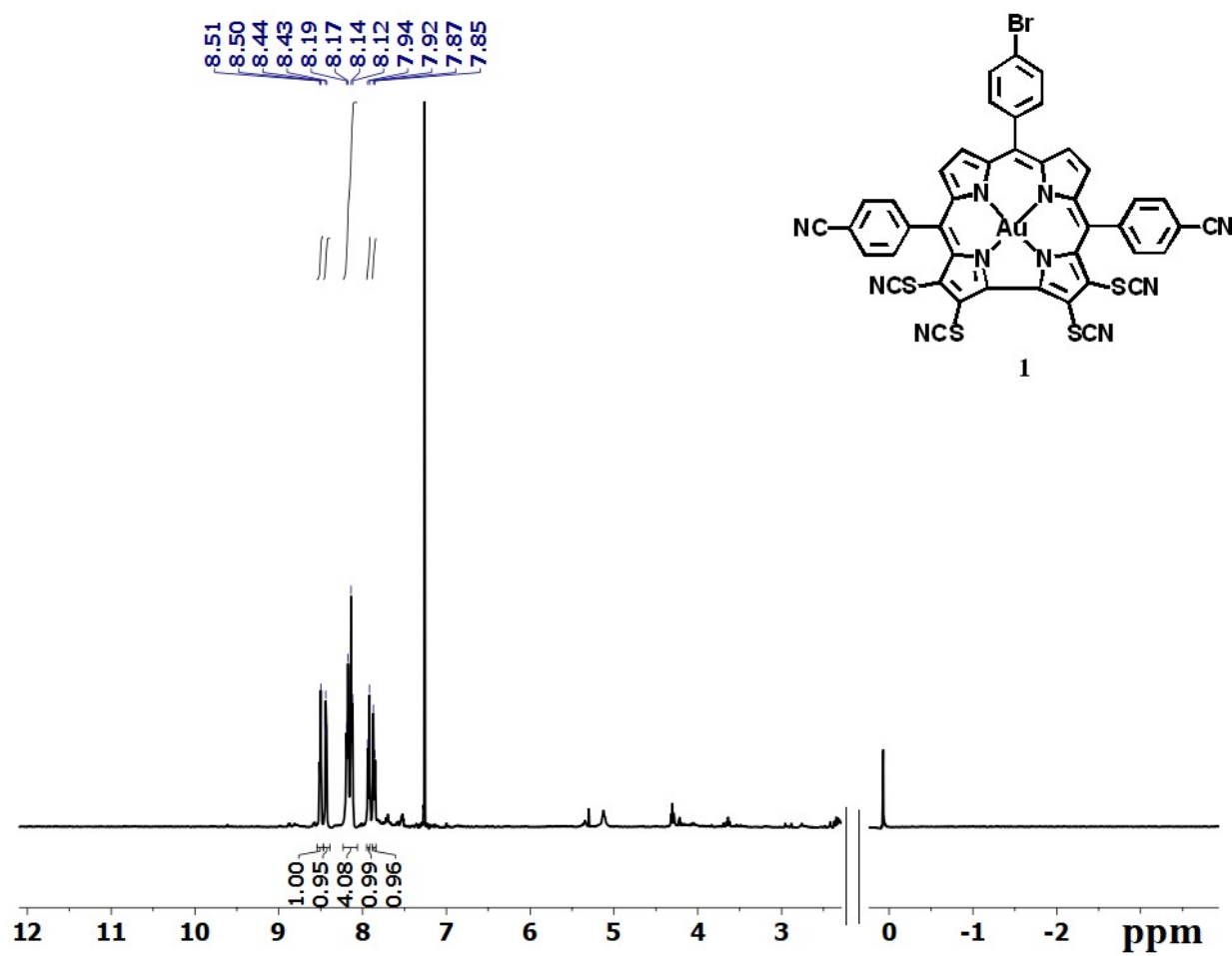


Fig. S9 ^1H NMR (400 MHz) spectrum of **1** in CDCl_3 .

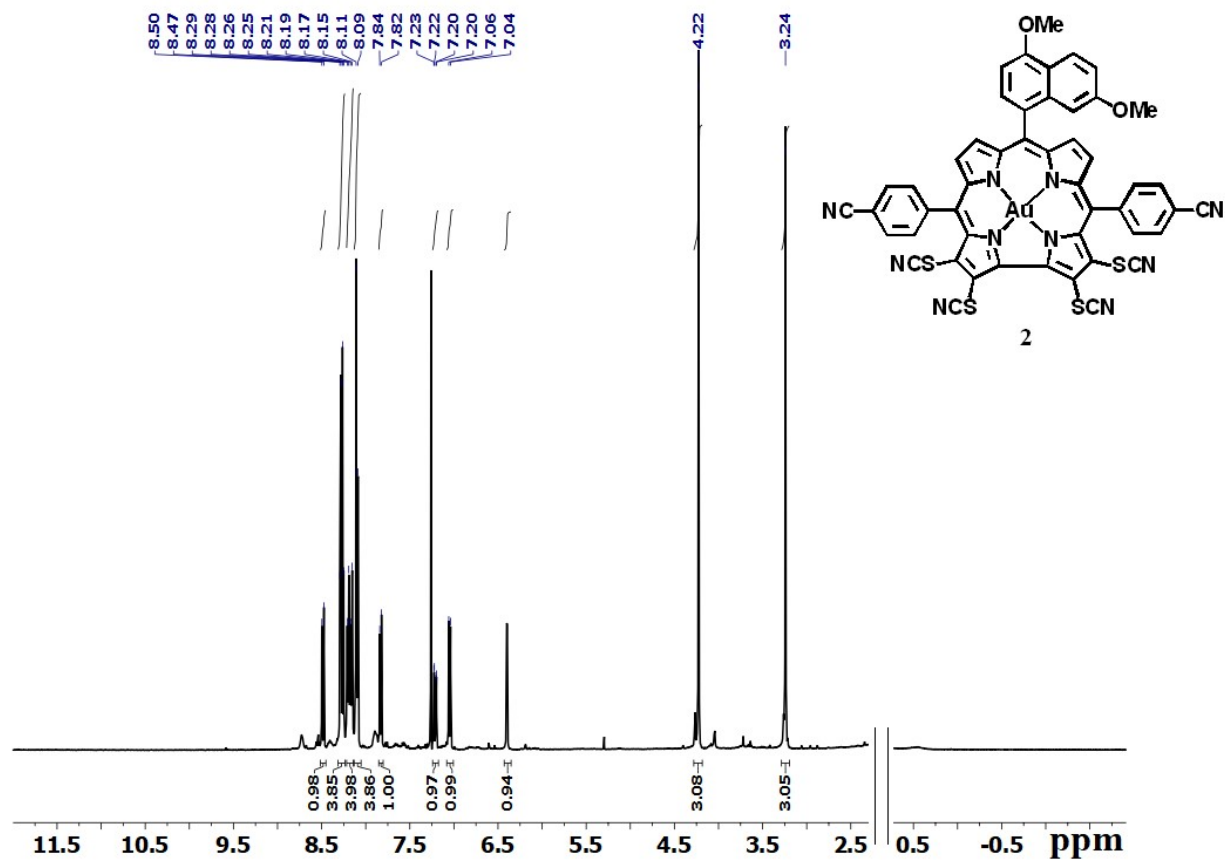


Fig. S10 ^1H NMR (400 MHz) spectrum of **2** in CDCl_3 .

Optimized Cartesian coordinates (Å)

All compounds were optimized the ZORA Hamiltonian, ZORA/TZ2P basis set, all electron, B3LYP* functional and the Grimme's D3 dispersion correction in the gas phase.

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1. Au[TPC] neutral

Au	0.000000000	0.000000000	0.119826000
N	1.387793000	-0.430310000	-1.207558000
N	-1.387793000	0.430310000	-1.207558000
N	-1.183226000	0.419214000	1.610131000
N	1.183226000	-0.419214000	1.610131000
C	2.652323000	-0.898745000	-0.886863000
C	3.276527000	-1.204661000	-2.145453000
C	2.399357000	-0.914718000	-3.153351000
C	1.186841000	-0.415274000	-2.565452000
C	0.000000000	0.000000000	-3.209169000
C	-1.186841000	0.415274000	-2.565452000
C	-2.399357000	0.914718000	-3.153351000
C	-3.276527000	1.204661000	-2.145453000
C	-2.652323000	0.898745000	-0.886863000
C	-3.190925000	1.063587000	0.409652000
C	-2.482544000	0.823232000	1.613371000
C	-2.842876000	0.894181000	2.998862000
C	-1.740030000	0.533910000	3.760570000
C	-0.678175000	0.224102000	2.870466000
C	0.678175000	-0.224102000	2.870466000
C	1.740030000	-0.533910000	3.760570000
C	2.842876000	-0.894181000	2.998862000
C	2.482544000	-0.823232000	1.613371000
C	3.190925000	-1.063587000	0.409652000
C	4.598582000	-1.527350000	0.529434000
C	4.899367000	-2.722774000	1.190874000
C	6.214463000	-3.154043000	1.316415000
C	7.253391000	-2.396600000	0.785189000
C	6.967545000	-1.204283000	0.128136000
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C	0.000000000	0.000000000	-4.699407000
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C	0.000000000	0.000000000	-7.504495000
C	-0.860069000	-0.840027000	-6.804448000
C	-0.858651000	-0.840232000	-5.414522000
C	-4.598582000	1.527350000	0.529434000
C	-5.652115000	0.773992000	0.001181000
C	-6.967545000	1.204283000	0.128136000
C	-7.253391000	2.396600000	0.785189000
C	-6.214463000	3.154043000	1.316415000
C	-4.899367000	2.722774000	1.190874000
H	4.091511000	-3.319901000	1.596698000
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H	1.521819000	1.503405000	-4.871555000
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H	-1.529558000	-1.502344000	-7.341104000
H	-4.091511000	3.319901000	1.596698000
H	-6.427156000	4.087073000	1.825626000
H	-8.279131000	2.732561000	0.883869000
H	-7.771106000	0.602892000	-0.281419000
H	-5.433443000	-0.161828000	-0.499448000
H	-4.269021000	1.611509000	-2.252301000
H	-2.561336000	1.046541000	-4.210645000
H	2.561336000	-1.046541000	-4.210645000
H	4.269021000	-1.611509000	-2.252301000
H	3.814373000	-1.174365000	3.373223000
H	1.694186000	-0.488881000	4.837674000
H	-1.694186000	0.488881000	4.837674000
H	-3.814373000	1.174365000	3.373223000

2. Au[TPC] anion

Au	0.000000000	0.000000000	0.132052000
N	1.403401000	-0.416291000	-1.201251000
N	-1.403401000	0.416291000	-1.201251000
N	-1.191845000	0.428995000	1.624300000
N	1.191845000	-0.428995000	1.624300000
C	2.666439000	-0.892577000	-0.886549000
C	3.274163000	-1.215279000	-2.149633000
C	2.386582000	-0.925623000	-3.156746000
C	1.190288000	-0.413711000	-2.569026000
C	0.000000000	0.000000000	-3.205521000
C	-1.190288000	0.413711000	-2.569026000
C	-2.386582000	0.925623000	-3.156746000
C	-3.274163000	1.215279000	-2.149633000
C	-2.666439000	0.892577000	-0.886549000
C	-3.214805000	1.063704000	0.409525000
C	-2.494670000	0.828324000	1.633081000
C	-2.853906000	0.887811000	3.004667000
C	-1.733017000	0.518688000	3.775054000
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C	0.687021000	-0.223972000	2.890742000
C	1.733017000	-0.518688000	3.775054000
C	2.853906000	-0.887811000	3.004667000
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C	3.214805000	-1.063704000	0.409525000

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C	-0.882835000	-0.812108000	-5.415521000
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C	-5.664853000	0.864047000	-0.134662000
C	-6.979510000	1.297261000	-0.018537000
C	-7.291742000	2.400389000	0.771347000
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H	1.567080000	1.451115000	-4.869982000
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H	0.000000000	0.000000000	-8.592901000
H	-1.577630000	-1.452259000	-7.342155000
H	-4.160105000	3.160715000	1.836532000
H	-6.490035000	3.927793000	2.057258000
H	-8.318242000	2.737604000	0.865052000
H	-7.767076000	0.761641000	-0.538739000
H	-5.436001000	-0.008334000	-0.734968000
H	-4.258209000	1.639267000	-2.266560000
H	-2.541888000	1.073064000	-4.213709000
H	2.541888000	-1.073064000	-4.213709000
H	4.258209000	-1.639267000	-2.266560000
H	3.826086000	-1.156956000	3.385587000
H	1.686862000	-0.466727000	4.852528000
H	-1.686862000	0.466727000	4.852528000
H	-3.826086000	1.156956000	3.385587000

3. Au[TPC] cation

Au	0.000000000	0.000000000	0.116982000
N	1.395230000	-0.421615000	-1.210958000
N	-1.395230000	0.421615000	-1.210958000

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N	1.183004000	-0.423309000	1.607590000
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C	0.000000000	0.000000000	-3.215172000
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C	0.686936000	-0.226370000	2.858658000
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C	-0.949186000	-0.745028000	-5.407489000
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C	-5.630791000	0.817765000	-0.107885000
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H	7.738184000	-0.669732000	-0.460031000
H	5.398916000	0.070611000	-0.682814000
H	-1.676363000	-1.339754000	-4.867935000
H	1.676363000	1.339754000	-4.867935000
H	1.668083000	1.347486000	-7.333648000

H	0.000000000	0.000000000	-8.575825000
H	-1.668083000	-1.347486000	-7.333648000
H	-4.129242000	3.210098000	1.777499000
H	-6.470887000	3.952589000	1.990911000
H	-8.284068000	2.686277000	0.873456000
H	-7.738184000	0.669732000	-0.460031000
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H	-4.240419000	1.684214000	-2.245750000
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H	2.534236000	-1.123528000	-4.209014000
H	4.240419000	-1.684214000	-2.245750000
H	3.822814000	-1.140357000	3.382870000
H	1.692734000	-0.466721000	4.836129000
H	-1.692734000	0.466721000	4.836129000
H	-3.822814000	1.140357000	3.382870000

4. Au[TPC(SCN)₄] neutral

Au	0.000000000	0.000000000	0.638463000
C	0.000000000	0.000000000	3.979289000
C	0.000000000	0.000000000	5.472628000
C	0.000000000	0.000000000	8.268736000
C	0.064467000	-1.201358000	7.571324000
C	0.066261000	-1.201437000	6.180809000
C	0.712840000	-0.103893000	-2.114371000
C	1.235360000	-0.179119000	3.331219000
C	1.334725000	-1.698640000	-5.182199000
C	1.803389000	-0.272279000	-2.999061000
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C	2.758753000	-0.398969000	1.658393000
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C	3.450722000	-0.459976000	2.923791000
C	4.812323000	-0.654160000	0.344739000
C	5.235804000	0.637217000	-3.094142000
C	5.384147000	-1.914353000	0.524984000
C	5.641568000	0.454085000	0.173402000
C	6.765760000	-2.064321000	0.520530000
C	7.022943000	0.303007000	0.169301000
C	7.587345000	-0.955745000	0.342052000
C	-0.064467000	1.201358000	7.571324000
C	-0.066261000	1.201437000	6.180809000
C	-0.712840000	0.103893000	-2.114371000
C	-1.235360000	0.179119000	3.331219000
C	-1.334725000	1.698640000	-5.182199000

C	-1.803389000	0.272279000	-2.999061000
C	-2.538455000	0.328243000	3.926260000
C	-2.600812000	0.391226000	-0.842053000
C	-2.758753000	0.398969000	1.658393000
C	-2.965593000	0.460456000	-2.224825000
C	-3.329022000	0.482692000	0.381607000
C	-3.450722000	0.459976000	2.923791000
C	-4.812323000	0.654160000	0.344739000
C	-5.235804000	-0.637217000	-3.094142000
C	-5.384147000	1.914353000	0.524984000
C	-5.641568000	-0.454085000	0.173402000
C	-6.765760000	2.064321000	0.520530000
C	-7.022943000	-0.303007000	0.169301000
C	-7.587345000	0.955745000	0.342052000
H	0.000000000	0.000000000	9.352488000
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H	0.115112000	-2.137702000	5.636664000
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H	4.516726000	-0.582658000	3.025775000
H	4.742640000	-2.777316000	0.661102000
H	5.204248000	1.435143000	0.031342000
H	7.200874000	-3.047519000	0.656553000
H	7.655124000	1.170444000	0.022110000
H	8.664801000	-1.073101000	0.337058000
H	-0.111684000	2.140822000	8.109708000
H	-0.115112000	2.137702000	5.636664000
H	-2.728448000	0.325459000	4.987472000
H	-4.516726000	0.582658000	3.025775000
H	-4.742640000	2.777316000	0.661102000
H	-5.204248000	-1.435143000	0.031342000
H	-7.200874000	3.047519000	0.656553000
H	-7.655124000	-1.170444000	0.022110000
H	-8.664801000	1.073101000	0.337058000
N	1.015018000	-2.761619000	-5.510142000
N	1.252523000	-0.184677000	-0.854916000
N	1.419702000	-0.230173000	1.975736000
N	5.752270000	1.664581000	-3.225799000
N	-1.015018000	2.761619000	-5.510142000
N	-1.252523000	0.184677000	-0.854916000
N	-1.419702000	0.230173000	1.975736000
N	-5.752270000	-1.664581000	-3.225799000
S	1.798217000	-0.124468000	-4.761382000
S	4.535659000	-0.894456000	-2.914018000
S	-1.798217000	0.124468000	-4.761382000
S	-4.535659000	0.894456000	-2.914018000

5. Au[TPC(SCN)₄] anion

Au	0.000000000	0.000000000	0.661742000
C	0.000000000	0.000000000	4.018035000
C	0.000000000	0.000000000	5.507176000
C	0.000000000	0.000000000	8.314683000
C	0.327939000	-1.155109000	6.223609000
C	0.328305000	-1.156277000	7.614075000
C	0.715101000	-0.118950000	-2.104395000
C	1.233878000	-0.208881000	3.374585000
C	1.528377000	-1.623185000	-5.296355000
C	1.788257000	-0.283892000	-2.985866000
C	2.531582000	-0.352127000	3.956657000
C	2.599844000	-0.444744000	-0.827667000
C	2.749311000	-0.460745000	1.686963000
C	2.964363000	-0.507489000	-2.203659000
C	3.325405000	-0.548900000	0.403854000
C	3.443934000	-0.503325000	2.946495000
C	4.807766000	-0.710309000	0.365288000
C	5.260479000	0.501662000	-3.195008000
C	5.402509000	-1.941535000	0.650910000
C	5.633717000	0.378532000	0.077212000
C	6.784996000	-2.084866000	0.632927000
C	7.015832000	0.237429000	0.053004000
C	7.596184000	-0.995535000	0.329980000
C	-0.327939000	1.155109000	6.223609000
C	-0.328305000	1.156277000	7.614075000
C	-0.715101000	0.118950000	-2.104395000
C	-1.233878000	0.208881000	3.374585000
C	-1.528377000	1.623185000	-5.296355000
C	-1.788257000	0.283892000	-2.985866000
C	-2.531582000	0.352127000	3.956657000
C	-2.599844000	0.444744000	-0.827667000
C	-2.749311000	0.460745000	1.686963000
C	-2.964363000	0.507489000	-2.203659000
C	-3.325405000	0.548900000	0.403854000
C	-3.443934000	0.503325000	2.946495000
C	-4.807766000	0.710309000	0.365288000
C	-5.260479000	-0.501662000	-3.195008000
C	-5.402509000	1.941535000	0.650910000
C	-5.633717000	-0.378532000	0.077212000
C	-6.784996000	2.084866000	0.632927000
C	-7.015832000	-0.237429000	0.053004000
C	-7.596184000	0.995535000	0.329980000
H	0.000000000	0.000000000	9.398924000
H	0.577435000	-2.058049000	5.678798000
H	0.580303000	-2.064192000	8.150911000

H	2.736289000	-0.327215000	5.014936000
H	4.510200000	-0.622608000	3.049249000
H	4.769155000	-2.791604000	0.877592000
H	5.184757000	1.338841000	-0.147176000
H	7.229439000	-3.050155000	0.849424000
H	7.636381000	1.090938000	-0.194096000
H	8.674474000	-1.107630000	0.307684000
H	-0.577435000	2.058049000	5.678798000
H	-0.580303000	2.064192000	8.150911000
H	-2.736289000	0.327215000	5.014936000
H	-4.510200000	0.622608000	3.049249000
H	-4.769155000	2.791604000	0.877592000
H	-5.184757000	-1.338841000	-0.147176000
H	-7.229439000	3.050155000	0.849424000
H	-7.636381000	-1.090938000	-0.194096000
H	-8.674474000	1.107630000	0.307684000
N	1.252726000	-0.222413000	-0.838562000
N	1.353371000	-2.678187000	-5.741574000
N	1.415223000	-0.285132000	2.005001000
N	5.820141000	1.491909000	-3.415591000
N	-1.252726000	0.222413000	-0.838562000
N	-1.353371000	2.678187000	-5.741574000
N	-1.415223000	0.285132000	2.005001000
N	-5.820141000	-1.491909000	-3.415591000
S	1.788049000	-0.045192000	-4.728958000
S	4.504388000	-0.990750000	-2.895707000
S	-1.788049000	0.045192000	-4.728958000
S	-4.504388000	0.990750000	-2.895707000

6. Au[TPC(SCN)₄] cation

Au	0.000000000	0.000000000	0.687296000
C	0.000000000	0.000000000	4.032605000
C	0.000000000	0.000000000	5.508048000
C	0.000000000	0.000000000	8.305129000
C	0.275015000	-1.994771000	-4.630479000
C	0.600356000	-1.044856000	7.608449000
C	0.611542000	-1.041898000	6.221775000
C	0.704746000	-0.173472000	-2.054197000
C	1.254898000	-0.130239000	3.377132000
C	1.717254000	-0.639195000	-2.931175000
C	2.561447000	-0.111117000	3.957944000
C	2.574238000	-0.526401000	-0.799184000
C	2.764354000	-0.364322000	1.709196000
C	2.873208000	-0.862536000	-2.164440000
C	3.329506000	-0.521814000	0.406244000
C	3.475085000	-0.246407000	2.947049000

C	4.799821000	-0.600042000	0.323251000
C	5.106420000	-0.479042000	-3.567320000
C	5.494628000	0.362077000	-0.423165000
C	5.521508000	-1.591588000	1.002392000
C	6.878907000	0.338882000	-0.480044000
C	6.904928000	-1.625937000	0.919461000
C	7.586563000	-0.657746000	0.185614000
C	-0.275015000	1.994771000	-4.630479000
C	-0.600356000	1.044856000	7.608449000
C	-0.611542000	1.041898000	6.221775000
C	-0.704746000	0.173472000	-2.054197000
C	-1.254898000	0.130239000	3.377132000
C	-1.717254000	0.639195000	-2.931175000
C	-2.561447000	0.111117000	3.957944000
C	-2.574238000	0.526401000	-0.799184000
C	-2.764354000	0.364322000	1.709196000
C	-2.873208000	0.862536000	-2.164440000
C	-3.329506000	0.521814000	0.406244000
C	-3.475085000	0.246407000	2.947049000
C	-4.799821000	0.600042000	0.323251000
C	-5.106420000	0.479042000	-3.567320000
C	-5.494628000	-0.362077000	-0.423165000
C	-5.521508000	1.591588000	1.002392000
C	-6.878907000	-0.338882000	-0.480044000
C	-6.904928000	1.625937000	0.919461000
C	-7.586563000	0.657746000	0.185614000
H	0.000000000	0.000000000	9.388505000
H	1.056545000	-1.866320000	8.147552000
H	1.065183000	-1.865317000	5.683952000
H	2.772991000	0.019934000	5.005900000
H	4.547491000	-0.243447000	3.045099000
H	4.947000000	1.138271000	-0.943804000
H	4.992328000	-2.352953000	1.562691000
H	7.402893000	1.093000000	-1.053940000
H	7.454363000	-2.410776000	1.425131000
H	8.668201000	-0.682847000	0.129694000
H	-1.056545000	1.866320000	8.147552000
H	-1.065183000	1.865317000	5.683952000
H	-2.772991000	-0.019934000	5.005900000
H	-4.547491000	0.243447000	3.045099000
H	-4.947000000	-1.138271000	-0.943804000
H	-4.992328000	2.352953000	1.562691000
H	-7.402893000	-1.093000000	-1.053940000
H	-7.454363000	2.410776000	1.425131000
H	-8.668201000	0.682847000	0.129694000
N	0.647034000	2.692951000	-4.614787000
N	1.258721000	-0.160466000	-0.810680000

N	1.425144000	-0.276922000	2.024771000
N	5.687619000	0.352738000	-4.122641000
N	-0.647034000	-2.692951000	-4.614787000
N	-1.258721000	0.160466000	-0.810680000
N	-1.425144000	0.276922000	2.024771000
N	-5.687619000	-0.352738000	-4.122641000
S	1.607922000	-0.950226000	-4.666933000
S	4.300744000	-1.727393000	-2.756476000
S	-1.607922000	0.950226000	-4.666933000
S	-4.300744000	1.727393000	-2.756476000