

MS20 Electric, opto-electronic and magnetic properties from elastic and inelastic scattering plus properties of materials from quantum crystallography

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Influence of non-covalent interactions on solid-state emission of halogenated diphenyl phosphanyl anthracenes

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Abstract

With applications in OLEDs, sensors, and field-effect transistors, organic solid-state luminescent materials have drawn a great deal of attention of the past two decades as alternatives to inorganic luminophores. One challenge still to overcome is the observed, dramatic quenching of their emission when passing from dilute solutions to solid-state. An avenue to reduce the quenching lies in intramolecular modification of a fluorophore or by controlling the formation of weak non-covalent intermolecular interactions in a crystalline phase, with halogenation as a potential modification. In certain chromophores, halogens atoms substituted along the heavy atom backbone promote intermolecular halogen bonding and, in turn, can increase the mixing of the singlet and triplet states of the excited chromophore and enhance intersystem crossing.

In this work,^[1] we present three newly synthesized halogenated anthracene derivatives, 9-PPh₂-10-Cl-(C₁₄H₈) (**1**), 9-PPh₂-10-I-(C₁₄H₈) (**2**) and 9-PPh₂-10-Br-(C₁₄H₈) (**3**), that exhibit solid-state luminescence, enhanced by the presence of halogen atoms. By introducing halogen substituents, we observe a significant red-shift of emission when comparing to other photoactive non-halogenated anthracene derivatives.^[2,3] In particular, for compound **3** a maximum emission wavelength of 452 nm was observed, whereas compound **1** was red-shifted to 552 nm (Figure 1). We will discuss the structure-property correlation in the studied systems supported by X-ray diffraction experiments and quantum crystallography tools with a special focus on C-X... π and X...X interactions (X = Cl, Br, I) considered as main driving force promoting Aggregation-Induced-Emission (AIE).

References

[1] T. Patten, N. Graw, S. Friedl, A. Krawczuk, D. Stalke, To be submitted, 2022; [2] T. Schillmöller, P. N. Ruth, R. Herbst-Irmer, D. Stalke, *Chem. Eur. J.*, 2020, **26**, 17390-17398; [3] T. Schillmöller, R. Herbst-Irmer, D. Stalke, *Adv. Optical Mater.*, 2021, **9**, 2001814.

Solid-state luminescence spectra of **1** and **3**

