

Luminescence studies of new [C,N,N'] cyclometallated platinum(II) and platinum(IV) compounds

Ariadna Lázaro,^a Oriol Serra,^a Laura Rodríguez,^{a,b} Margarita Crespo,^{a,c} and Mercè Font-Bardia^d

^a *Departament de Química Inorgànica i Orgànica, Secció de Química Inorgànica, Facultat de Química, Universitat de Barcelona, Martí i Franquès, 1-11, 08028-Barcelona (Spain)*

^b *Institut de Nanociència i Nanotecnologia (IN2UB). Universitat de Barcelona, 08028-Barcelona (Spain)*

^c *Institut de Biomedicina de la Universitat de Barcelona (IBUB). 08028-Barcelona (Spain)*

^d *Unitat de Difracció de RX, Centres Científics i Tecnològics de la Universitat de Barcelona (CCiTUB), Universitat de Barcelona, Solé i Sabarís 1-3, 08028-Barcelona (Spain)*

Supporting Information

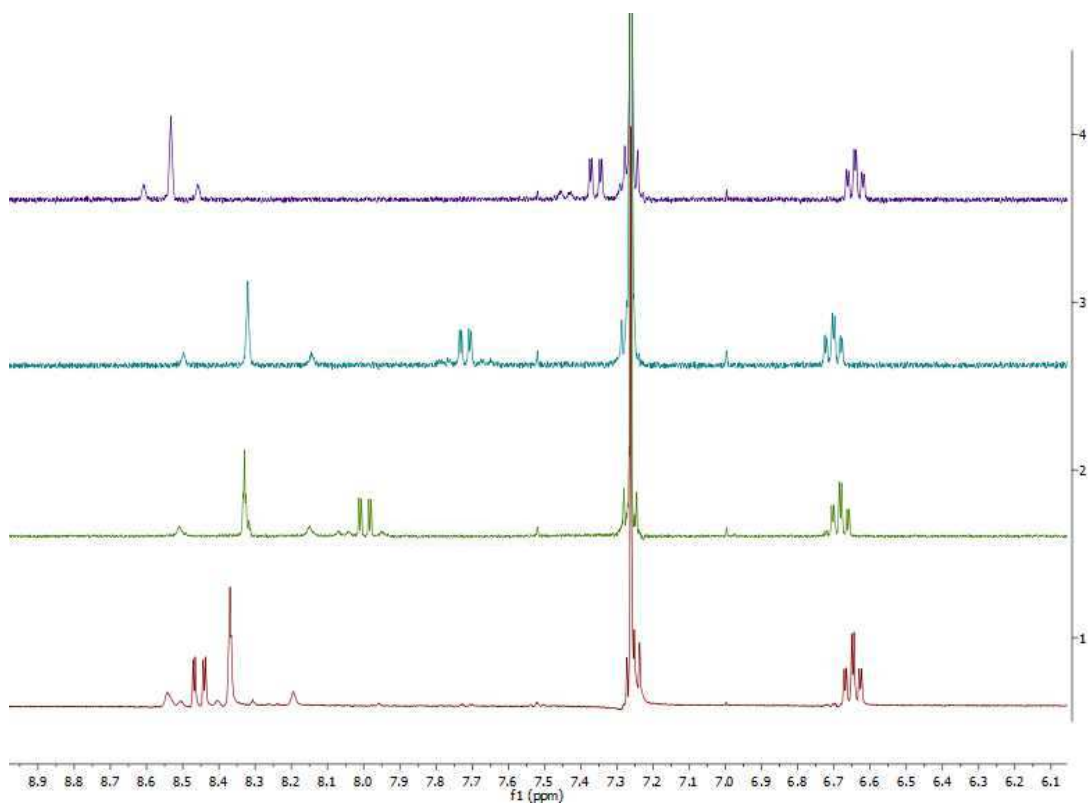


Figure S1. Aromatic region of the ^1H -NMR spectra in CDCl_3 of the cyclometallated platinum(II) compounds: **1** (purple), **2a** (blue), **2b** (green), **2c** (red).

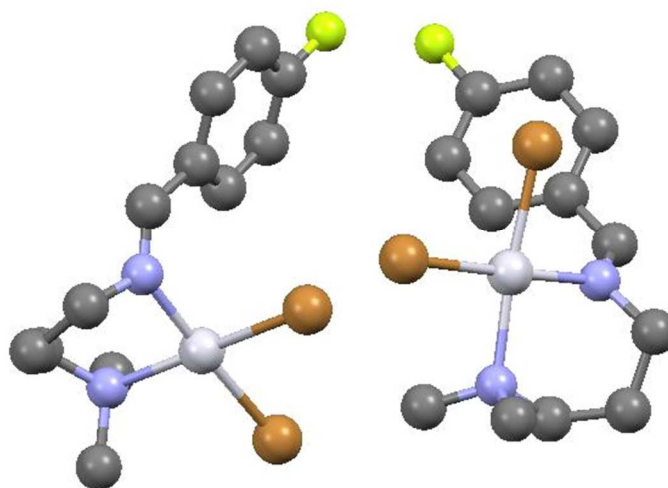


Figure S2. Unit cell of compound **1b** showing the presence of two independent molecules without any $\text{Pt}\cdots\text{Pt}$ contact (distance: 7.165 Å). Grey: platinum; blue: nitrogen; green: fluorine; brown: bromide; Hydrogens have been omitted for clarity.

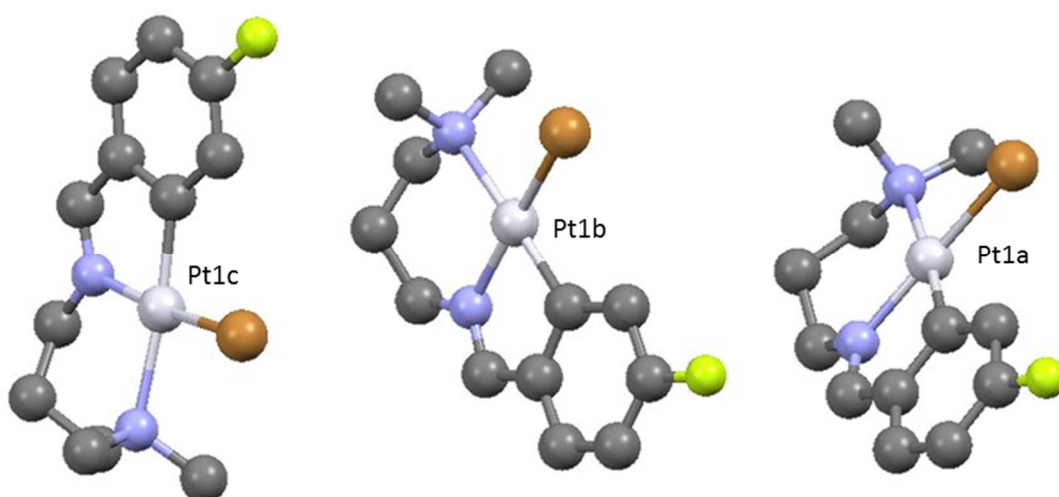


Figure S3. Unit cell of compound **2b** showing the presence of three independent molecules without any Pt...Pt contact (Pt1a-Pt1b distance: 8.329 and Pt1b-Pt1c distance: 7.892 Å). Grey: platinum; blue: nitrogen; green: fluorine; brown: bromide; Hydrogens have been omitted for clarity.

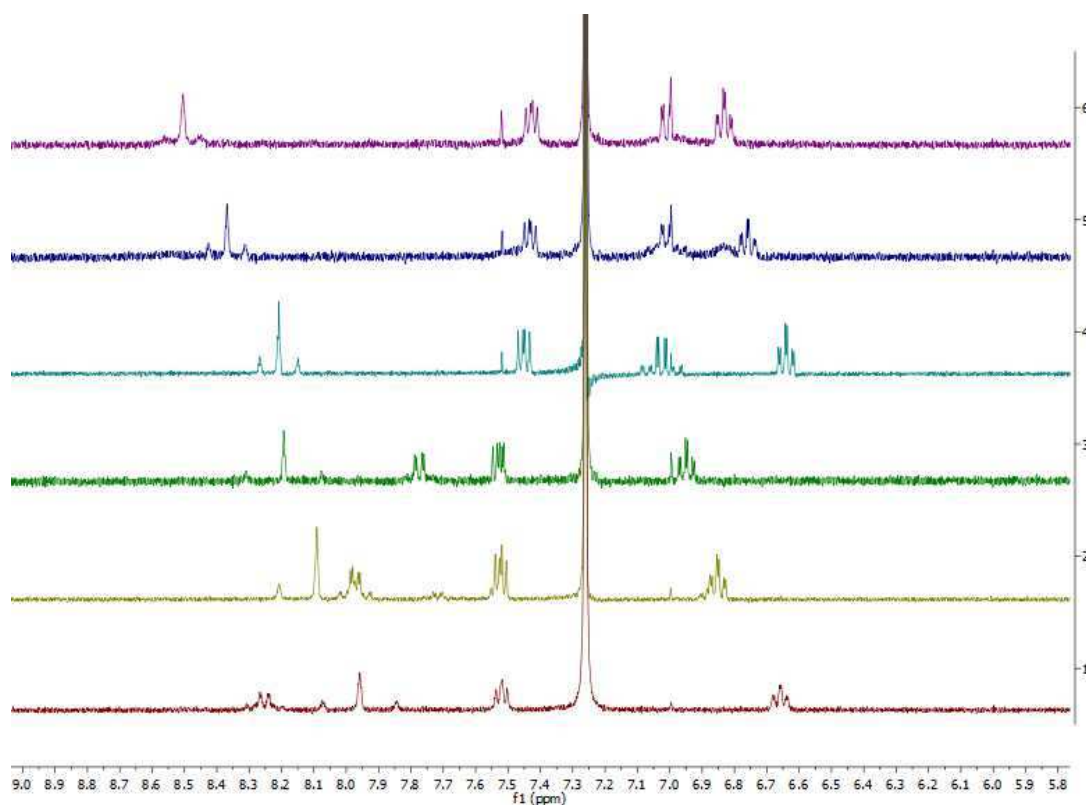
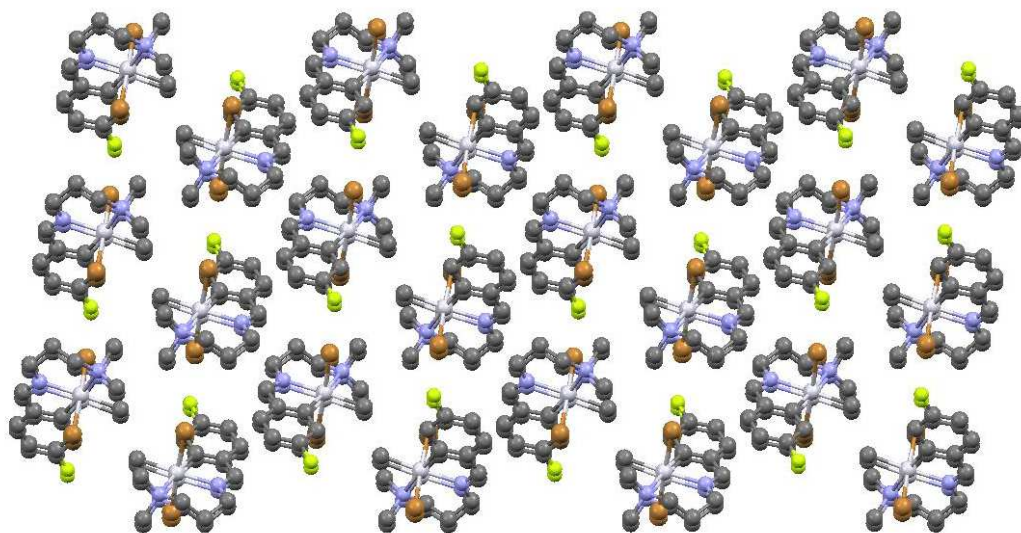
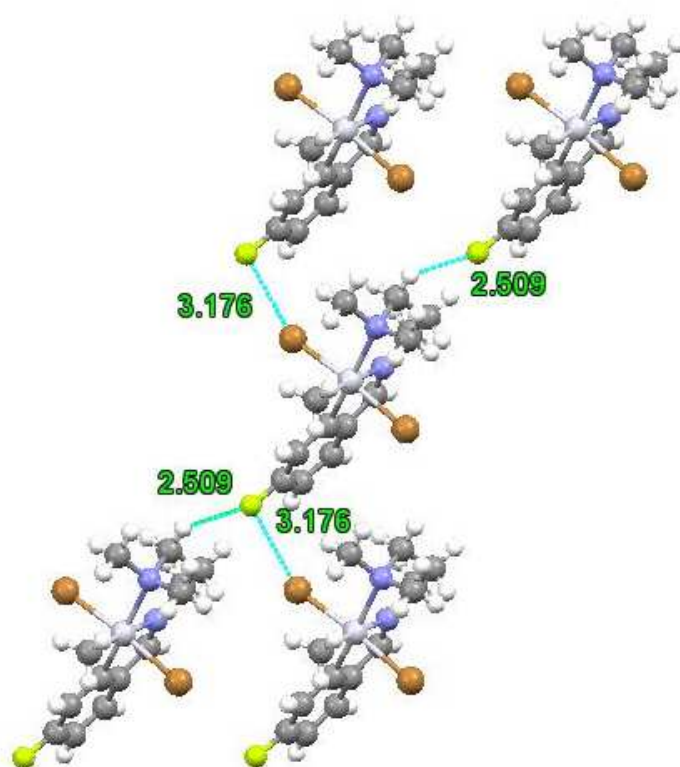


Figure S4. Aromatic region of the ^1H -NMR spectra in CDCl_3 of the cyclometallated platinum(IV) compounds: **3a** (purple), **3b** (dark blue), **3c** (light blue), **4a** (dark green), **4b** (light green), **4c** (red).

A)



B)



C)

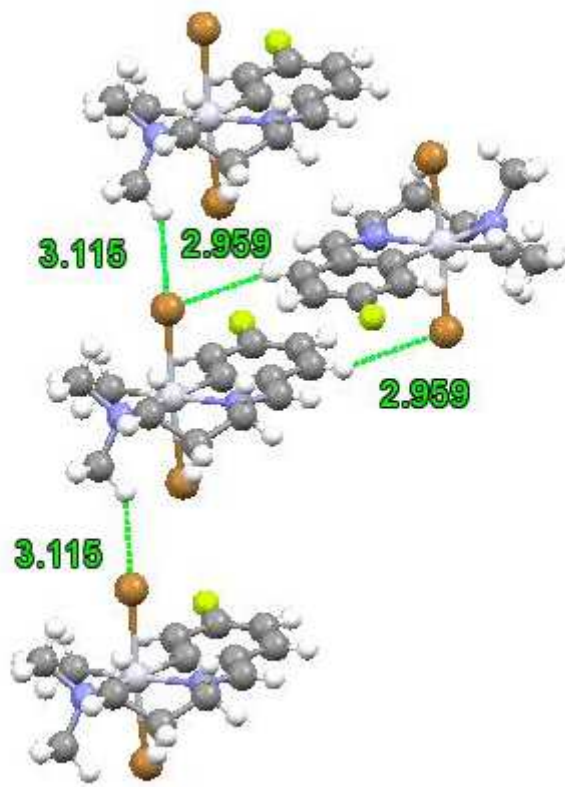
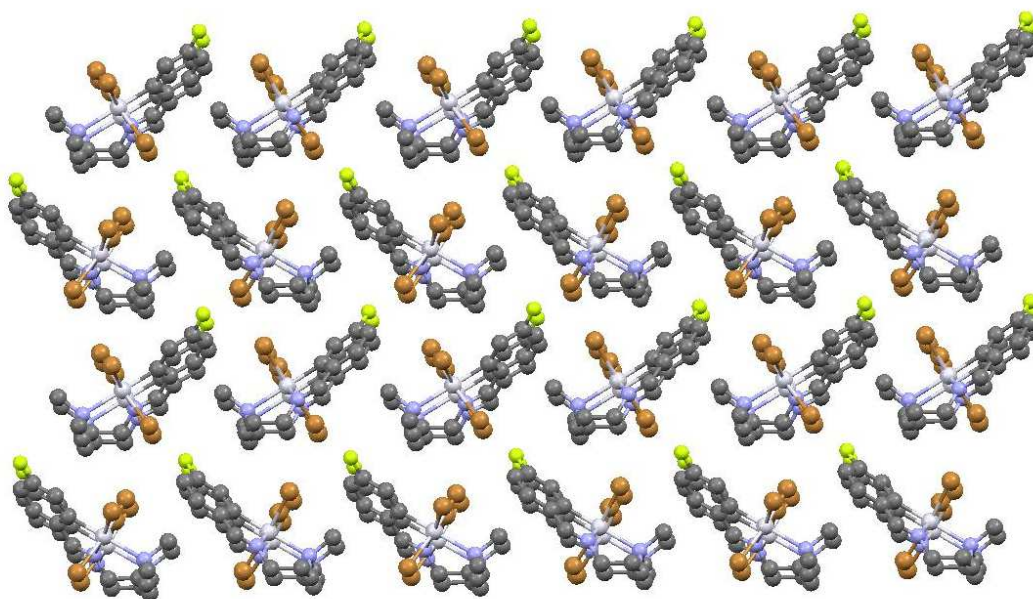
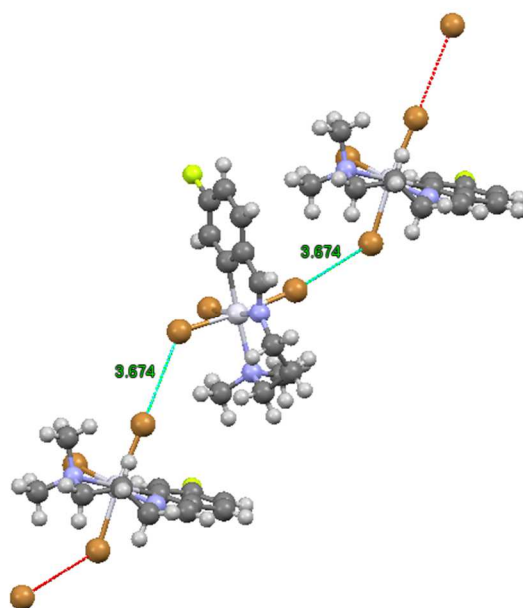


Figure S5. A) 3D packing of compound **3b**. Grey: platinum; blue: nitrogen; green: fluorine; brown: bromide; Hydrogens have been omitted for clarity. **B)** Figure highlighting the intramolecular C-F $\cdots$ Br-Pt and C-F $\cdots$ H₃CN interactions. **C)** Figure highlighting the intramolecular Br $\cdots$ H(aromatic) and Br $\cdots$ H(methyl) interactions.

A)



B)



C)

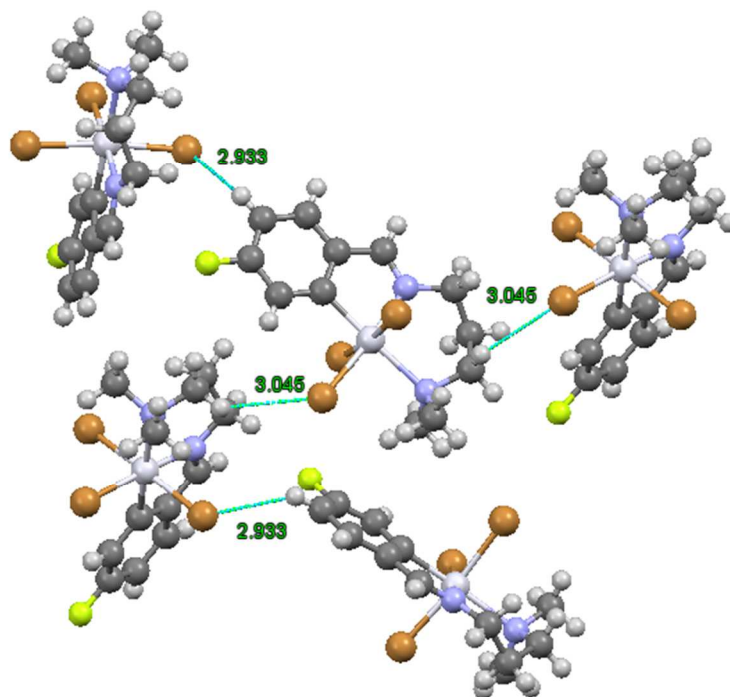


Figure S6. A) 3D packing of compound **4b**. Grey: platinum; blue: nitrogen; green: fluorine; brown: bromide; Hydrogens have been omitted for clarity. **B)** Figure highlighting the intramolecular Br $\cdots$ Br interactions. **C)** Figure highlighting the intramolecular Br $\cdots$ H(aromatic) and Br $\cdots$ H(methylene) interactions.

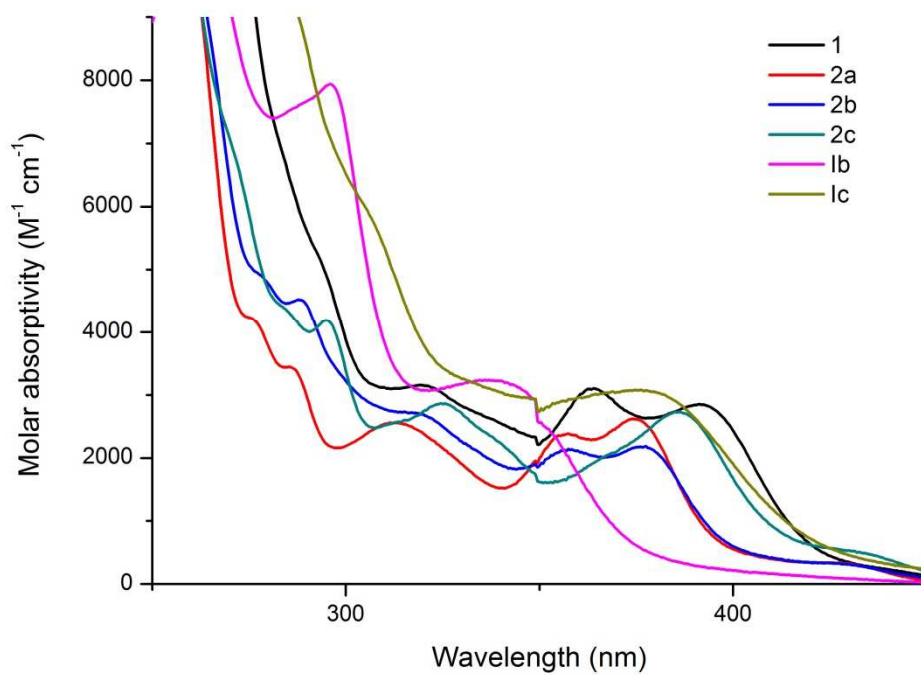


Figure S7. Absorption spectra of 10^{-4} M dichloromethane solution of Pt(II) compounds at 298 K.

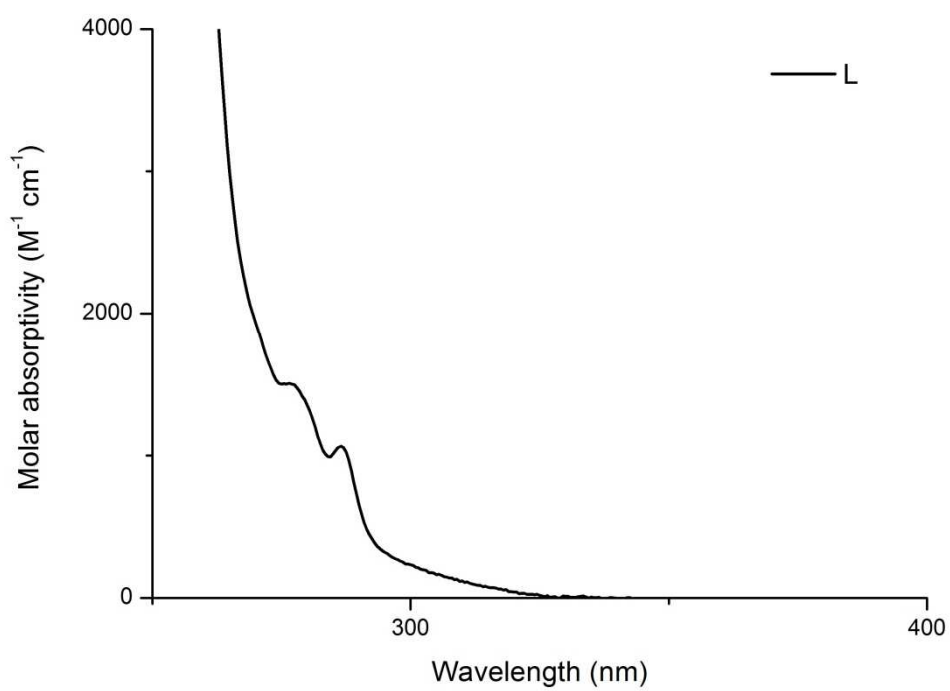


Figure S8. Absorption spectra of 10^{-4} M dichloromethane solution of the ligand **L** at 298 K.

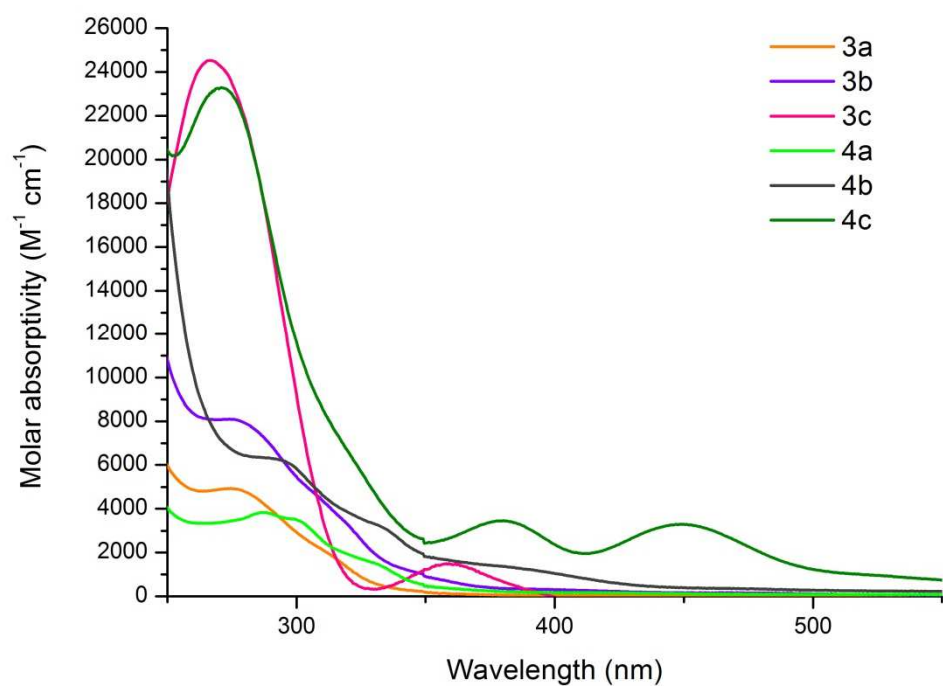


Figure S9. Absorption spectra of 10^{-4} M dichloromethane solution of platinum(IV) compounds at 298 K.

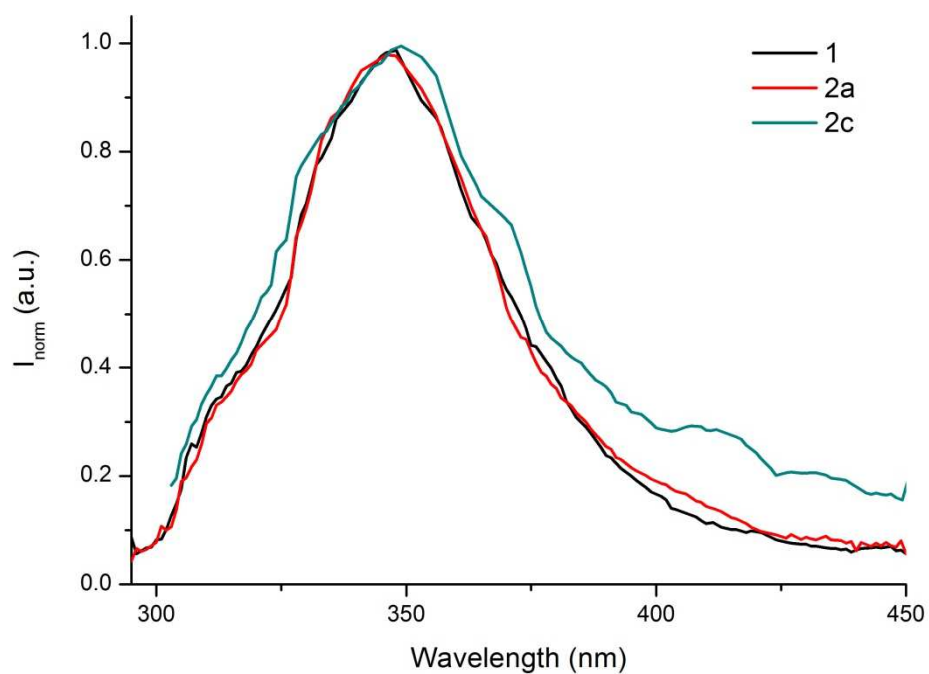


Figure S10. Emission spectra of platinum(II) compounds in dichloromethane solution at 298 K. λ_{exc} (nm) = 285 (**1**), 285 (**2a**), 295 (**2c**).

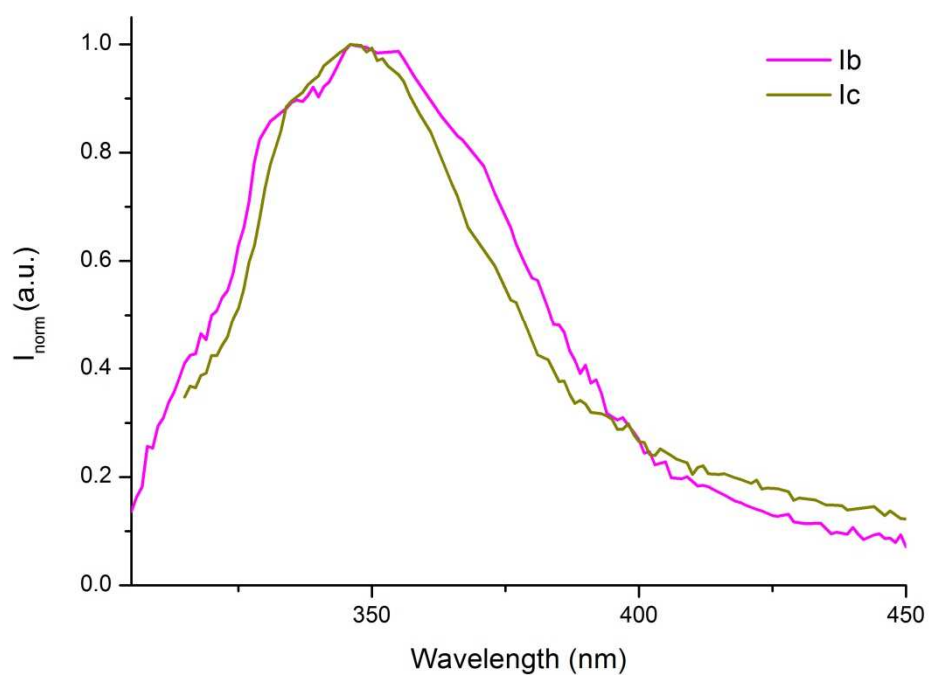


Figure S11. Emission spectra of platinum(II) coordination compounds in dichloromethane solution at 298 K. λ_{exc} (nm) = 295 (**Ib**), 305 (**Ic**).

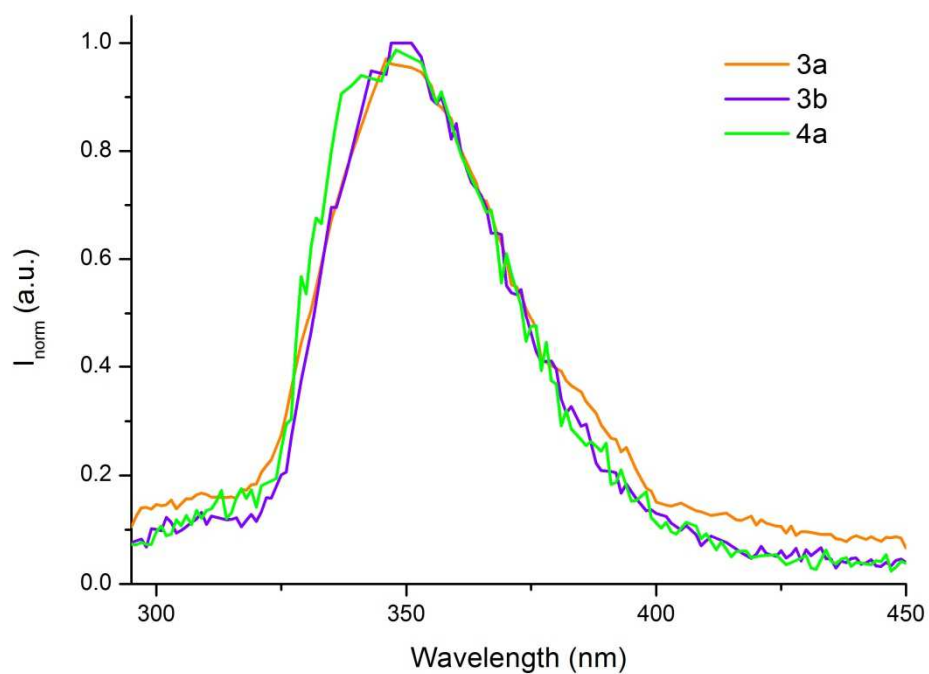


Figure S12. Emission spectra of platinum(IV) compounds in dichloromethane solution at 298 K. λ_{exc} (nm) = 275 (**3a**), 275 (**3b**), 295 (**4b**).

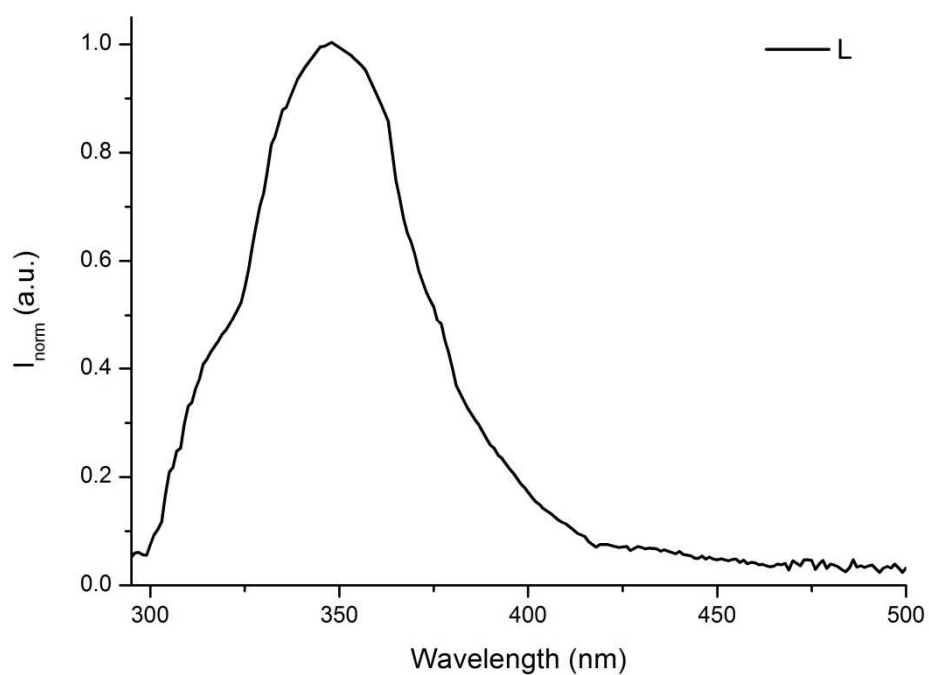


Figure S13. Emission spectra of the ligand **L** in dichloromethane solution at 298 K. λ_{exc} (nm) = 285.

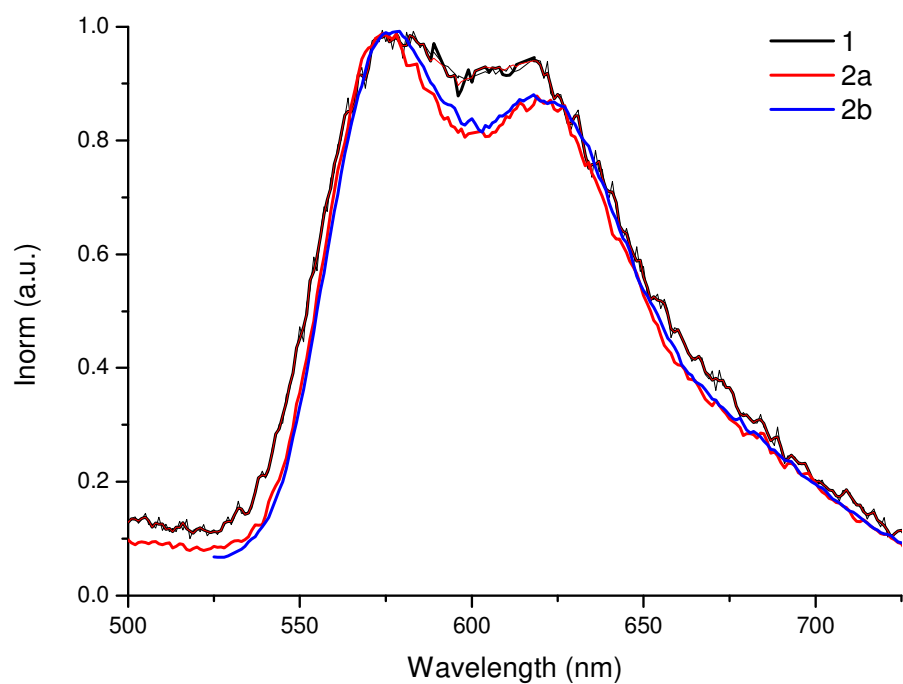


Figure S14. Emission spectra of platinum(II) compounds in dichloromethane solution at 298 K: λ_{exc} (nm) = 375 (**1**), 390 (**2a**).

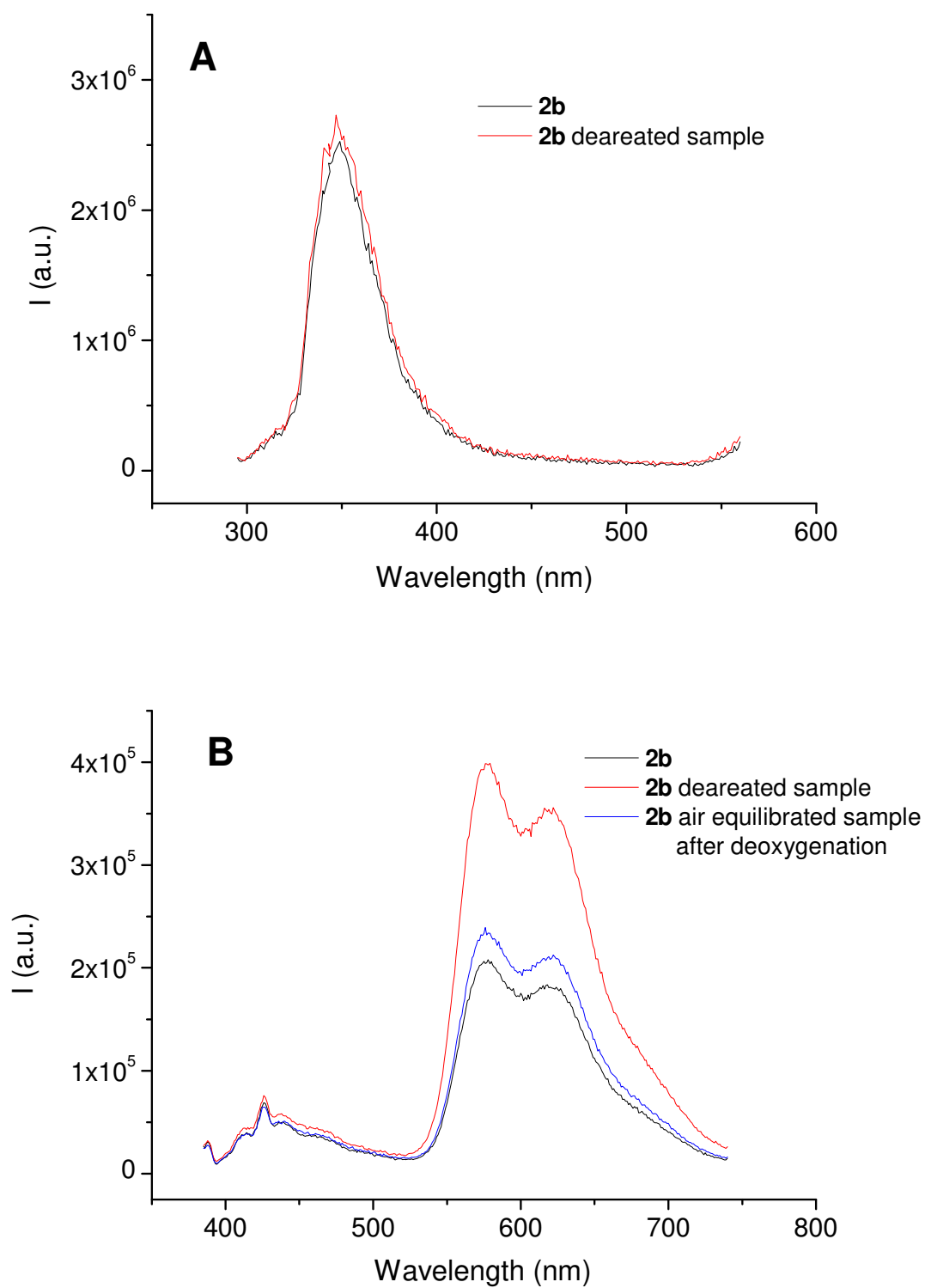


Figure S15. Emission spectra of **2b** in the presence and in the absence of oxygen and upon excitation the sample at 285 nm (A) and 375 nm (B).