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BOOK OF ABSTRACTS



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SPONTANEOUS *IN SITU* GENERATION OF HIGHLY PHOTOEMISSIVE DIAURACYCLES IN WATER SOLUTION BASED ON THE 2-THIOCYTOSINE LIGAND

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A feature that attracts the attention of inorganic chemists towards the production of water-soluble gold(I) complexes is the dynamic behaviour that, in some instances, they manifest in solution because of aurophilicity, it is, the self-aggregation of gold(I) at sub-van der Waals distances.

As devoted “aurophilic” chemists ourselves, we have considered in the recent years natural nucleobases as surprising ligands for the stabilization of molecular gold(I) compounds. In those, the co-existence of strong aurophilic interactions and numerous hydrogen bonds in an “orthogonal” fashion allows their effective self-aggregation in water and, hence, the design of low-molecular-weight gelators^[1] and/or luminophores.^[2]

Thiol-functionalized nucleobases are interesting polydentate *S,N*-donor heterocycles and, so, they had been considered for achieving the main goals of nowadays’ gold(I) chemistry.^[3] Hence, recalling our recent results, which we have reported for extremely simple complexes featuring the natural nucleobase adenine, and the potential ones shown by thiolated nucleobases, we are reporting in here a full study of the unexpected time-dependent photophysical behaviour that (2-thiocytosine)-based gold(I) complexes display in aqueous solution. As it will be explained, the new absorption and emission bands seem to be originated in a molecular rearrangement towards the formation of neutral diauracycles.

References

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- [3] See for example: (a) Lee, Y.-A.; Eisenberg, R. *J. Am. Chem. Soc.*, **2003**, 125, 7778-7779. (b) Abás, E.; Pena-Martínez, R.; Aguirre-Ramírez, D.; Rodríguez-Diéguez, A.; Laguna M.; Grasa, L. *Dalton Trans.*, **2020**, 49, 1915-1927.