
STRUCTURAL SCIENCE
CRYSTAL ENGINEERING
MATERIALS

**Volume 78 (2022)**

**Supporting information for article:**

# A new linear phenyloxazole-benzothiadiazole luminophore: crystals growth, structure and fluorescence properties

**Valery A. Postnikov, Natalia I. Sorokina, Artem A. Kulishov, Maria S. Lyasnikova, Timofei A. Sorokin, Alexandra Ya. Freidzon, Anastasia S. Stepko, Oleg V. Borshchev, Maxim S. Skorotetsky, Nikolay M. Surin, Evgeniya A. Svidchenko and Sergey A. Ponomarenko**

## S1. Gel permeation chromatography

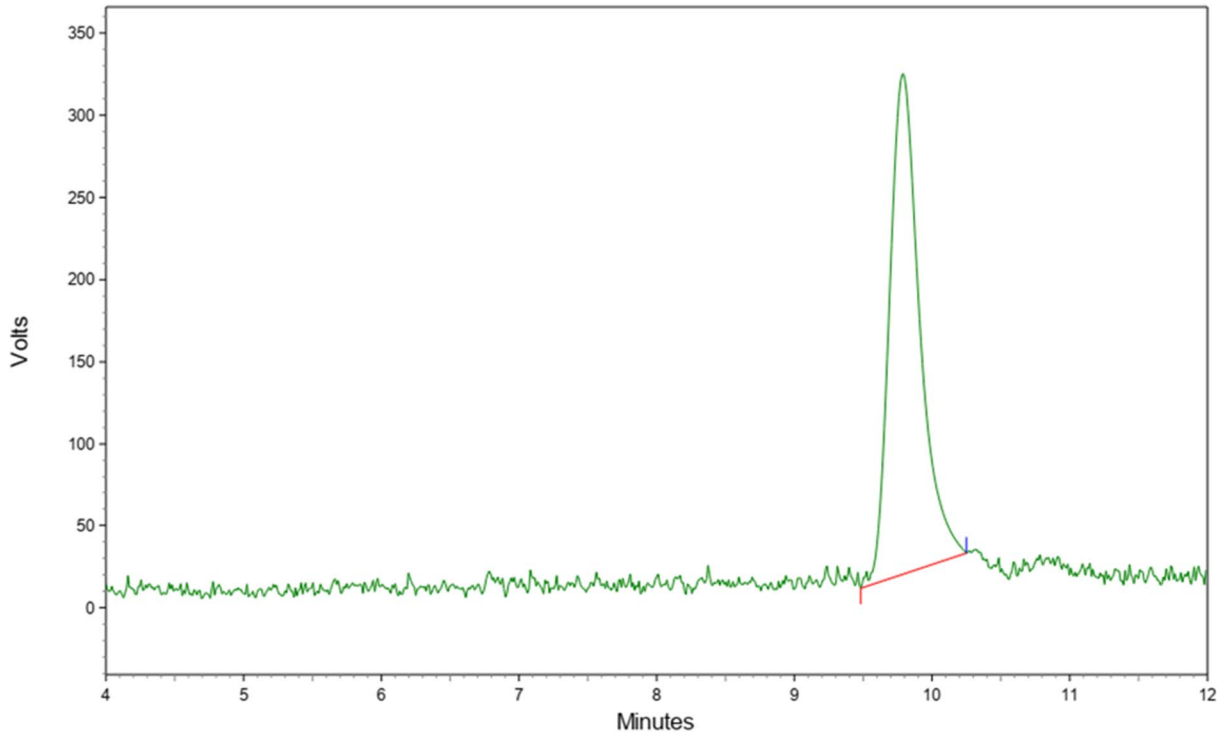



**Figure S1** GPC curve of $BTD(PO)_2$ after purification.

## S2. IR spectroscopy

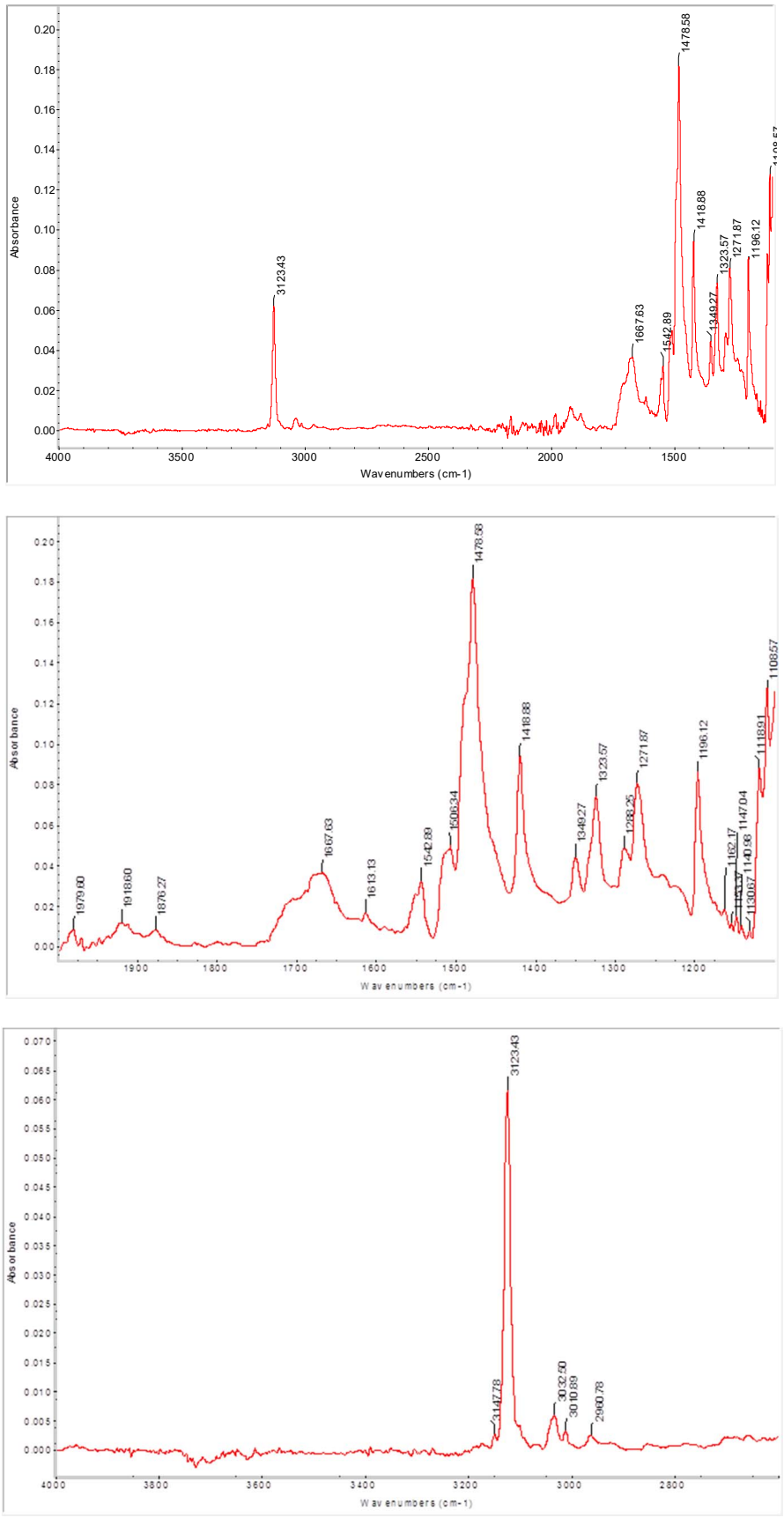



**Figure S2** IR spectra of **BTD(PO)$_2$** (crystalline powder).

**S3. Mass Spectrometry**

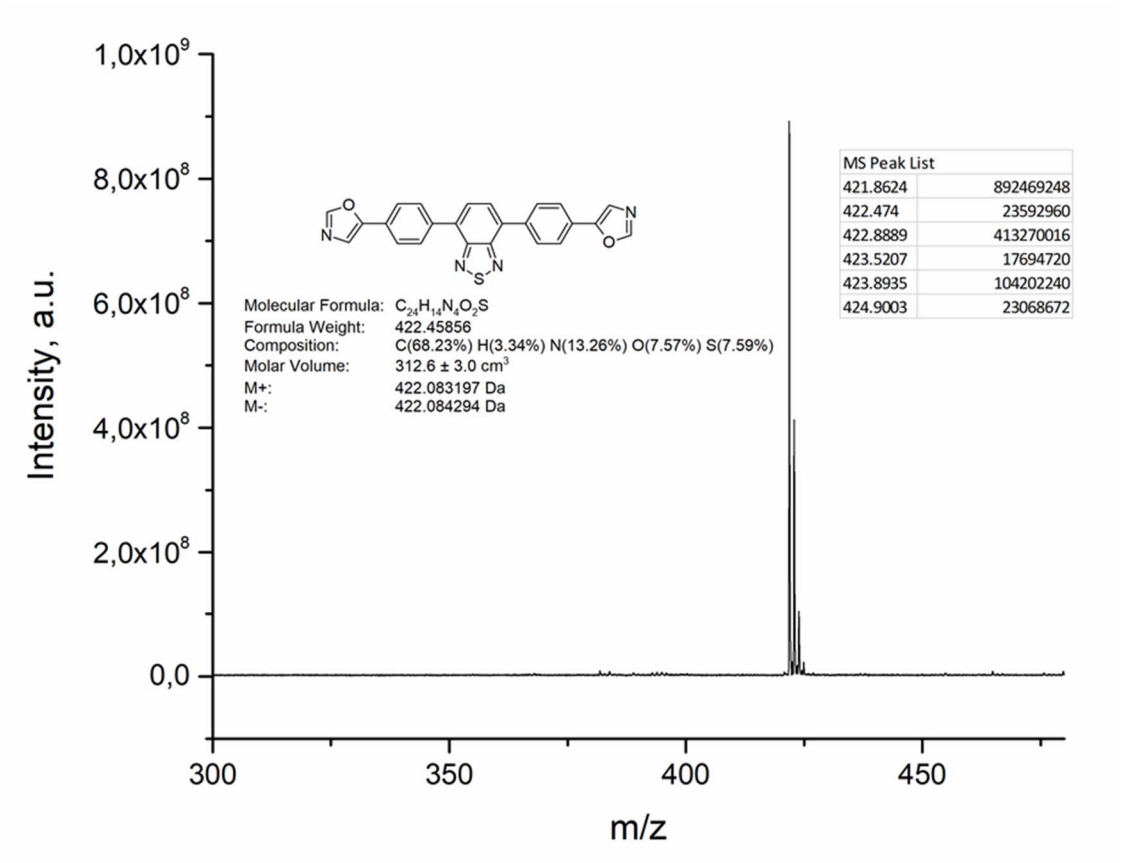



**Figure S3** MALDI-MS spectrum of **BTD(PO)$_2$**.

**S4. In situ polarizing microscopy in various phases**

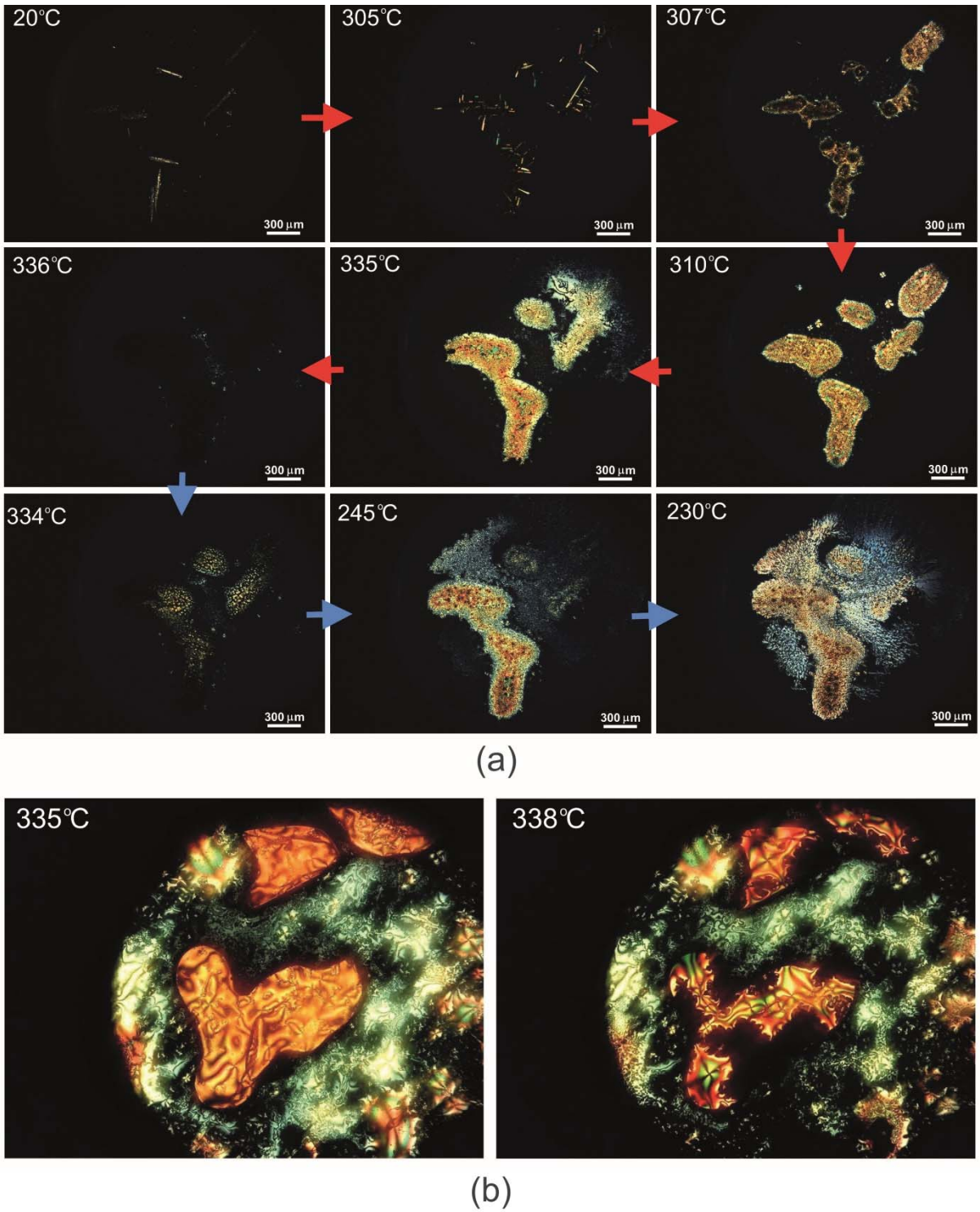
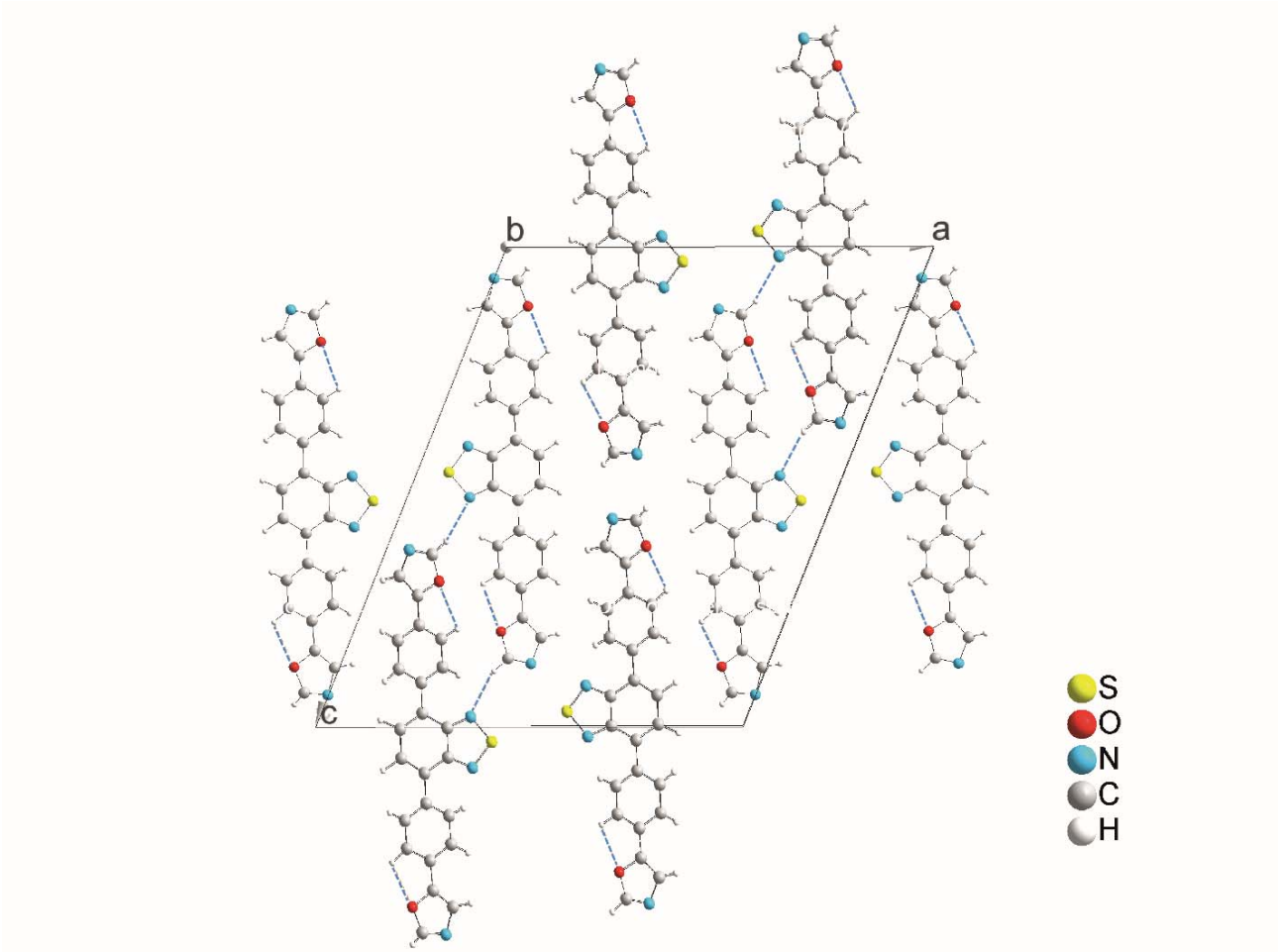
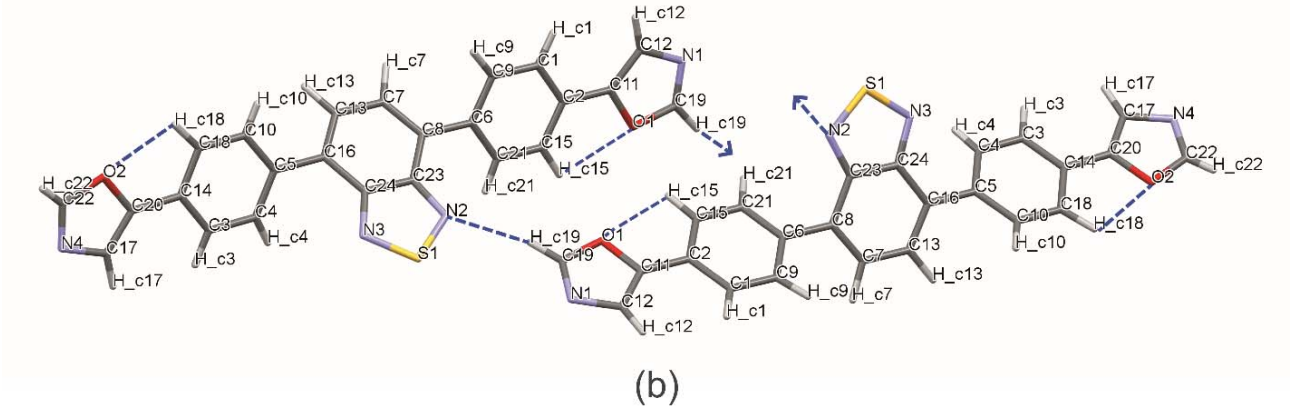



**Figure S4** Polarizing microphotographs of **BTD(PO)$_2$** at different temperatures during heating (red arrows) and cooling (blue arrows) (a) and mesophase near the transition temperature to the isotropic liquid state (b).

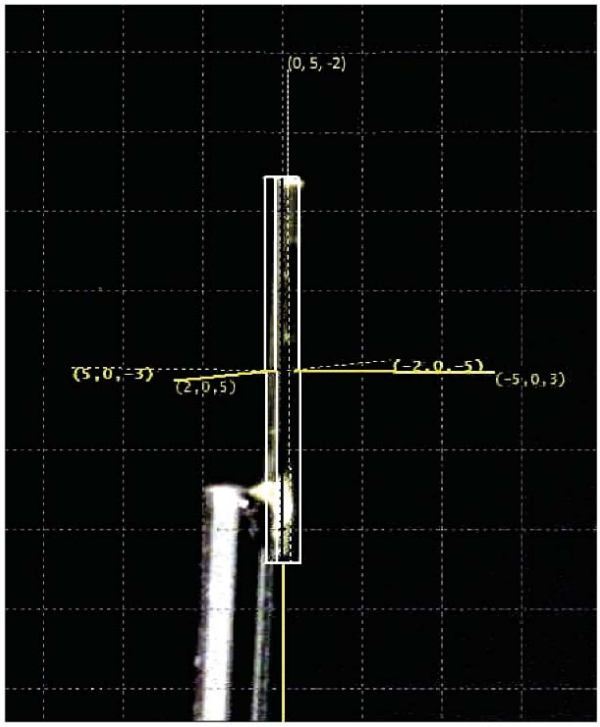
## S5. Crystal structure and habit




(a)




(b)




(c)

**Figure S5** Unit cell projection (a) and the position of the nearest molecules in the crystal (b), indicating the intramolecular and intermolecular H-bonds (blue dotted lines); (c) photographic image of a single crystal with face indices determined in the X-ray diffraction experiment.

## S6. Quantum chemical calculation

**Table S1** Calculated and experimental absorption / luminescence bands and FMO levels of the **BTD(PO)$_2$**.

| | Calculated | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|
| | Abs $\lambda_{max}$ (nm) | Abs $f_{osc}$ | Lum $\lambda_{max}$ (nm) | Lum $f_{osc}$ | 0-0 transition (nm) | 0-0 transition ($cm^{-1}$) | Orbitals | HOMO (eV) | LUMO (eV) |
| hexane | 380/279 | 0.93/1.29 | 515 | 1.01 | 441 | 22678 | H→L/H→L+1 | -6.88 | -1.44 |
| toluene | 381/280 | 0.95/1.31 | 520 | 1.03 | 443 | 22578 | | -6.88 | -1.43 |
| THF | 380/279 | 0.91/1.31 | 519 | 1.03 | 452 | 22108 | | -6.87 | -1.41 |
| | Experimental | | | | | | | | |
| | Abs $\lambda_{max}$ (nm) | $f_{osc.}$ abs | Lum $\lambda_{max.}$ (nm) | Lum QY (%) | 0-0 transition (nm) | 0-0 transition ($cm^{-1}$) | | | |
| hexane | 400/306 | - | 503 | 66 | 451 | 22170 | | | |
| toluene | 404/310 | 0.63/1.38 | 510 | 87 | 459 | 21790 | | | |
| THF | 402/308 | 0.64/1.37 | 517 | 96 | 463 | 21600 | | | |

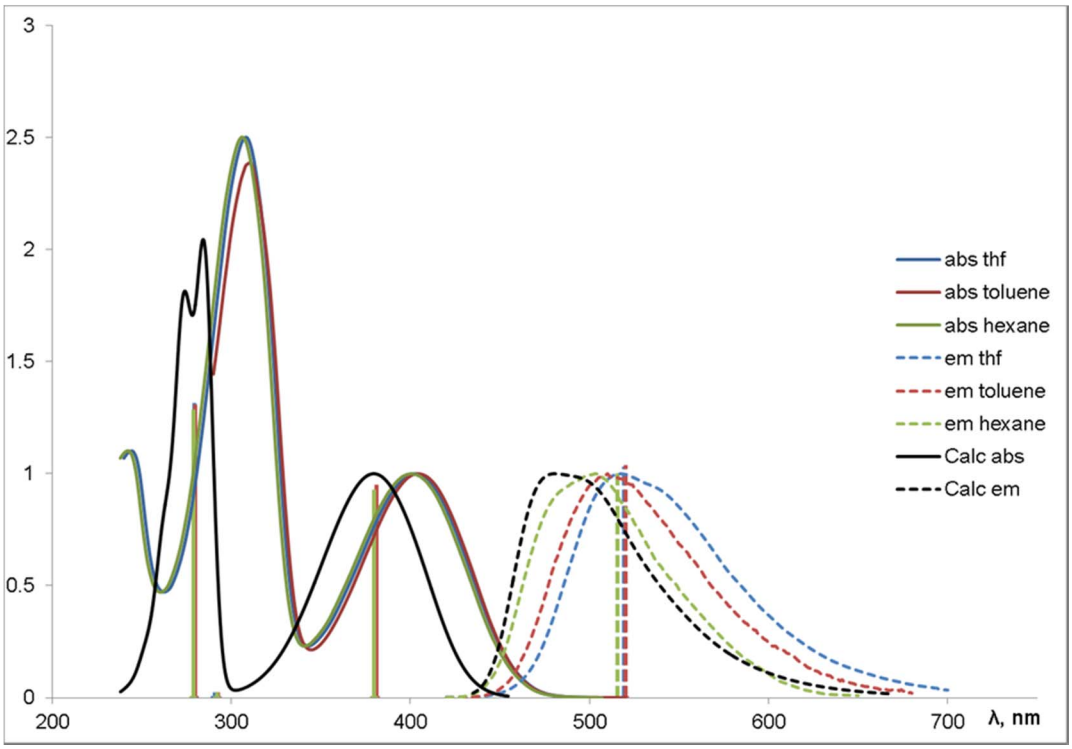



**Figure S6** Absorption (solid lines) and emission (dashed lines) spectra of **BTD(PO)$_2$** calculated using the vibronic model (black) and experimental in THF (blue), toluene (red), and hexane (green). Vertical lines correspond to the vertical electronic transitions.