Electronic Supplementary Material (ESI) for Journal of Materials Chemistry C.


# Hiding and reading of information in a mechanochromic system of 2,5-dicarbazole-substituted terephthalate derivative

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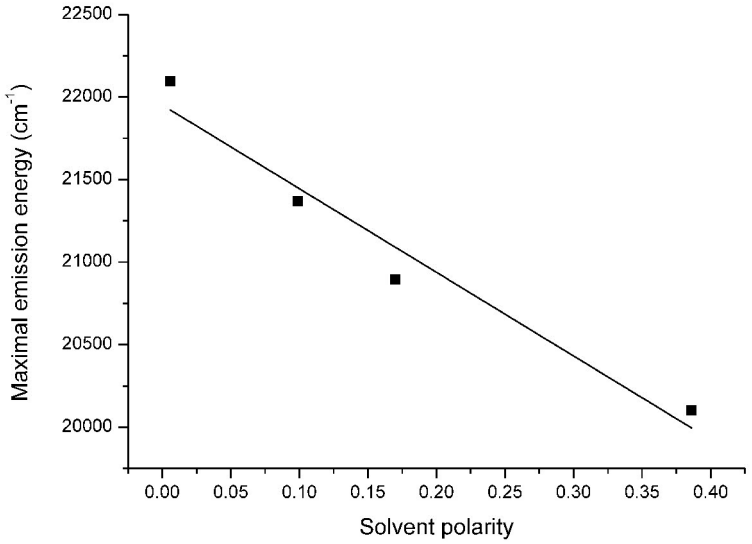


**Fig. S1** Lippert–Mataga plot: fluorescence emission maximum energy of BOCTA as a function of solvent polarity.

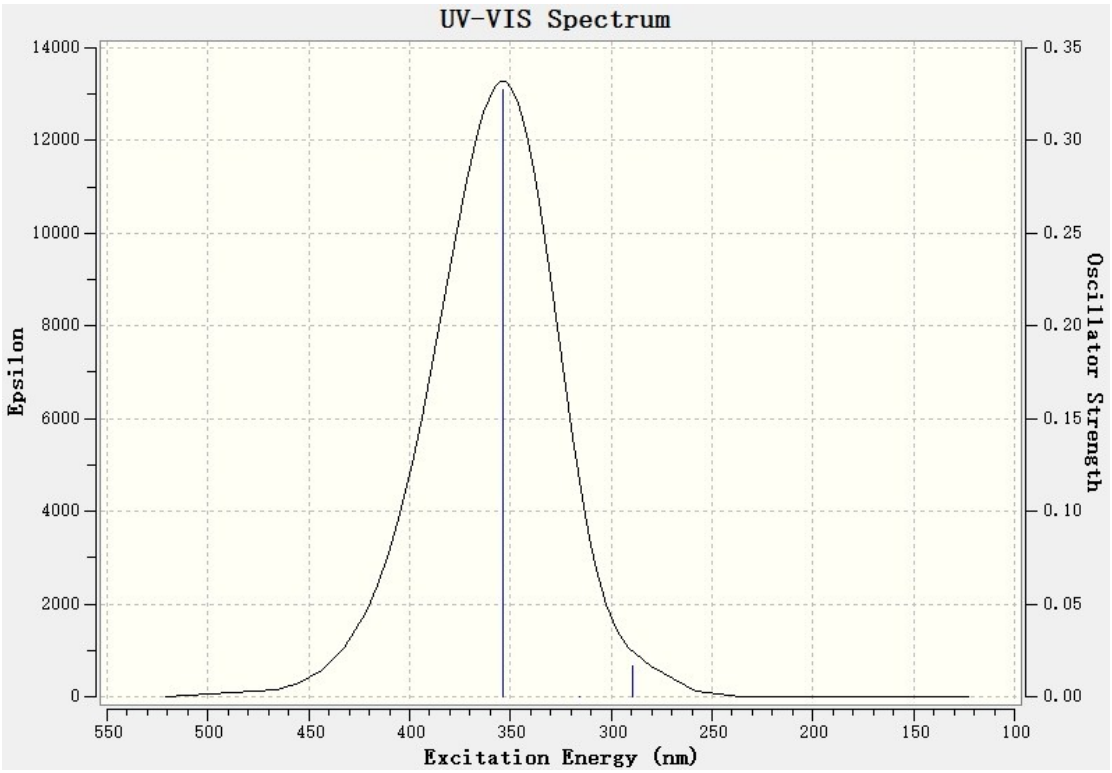


**Fig. S2** Simulated absorption spectrum of BOCTA by the TD/DFT-CAM-B3LYP/6-31G(d) calculation.

**Table S1.** Photophysical data of BOCTA obtained by quantum chemical calculation.

| | Transition assignment | E (eV) | $\lambda_{abs}$ (nm) | Oscillator strength |
|---|---|---|---|---|
| BOCTA | HOMO-4→LUMO (7.8%)<br>HOMO-2→LUMO (4.6%)<br>HOMO→LUMO (81.8%) | 3.5037 eV | 353.87 nm | 0.3277 |

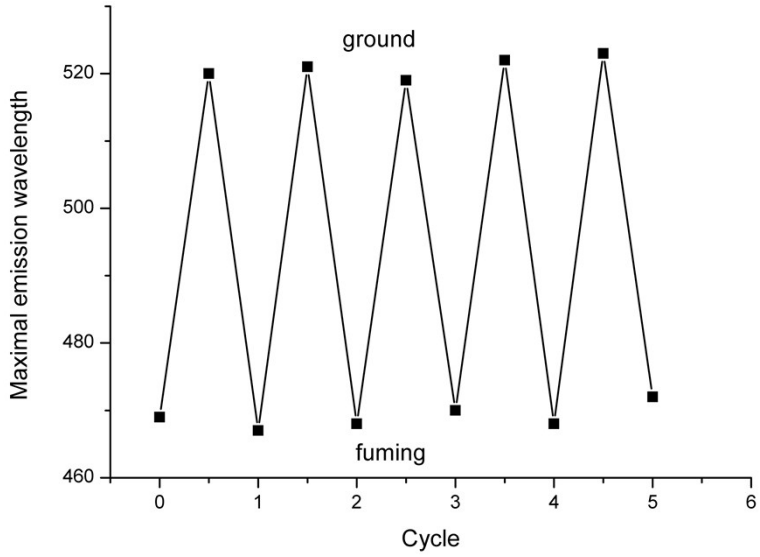


**Fig. S3** Change of maximal emission wavelength during the grinding-fuming cycle.

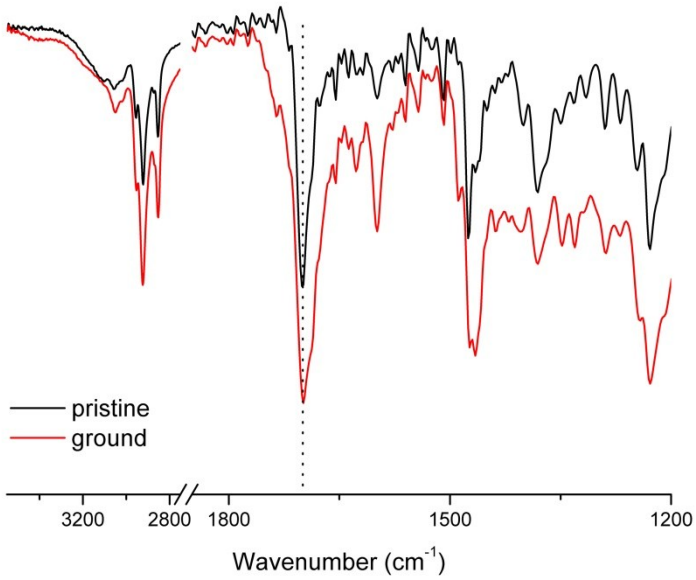


**Fig. S4** FT-IR spectra of pristine and ground solids.

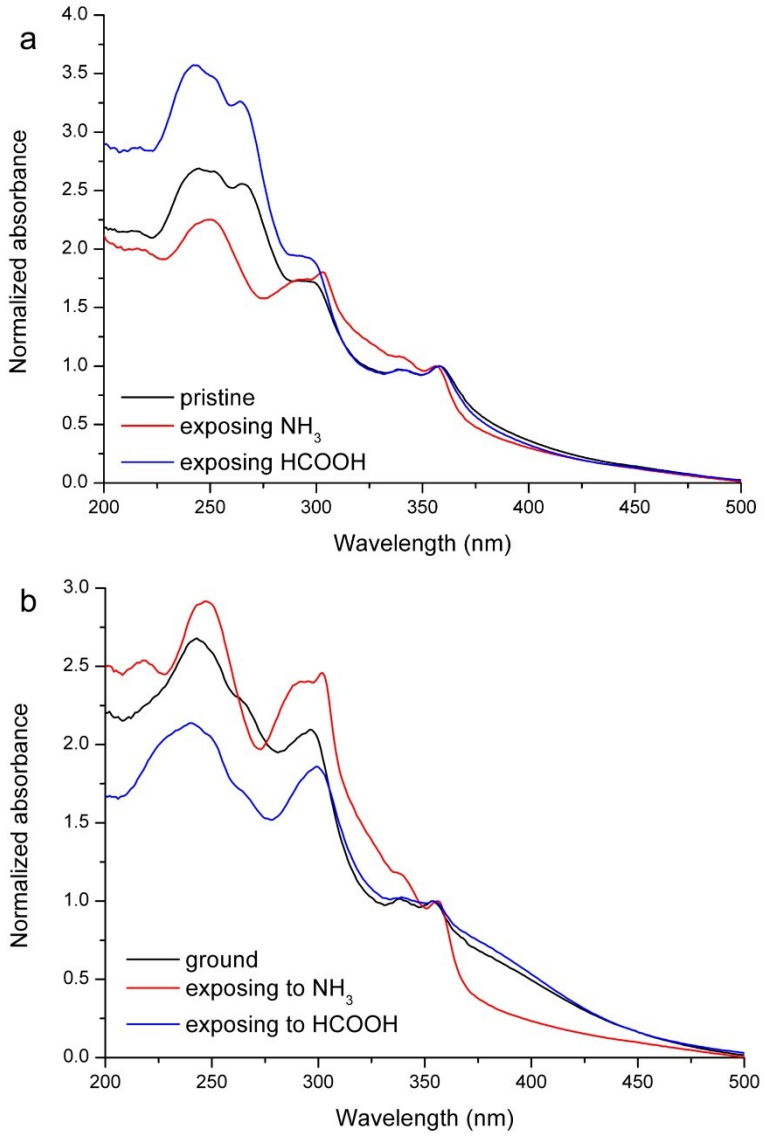


**Fig. S5** UV-vis absorption spectra of (a) pristine and (b) solids upon exposure to $NH_3$ and then formic acid vapors.

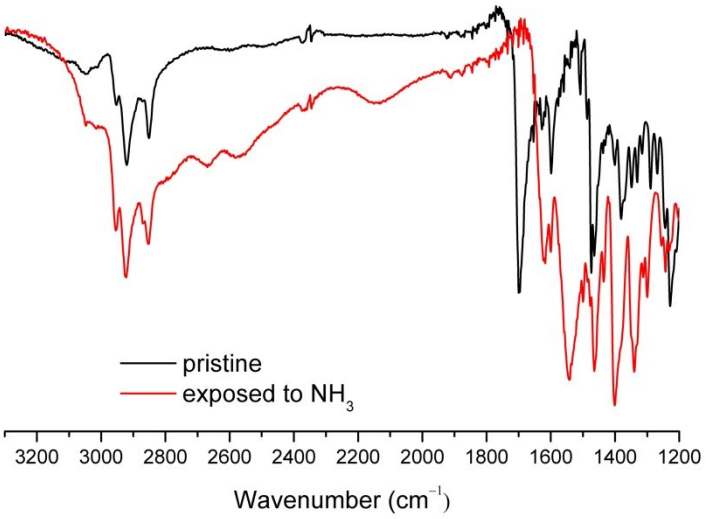


**Fig. S6** FT-IR spectra of pristine and fumed solids.

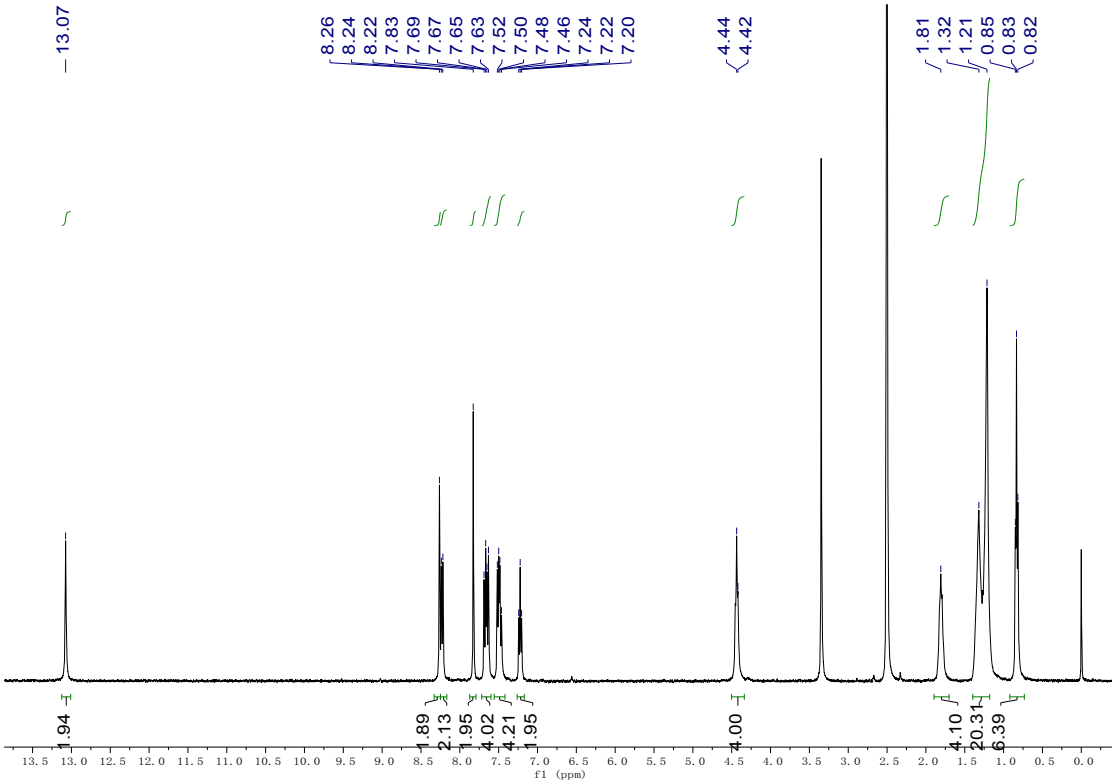


**Fig. S7** $^{1}$H NMR spectrum of BOCTA in $D_6$-DMSO.

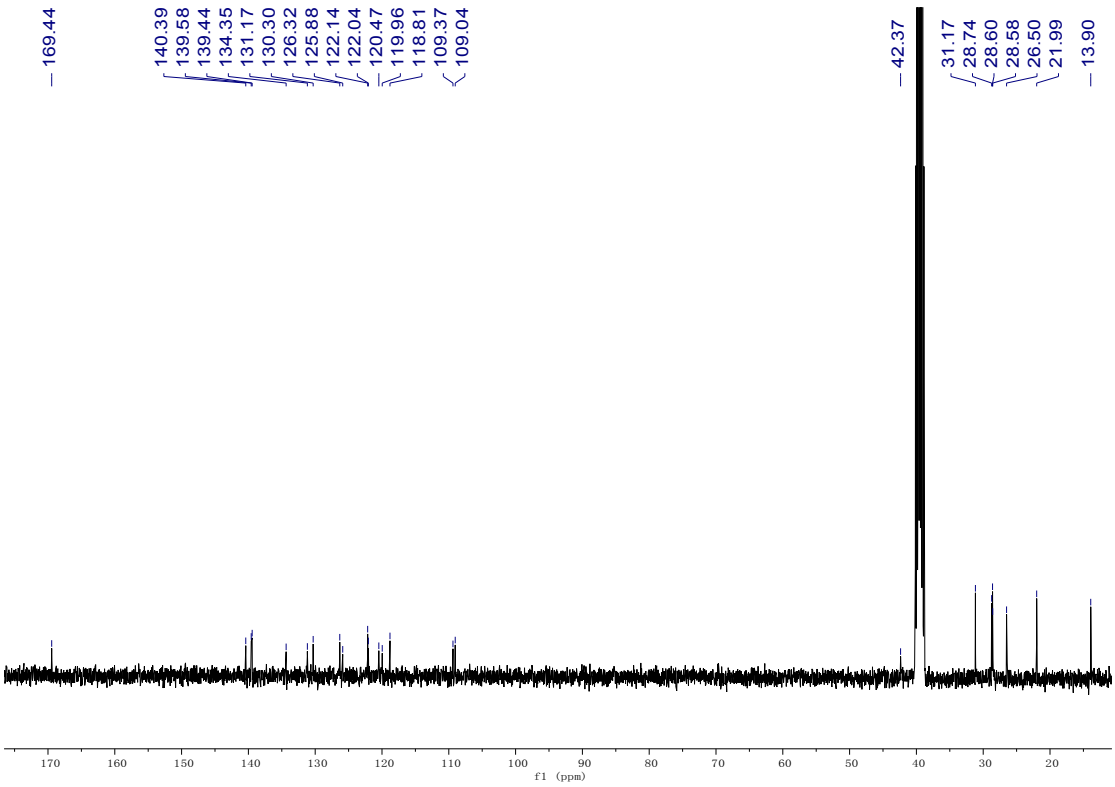


**Fig. S8** $^{13}$C NMR spectrum of BOCTA in $D_6$-DMSO.

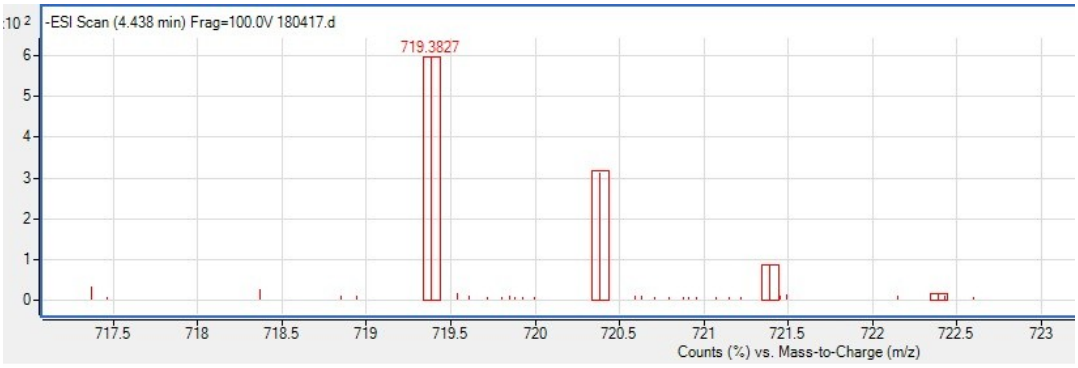


**Fig. S9** HRMS spectrum of BOCTA as anion.