Selective Turn-Off Phosphorescent and Colorimetric Detection of Mercury(II) in Water by Half-Lantern Platinum (II) Complexes.

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SUPPORTING INFORMATION

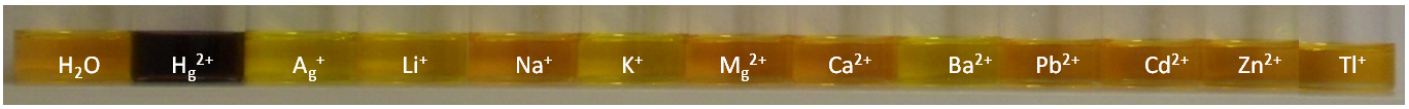


Figure S1. Photographs of **B** in DMSO (5 mL, 2 x 10^{-4} M) upon addition of 0.5 mL of H_2O or aqueous solutions of every metal ion (0.01 M for Hg^{2+}, Ca^{2+} and 0.1 M, for the rest of the cations).

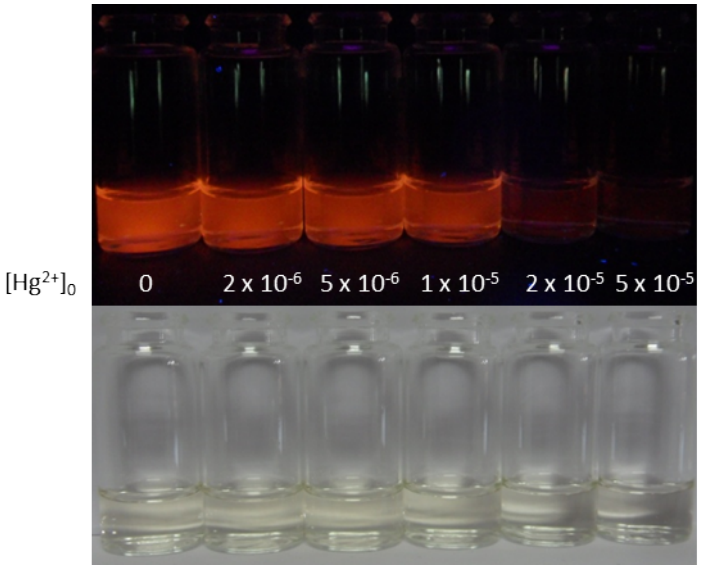


Figure S2. Lower picture: photographs of **B** (1 mL, 2 x 10^{-5} M in DMSO) after addition of 3 mL of aqueous solutions of Hg^{2+} with different concentrations. Upper picture: photographs of these solutions irradiated with UV light at λ = 365 nm.

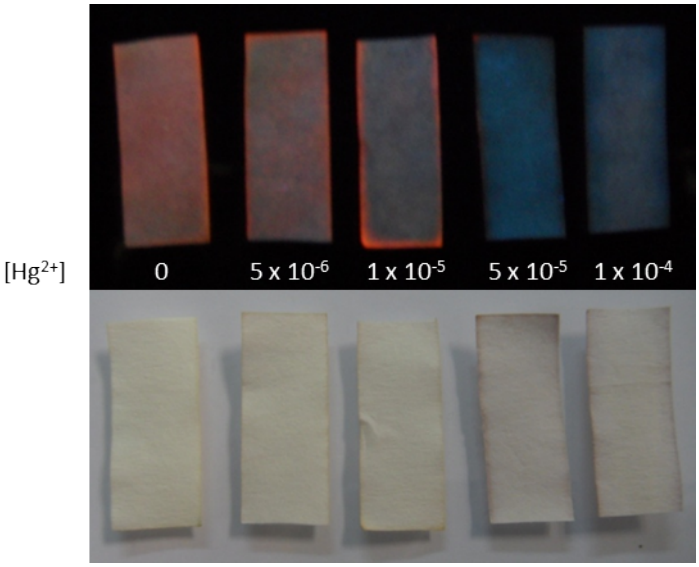


Figure S3. Lower picture: Photographs of dried test strips of **A** (DMSO, 2 x 10^{-4} M) after immersion in water and aqueous solutions of Hg^{2+} with different concentrations. Upper picture: photographs of these test strips irradiated with UV light at λ = 365 nm.

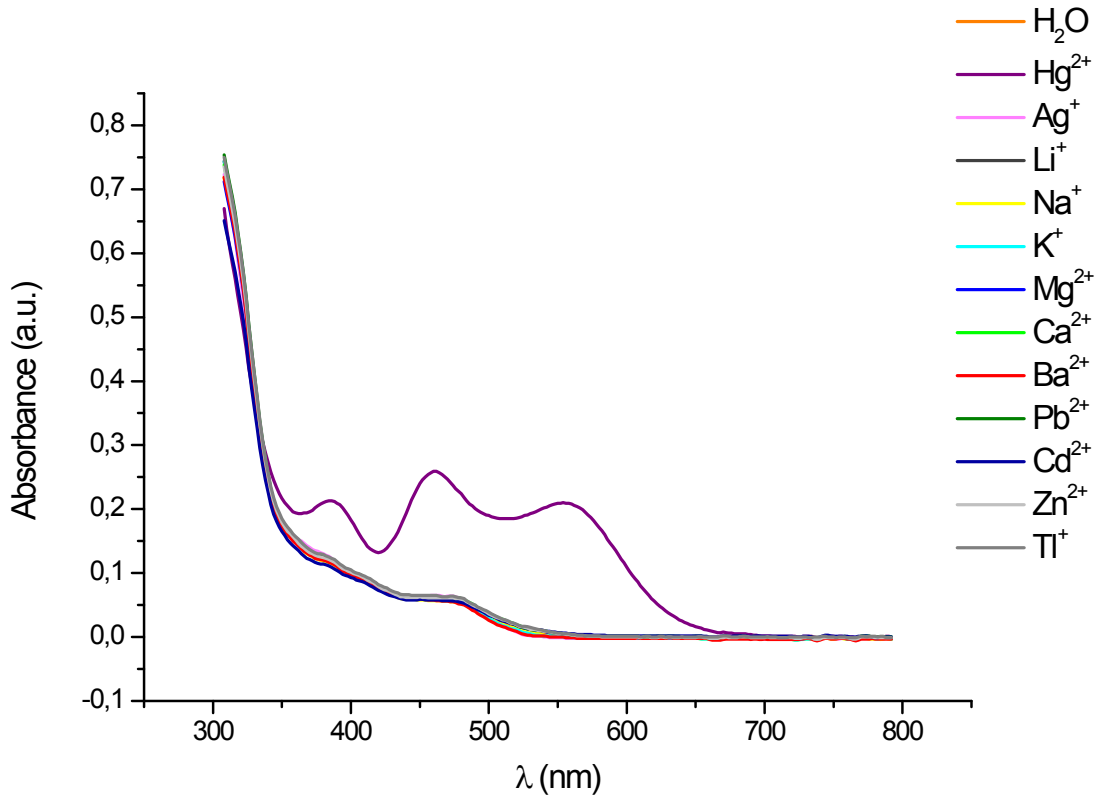


Figure S4. Absorption spectra of **B** in DMSO (5 mL, 2 x 10^{-4} M) upon the addition of

0.5 mL of water or aqueous solutions of every metal ion (0.01 M for Hg^{2+}, Ca^{2+} and 0.1 M, for the rest of the cations).

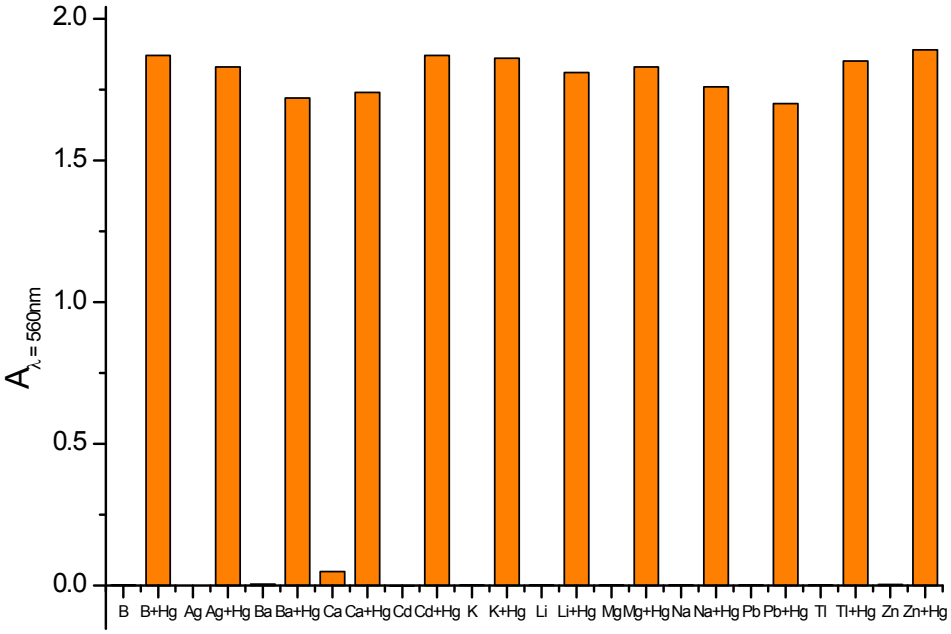


Figure S5.Absorption response of **B** in DMSO (5 mL, 2 x 10^{-4} M) to the presence of several metal ions (0.5 mL, 0.1 M in H_2O) with (0.5 mL, 0.01 M in H_2O) and without Hg^{2+}.

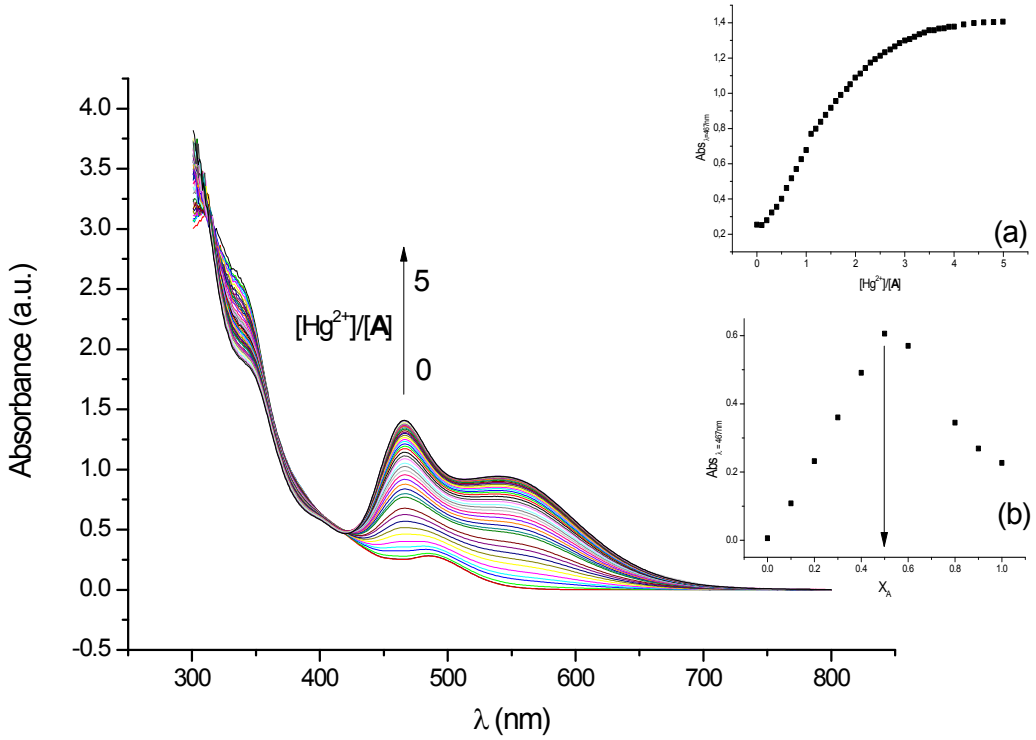


Figure S6.Changes in the UV-Vis absorption spectra of **A** in DMSO (3 mL, 10^{-4} M) upon addition of Hg^{2+} (n x 10μL, 3 x 10^{-3} M; 0-5 **A**:Hg^{2+} molar ratio) in buffer aqueous solution (HEPES, 20mM, pH = 7.0). Inset: a) Titration curve of **A** with Hg^{2+} b) Job's plot for determining the stoichiometry of the complex [**A**-Hg^{2+}] $^{+}$ in DMSO / H_2O (1:0.1, v/v).

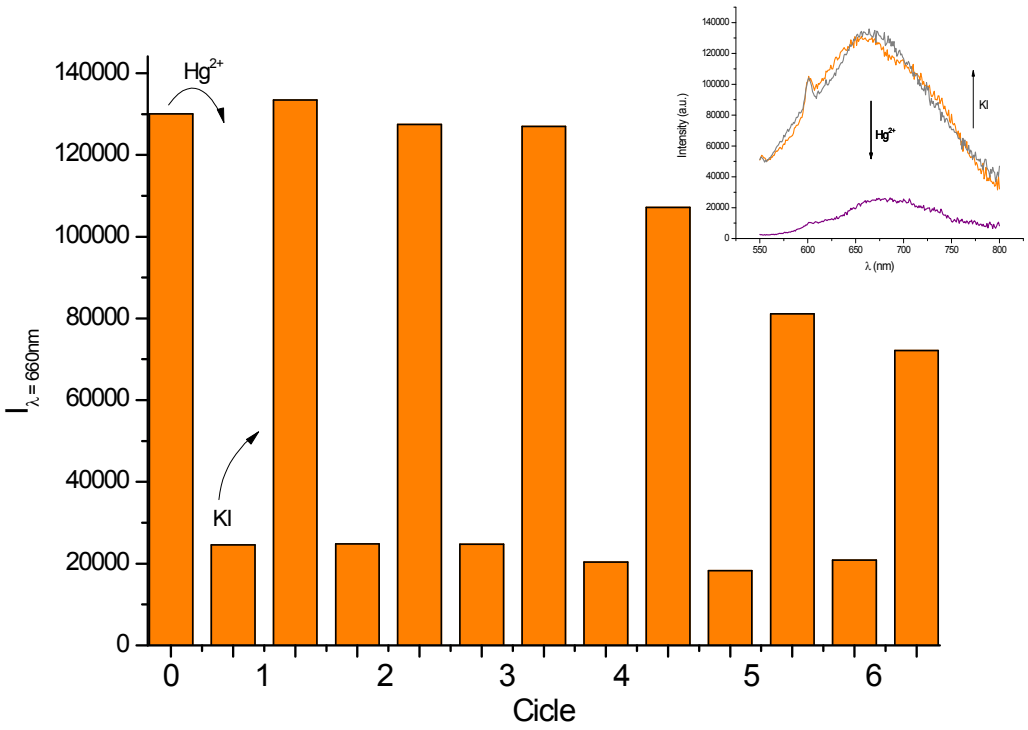
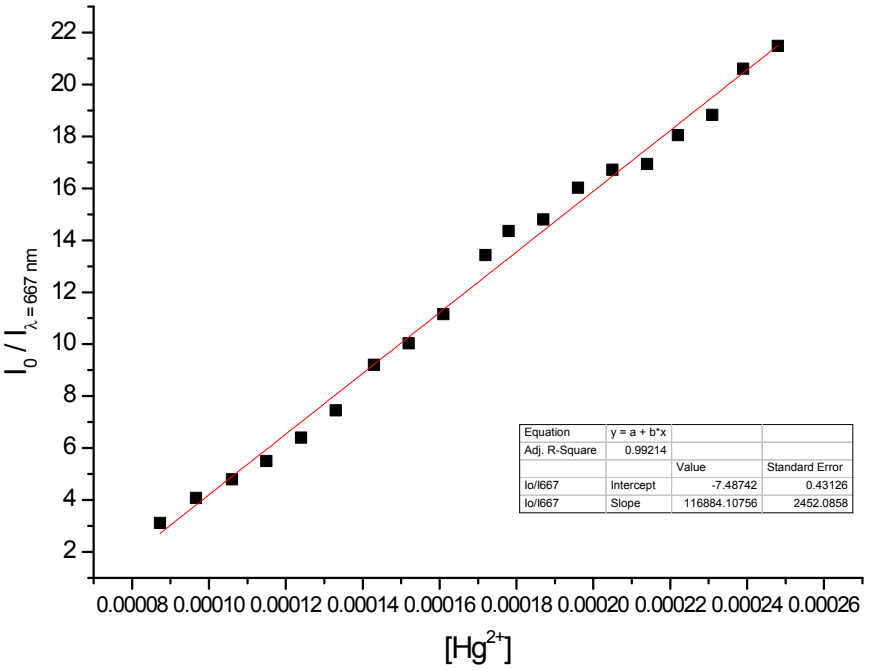


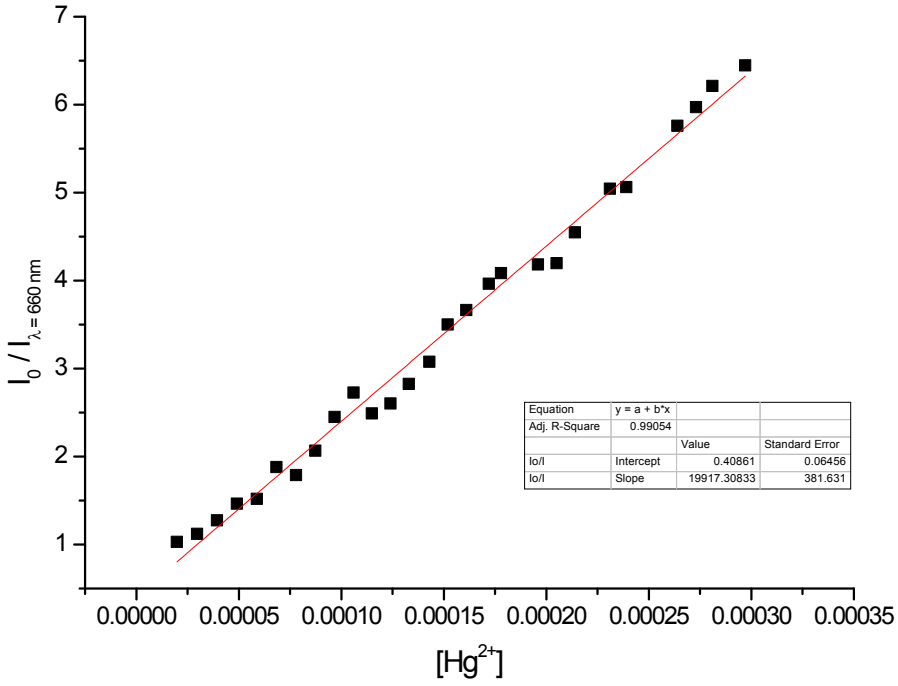
Figure S7.Reversible Hg^{2+} complexation to **B** by addition of KI followed by luminescence. Inset: Orange line, free **B** (2 x 10^{-4}M, DMSO); violet line: **B** + Hg^{2+} (1:1); grey line: **B** + Hg^{2+} + KI (1:1:2).

Table S1.Emission lifetimes of mixtures **A**/ Hg^{2+} (DMSO/H_2O).

[Hg^{2+}]/[**A**]	0	0.2	0.4	0.6	0.8	1
τ (ns)	25.2	27.7	26.4	26.7	26.8	27.3



(a)



(b)

Figure S8: Stern-Volmer plot for the titration of: a) **A** in DMSO (3 mL, 10^{-4} M) with Hg^{2+}; b) **B** in DMSO (3 mL, 10^{-4} M) with Hg^{2+}.

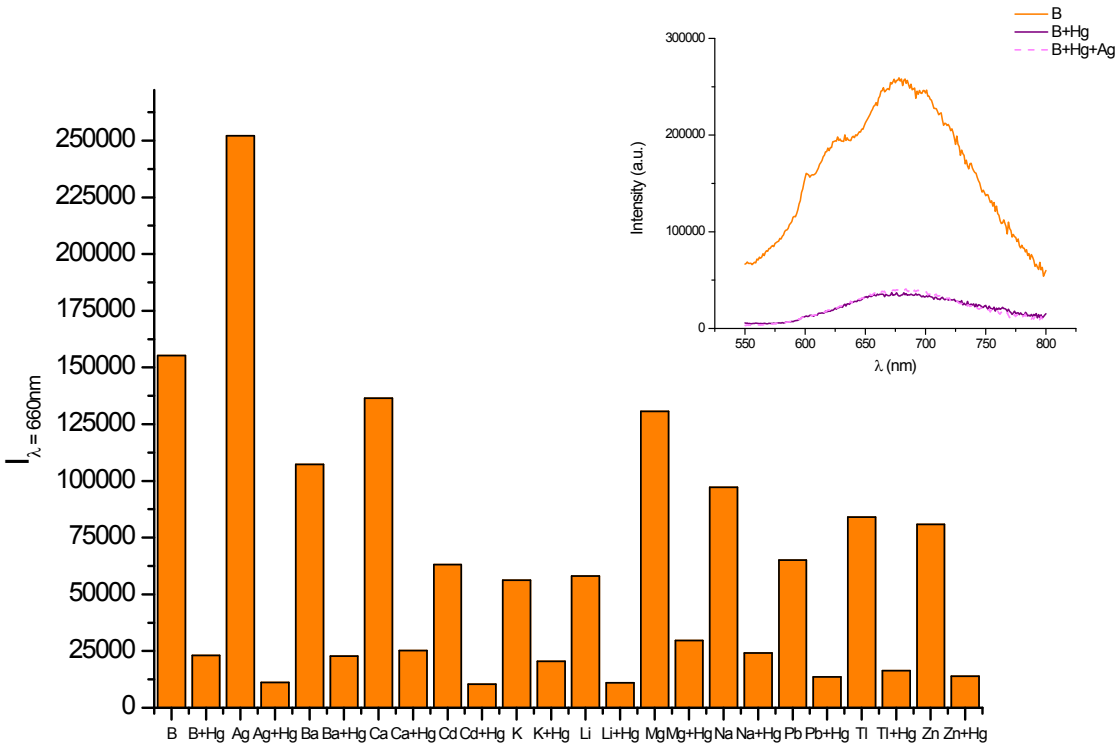


Figure S9.Luminescence response of **B** (5 mL, 2 x 10^{-4}M in DMSO) to the presence of several metal ions (0.5 mL, 0.1 M in H_2O) before and after addition of Hg^{2+} (0.5 mL, 0.01 M in H_2O). Inset: emission intensity of **B** (λ_{exc} = 510 nm) in DMSO, **B**+Hg^{2+} and **B**+Hg^{2+}+Ag^{+}

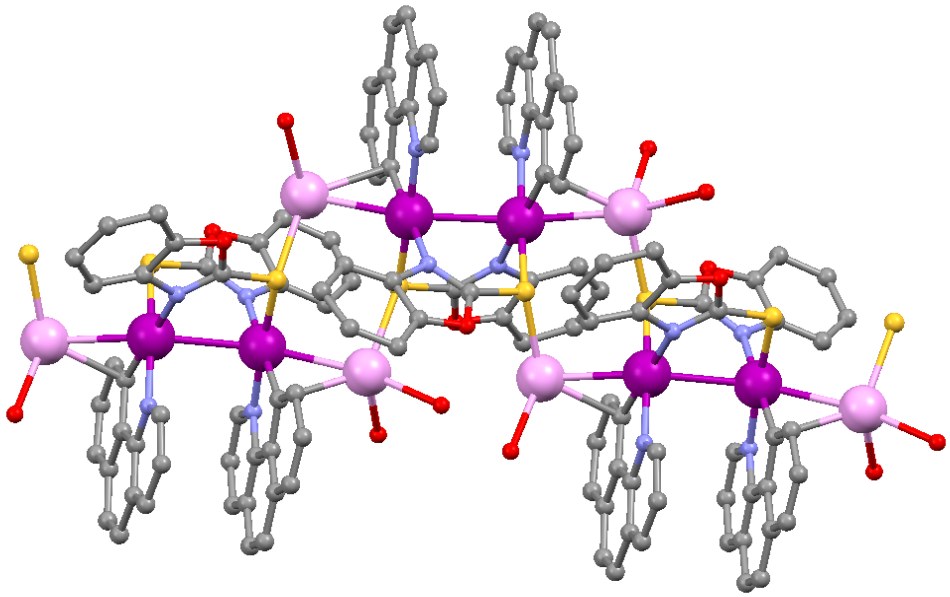


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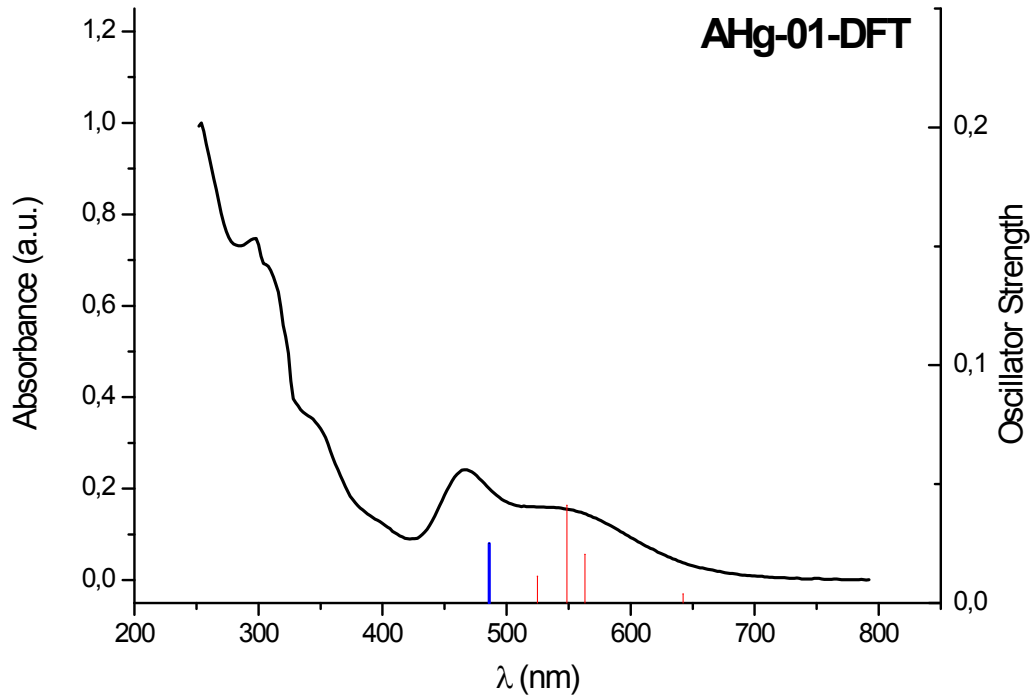
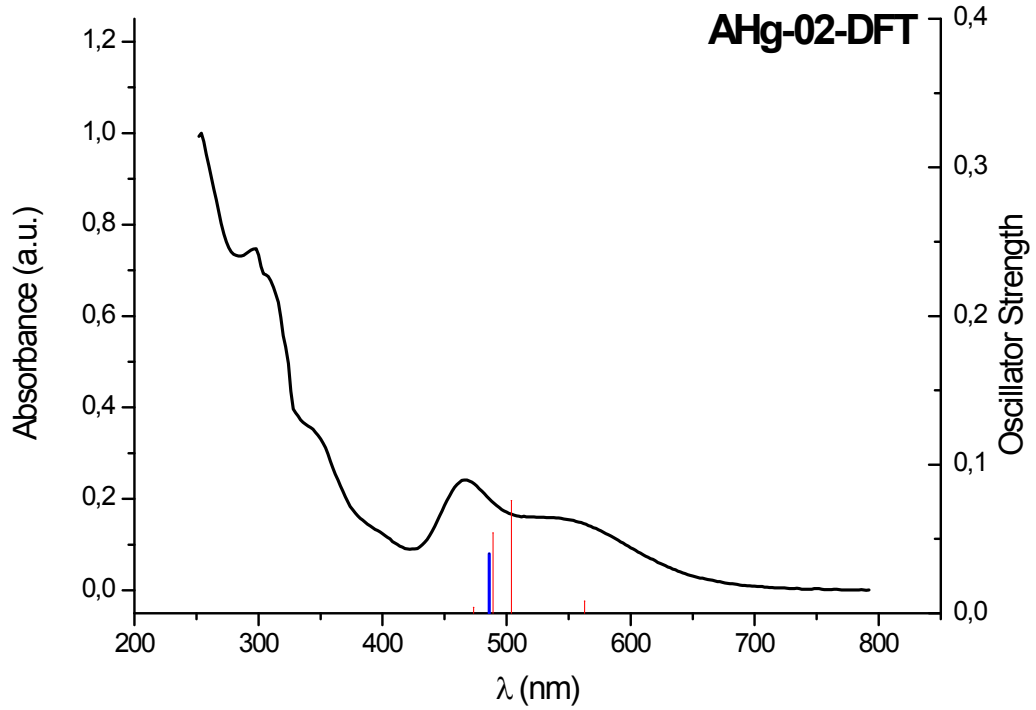
Figure S10. Molecular structure of the adduct **B**: $2Ag^{+}$ based on single crystal data from poorly diffracting crystals.


AHg-01-DFT
Absorbance (a.u.)
Oscillator Strength
λ (nm)
1,2
1,0
0,8
0,6
0,4
0,2
0,0
0,2
0,1
0,0
200
300
400
500
600
700
800


AHg-02-DFT
Absorbance (a.u.)
Oscillator Strength
λ (nm)
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1,0
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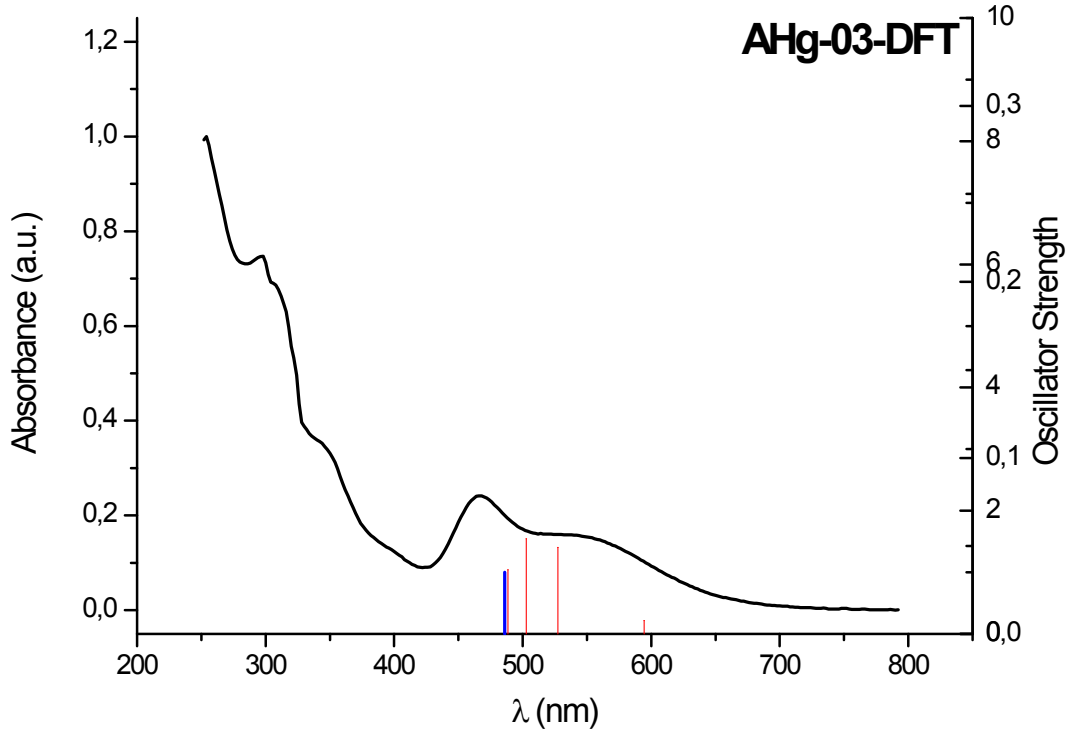
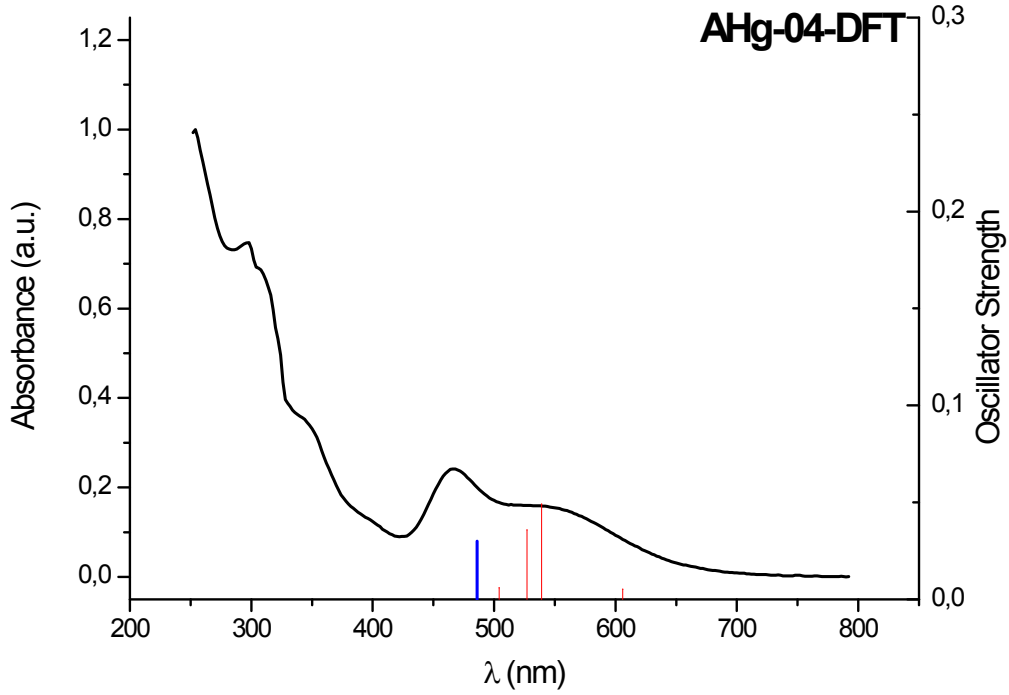
0,6
0,4
0,2
0,0
0,4
0,3
0,2
0,1
0,0
200
300
400
500
600
700
800


AHg-03-DFT
Absorbance (a.u.)
Oscillator Strength
λ (nm)
1,2
1,0
0,8
0,6
0,4
0,2
0,0
10
8
6
4
2
0,0
0,3
0,2
0,1
200
300
400
500
600
700
800


AHg-04-DFT
Absorbance (a.u.)
Oscillator Strength
λ (nm)
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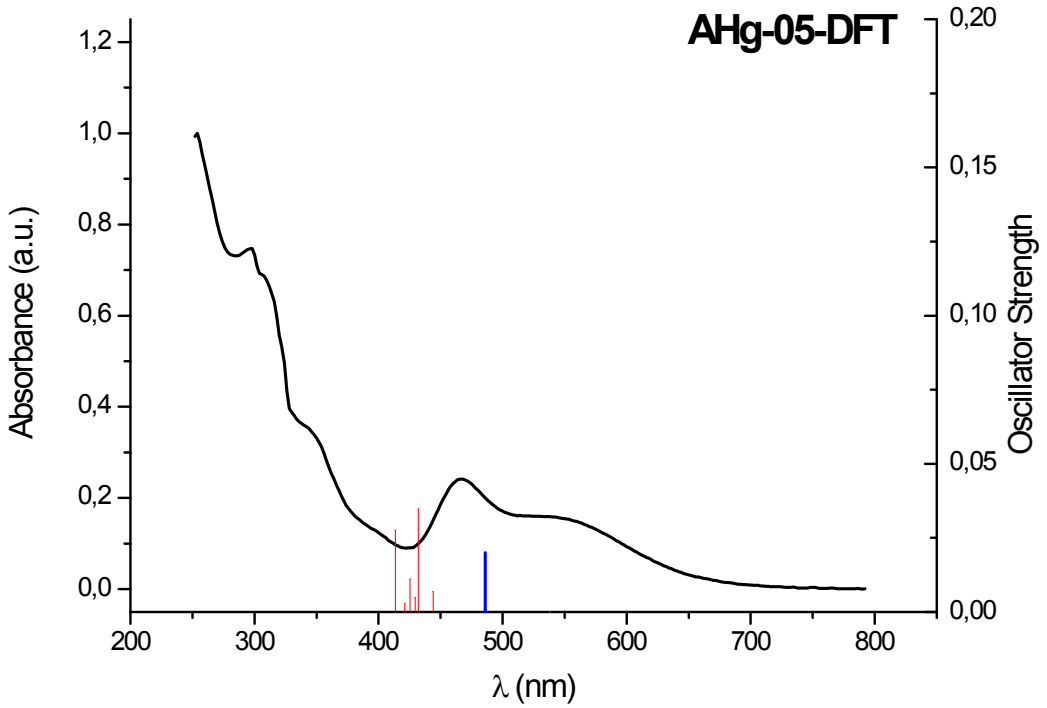
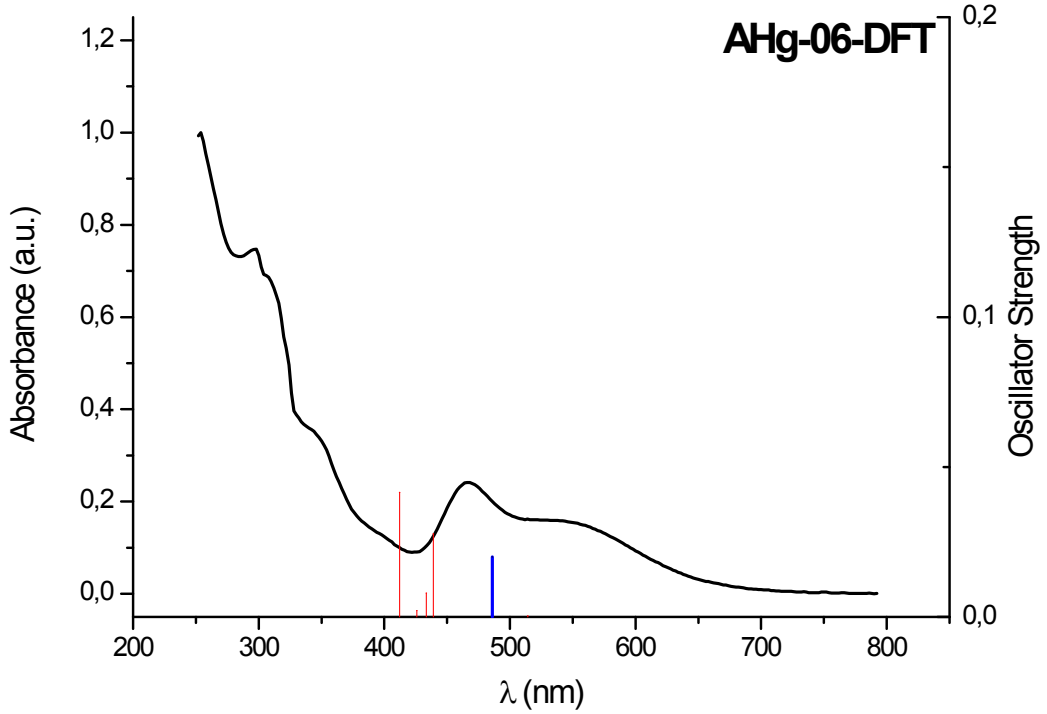
0,4
0,2
0,0
0,3
0,2
0,1
0,0
200
300
400
500
600
700
800


AHg-05-DFT
Absorbance (a.u.)
Oscillator Strength
λ (nm)
1,2
1,0
0,8
0,6
0,4
0,2
0,0
0,20
0,15
0,10
0,05
0,00
200
300
400
500
600
700
800


AHg-06-DFT
Absorbance (a.u.)
Oscillator Strength
λ (nm)
1,2
1,0
0,8
0,6
0,4
0,2
0,0
0,2
0,1
0,0
200
300
400
500
600
700
800

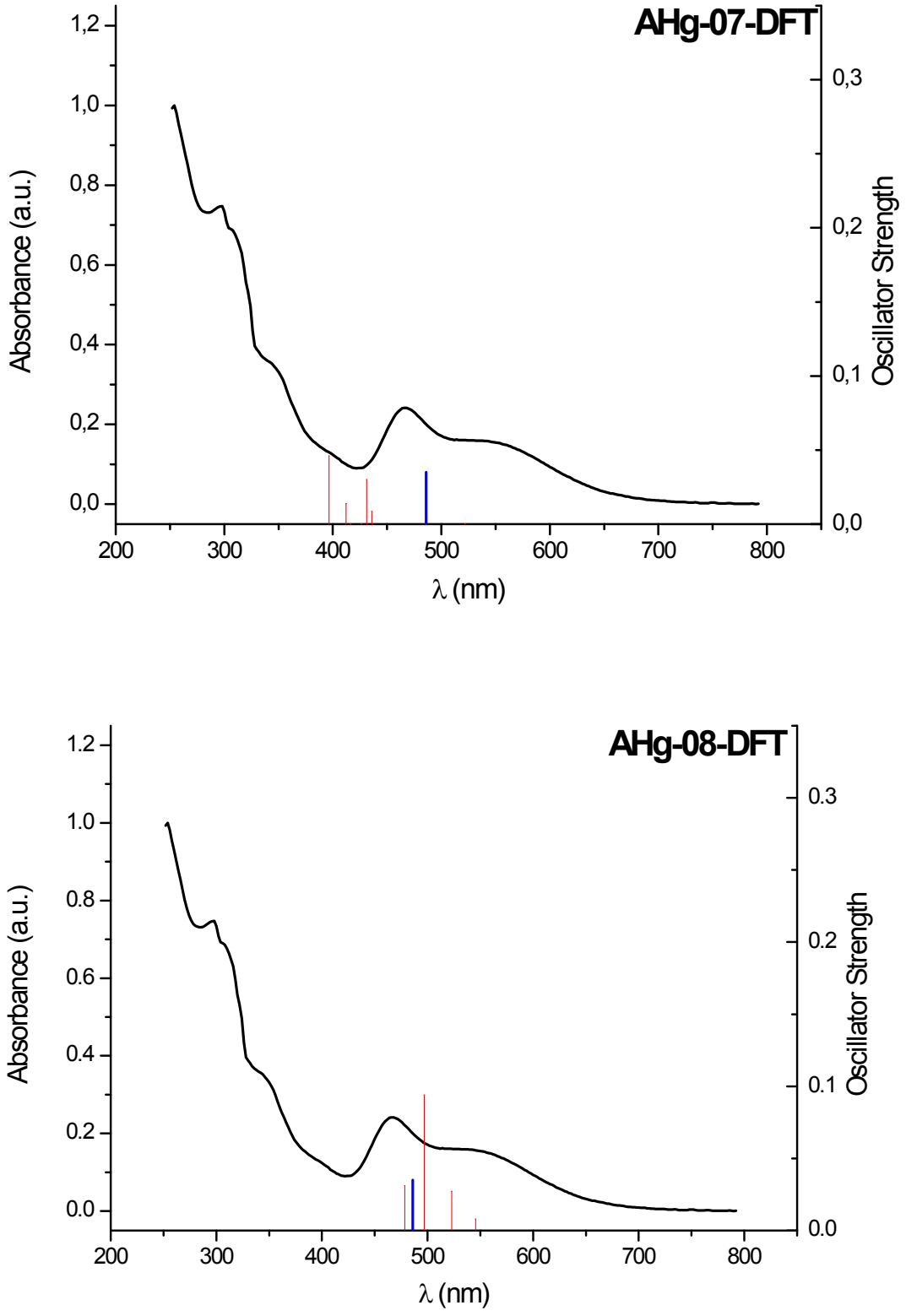


Figure S11. Comparison of the experimental absorption spectrum of **A**: Hg^{2+} (1:5) in

DMSO/H_2O (black line) with the ^{1}MMLCT absorption of **A** (blue bar) and the low-energy calculated absorption frequencies (red bars) of the different proposed structures.