New Au(I)-Cu(I) heterometallic complexes: role of bridging pyridazine ligands in the presence of unsupported metallophilic interactions

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ELECTRONIC SUPPLEMENTARY INFORMATION

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I. Characterization of the complexes **1, 3-6**

1. IR spectra

Infrared spectra were recorded in the 4000-200cm^{-1} range on a Perkin-Elmer FT-IR Spectrum 1000 spectrophotometer using Nujol mulls between polyethylene sheets.

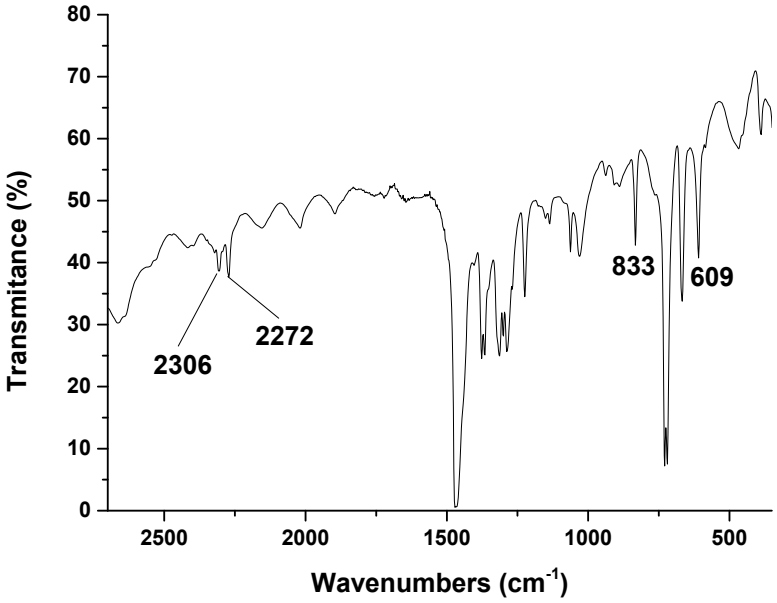

Figure 1. FT-IR spectrum of complex **1** in Nujol mulls

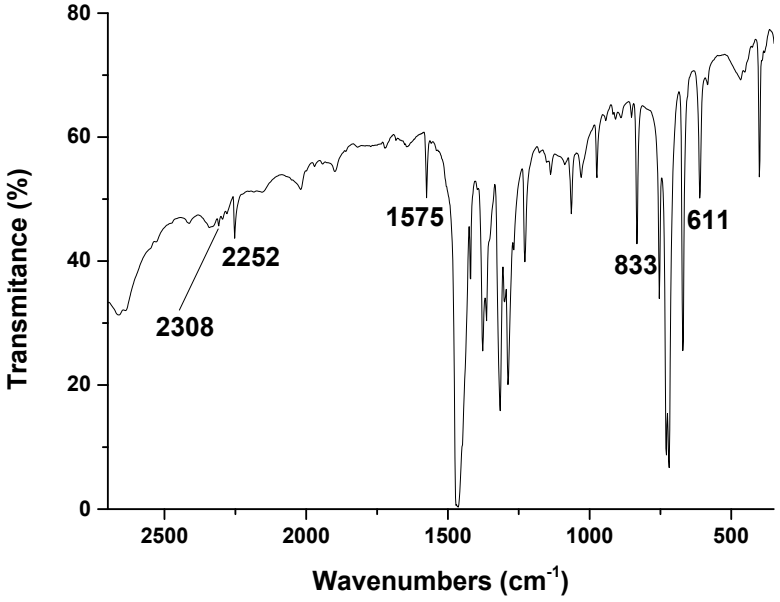

Figure 2. FT-IR spectrum of complex **3** in Nujol mulls

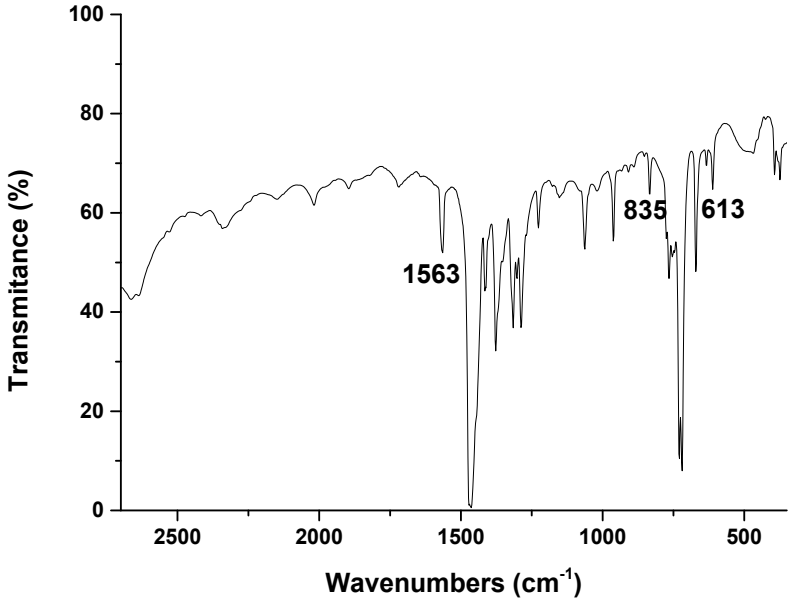

Figure 3. FT-IR spectrum of complex **4** in Nujol mulls

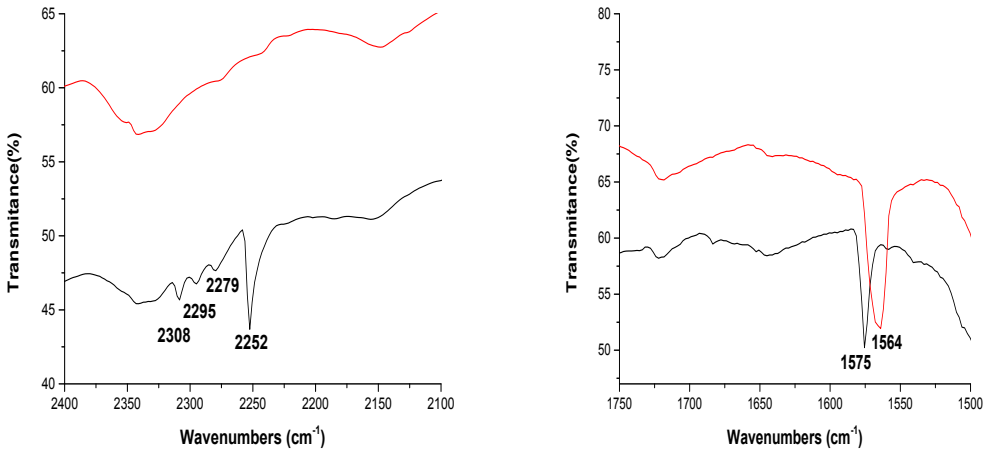

Figure 4. FT-IR spectra of complexes **3** (black) and **4** (red) in Nujol mulls corresponding to the range of ν(C ≡ N) of nitrile ligand (left) and ν(C=N) of pyridazine ligand (right).

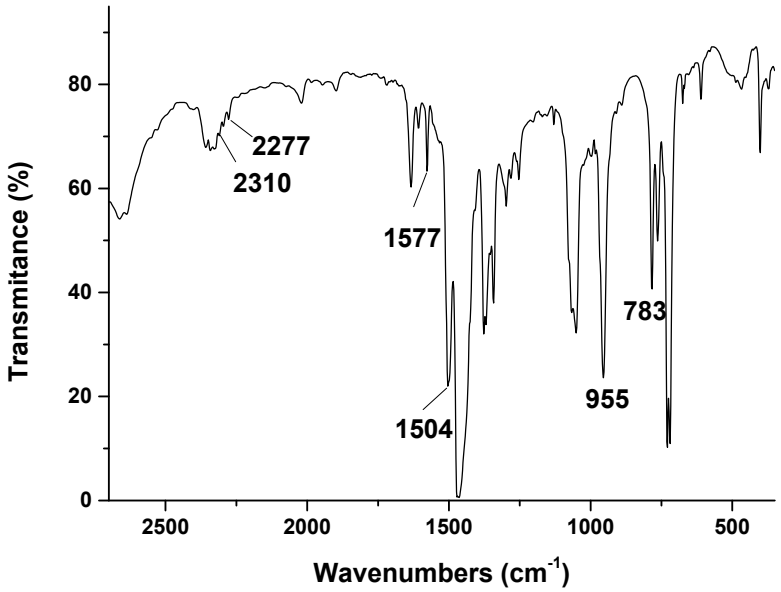

Figure 5. FT-IR spectrum of complex **5** in Nujol mulls

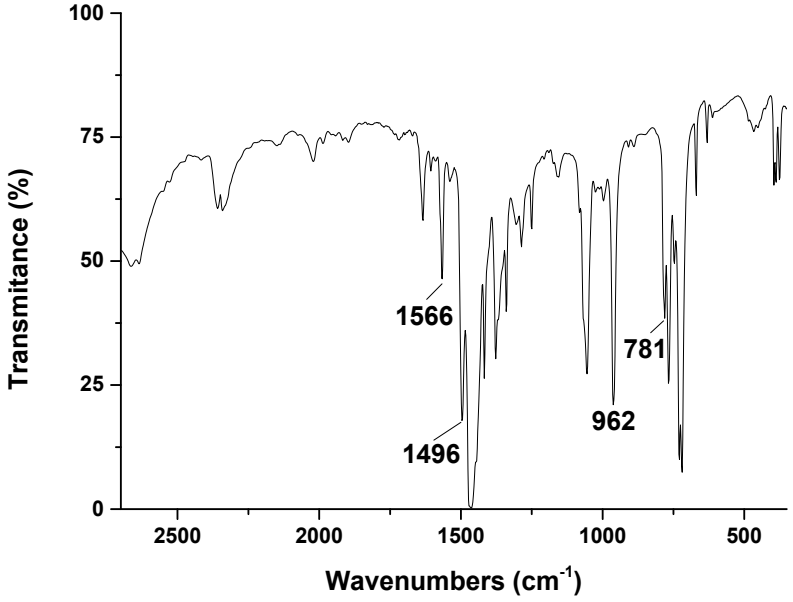

Figure 6. FT-IR spectrum of complex **6** in Nujol mulls

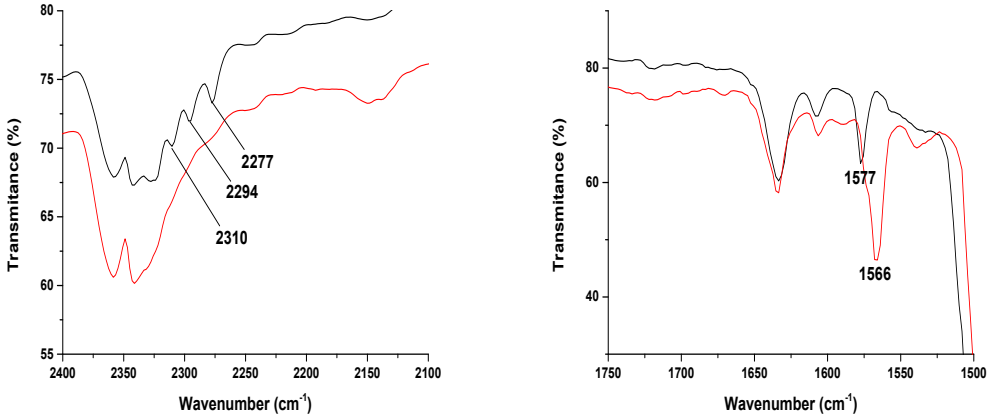

Figure 7. FT-IR spectra of complexes **5** (black) and **6** (red) in Nujol mulls corresponding to the range of ν(C ≡ N) of nitrile ligand (left) and ν(C=N) of pyridazine ligand (right).

2. Liquid ^{1}H and $^{19}F\{^{1}H\}$ NMR spectra (300 MHz, 25ºC)

^{1}H and ^{19}F spectra were recorded on a Bruker ARX 300 in CD_3CN. Chemical shifts are quoted relative to $SiMe_4$ (^{1}H external) and $CFCl_3$ (^{19}F external)

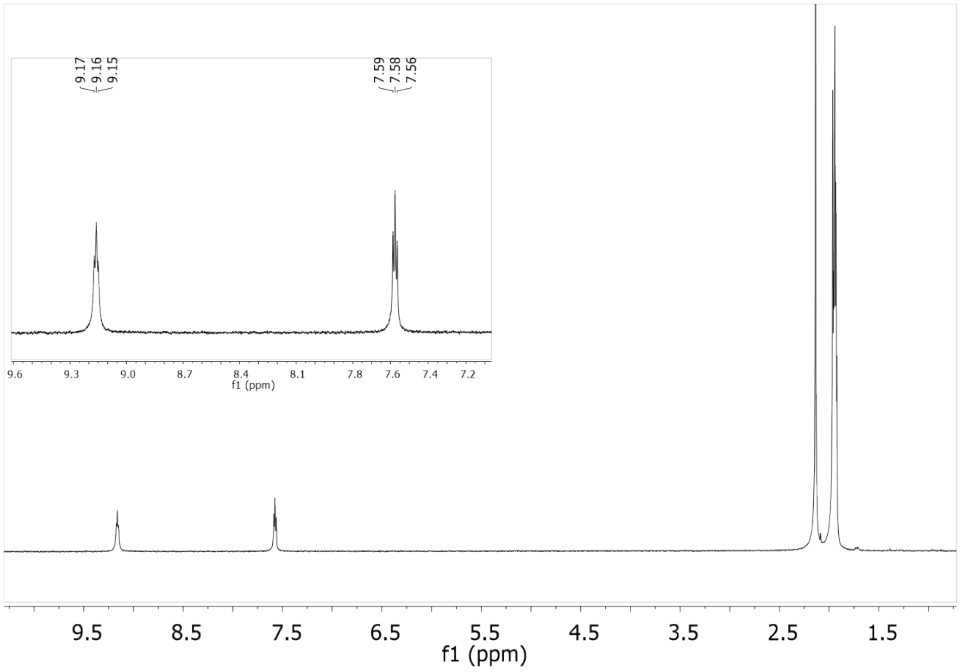

Figure 8. ^{1}H NMR spectrum of complex **3** in CD_3CN.

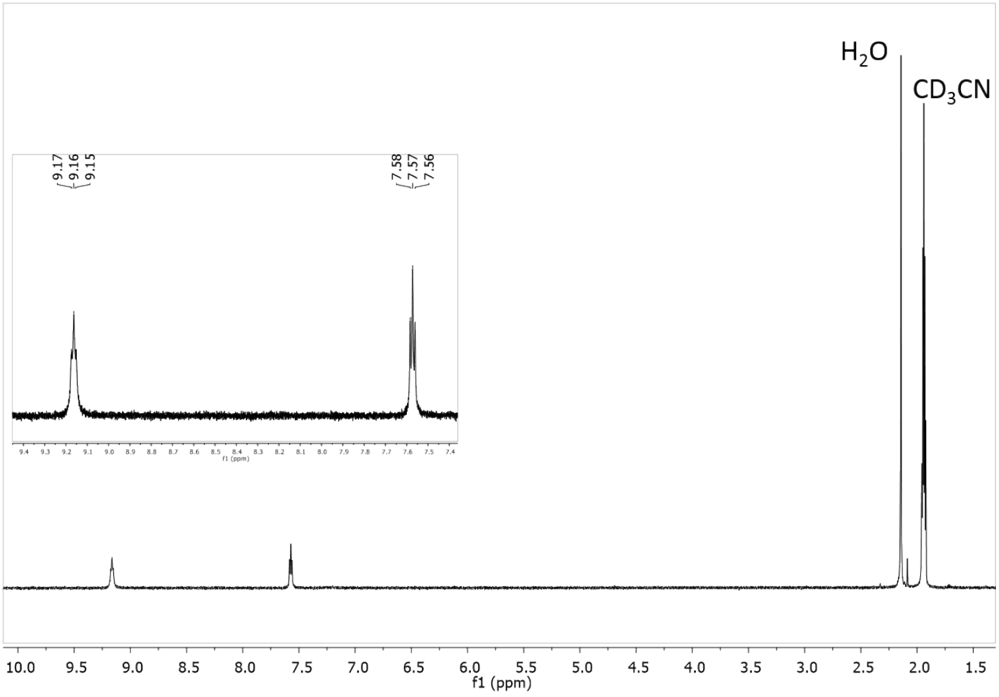

Figure 9. ^{1}H NMR spectrum of complex **4** in CD_3CN.

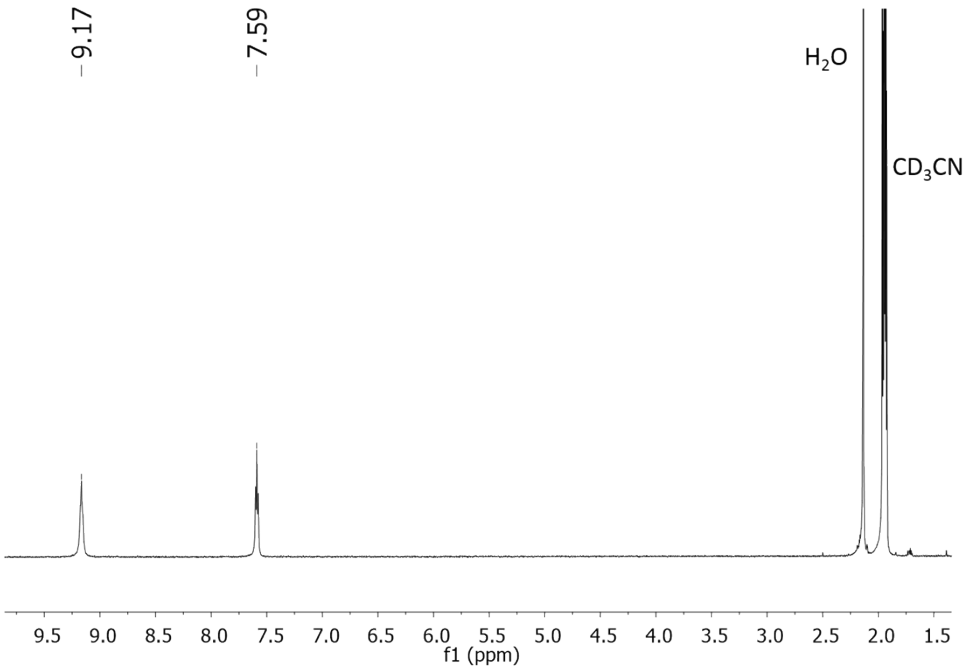

Figure 10. ^{1}H NMR spectrum of complex **5** in CD_3CN.

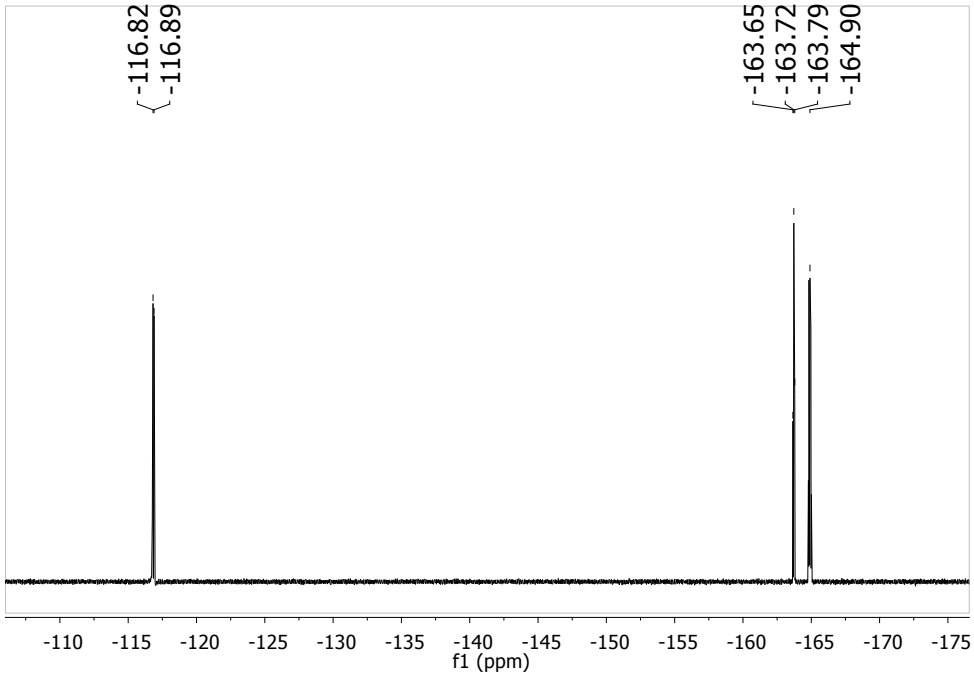

Figure 11. $^{19}F\{^{1}H\}$ NMR spectrum of complex **5** in CD_3CN.

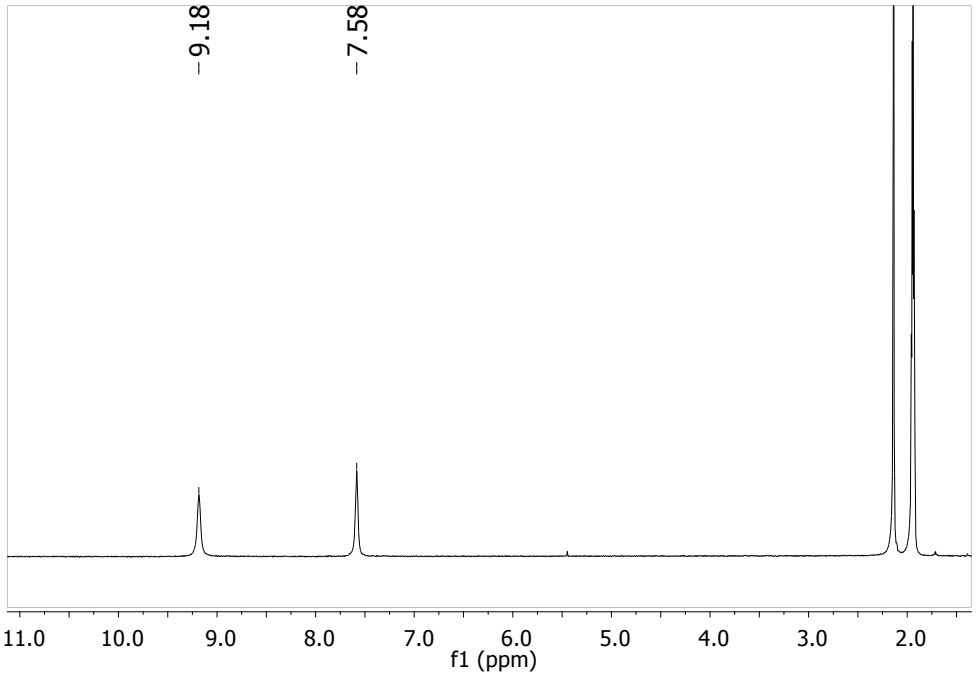

Figure 12. ^{1}H NMR spectrum of complex **6** in CD_3CN.

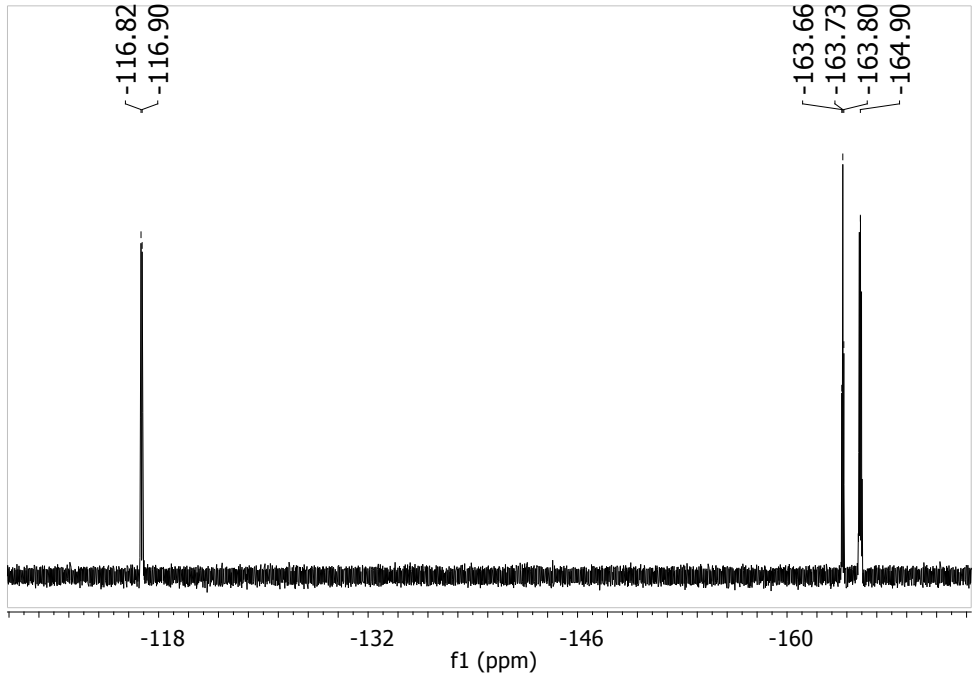

Figure 13. $^{19}F\{^{1}H\}$ NMR spectrum of complex **6** in CD_3CN.

II. Optical properties

1. UV-Vis absorption spectra:

Absorption spectra in solution were recorded on a Hewlett-Packard 8453 diode array UV-Vis spectrophotometer. Diffuse reflectance UV-Vis spectra of pressed powder samples diluted with KBr were recorded on a Shimadzu (UV-3600 spectrophotometer with a Harrick Praying Mantis accessory) and recalculated following the Kubelka-Munk function.

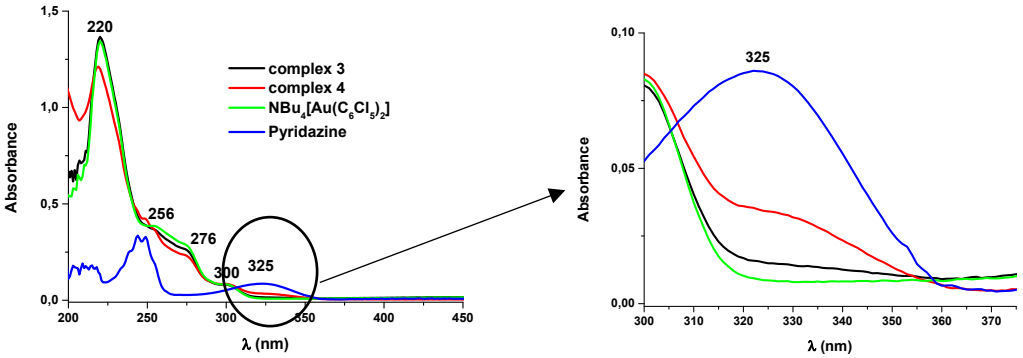

Figure 14. UV-Vis spectra for complexes **3** (9.08×10^{-6} M), **4** (8.70×10^{-6} M), $NBu_4[Au(C_6Cl_5)_2]$ (5.17×10^{-5} M) and pyridazine (2×10^{-4} M) in acetonitrile.

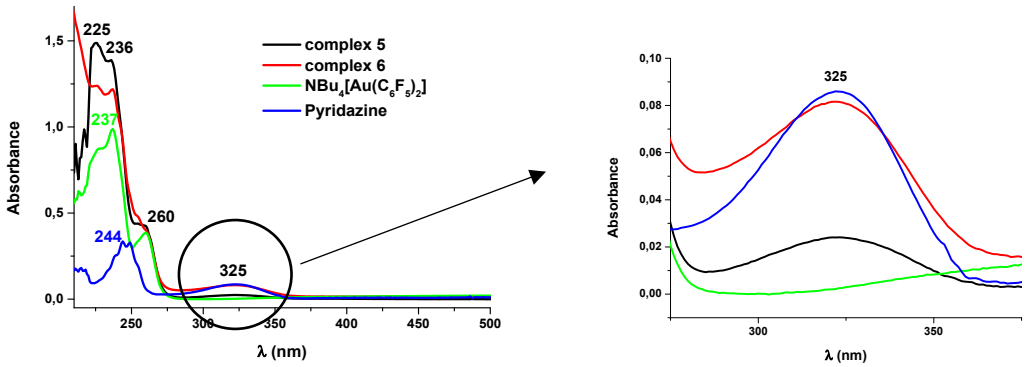

Figure 15. UV-Vis spectra for complexes **5** (2.64×10^{-5} M), **6** (2.65×10^{-5} M), $NBu_4[Au(C_6F_5)_2]$ (5.17×10^{-5} M) and pyridazine (2×10^{-4} M) in acetonitrile.

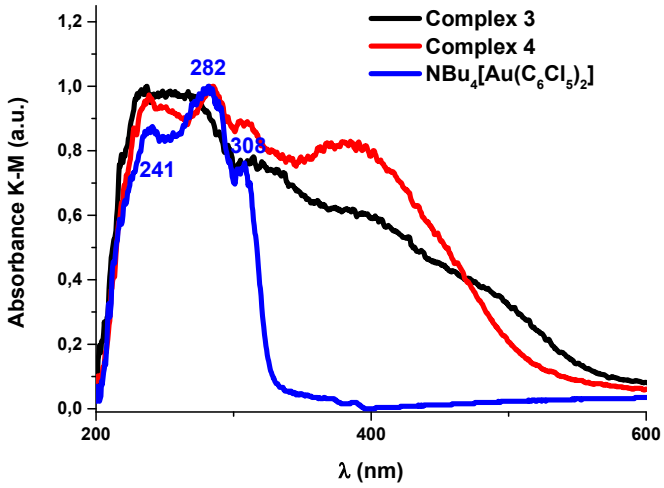

Figure 16. UV-Vis absorption spectra in solid state for complexes **3** (black), **4** (red) and $NBu_4[Au(C_6Cl_5)_2]$ diluted with KBr.

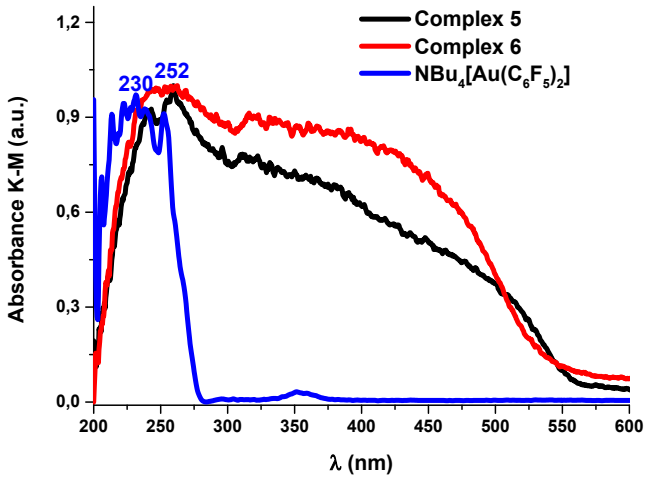

Figure 17. UV-Vis absorption spectra in solid state for complexes **5** (black), **6** (red) and $NBu_4[Au(C_6F_5)_2]$ (blue) diluted with KBr.

2. Life time measurement:

Complex 1:

Emission centred at **490nm**, excitation led of **370nm**:

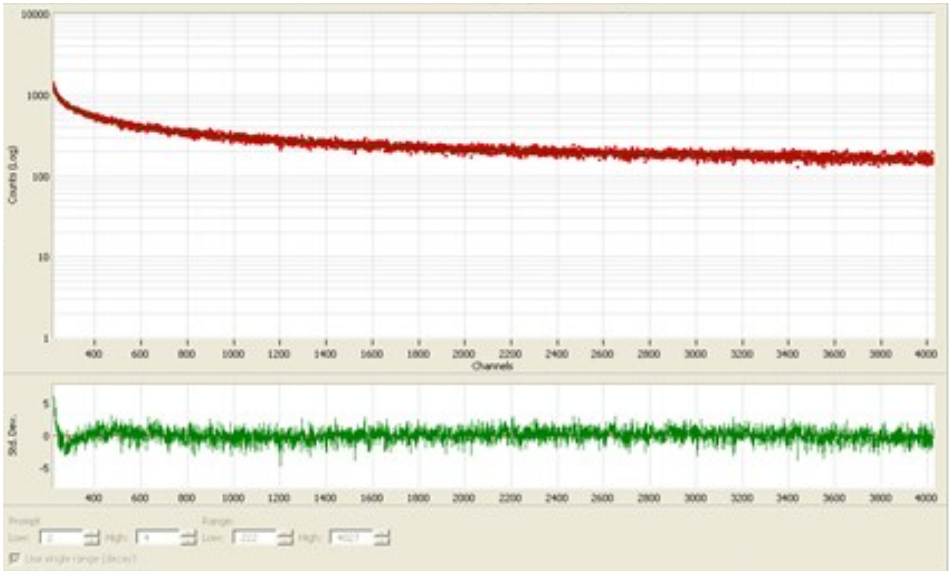

Figure 18. Lifetime decay.

Fitted parameters obtained:

SHIFT = 0 ch

T1 = 99.64665 ch

4.374064E-08 sec

S.Dev = 1.173863E-09 sec

T2 = 937.8336 ch

4.11669E-07 sec

S.Dev = 4.918362E-09 sec

A = 161.1211

S.Dev = 0.3305739

B1 = 553.5693

[15.14 Rel.Ampl]

S.Dev = 4.763408

B2 = 329.7734

[84.86 Rel.Ampl]

S.Dev = 1.438369

CHISQ = 1.14678