

Fine-tuning solid state luminescence properties of molecular crystals via solid solution formation

Kristaps Saršūns¹, Kaspars Leduskrasts², Toms Reķis¹, Agris Bērziņš¹

¹Department of Physical Chemistry, Faculty of Chemistry, University of Latvia, kristaps.sarsuns@lu.lv, Riga, Latvia, ²Latvian Institute of Organic Synthesis, Riga, Latvia

Approaches and tools of crystal engineering is developed to allow employing the knowledge of intermolecular interaction preferences to predict crystal structure formation and therefore crystal properties. For example, solid solutions, for which the component ratios can be varied in continuum [1]. Along with the composition, also properties of solid solutions are modulated. Therefore, they hold a potential for tuning molecular crystal material properties in a smooth fashion. The question, however, is whether the response of a wanted property is sensitive enough to the varying component ratio. The properties may include solid-state luminescence and phosphorescence properties [2].

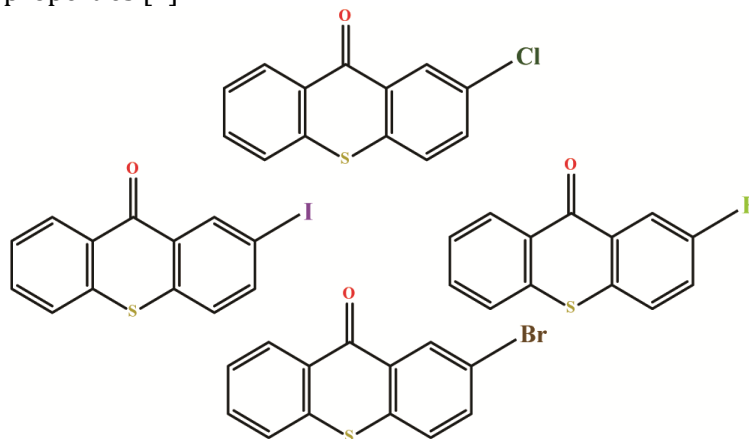


Fig 1. Molecular structures of thioxanthone halogenated derivatives

In this study we explored the solid solution formation between thioxanthone halogenated derivatives (Fig 1., TX-R, R = Cl, F, Br, I). The compounds have been selected based on reported room-temperature solid-state luminescence phenomena [3] and chemically similar structures, in which the different atom (R) may not significantly affect the dominant intermolecular interactions. Solid solutions have been identified and characterized using powder X-ray diffraction and thermal methods of analysis. Their composition limits are summarized in respective two component phase diagrams. Photoluminescence spectra of all crystalline phases in powder form were recorded to see how they change with respect to those of the pure substances known from the literature [3]. As a result, this confirmed that fine-tuning solid state luminescence properties of molecular crystals can be modulated via solid solution formation.

- [1] Lusi M. Engineering Crystal Properties through Solid Solutions. *Crystal Growth & Design*, 18(6), 3704-3712 (2018)
- [2] Saršūns K, Bērziņš A, Reķis T. Solid Solutions in Xanthone – Thioxanthone Binary System: How Well are Similar Molecules Discriminated in the Solid State? *Crystal Growth & Design*, 20(12), 7997-8004 (2020)
- [3] Wen Y, Liu H, Zhang S, Gao Y, Yan Y, Yang B. One-dimensional π - π stacking induces highly efficient pure organic room-temperature phosphorescence and ternary-emission single-molecule white light. *J. Mater. Chem. C*, 7, 12502-12508 (2019).

A.K.A. acknowledges support by European Social Fund, project “Strengthening of the capacity of doctoral studies at the University of Latvia within the framework of the new doctoral model”, identification No. 8.2.2.0/20/I/006 and University of Latvia foundation through “Mikrotīkls” doctoral scholarship in the field of natural and medical sciences.