Electronic Supplementary Material (ESI) for Dalton Transactions.

Development of gold(I) phosphorescent tweezer for sensing applications

Araceli de Aquino,[a,b] Francisco J. Caparrós,[a,b] Gabriel Aullón,[a,c] Khai-Nghi Truong,[d] Kari Rissanen,[d] João Carlos Lima,[e,*] Laura Rodríguez[a,b,*]

[a] *Departament de Química Inorgànica i Orgànica. Secció de Química Inorgànica. Universitat de Barcelona, Martí i Franquès 1-11, 08028 Barcelona, Spain. e-mail: laura.rodriguez@qi.ub.es*

[b] *Institut de Nanociència i Nanotecnologia (IN^{2}UB). Universitat de Barcelona, 08028 Barcelona (Spain)*

[c] *Department of Chemistry, University of Jyväskyla, 40014 Jyväskylä (Finland)*

[d] *Samsung Advanced Institute of Technology, Samsung Electronics Co. Ltd., 130 Samsung-ro, Yeongtong-gu, Suwon-si, Gyeonggi-do, 16678, Republic of Korea*

[e] *LAQV-REQUIMTE, Departamento de Química, Universidade Nova de Lisboa, 2829-516 Caparica, Portugal. e-mail: lima@fct.unl.pt*

Supporting Information

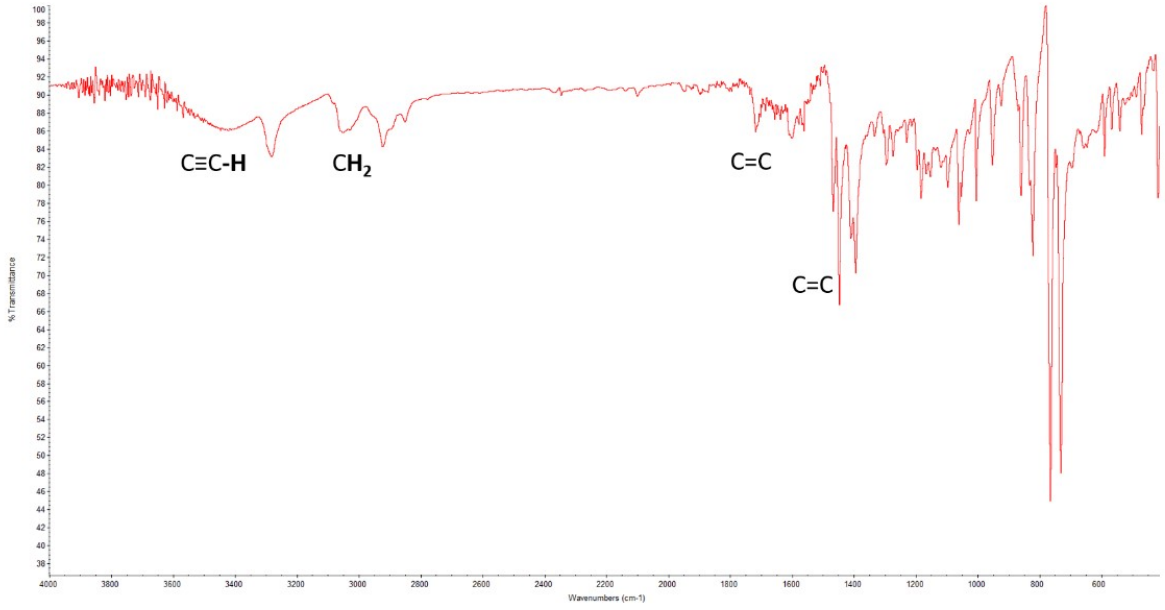


Figure S1. IR spectra of **L**.

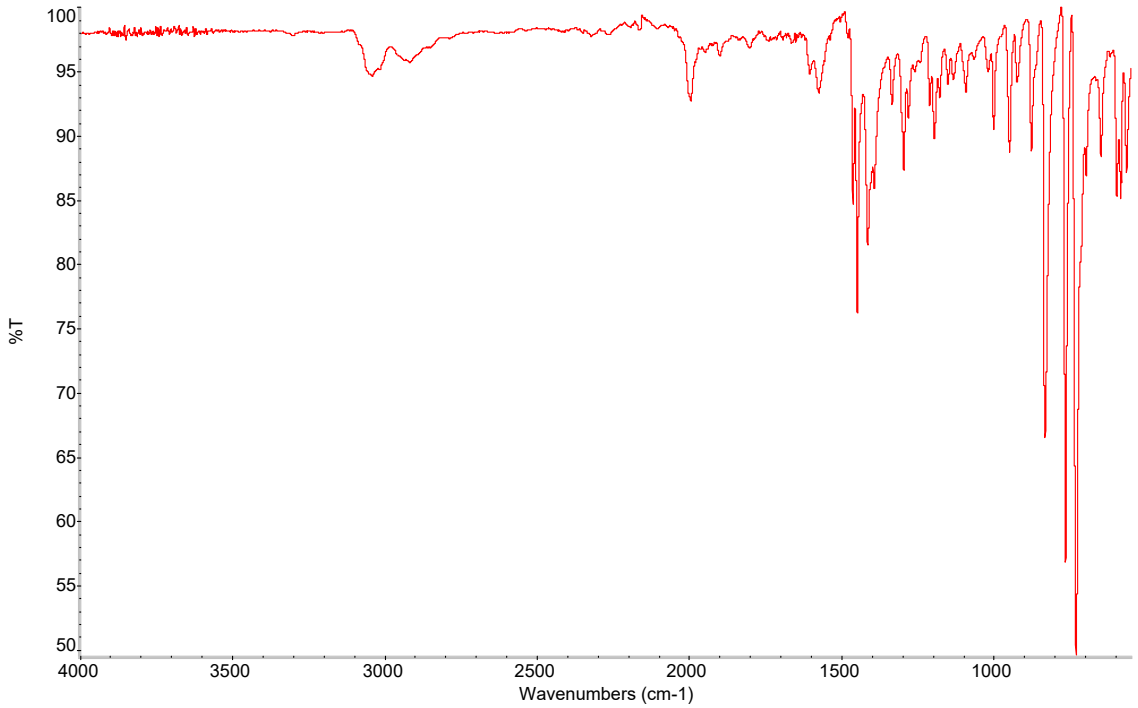


Figure S2. IR spectra of **1**.

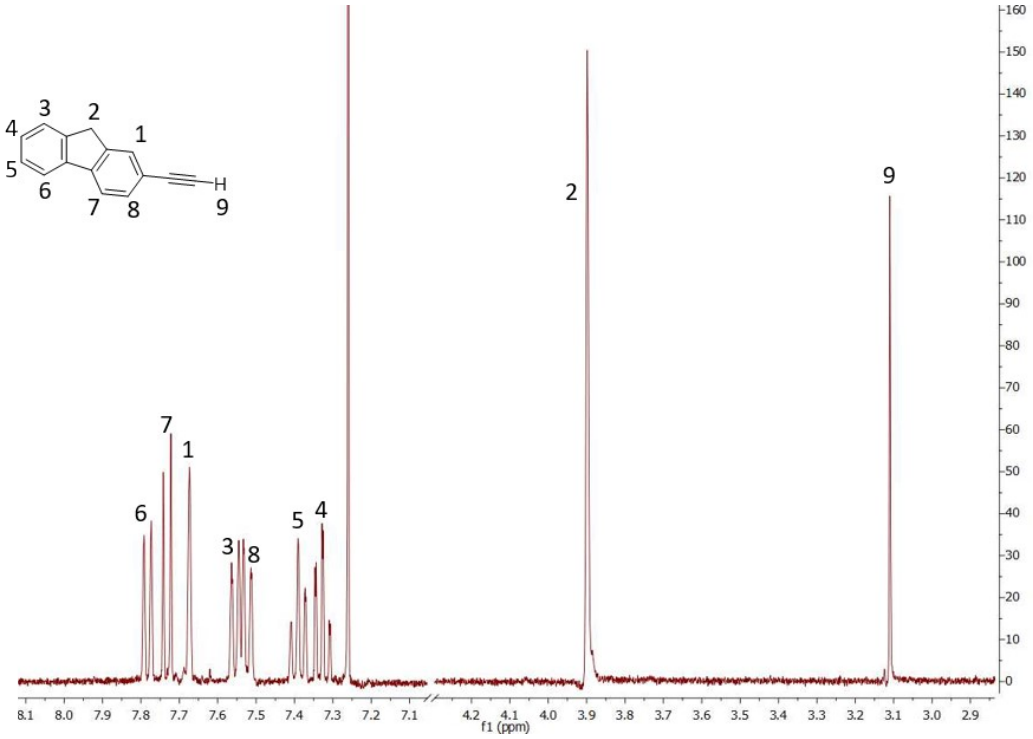


Figure S3. ^{1}H NMR spectrum of **L** in $CDCl_3$.

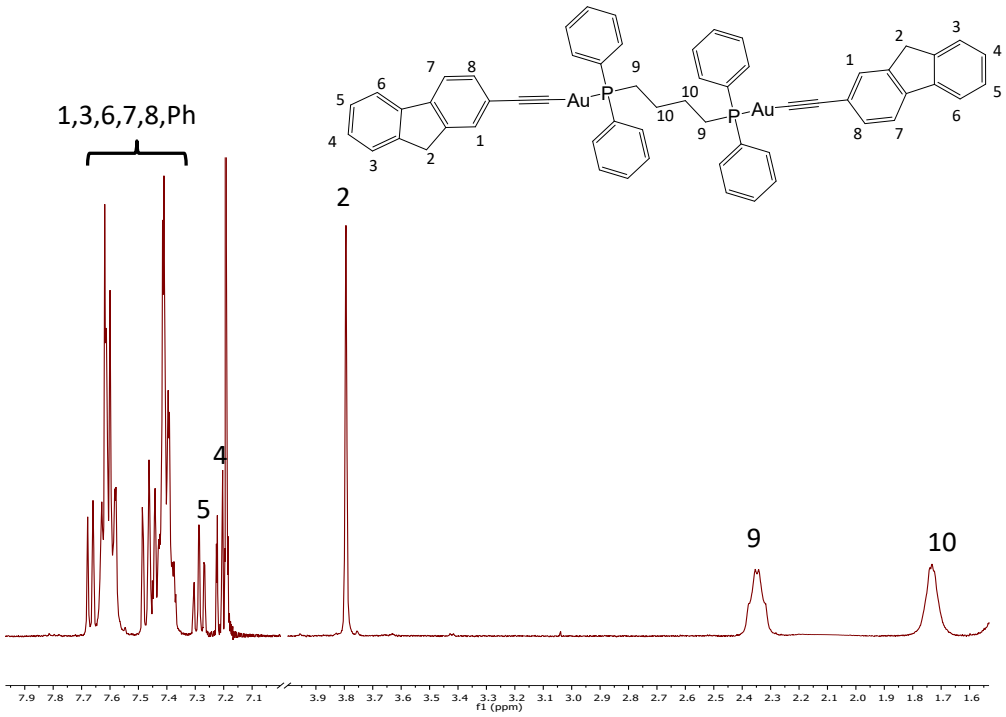


Figure S4. ^{1}H NMR spectrum of **2** in $CDCl_3$.

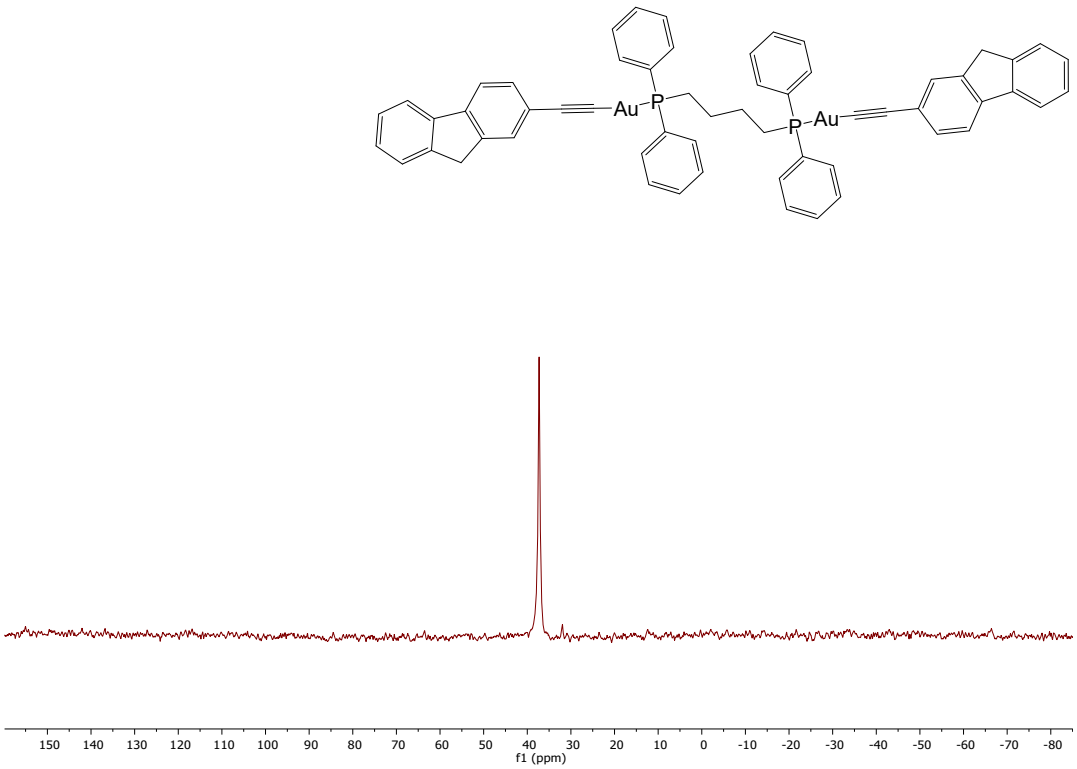


Figure S5. ^{31}P NMR spectrum of **2** in $CDCl_3$.

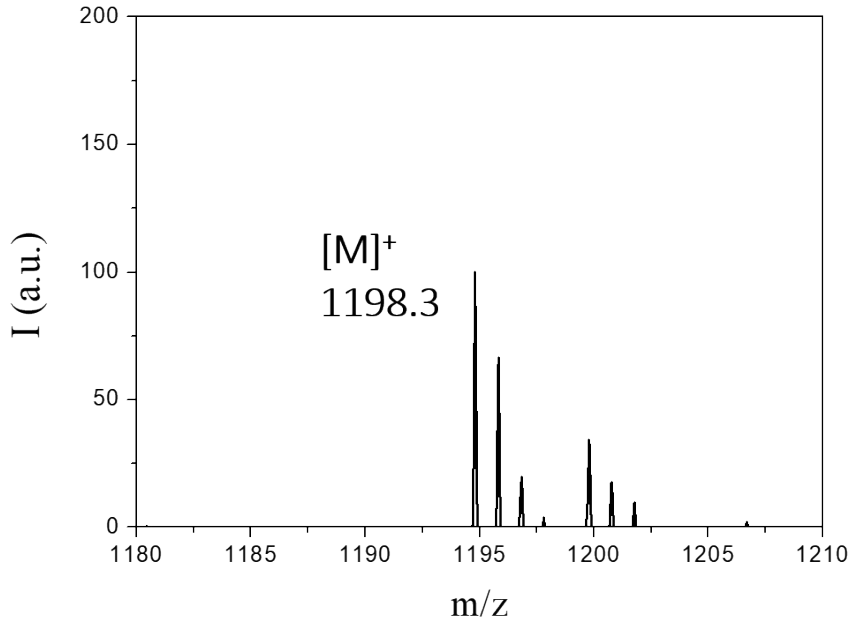


Figure S6. MALDI-TOF MS(+) spectrum of **2**.

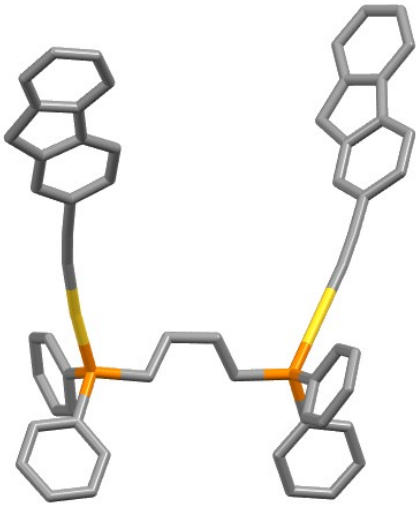


Figure S7. Boat-like conformation of compound **2**.

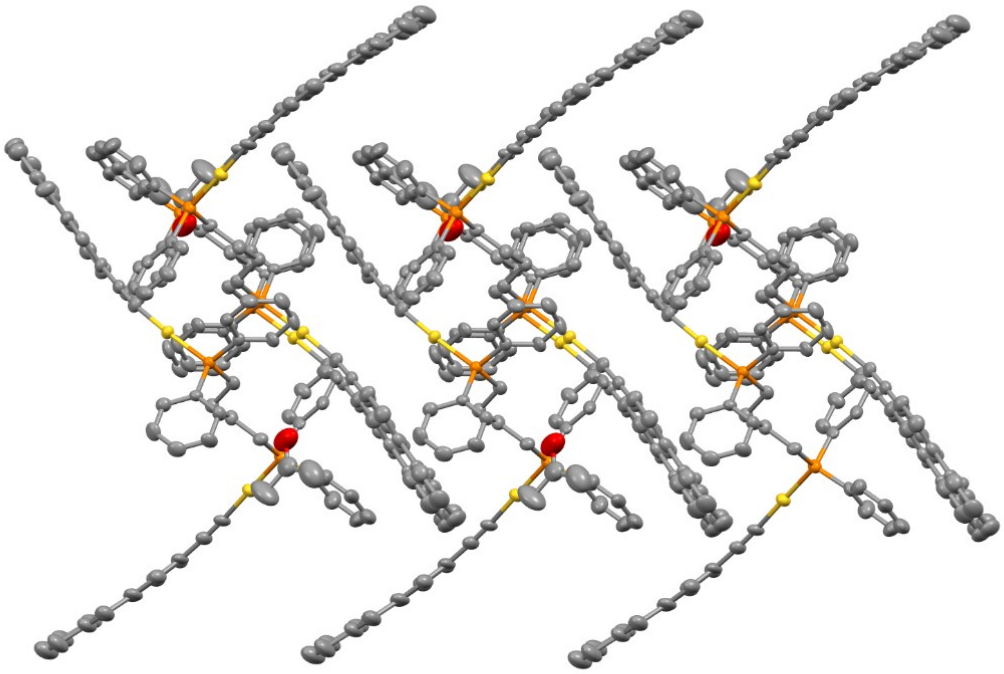


Figure S8. Packing of compound **2**. Yellow: gold; orange: phosphorus; grey: carbon; red: oxygen. Hydrogens have been omitted for clarity.

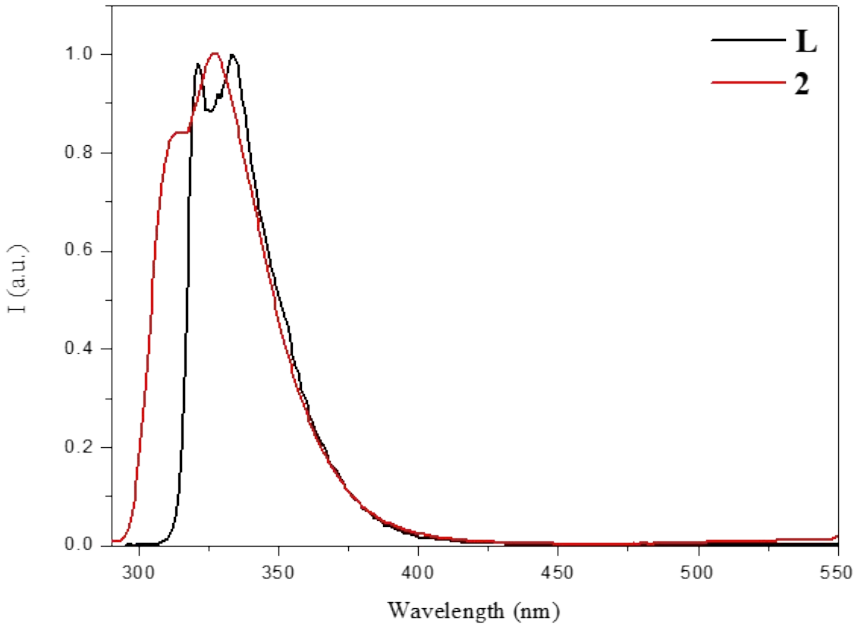


Figure S9. Emission spectra of 1×10^{-5} M solutions of the compounds **L** and **2** in acetonitrile in air-equilibrated samples at room temperature.

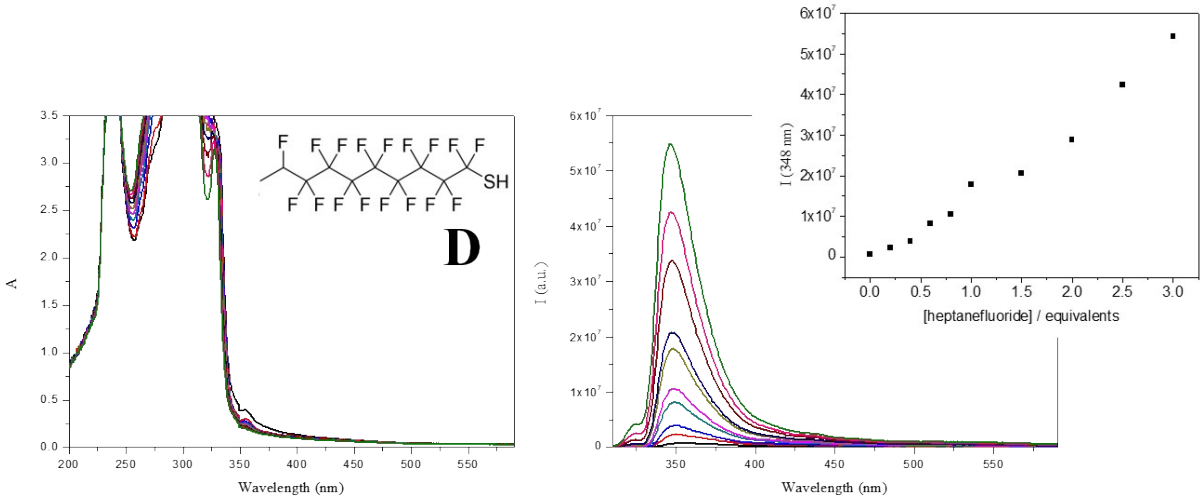


Figure S10. Absorption (left) and emission (right) spectra of the compound **2** in the presence of different amounts of heptane fluoride (**D**) at room temperature. λ_{exc} = 300 nm.

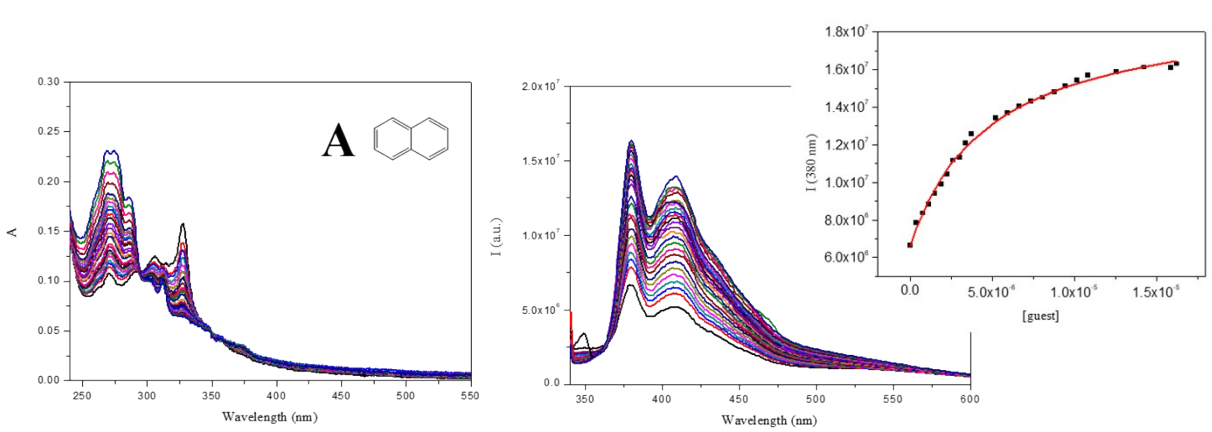


Figure S11. Absorption (left) and emission (right) spectra of the compound **2** in the presence of different amounts of naphthalene (**A**) at room temperature. λ_{exc} = 330 nm.

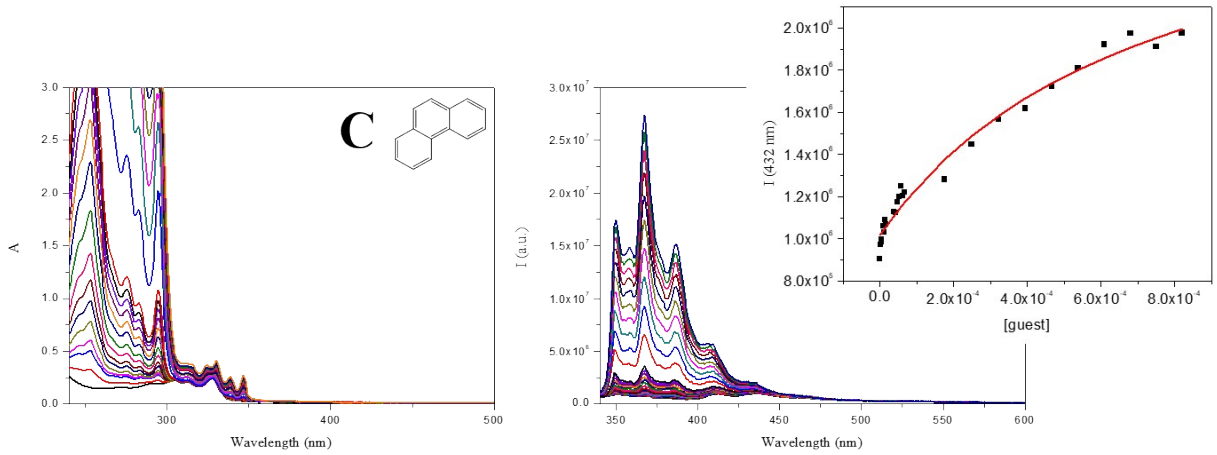


Figure S12. Absorption (left) and emission (right) spectra of the compound **2** in the presence of different amounts of phenanthrene (**C**) at room temperature. λ_{exc} = 330 nm.

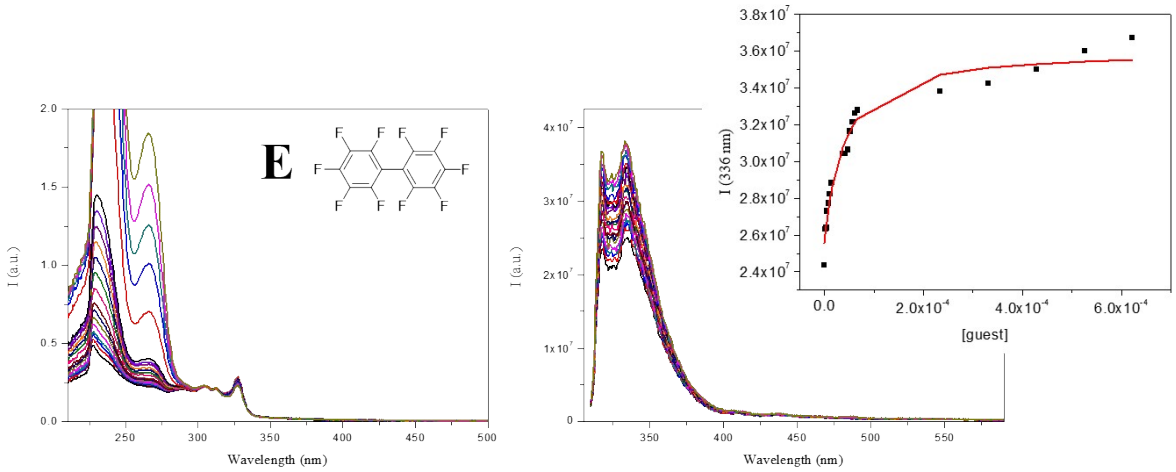


Figure S13. Absorption (left) and emission (right) spectra of the compound **2** in the presence of different amounts of diphenyl fluoride (**E**) at room temperature. λ_{exc} = 300 nm.

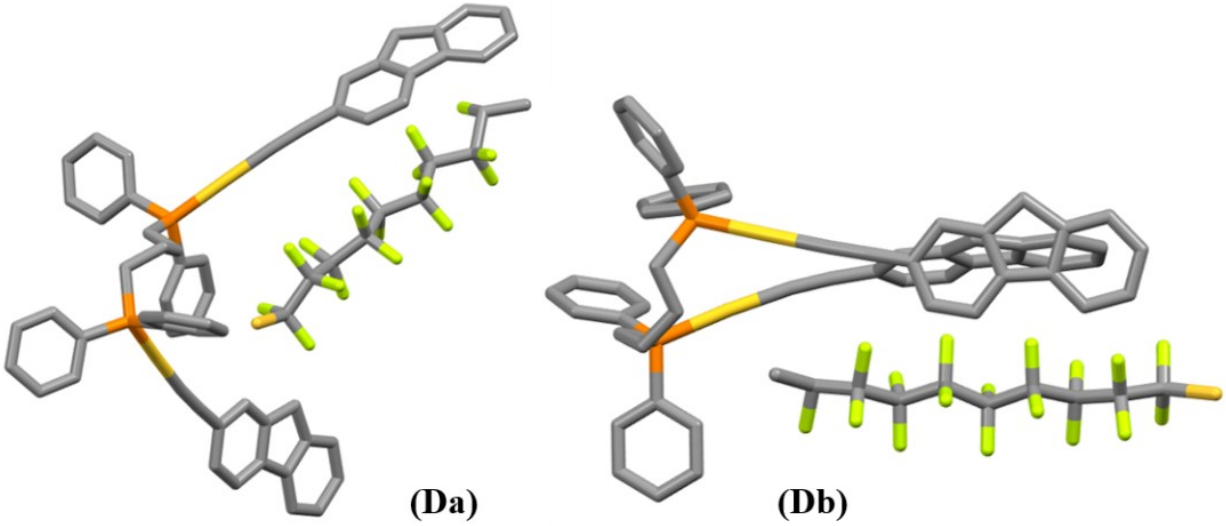
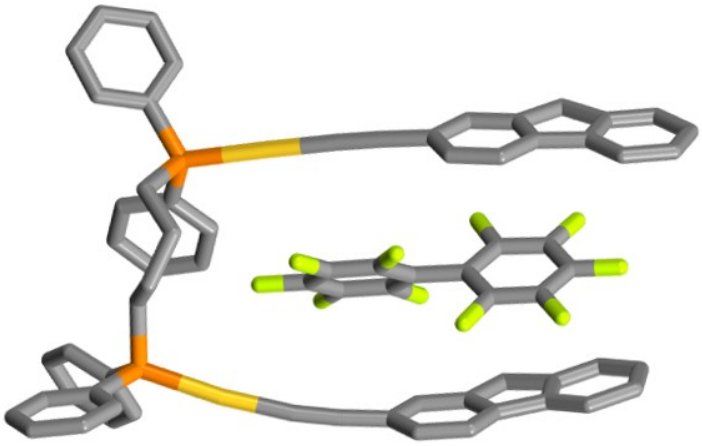


Figure S14. Calculated host-guest structures of the gold(I) complex and the heptadecafluoro-1-decanethiol with two different orientations.



(E)

Figure S15. Calculated host-guest structures of the gold(I) complex and the diphenyl fluoride.

Table S1. Calculated host-guest energies (in kcal·mol^{-1}) of the gold(I) complex and the adducts obtained with naphthalene (**A**), anthracene (**B**), phenanthrene (**C**), heptane fluoride **(D)** and diphenyl fluoride (**E**).

Adduct	Corrected formation	Host deformation	Guest deformation	BSSE-corrected interaction	Non-corrected formation
Naphthalene (**A**)	-8.2	8.9	0.1	17.2	-10.1
Anthracene (**B**)	-10.7	10.0	0.1	20.8	-12.9
Phenanthrene (**C**)	-5.2	18.4	0.3	23.9	-7.1
Heptane fluoride (**D**)	-12.7	22.9	9.3	0.9	-15.2
Diphenyl fluoride (**E**)	-14.6	32.9	17.0	1.3	-19.2

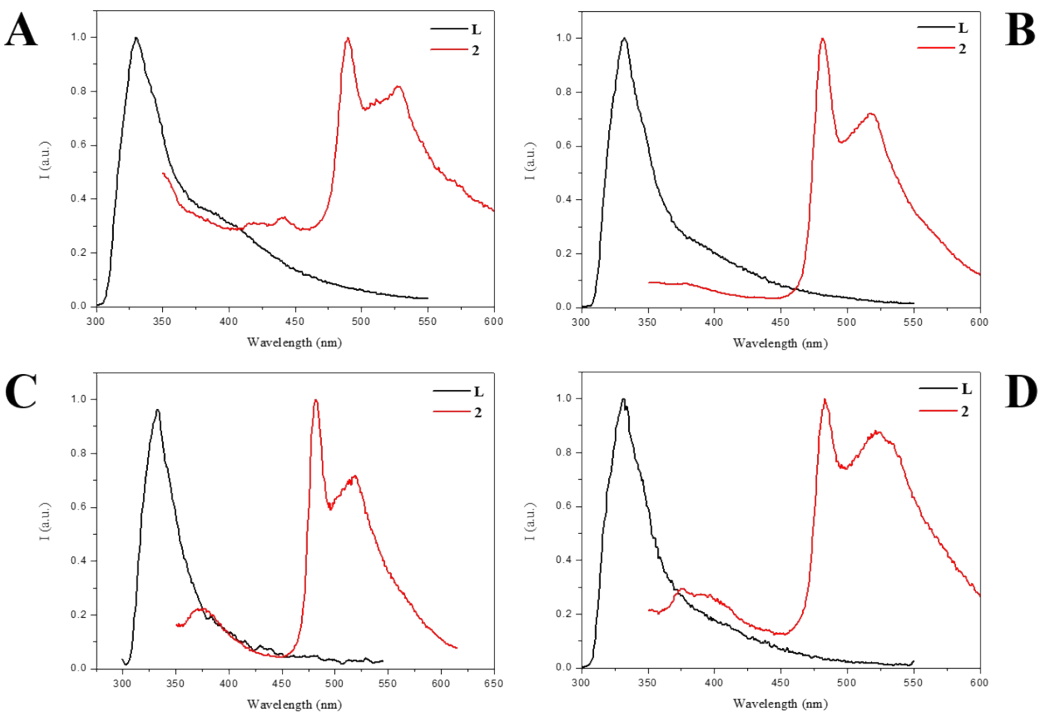


Figure S16. Emission spectra of the compounds **L** and **2** immobilized in Cellulose (**A**), PMMA (**B**), PS (**C**) and Zeonex (**D**) with air-equilibrated samples at room temperature. λ_{exc} = 335 nm for **2**, **3** and **4**. λ_{exc} = 285 nm for **L**.

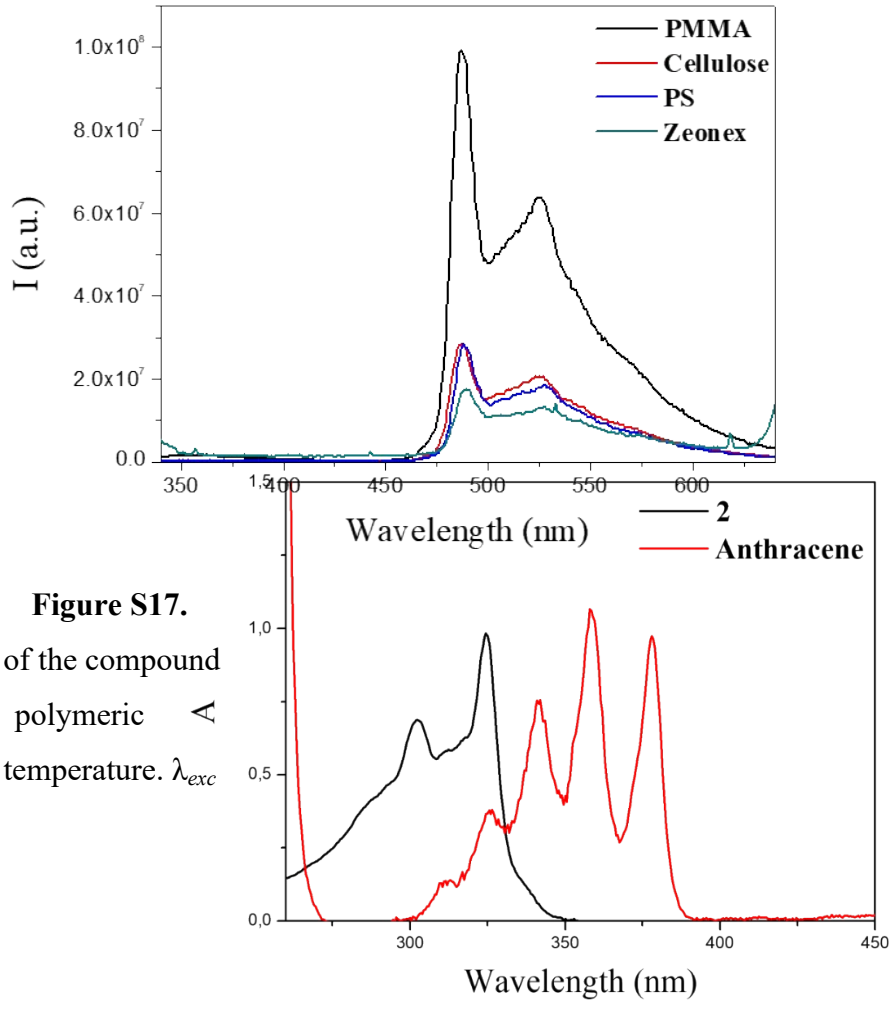


Figure S17. Emission spectra of the compound **2** in different polymeric matrixes at room temperature. λ_{exc} = 330 nm.

Figure S19. Absorption spectra of compound **2** and an anthracene solution in 1×10^{-5}M dichloromethane solutions at room temperature.

Table S2. Crystal data and structure refinement for **2**.

Compound	**2**
Formula	$C_{58}H_{46}Au_2P_2 \cdot C_3H_6O$
Crystal size, mm	0.24 x 0.27 x 0.28
Fw	1256.90
Temp., K	170(2)
Wavelenght, Å	0.71073
Crystal system	triclinic
Space group	$P\bar{1}$
a, Å	11.4012(2)
b, Å	12.0453(3)
c, Å	22.9156(7)
α, °	98.2270(10)
β, °	95.3860(10)
γ, °	117.227(2)
Volume, Å^3	2723.73(13)
Z	2
$D_{calc.}$, mg m^{-3}	1.533
Abs. coef., mm^{-1}	5.477
F(000)	1228
θ range for data coll, °	1.945 to 26.250
Refins coll./independent	22153/10958
Data/restraint/parameters	10958/33/597
GOF on F^2	1.042
Final *R* index ($I > 2\sigma(I)$)	R1 = 0.0449, wR2 = 0.0831
R index (all data)	R1 = 0.0741, wR2 = 0.0905
Peak and hole, e Å^{-3}	1.250 and -0.757
CCDC	2194275

Table S3. Phosphorescent quantum yields of **L** and **2** in Cellulose, PMMA, PS and Zeonex with air-equilibrated samples.

Compound	ΦFl				ΦPh			
	Cellulose	**PMMA**	**PS**	**Zeonex**	**Cellulose**	**PMMA**	**PS**	**Zeonex**
L	0.12	0.055	0.16	0.12	-	-	-	-
2	0.001	0.002	0.003	0.004	0.011	0.02	0.015	0.014