README FILE

Dataset Title: Dataset of "***Polymorphism-Dependent Room-Temperature Phosphorescence of a Persulfurated Benzene***"

Dataset Authors: **Simone d'Agostino,[a] Andrea Vitale,[a] Yashraj Kapadiya,[b] Marc Gingras,[b] Fabrizia Negri,[a] Paola Ceroni[a] and Andrea Fermi[a]**

Affiliations: [a] Department of Chemistry "Giacomo Ciamician", University of Bologna, via Gobetti, 85 – 40129 Bologna, Italy;
[b] Aix Marseille Univ., CNRS, CINAM, Marseille, France.

Dataset contact person: Andrea Fermi, Department of Chemistry "Giacomo Ciamician", University of Bologna, Via P. Gobetti 85, 40129 Bologna, Italy (andrea.fermi2@unibo.it).

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Dataset contents

The dataset consists of:
• 1 compressed folder named **emission-data.zip** containing 2 subfolders named:

emission-data_X

(with X = 1 or 2)

the two subfolders contain emission spectra (X=1) and emission decays (X=2, with associated fitting functions) in .txt format for the analysed substances;
• 1 readme file in .pdf format

readme_file.pdf

Dataset documentation

Abstract

The dataset contains *i*) emission spectra recorded at room temperature from solid samples of two distinct polymorphs of 1,2,3,4,5,6-hexakis((4-isopropylphenyl)thio)benzene and *ii*) the associated emission decays in the same experimental conditions.

Content of the files

The attached dataset includes:
• a folder labelled as "Emission-data_1", containing the emission spectrum recorded on solid samples at RT for each polymorph of the analysed substance (named "P1" and "P2" for polymorph in form 1 and 2, respectively). The data consist of two columns for each spectrum (wavelength in nanometers vs. normalised emission intensity), in a .txt file.
• a folder labelled as "Emission-data_2", containing the emission decays at specific wavelenghts for each polymorph (1 and 2). The data consist of two columns for each decay (time in nanoseconds vs. normalised emission intensity decay) recorded for a given polymorph. In addition, two additional data columns are present, containing biexponential functions for the two decays reported.

Methodologies

All emission spectra were recorded on solid samples at RT, unless otherwise specified, with a a Varian Cary Eclipse spectrofluorometer. In a typical setup, ca. 1 mg of material is placed between two glass slides and placed in a 45° configuration within the instrument's sample holder. Lifetimes >10 µs are recorded on the same instrument using gated detection and a mono- or biexponential function to fit the emission decay. Alternatively, lifetimes <10 µs are recorded on a Edinburgh FLS920 fluorometer (equipped with a Hamamatsu Photomultiplier R928P phototube) by time-correlated single-photon counting (TCSPC) technique. The estimated experimental errors are 2 nm on the band maximum, 5% luminescence lifetime.

References

Simone d'Agostino, Andrea Vitale, Yashraj Kapadiya, Marc Gingras, Fabrizia Negri, Paola Ceroni, Andrea Fermi, "Polymorphism-Dependent Room-Temperature Phosphorescence of a Persulfurated Benzene", *Chem. Commun.* **2026**, submitted.