

## Electronic Supplementary Information (ESI)

### Terpyridine Isomerism as a Tool for Tuning of the Red-to-NIR Emissive Properties in Heteronuclear Gold(I)-Thallium(I) Complexes

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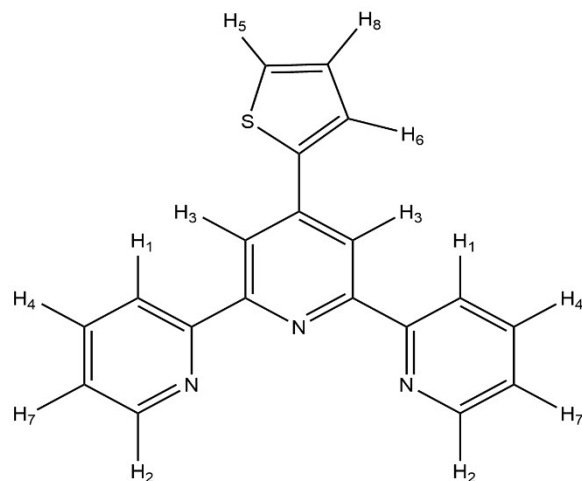
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#### Table of Contents

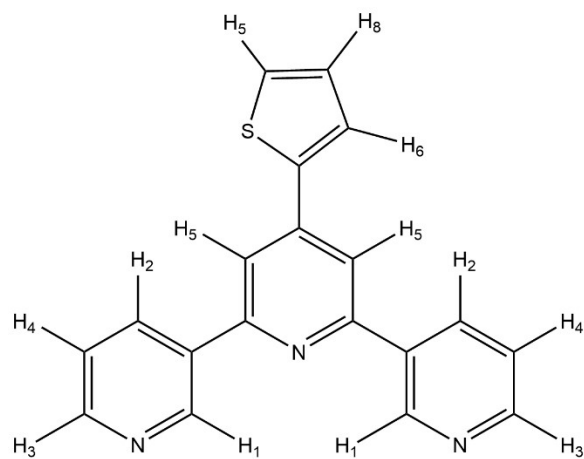
|  |           |
|--|-----------|
| <b>1. Characterization of the complexes.....</b>   | <b>2</b>  |
| 1. <sup>1</sup> H NMR signal assignment complexes.....   | 2         |
| 2. <sup>1</sup> H NMR of L <sub>1</sub> , L <sub>2</sub> and L <sub>3</sub> (600 MHz).....                       | 3         |
| 3. <sup>1</sup> H NMR spectra of complexes 1, 2 and 3 (300 MHz, 298K).....                                       | 4         |
| 4. Single crystal analysis of compounds 1-3. ....  | 6         |
| 5. IR spectra.....   | 8         |
| <b>2. Optical properties.....</b>  | <b>9</b>  |
| 1. UV-Vis absorption spectra in solution .....   | 9         |
| 2. Experimental UV-vis solid state absorption and TD-DFT singlet-singlet and singlet-triplet for complexes. .... | 11        |
| <b>3. Computational studies.....</b>   | <b>12</b> |
| 1. xyz for complex 1.....  | 12        |
| 2. xyz for complex 2.....  | 14        |

## 1. Characterization of the complexes

### 1. $^1\text{H}$ NMR signal assignment complexes.



**Figure S1:**  $^1\text{H}$  NMR assignment of ligand **L<sub>1</sub>**.



**Figure S2:**  $^1\text{H}$  NMR assignment of ligand **L<sub>2</sub>**.

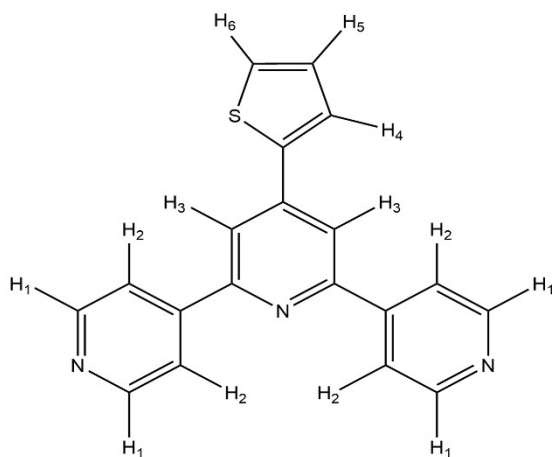
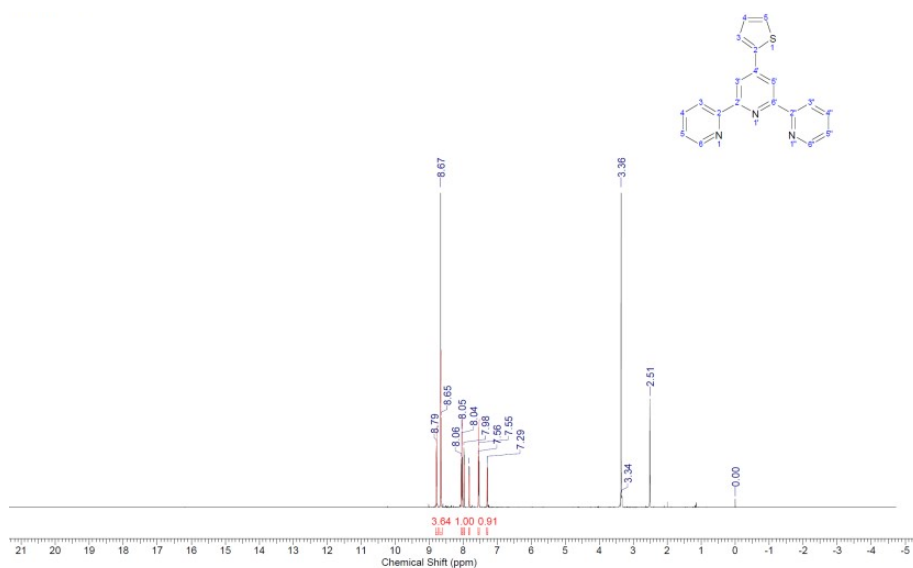


Figure S3:  $^1\text{H}$  NMR assignment of ligand  $\text{L}_3$ .

## 2. $^1\text{H}$ NMR of $\text{L}_1$ , $\text{L}_2$ and $\text{L}_3$ (600 MHz).



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Figure S4 :  $^1\text{H}$  NMR spectrum of  $\text{L}_1$  in  $[\text{D}_6]\text{-DMSO}$ .

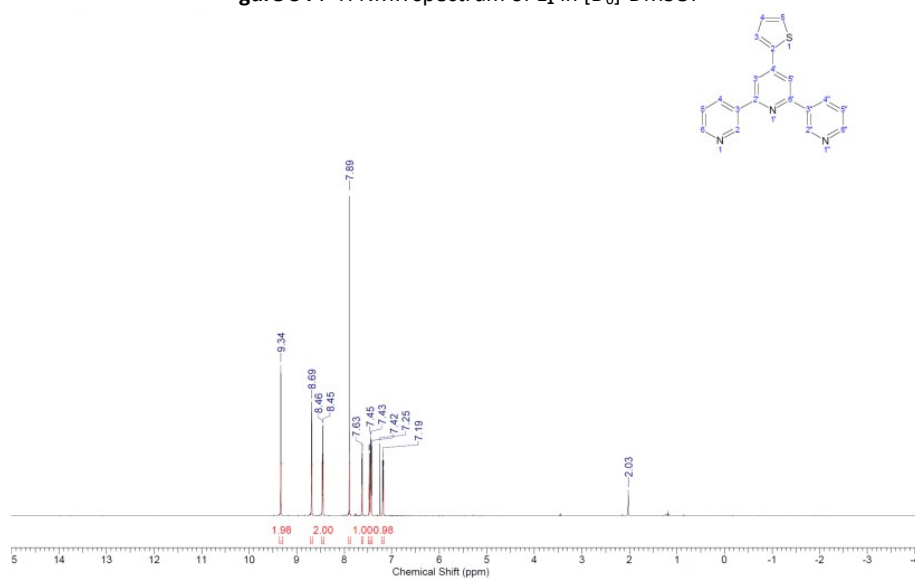


Figure S5 :  $^1\text{H}$  NMR spectrum of  $\text{L}_2$  in  $\text{CDCl}_3$ .

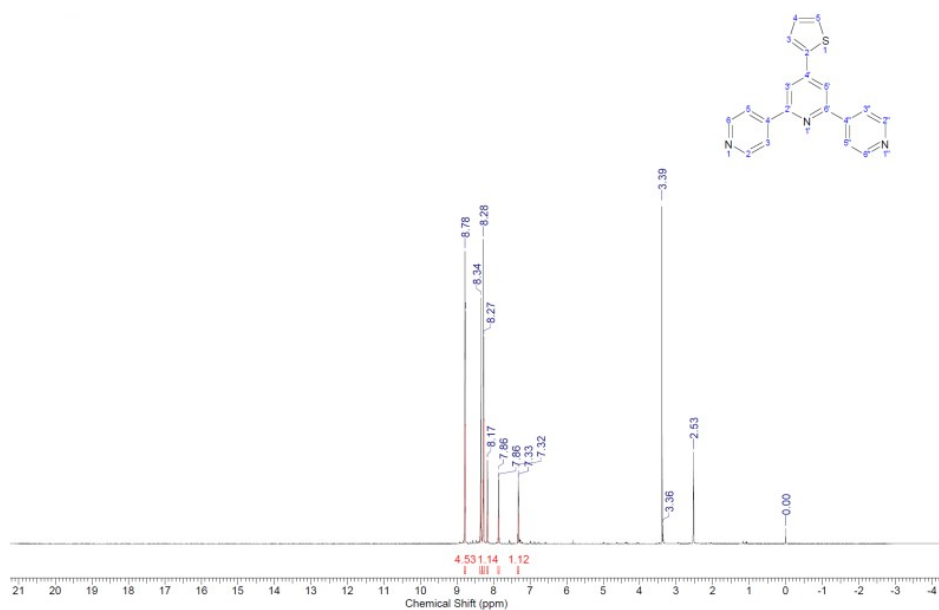


Figure S6 :  $^1\text{H}$  NMR spectrum of  $\text{L}_3$  in  $[\text{D}_6]$ -DMSO.

### 3. $^1\text{H}$ NMR spectra of complexes 1, 2 and 3 (300 MHz, 298K)

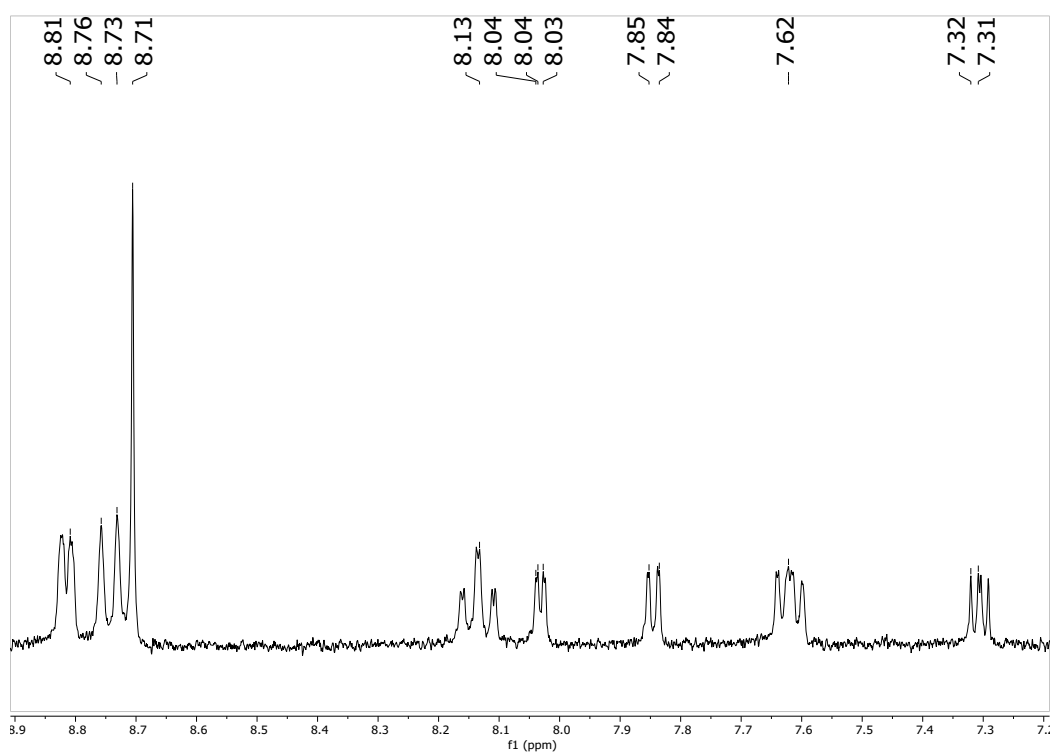


Figure S7:  $^1\text{H}$  NMR spectrum of complex 1 in  $[\text{D}_6]$ -DMSO.

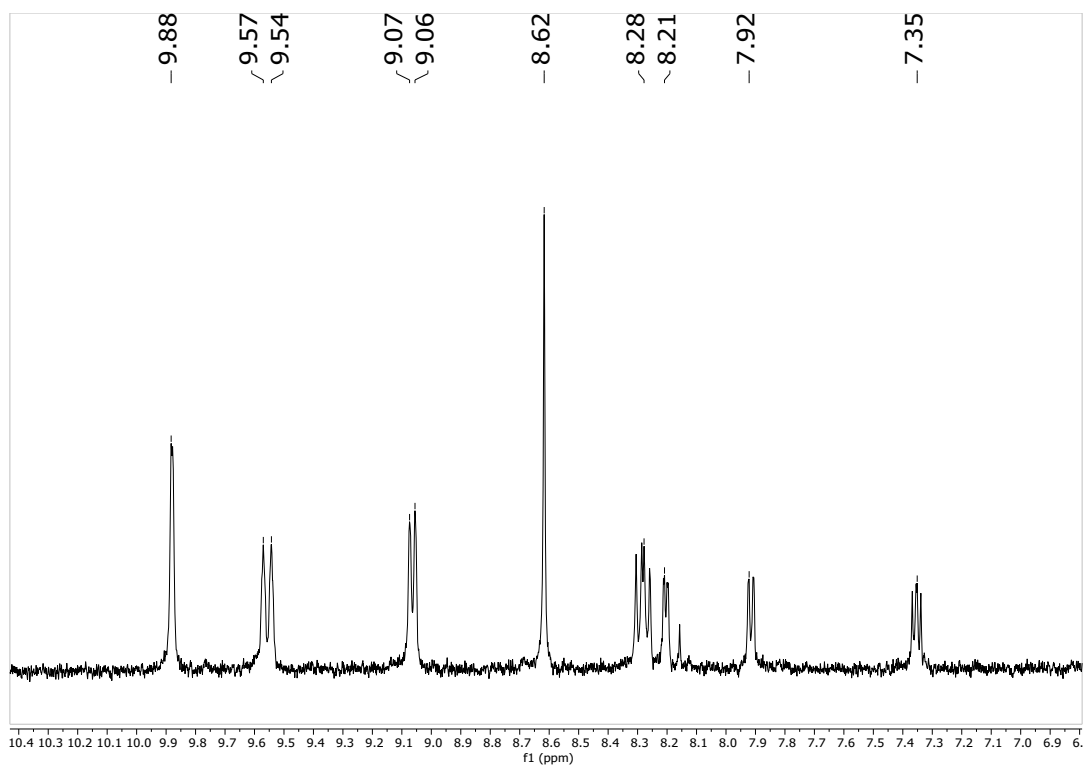


Figure S8:  $^1\text{H}$  NMR spectrum of complex **2** in  $[\text{D}_6]\text{-DMSO}$ .

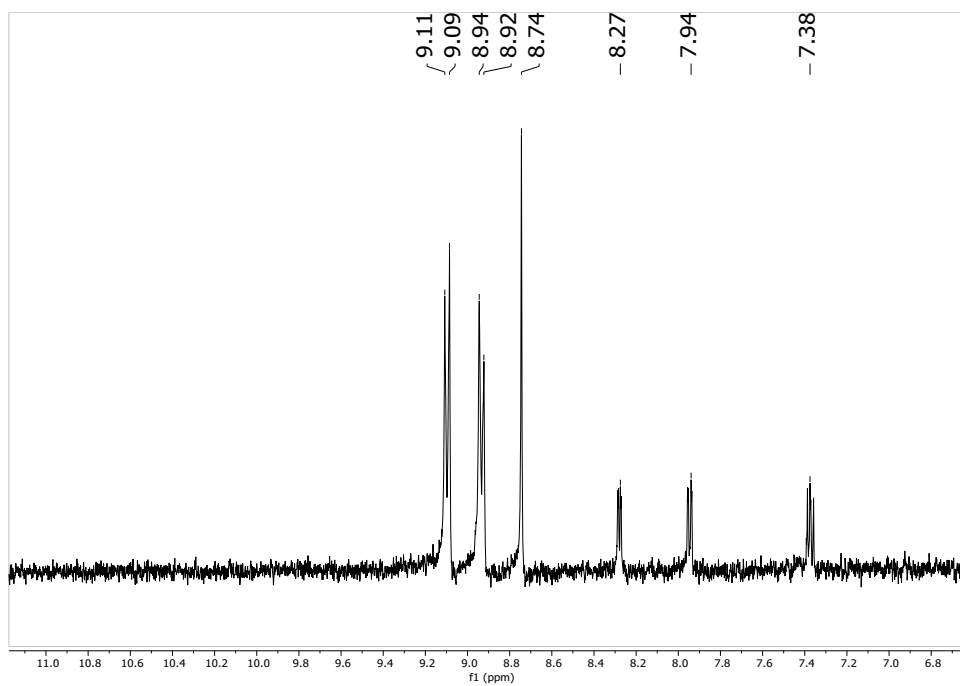
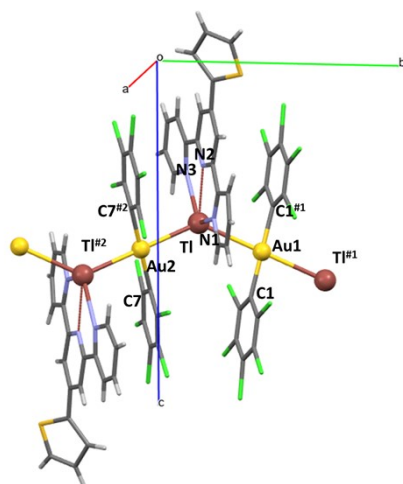


Figure S9:  $^1\text{H}$  NMR spectrum of complex **3** in  $[\text{D}_6]\text{-DMSO}$ .

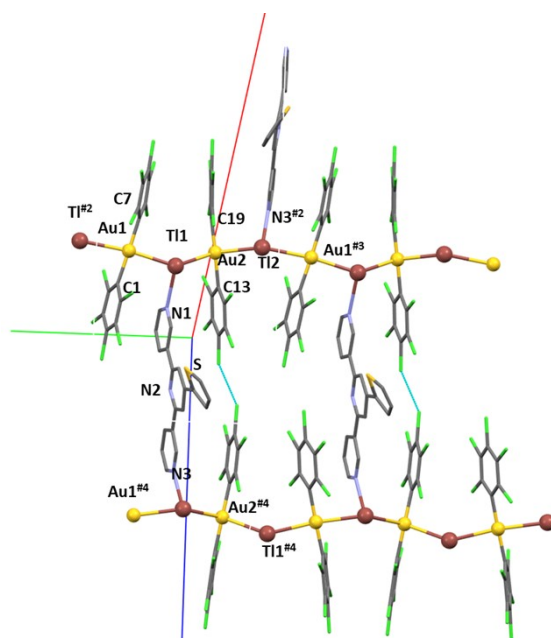
#### 4. Single crystal analysis of compounds 1-3.

**Table S1** : Data collection and structure refinement details for 2-4

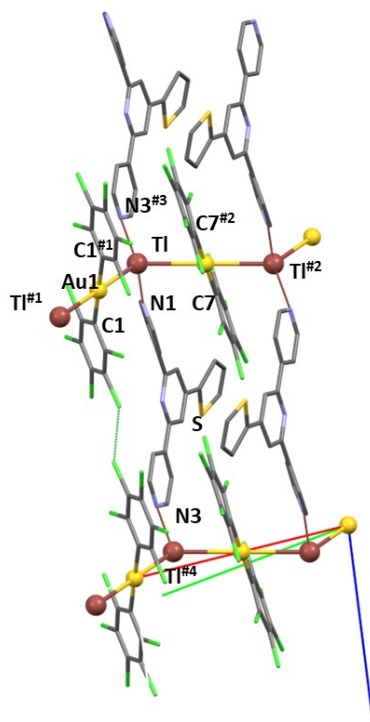
|  | <b>1</b>  | <b>2</b>  | <b>3</b>  |
|--|---|---|---|
| Chemical Formula   | C <sub>31</sub> H <sub>13</sub> Au Cl <sub>10</sub> N <sub>3</sub> S TI | C <sub>43</sub> H <sub>13</sub> Au <sub>2</sub> Cl <sub>20</sub> N <sub>3</sub> S TI <sub>2</sub> | C <sub>31</sub> H <sub>13</sub> Au Cl <sub>10</sub> N <sub>3</sub> S TI |
| Crystal habit  | Dark-Green plate  | Red plate   | Orange prism  |
| Crystal size/mm  | 0.166x0.037x0.017   | 0.121x0.106x0.016   | 0.121x0.x121x0.046  |
| Crystal system   | Triclinic   | Monoclinic  | Triclinic   |
| Space group  | P-1   | C 2/c   | P -1  |
| a/Å  | 10.5516(8)  | 44.5975(15)   | 11.2372(4)  |
| b/Å  | 10.9165(9)  | 10.7247(3)  | 12.8751(4)  |
| c/Å  | 15.3597(13)   | 30.8509(10)   | 13.5564(6)  |
| α/°  | 89.270(3)°  | 90  | 76.6270(10)   |
| β/°  | 86.508(3)°  | 124.1240(10)  | 85.9050(10)   |
| γ/°  | 88.089(3)°  | 90  | 69.1070(10)°  |
| V/Å <sup>3</sup>   | 1764.9(2)   | 12215.2(7)  | 1782.56(12)   |
| Z  | 2   | 8   | 2   |
| D <sub>c</sub> /g cm <sup>-3</sup>                               | 2.287   | 2.300   | 2.264   |
| M  | 1215.34   | 2115.30   | 1215.34   |
| F(000)   | 1132  | 7744  | 1129  |
| T/°C   | 26  | 22  | 26  |
| 2θmax/°  | 53  | 56  | 56  |
| μ(Mo-Kα)/mm <sup>-1</sup>  | 9.557   | 10.993  | 9.464   |
| No. refl. Measured   | 38612   | 137038  | 41470   |
| No. unique refl.   | 7481  | 14581   | 8531  |
| R <sub>int</sub>   | 0.0834  | 0.0871  | 0.0315  |
| R[F>2σ(F)][a]  | 0.0589  | 0.0696  | 0.0277  |
| wR[F 2 , all refl.][b]   | 0.1548  | 0.2312  | 0.0545  |
| No. of refl. Used<br>[F>2σ(F)]                                   | 7481  | 14581   | 8531  |
| No. of parameters  | 423   | 613   | 519   |
| No. of restraints  | 20  | 103   | 134   |
| S <sup>[c]</sup>   | 1.021   | 1.020   | 1.071   |
| Max. residual electron<br>density/e <sup>-</sup> Å <sup>-3</sup> | 1.486   | 2.219   | 0.66  |



**Figure S10:** Partial view of the polymeric chain in the crystal structure of **1** formed via Au...Tl interactions with the labelling scheme for the atom positions and crystallographic axes (red *a*, green *b* and blue *c*). Hydrogen atoms have been omitted for clarity. #1:  $-x+1, -y+1, -z+1$ ; #2:  $-x+1, -y, -z+1$ .

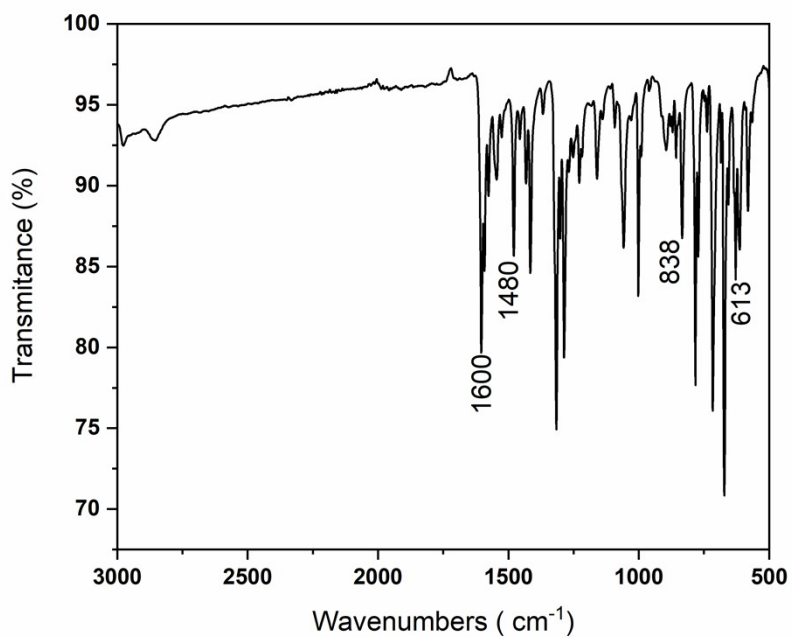


**Figure S11:** Partial view of the 2D network in the crystal structure of **2** formed via Au...Tl interactions and bridging  $L_2$  ligands with the labelling scheme for the atom positions and crystallographic axes (red *a*, green *b* and blue *c*). Hydrogen atoms have been omitted for clarity. #1:  $x, y+1, z$ ; #2:  $x, -y, z-1/2$ ; #3:  $x, y-1, z$ ; #4:  $x, -y, z+1/2$



**Figure S12:** Partial view of the 2D network in the crystal structure of **3** formed via Au $\cdots$ Tl interactions and bridging  $L_3$  ligands with the labelling scheme for the atom positions and crystallographic axes (red  $a$ , green  $b$  and blue  $c$ ). Hydrogen atoms have been omitted for clarity. #1:  $-x+2,-y,-z$ ; #2:  $-x+1,-y,-z$ ; #3:  $x,y,z-1$ ; #4:  $-x+2,-y,-z+1$ .

## 5. IR spectra



**Figure S13:** FT-IR spectrum of complex **1**.



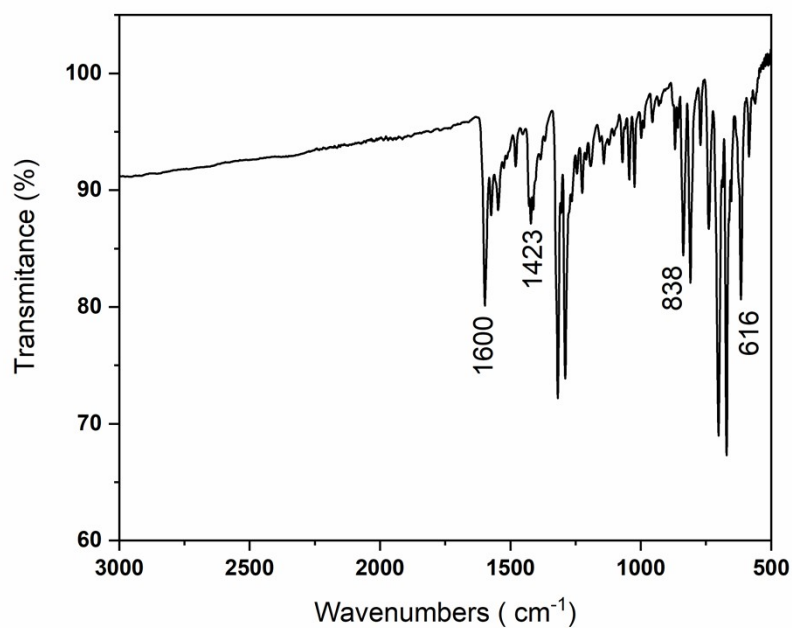


Figure S14: FT-IR spectrum of complex 2.

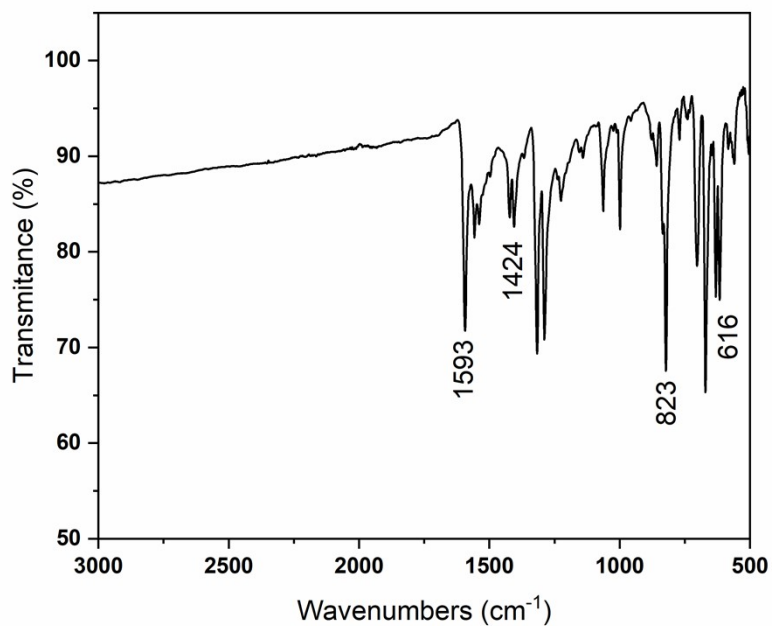
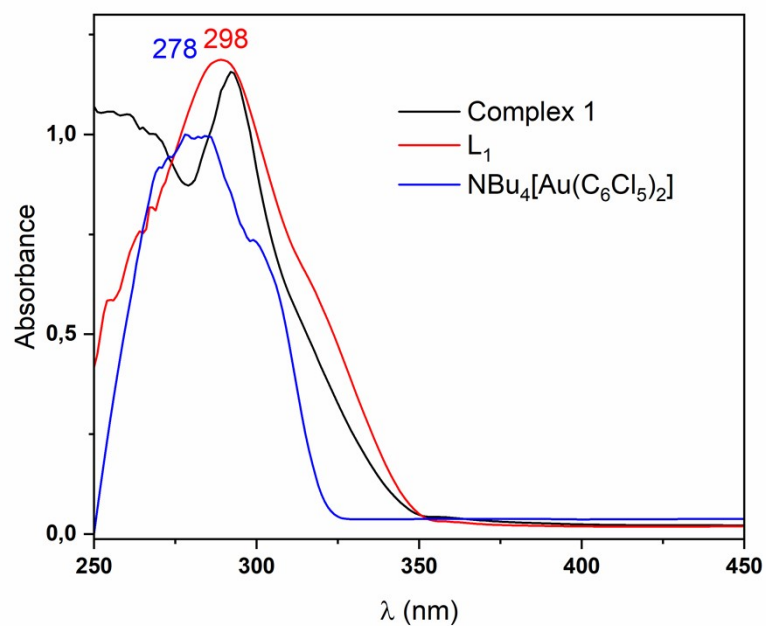


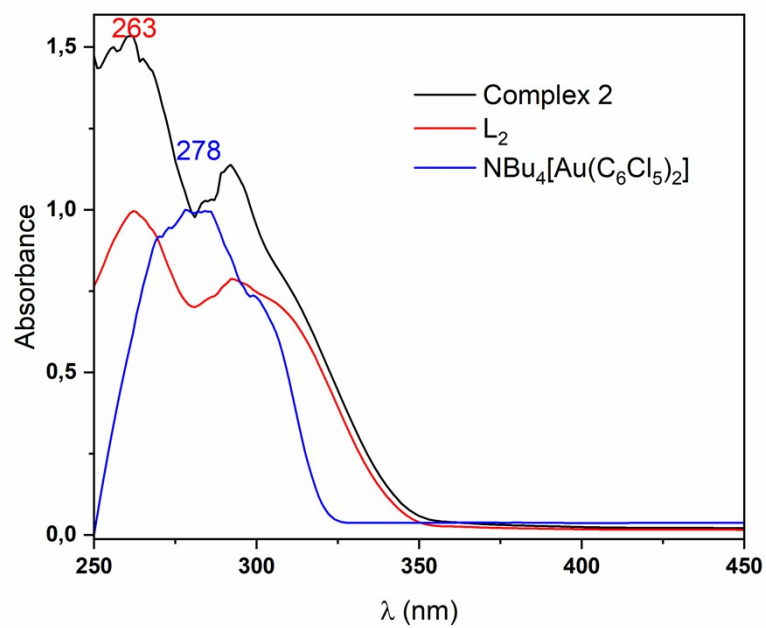
Figure S15: FT-IR spectrum of complex 3.

## 2. Optical properties

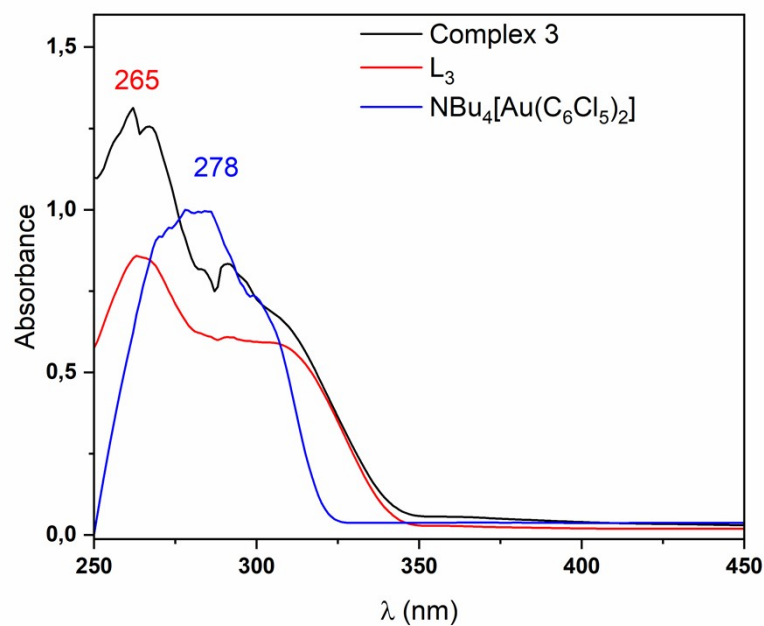
### 1. UV-Vis absorption spectra in solution



**Figure S16:** UV-Vis absorption spectra in DMSO solution of complex 1 ( $2.96 \cdot 10^{-5}$  M), L<sub>1</sub> ( $1.9 \cdot 10^{-5}$  M) and [NBu<sub>4</sub>][Au(C<sub>6</sub>Cl<sub>5</sub>)<sub>2</sub>] ( $3.39 \cdot 10^{-5}$  M).

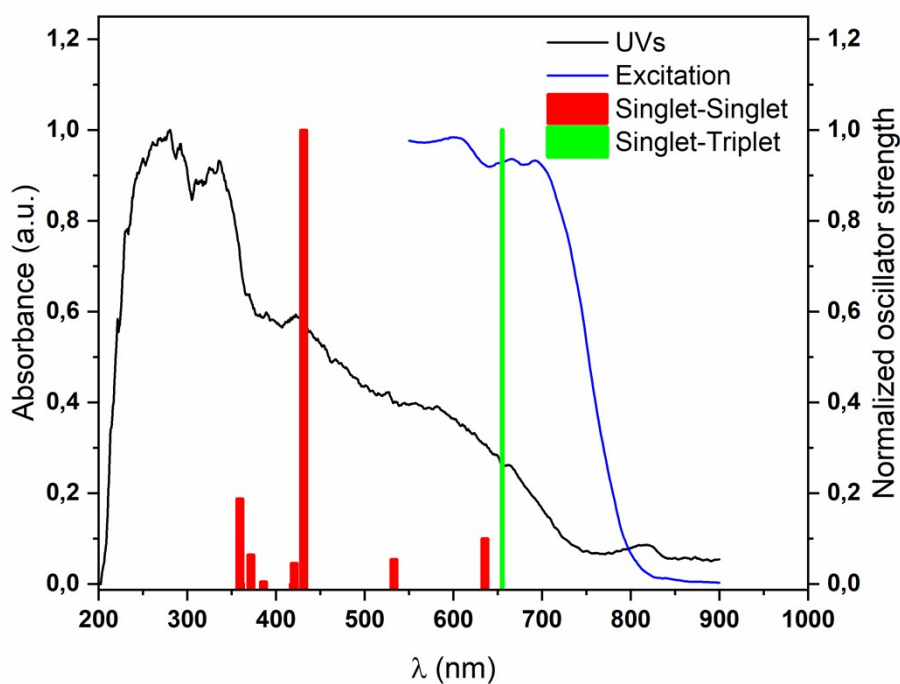


**Figure S17:** UV-Vis absorption spectra in DMSO solution of complex 2 ( $4.28 \cdot 10^{-5}$  M), L<sub>2</sub> ( $2.71 \cdot 10^{-5}$  M) and [NBu<sub>4</sub>][Au(C<sub>6</sub>Cl<sub>5</sub>)<sub>2</sub>] ( $3.39 \cdot 10^{-5}$  M).



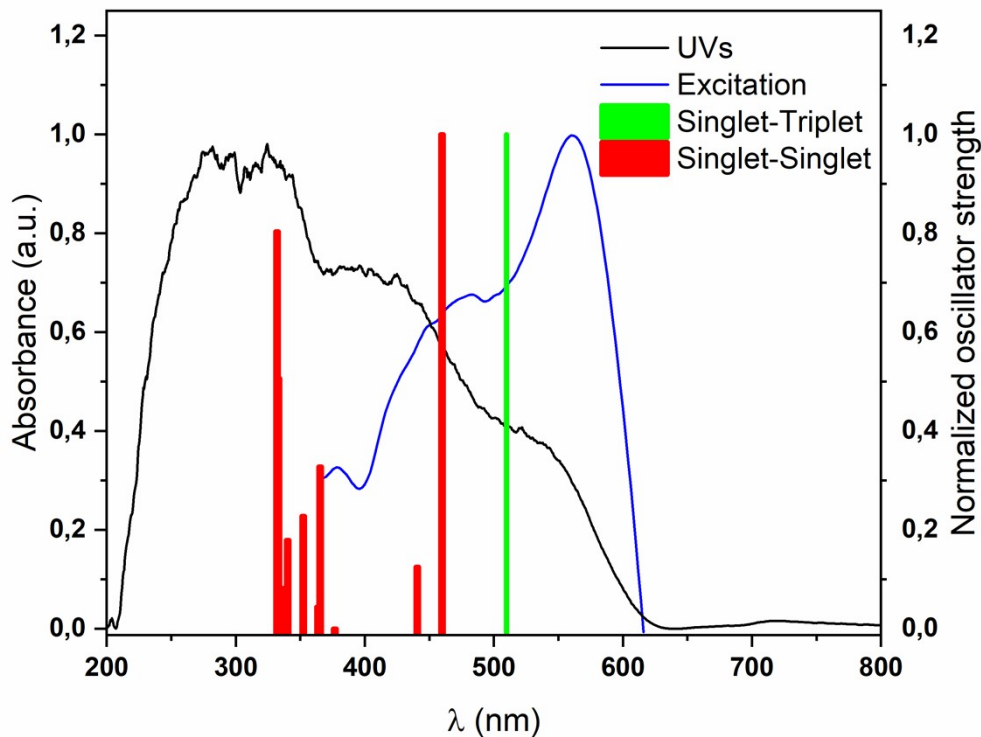
**Figure S18:** UV-Vis absorption spectra in DMSO solution of complex **3** ( $3.75 \cdot 10^{-5}$  M),  $L_3$  ( $2.03 \cdot 10^{-5}$  M) and  $[NBu_4][Au(C_6Cl_5)_2]$  ( $3.39 \cdot 10^{-5}$  M).

## 2. Experimental UV-vis solid state absorption and TD-DFT singlet-singlet and singlet-triplet for complexes.



**Figure S19:** Experimental UV-vis solid state absorption spectrum (black line), excitation (blue), TD-DFT singlet-singlet excitations (red bars) and singlet-triplet (green bars) for complex **1**. The green bar only represents the energy

of the lowest singlet-Triplet transitions since the oscillator strength cannot be calculated.



**Figure S20:** Experimental UV-vis solid state absorption spectrum (black line) , excitation (blue) ,TD-DFT singlet–singlet excitations (red bars) and singlet-triplet (green bars) for complex **2**. The green bar only represents the energy of the lowest singlet-Triplet transitions since the oscillator strength cannot be calculated.

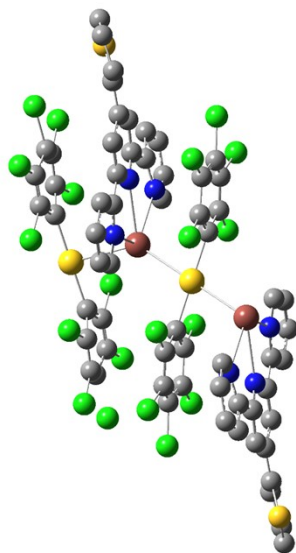
### 3. Computational studies

#### 1. xyz for model 1a

|    |             |            |             |    |             |            |             |
|----|-------------|------------|-------------|----|-------------|------------|-------------|
| Tl | 10.60940000 | 4.40310000 | 0.91970000  | C  | 7.74550000  | 2.87940000 | 2.29790000  |
| Au | 7.85850000  | 5.04140000 | 0.00000000  | C  | 7.78980000  | 2.64250000 | 3.64130000  |
| Au | 13.27210000 | 5.04140000 | 0.00000000  | C  | 12.13540000 | 5.96810000 | -2.75750000 |
| Cl | 7.95370000  | 1.81210000 | 1.09240000  | C  | 11.96220000 | 5.99880000 | -4.04780000 |
| Cl | 11.54330000 | 7.38260000 | -4.95110000 | C  | 12.49270000 | 3.63020000 | -3.97710000 |
| Cl | 6.93240000  | 6.90040000 | 2.57010000  | C  | 12.33270000 | 4.90350000 | -4.61350000 |
| Cl | 7.64240000  | 3.11550000 | 6.32810000  | C  | 7.43880000  | 3.64740000 | 4.68420000  |
| Cl | 7.15970000  | 6.10890000 | 5.55560000  | C  | 7.46620000  | 4.35720000 | 1.90900000  |
| Cl | 12.06860000 | 7.55230000 | -1.89310000 | C  | 7.33090000  | 5.26610000 | 2.93420000  |
| Cl | 11.95170000 | 4.68310000 | -6.45180000 | C  | 12.64980000 | 3.69500000 | -2.70450000 |
| Cl | 7.94950000  | 0.97080000 | 4.09030000  | Cl | 12.99190000 | 2.22580000 | -1.78000000 |
| Cl | 12.60890000 | 2.10930000 | -4.86630000 | Tl | 5.10750000  | 5.67960000 | -0.91970000 |
| C  | 12.69640000 | 4.85280000 | -1.96210000 | Cl | 7.76320000  | 8.27060000 | -1.09240000 |
| C  | 7.45310000  | 4.81340000 | 4.36600000  | Cl | 8.78450000  | 3.18230000 | -2.57010000 |

|    |             |             |             |   |             |             |             |
|----|-------------|-------------|-------------|---|-------------|-------------|-------------|
| CI | 8.07450000  | 6.96720000  | -6.32810000 | C | 11.91210000 | 1.11870000  | 4.41900000  |
| CI | 8.55720000  | 3.97380000  | -5.55560000 | H | 12.20190000 | 1.15360000  | 5.32150000  |
| CI | 7.76750000  | 9.11190000  | -4.09030000 | C | 10.22900000 | 7.46920000  | 1.14900000  |
| C  | 8.26380000  | 5.26930000  | -4.36600000 | H | 10.32000000 | 7.19710000  | 0.23730000  |
| C  | 7.97140000  | 7.20330000  | -2.29790000 | C | 10.70970000 | 5.98660000  | 8.69670000  |
| C  | 7.92710000  | 7.44020000  | -3.64130000 | H | 10.08000000 | 6.63750000  | 8.42230000  |
| C  | 8.27810000  | 6.43530000  | -4.68420000 | C | 11.33670000 | 3.66020000  | 5.81550000  |
| C  | 8.25070000  | 5.72560000  | -1.90900000 | H | 11.59280000 | 2.89380000  | 6.31410000  |
| C  | 8.38600000  | 4.81660000  | -2.93420000 | C | 11.22910000 | 5.89130000  | 10.07540000 |
| CI | 15.00100000 | 2.70020000  | 4.95110000  | H | 11.06470000 | 6.56610000  | 10.72570000 |
| CI | 14.47560000 | 2.53050000  | 1.89310000  | C | 11.73790000 | 0.00540000  | 2.26250000  |
| CI | 14.59260000 | 5.39960000  | 6.45180000  | H | 11.89080000 | -0.76280000 | 1.72810000  |
| CI | 13.93540000 | 7.97350000  | 4.86630000  | C | 11.85960000 | 4.90120000  | 10.34060000 |
| C  | 13.84790000 | 5.22990000  | 1.96210000  | H | 12.14910000 | 4.66970000  | 11.21600000 |
| C  | 14.40880000 | 4.11470000  | 2.75750000  | C | 12.02010000 | -0.11530000 | 3.62360000  |
| C  | 14.58200000 | 4.08390000  | 4.04780000  | H | 12.27420000 | -0.94370000 | 4.01430000  |
| C  | 14.05150000 | 6.45250000  | 3.97710000  | C | 11.23990000 | 5.06510000  | 7.90120000  |
| C  | 14.21150000 | 5.17920000  | 4.61350000  | C | 11.21930000 | 3.62970000  | 4.45440000  |
| C  | 13.89440000 | 6.38770000  | 2.70450000  | C | 10.31560000 | 6.99630000  | 3.46450000  |
| CI | 13.55240000 | 7.85690000  | 1.78000000  | S | 3.52560000  | 6.14370000  | -8.89460000 |
| S  | 12.19130000 | 3.93900000  | 8.89460000  | N | 4.83040000  | 5.55960000  | -3.65900000 |
| N  | 10.88650000 | 4.52310000  | 3.65900000  | N | 4.71410000  | 7.94260000  | -2.45700000 |
| N  | 11.00280000 | 2.14010000  | 2.45700000  | C | 4.92090000  | 4.09500000  | -5.67410000 |
| C  | 10.79600000 | 5.98780000  | 5.67410000  | H | 5.06400000  | 3.25400000  | -6.08520000 |
| H  | 10.65290000 | 6.82870000  | 6.08520000  | C | 4.42330000  | 9.03510000  | -1.69690000 |
| C  | 11.29360000 | 1.04760000  | 1.69690000  | H | 4.54350000  | 9.02110000  | -0.74930000 |
| H  | 11.17340000 | 1.06160000  | 0.74930000  | C | 5.02100000  | 4.24130000  | -4.33070000 |
| C  | 10.69590000 | 5.84150000  | 4.33070000  | C | 4.61400000  | 5.23080000  | -6.43410000 |
| C  | 11.10290000 | 4.85200000  | 6.43410000  | N | 5.34780000  | 3.27310000  | -2.12110000 |
| N  | 10.36910000 | 6.80970000  | 2.12110000  | C | 5.86360000  | 1.09440000  | -1.74990000 |
| C  | 9.85340000  | 8.98840000  | 1.74990000  | H | 6.08640000  | 0.41550000  | -1.11770000 |
| H  | 9.63060000  | 9.66720000  | 1.11770000  | C | 4.37490000  | 7.83230000  | -3.74730000 |
| C  | 11.34200000 | 2.25050000  | 3.74730000  | C | 5.58770000  | 1.80520000  | -3.97710000 |
| C  | 10.12920000 | 8.27750000  | 3.97710000  | H | 5.52740000  | 1.63250000  | -4.90120000 |
| H  | 10.18950000 | 8.45020000  | 4.90120000  | C | 5.87040000  | 0.77710000  | -3.05800000 |
| C  | 9.84650000  | 9.30560000  | 3.05800000  | H | 6.06060000  | -0.10270000 | -3.34680000 |
| H  | 9.65640000  | 10.18540000 | 3.34680000  | C | 3.80480000  | 8.96400000  | -4.41900000 |

|   |            |            |              |   |            |             |              |
|---|------------|------------|--------------|---|------------|-------------|--------------|
| H | 3.51500000 | 8.92920000 | -5.32150000  | C | 3.97900000 | 10.07730000 | -2.26250000  |
| C | 5.48790000 | 2.61360000 | -1.14900000  | H | 3.82610000 | 10.84560000 | -1.72810000  |
| H | 5.39690000 | 2.88560000 | -0.23730000  | C | 3.85730000 | 5.18160000  | -10.34060000 |
| C | 5.00720000 | 4.09610000 | -8.69670000  | H | 3.56780000 | 5.41310000  | -11.21600000 |
| H | 5.63690000 | 3.44520000 | -8.42230000  | C | 3.69680000 | 10.19810000 | -3.62360000  |
| C | 4.38020000 | 6.42250000 | -5.81550000  | H | 3.44270000 | 11.02640000 | -4.01430000  |
| H | 4.12410000 | 7.18890000 | -6.31410000  | C | 4.47700000 | 5.01760000  | -7.90120000  |
| C | 4.48780000 | 4.19140000 | -10.07540000 | C | 4.49760000 | 6.45300000  | -4.45440000  |
| H | 4.65220000 | 3.51660000 | -10.72570000 | C | 5.40130000 | 3.08650000  | -3.46450000  |



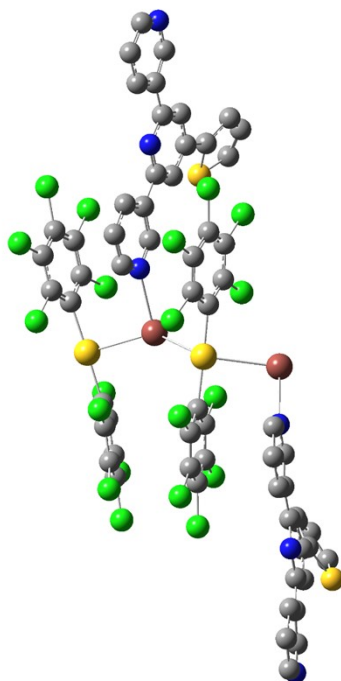
**Figure S21:** Model 1a. Color code: yellow (gold), grey (carbon), blue (nitrogen), orange (sulfur), brown (thallium) and green (chlorine).

## 2. xyz for model 2a

|    |             |             |            |    |             |             |             |
|----|-------------|-------------|------------|----|-------------|-------------|-------------|
| Au | 12.91460000 | 0.47210000  | 3.06930000 | Cl | 8.18870000  | -0.12870000 | 7.63650000  |
| Au | 14.17810000 | 5.76410000  | 4.07020000 | Cl | 15.71260000 | 4.23090000  | -1.20700000 |
| Tl | 14.41300000 | -2.06080000 | 3.65180000 | Cl | 18.26990000 | 1.20970000  | 1.16280000  |
| Tl | 13.55200000 | 2.95960000  | 4.58610000 | Cl | 12.24630000 | 0.59410000  | -0.16290000 |
| Cl | 16.21020000 | 1.00810000  | 3.43940000 | Cl | 17.35980000 | 0.98130000  | -1.79110000 |
| Cl | 13.60580000 | 4.48610000  | 1.04170000 | Cl | 13.39880000 | -0.25850000 | 6.38170000  |
| Cl | 11.15730000 | -0.51590000 | 8.48050000 | Cl | 18.69940000 | 4.69530000  | -0.60040000 |

|    |             |             |             |   |             |            |             |
|----|-------------|-------------|-------------|---|-------------|------------|-------------|
| CI | 9.73740000  | 0.73460000  | 2.57920000  | C | 11.47850000 | 6.64930000 | 5.09510000  |
| CI | 14.33240000 | 0.69280000  | -2.45690000 | C | 16.60600000 | 1.01990000 | 0.79940000  |
| CI | 9.44630000  | 6.96030000  | 8.51120000  | C | 6.30680000  | 2.95040000 | 11.20660000 |
| CI | 11.09190000 | 6.81020000  | 3.39440000  | H | 6.42100000  | 3.11720000 | 10.29800000 |
| CI | 8.84040000  | 7.27460000  | 5.47300000  | C | 9.83040000  | 2.41200000 | 12.21280000 |
| CI | 7.48540000  | 0.46010000  | 4.69080000  | H | 9.71730000  | 2.23030000 | 13.11890000 |
| CI | 12.33490000 | 6.29110000  | 9.43770000  | C | 11.11080000 | 2.43670000 | 11.63310000 |
| CI | 19.57640000 | 5.62830000  | 2.20150000  | C | 10.04890000 | 2.91500000 | 9.55420000  |
| CI | 14.54600000 | 5.77850000  | 7.34970000  | C | 12.37240000 | 1.44350000 | 13.75280000 |
| CI | 17.44400000 | 6.08950000  | 4.41570000  | H | 11.66700000 | 1.03480000 | 14.19460000 |
| S  | 13.89140000 | 2.77770000  | 12.12340000 | C | 10.15690000 | 3.47270000 | 5.40660000  |
| C  | 14.29670000 | 0.80440000  | 1.56810000  | H | 10.18190000 | 3.57400000 | 4.48320000  |
| C  | 8.74850000  | 2.66620000  | 11.40070000 | C | 16.95370000 | 5.49100000 | 2.88590000  |
| C  | 13.91650000 | 0.71860000  | 0.22730000  | C | 11.20370000 | 2.73800000 | 10.27180000 |
| C  | 10.74840000 | -0.21340000 | 6.82410000  | H | 12.03230000 | 2.81810000 | 9.86200000  |
| C  | 11.45980000 | 0.16410000  | 4.49740000  | C | 12.96460000 | 6.22030000 | 6.81130000  |
| C  | 16.21840000 | 0.94380000  | -0.51080000 | C | 17.56460000 | 4.87970000 | 0.61550000  |
| N  | 11.33590000 | 3.24530000  | 6.04260000  | C | 12.31670000 | 2.14070000 | 12.53210000 |
| C  | 15.64120000 | 0.95240000  | 1.79540000  | C | 4.92910000  | 2.75410000 | 13.06840000 |
| C  | 12.74510000 | 6.31150000  | 5.43730000  | H | 4.08060000  | 2.76470000 | 13.44300000 |
| C  | 9.41710000  | -0.03110000 | 6.45890000  | C | 11.26910000 | 3.06510000 | 7.33230000  |
| C  | 9.13970000  | 0.23590000  | 5.13080000  | H | 12.05930000 | 2.86160000 | 7.77510000  |
| C  | 16.20330000 | 4.67490000  | 0.39330000  | C | 8.96130000  | 3.42550000 | 7.40120000  |
| N  | 5.91140000  | 2.52670000  | 13.84990000 | H | 8.16630000  | 3.52140000 | 7.87230000  |
| C  | 7.35340000  | 2.69080000  | 11.95230000 | C | 11.96820000 | 6.43050000 | 7.74860000  |
| C  | 15.24570000 | 4.80470000  | 1.39190000  | C | 8.94820000  | 3.56490000 | 5.99910000  |
| C  | 10.10330000 | 0.33890000  | 4.16290000  | H | 8.16170000  | 3.71010000 | 5.52090000  |
| C  | 11.73400000 | -0.09330000 | 5.84340000  | C | 5.02560000  | 2.98040000 | 11.74800000 |
| N  | 8.85170000  | 2.92680000  | 10.10330000 | H | 4.27410000  | 3.14790000 | 11.22400000 |
| C  | 10.42780000 | 6.88950000  | 5.99400000  | C | 17.95150000 | 5.30870000 | 1.88730000  |
| C  | 14.86100000 | 0.78400000  | -0.75850000 | C | 14.61780000 | 2.09130000 | 13.51280000 |
| C  | 15.59640000 | 5.26150000  | 2.68420000  | H | 15.51680000 | 2.16750000 | 13.73300000 |
| C  | 7.11000000  | 2.50310000  | 13.28550000 | C | 10.11840000 | 3.14980000 | 8.09590000  |
| H  | 7.84210000  | 2.34600000  | 13.83670000 | C | 13.76300000 | 1.49070000 | 14.18190000 |
| C  | 10.70790000 | 6.76190000  | 7.32460000  | H | 14.01710000 | 1.06070000 | 14.96820000 |

|   |             |             |             |   |             |             |             |
|---|-------------|-------------|-------------|---|-------------|-------------|-------------|
| N | 14.56490000 | -2.52670000 | 1.08030000  | C | 19.85720000 | -2.73800000 | -2.49770000 |
| S | 22.54480000 | -2.77770000 | -0.64610000 | H | 20.68580000 | -2.81810000 | -2.90760000 |
| C | 17.40200000 | -2.66620000 | -1.36890000 | C | 20.97010000 | -2.14070000 | -0.23750000 |
| N | 19.98940000 | -3.24530000 | -6.72700000 | C | 13.58260000 | -2.75410000 | 0.29880000  |
| C | 16.00690000 | -2.69080000 | -0.81730000 | H | 12.73410000 | -2.76470000 | 0.67340000  |
| N | 17.50520000 | -2.92680000 | -2.66630000 | C | 19.92260000 | -3.06510000 | -5.43730000 |
| C | 15.76350000 | -2.50310000 | 0.51590000  | H | 20.71280000 | -2.86160000 | -4.99440000 |
| H | 16.49560000 | -2.34600000 | 1.06710000  | C | 17.61480000 | -3.42550000 | -5.36830000 |
| C | 14.96020000 | -2.95040000 | -1.56300000 | H | 16.81980000 | -3.52140000 | -4.89730000 |
| H | 15.07450000 | -3.11720000 | -2.47160000 | C | 17.60160000 | -3.56490000 | -6.77040000 |
| C | 18.48390000 | -2.41200000 | -0.55680000 | H | 16.81520000 | -3.71010000 | -7.24870000 |
| H | 18.37080000 | -2.23030000 | 0.34940000  | C | 13.67910000 | -2.98040000 | -1.02160000 |
| C | 19.76420000 | -2.43670000 | -1.13650000 | H | 12.92760000 | -3.14790000 | -1.54560000 |
| C | 18.70230000 | -2.91500000 | -3.21540000 | C | 23.27130000 | -2.09130000 | 0.74320000  |
| C | 21.02590000 | -1.44350000 | 0.98330000  | H | 24.17020000 | -2.16750000 | 0.96350000  |
| H | 20.32040000 | -1.03480000 | 1.42500000  | C | 18.77180000 | -3.14980000 | -4.67370000 |
| C | 18.81030000 | -3.47270000 | -7.36290000 | C | 22.41650000 | -1.49070000 | 1.41230000  |
| H | 18.83540000 | -3.57400000 | -8.28640000 | H | 22.67060000 | -1.06070000 | 2.19860000  |



**Figure S22:** Model 2a. Color code: yellow (gold), grey (carbon), blue (nitrogen), orange (sulfur), brown (thallium) and green (chlorine).



