

Extended Structures Containing Pt(II)-Tl(I) Bonds. Effect of these interactions on the Luminescence of Cyclometalated Pt(II) Compounds.

Juan Forniés,*^[a] Sara Fuertes,^[a] Antonio Martín^[a] and Violeta Sicilia*^[b]

^[a] Departamento de Química Inorgánica, Instituto de Ciencia de Materiales de Aragón, Facultad de Ciencias, Universidad de Zaragoza-CSIC, Plaza. S. Francisco s/n 50009 Zaragoza (Spain). Fax: (+34)976-761159

E-mail: juan.fornies@unizar.es

^[b] Departamento de Química Inorgánica, Instituto de Ciencia de Materiales de Aragón, Escuela Universitaria de Ingeniería Técnica Industrial, Universidad de Zaragoza-CSIC, Campus Universitario del Actur, Edificio Torres Quevedo, 50018, Zaragoza (Spain).

Fax: (+34)976-762189

E-mail: sicilia@unizar.es

Belén Gil,^[c] and Elena Lalinde*^[c]

^[c] Departamento de Química - Grupo de Síntesis Química de La Rioja, UA-CSIC, Universidad de La Rioja, 26006, Logroño, Spain. Fax: (+34)941-299621

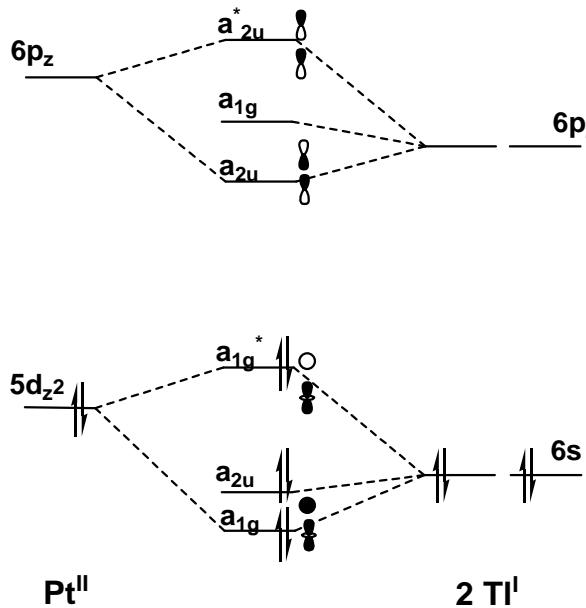


Chart 1: qualitative molecular orbital diagram for the Tl-Pt-Tl unit, proposed by Balch et al. for compound $\text{Tl}_2\text{Pt}(\text{CN})_4$. Ref: Nagle, J. K.; Balch, A. L.; Olmstead, M. M. *J. Am. Chem. Soc.* **1988**, *110*, 319.

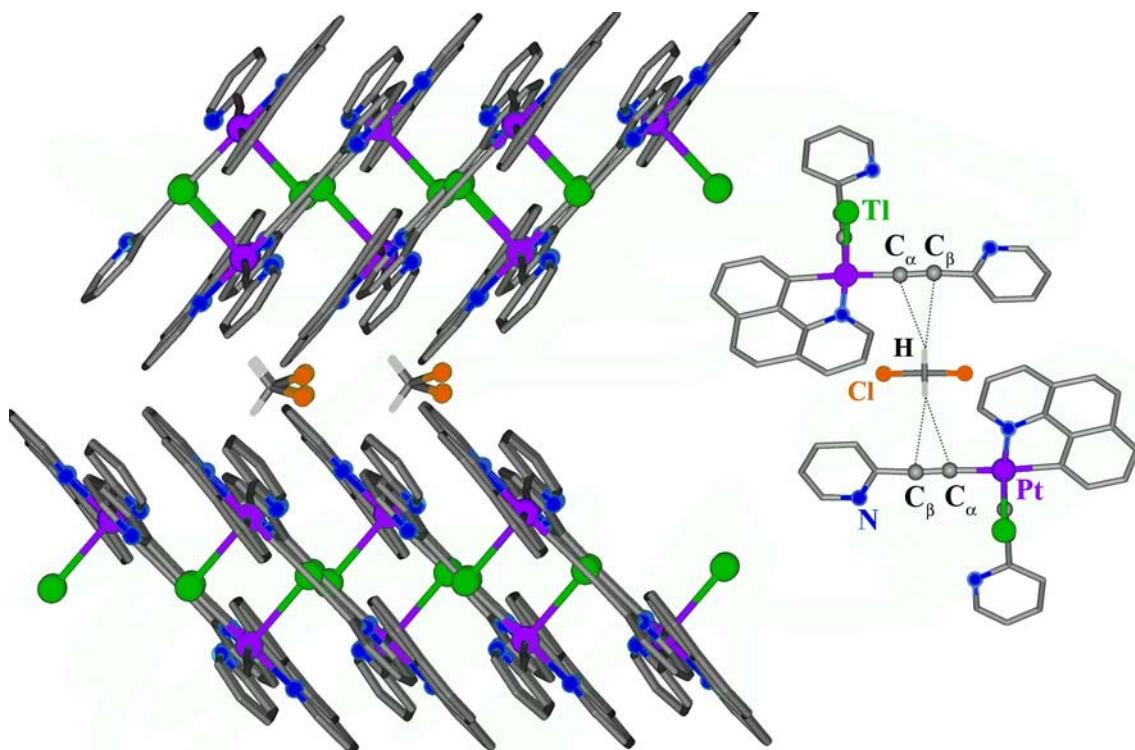


Figure S1: Supramolecular structure of the solvate **2** CH_2Cl_2 showing how each CH_2Cl_2 molecule is connecting two $[\text{PtTl}(\text{bzq})(\text{C}\equiv\text{C}-\text{C}_5\text{H}_4\text{N}-2)_2]$ motifs of different layers through weak $\text{C}-\text{H}\cdots\text{C}\equiv\text{C}$ interactions ($\text{CH}\cdots\text{C}\alpha$ 2.8747; $\text{CH}\cdots\text{C}\beta$ 2.8234 Å).

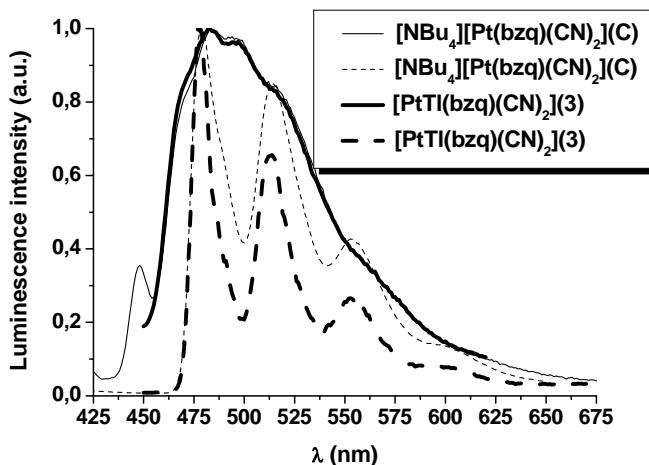


Figure S2. Normalized emission spectra in methanol (10^{-4} M) at 298K (—) and 77K (--) of **C** and **3**.

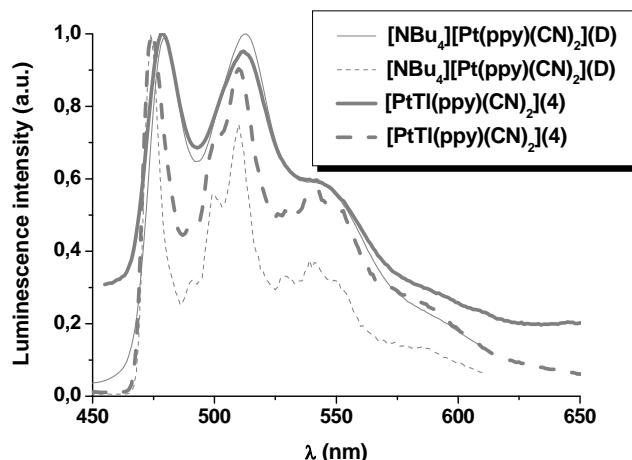


Figure S3. Normalized emission spectra in methanol (10^{-4} M) at 298K (—) and 77K (--) of **D** and **4**.

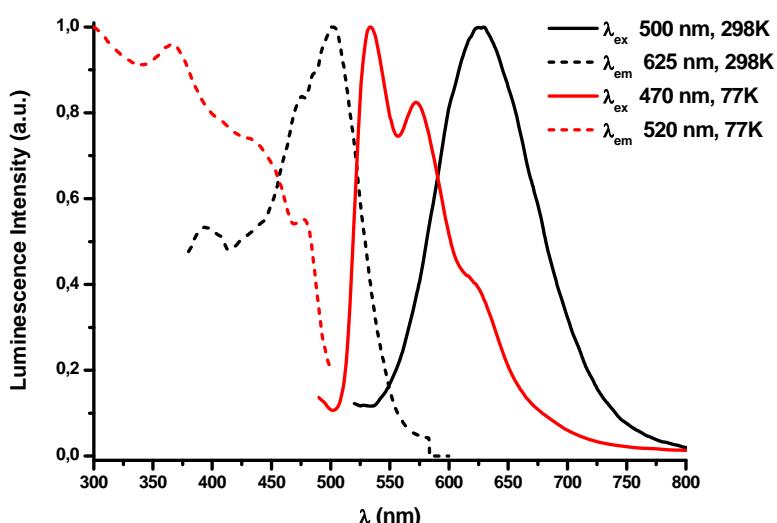


Figure S4. Normalized excitation and emission spectra in solid state of compound **1**.