Triazinone-Bridged Neutral Dinuclear Gold(I)-NHC Complex
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**Supporting Information**

**ABSTRACT:** We report the synthesis and characterization of a neutral pincer-type \( \mu^2-\eta^2(1\kappa\text{C}_\text{carbene}:2\kappa\text{C}_\text{carbene})-(\text{C}^*-\text{N}-\text{C}^*) \)-ligand-coordinated gold(I)-NHC complex with an emission wavelength of 452 nm. Solid-state structure analysis confirms the dinuclear structure of this complex.

**PHOTOLUMINESCENCE MEASUREMENTS**

The absorption and emission spectra of complex 2 are shown in Figures 3 and 4. The absorption maximum was observed at a wavelength of 220 nm independent from the measurement conditions (poly(methyl methacrylate) (PMMA) film (2%) or in the solid state (100% film)) (Figure 3).

The maxima of the emission wavelength (Figure 4) have been observed at 452 nm in PMMA (2%) and 464 nm in the

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solid state (100% film). The slightly bathochromic shift could be caused by a small increase of the intramolecular aurophilic interaction as a result of geometrical changes in the complex due to packing effects. Compared to previously reported intermolecular Au···Au interactions caused by aggregation of the metal centers with possible additional emission bands at higher wavelengths, this shift is not significant. Compared to the analogous silver complex, the emission wavelength maximum (417 nm) is significantly shifted toward higher wavelengths.

Figure 1. Molecular structure of compound 2 in C2/c. Hydrogen atoms have been omitted for clarity. Thermal ellipsoids are drawn at 50% probability. Selected distances (Å), angles (deg), and torsional angles (deg): Au1···Au2 3.2797(9); Au1−C1 2.046(8); C5−O1 1.228(9); Au2−C7 2.057(6); Au1−N3 2.879(6); Au2−N3 2.982(6); C1−Au1−C1′ 169.6(3); C7−Au2−C7′ 173.7(3); N4−C4−N2−C1 −166.2(7); N5−C6−N6−C7 −154.2(7).

Figure 2. Part of the unit cell of 2 showing intra- and intermolecular hydrogen bonds along the b- and c-axes (left) as well as the a-axis. Distances (in Å): I 2.493, II 2.712, III 2.949, IV 2.902, V 2.882, VI 2.438.

Figure 3. UV−vis absorption spectra of complex 2 in PMMA (2%) and 100% film.

Figure 4. Emission spectra of complex 2 (excitation wavelength, λexc 300 nm, room temperature). 2% in PMMA: XRGB 0.1826, YRGB 0.1898 (X and Y are CIE coordinates at room temperature); emission wavelength, λem 452 nm; quantum yield, radiant exposure under N2, ϕ 0.15; average decay lifetime, τM 1.64 μs; 100% film: XRGB 0.1983, YRGB 0.2413, λem 464 nm, ϕ 0.06.
CONCLUSION

We were able to synthesize and characterize the first example of a novel neutral dinuclear Au(I) complex with an anionic C*-N-C® NHC ligand. Each of the two gold centers is coordinated by both bidentate ligands, which are helically twisted around the metal–metal axis. The complex shows a strong photoluminescent emission in the blue region of the spectrum at 460 nm and no significant shift of the emission maximum due to aggregation.

EXPERIMENTAL SECTION

General Experimental Methods. All chemicals used were obtained from commercial suppliers and used without further purification. The silver(I)-NHC complex and Au(THT)Cl were synthesized according to published procedures. The NMR spectra were recorded with a Bruker AC 300 P spectrometer and referenced internally to the references of the solvent. 1H NMR spectra were recorded at 300.14 MHz; 13C NMR spectra at 75.475 MHz.

EXPERIMENTAL SECTION

Synthesis of Di[4,6-bis(1-tert-butylimidazoline-2-ylidine-3-yl)-5H-1,3,5-triazin-2-05-5-ide][diiodo](1). A 100 mg amount of silver(I)-NHC complex and 71.8 mg of Au(THT)Cl were stirred in 10 mL of acetonitrile at room temperature for 3 h under exclusion of light, whereupon the formed suspension is filtered through Celite and concentrated in vacuo. The raw product is precipitated by addition of about 20 mL of diethyl ether, filtered, washed twice with 10 mL of diethyl ether, then dried in vacuo to give the product as a white solid. Crystals suitable for X-ray diffraction were obtained by slow crystallization from diethyl ether, then dried in vacuo to give the product as a white solid.

Preliminary examination and data collection were carried out on a NONIUS Kappa CCD. Raw data were corrected for Lorentz polarization effects and, arising from the scaling procedure, for latent decay. An absorption correction was applied using SADABS. After merging, the independent reflections all were used to refine the structure. The structures were solved by a combination of direct methods and difference Fourier synthesis. All non-hydrogen atom positions were refined with anisotropic displacement parameters, while hydrogen atoms were placed in calculated positions and then refined using the SHELXL-97 riding model. Full-matrix least-squares calculations were performed with the programs COLLECT, DIRAX, EVALCCD, SIR92, SADABS, the SHELXL-97 package and ORTEP-III.

Graphics were generated and processed with the programs PLATON, MERCURY, and POVRAY.

ASSOCIATED CONTENT

Supporting Information

The crystallographic information files of complex 2 as well as the crystallographic details of the measurements are available free of charge via the Internet at http://pubs.acs.org.

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Notes

The authors declare no competing financial interest.

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REFERENCES


