Supplementary Information

Alkynyl-functionalized Gold NHC Complexes and Their Coinage

Metal Clusters

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Crystallographic appendix

Table S1: Crystal data and structure refinement for **2, 3, 4, 6, 7** and **8.**

Identification code	**2**	**3**	**4**	**6**	**7**	**8**
Empirical formula	$C_{21}H_{21}BrN_2$	$C_{21}H_{20}AuClN_2$	$C_{21}H_{20}AuBrN_2$	$C_{29}H_{25}AuN_2$	$C_{91}H_{72}Au_4Cl_2Cu_2N_4$	$C_{91}H_{72}Ag_2Au_4Cl_2N_4$
Formula weight	381.31	532.81	577.27	598.48	2207.37	2296.03
Temperature/K	100	200	200	150	150	200
Crystal system	monoclinic	monoclinic	monoclinic	monoclinic	triclinic	triclinic
Space group	$P2_1/c$	C2/c	I2/a	$P2_1/c$	P-1	P-1
a/Å	11.9360(5)	27.2118(10)	18.6744(7)	21.8656(19)	11.2232(18)	11.3173(6)
b/Å	17.1639(10)	10.5894(5)	10.5567(6)	25.3354(18)	11.3107(18)	11.3624(6)
c/Å	8.9095(3)	18.6024(7)	20.2408(8)	18.1177(15)	16.682(3)	16.9117(9)
α/°	90	90	90	90	106.416(13)	108.028(4)
β/°	91.527(3)	132.759(2)	91.555(3)	99.562(7)	96.847(13)	96.042(4)
γ/°	90	90	90	90	104.649(14)	105.373(4)
Volume/$Å^3$	1824.63(14)	3935.7(3)	3988.8(3)	9897.3(14)	1923.4(6)	1951.90(19)
Z	4	8	8	16	1	1
$\rho_{calc}g/cm^3$	1.388	1.798	1.923	1.607	1.906	1.953
μ/mm^{-1}	2.257	7.617	9.385	5.963	8.261	8.097
F(000)	784.0	2048.0	2192.0	4672.0	1054.0	1090.0
Crystal size/mm^3	0.575 × 0.241 × 0.06	0.094 × 0.047 × 0.019	0.299 × 0.23 × 0.166	0.412 × 0.312 × 0.174	0.48 × 0.299 × 0.073	0.214 × 0.113 × 0.05
Radiation	MoKα (λ = 0.71073)	MoKα (λ = 0.71073)	MoKα (λ = 0.71073)	MoKα (λ = 0.71073)	MoKα (λ = 0.71073)	MoKα (λ = 0.71073)
2Θ range for data collection/°	3.414 to 52.09	4.078 to 52.202	4.352 to 51.996	2.79 to 51.242	3.832 to 54.296	3.812 to 52.11
Index ranges	-14 ≤ h ≤ 11, -21 ≤ k ≤ 21, -11 ≤ l ≤ 10	-33 ≤ h ≤ 33, -13 ≤ k ≤ 13, -22 ≤ l ≤ 22	-20 ≤ h ≤ 22, -13 ≤ k ≤ 13, -24 ≤ l ≤ 24	-25 ≤ h ≤ 26, -30 ≤ k ≤ 30, -21 ≤ l ≤ 21	-14 ≤ h ≤ 14, -12 ≤ k ≤ 14, -21 ≤ l ≤ 21	-13 ≤ h ≤ 13, -12 ≤ k ≤ 14, -20 ≤ l ≤ 20
Reflections collected	9675	34765	13935	112058	17364	14184
Independent reflections	3586 [R_{int} = 0.0939, R_{sigma} = 0.0973]	3883 [R_{int} = 0.1391, R_{sigma} = 0.0784]	3881 [R_{int} = 0.0398, R_{sigma} = 0.0355]	18432 [R_{int} = 0.0559, R_{sigma} = 0.0393]	8344 [R_{int} = 0.0600, R_{sigma} = 0.0820]	7473 [R_{int} = 0.0625, R_{sigma} = 0.1002]
Data/restraints/parameters	3586/0/220	3883/0/229	3881/0/229	18432/0/1165	8344/0/526	7473/96/541
Goodness-of-fit on F^2	0.938	0.859	0.867	0.896	0.809	0.905
Final R indexes [I>=2σ (I)]	R_1 = 0.0595, wR_2 = 0.1367	R_1 = 0.0403, wR_2 = 0.0760	R_1 = 0.0203, wR_2 = 0.0375	R_1 = 0.0240, wR_2 = 0.0362	R_1 = 0.0297, wR_2 = 0.0475	R_1 = 0.0432, wR_2 = 0.0786
Final R indexes [all data]	R_1 = 0.0919, wR_2 = 0.1519	R_1 = 0.1096, wR_2 = 0.0943	R_1 = 0.0419, wR_2 = 0.0405	R_1 = 0.0434, wR_2 = 0.0390	R_1 = 0.0602, wR_2 = 0.0517	R_1 = 0.0940, wR_2 = 0.0904
Largest diff. peak/hole / e $Å^{-3}$	0.90/-0.85	1.18/-0.48	0.29/-0.91	1.06/-0.70	1.03/-1.26	1.00/-1.30

Complexes **7** and **8** both crystallized together with dichloromethane in the lattice.

Crystallographic data (excluding structure factors) for the structures reported in this paper have been deposited with the Cambridge Crystallographic Data Centre as a supplementary publication no. CCDC 1059550-1059555. Copies of the data can be obtained free of charge on application to CCDC, 12 Union Road, Cambridge CB21EZ, UK (fax: (+(44)1223-336-033; email: deposit@ccdc.cam.ac.uk).

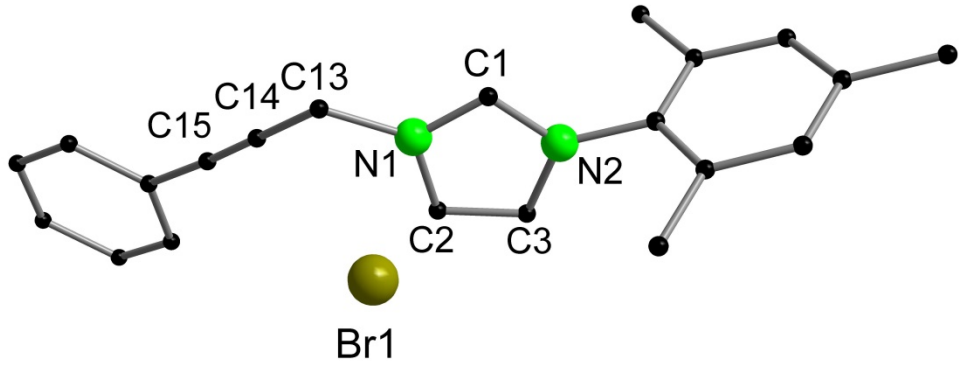
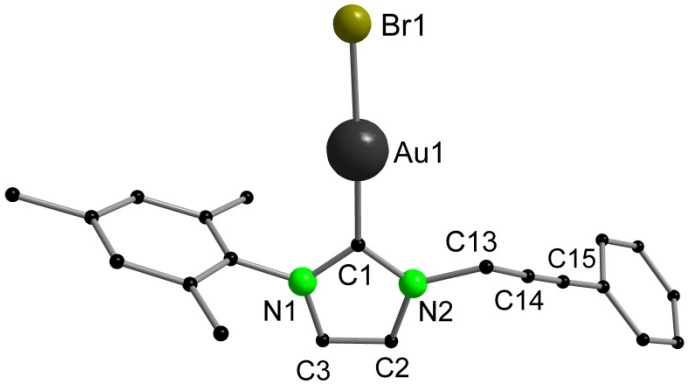


Fig. S1 Crystal structure of the imidazolium salt **2**.



Photoluminescence measurements

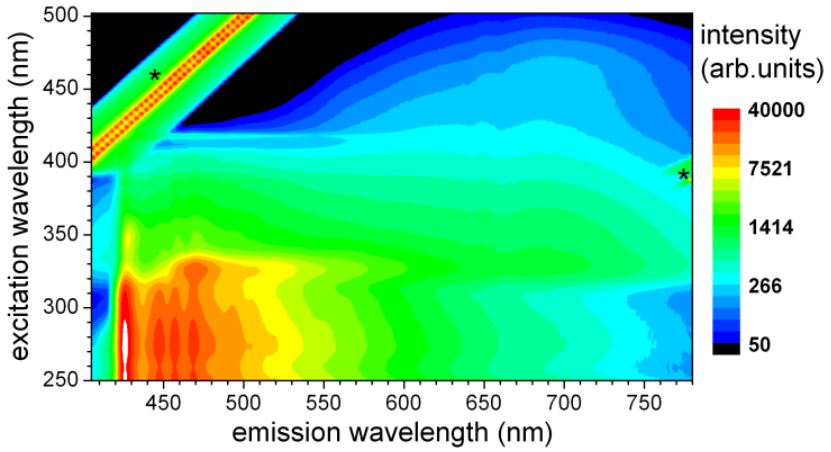


Fig. S2 Photoluminescence map (color-coded PL intensity vs. excitation and emission wavelengths) of solid complex **6** at T = 20 K. Emission was guided through a 400 nm longpass filter. The asterisks indicate the first and second order excitation lines above λ_{exc} ~ 400 nm.

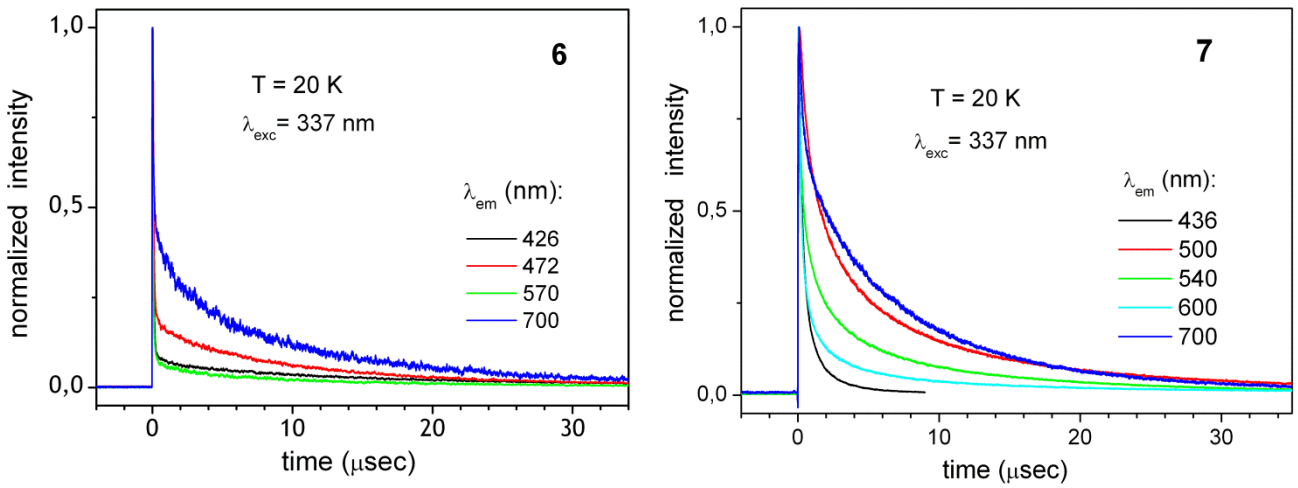


Fig. S3 PL decay curves recorded for solid **6** and **7** at different emission wavelengths under nsec-pulsed excitation at 337 nm (N_2 -laser) and T = 20 K.

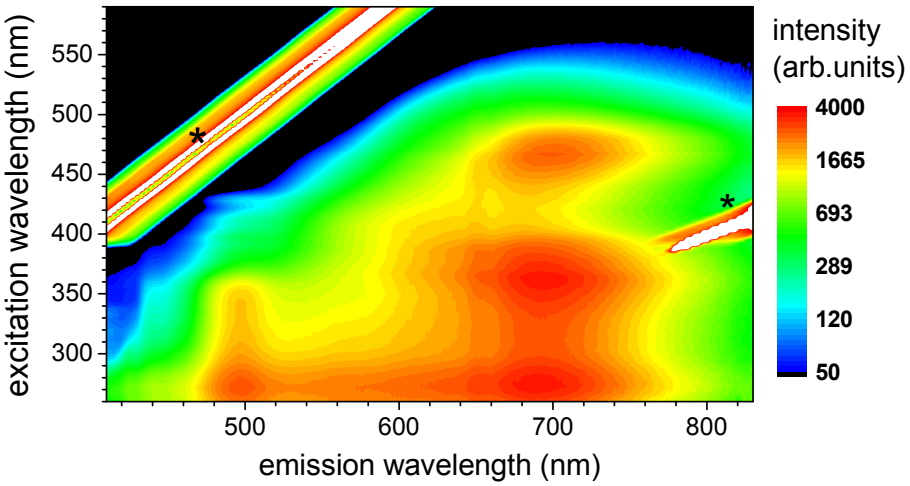


Fig. S4 Photoluminescence map (color-coded PL intensity vs. excitation and emission wavelengths) of solid complex **7** at T = 20 K. The map was recorded after several months storage of the sample (under ambient conditions, in dark) and reveals an enhanced red emission at ~700 nm as compared to the freshly prepared sample (cf. Fig. 7 in text). The asterisks indicate the first and second order excitation lines.