

Supplementary Information

Doping of charge-transfer molecules in cocrystals for the design of materials with novel piezo-activated luminescence

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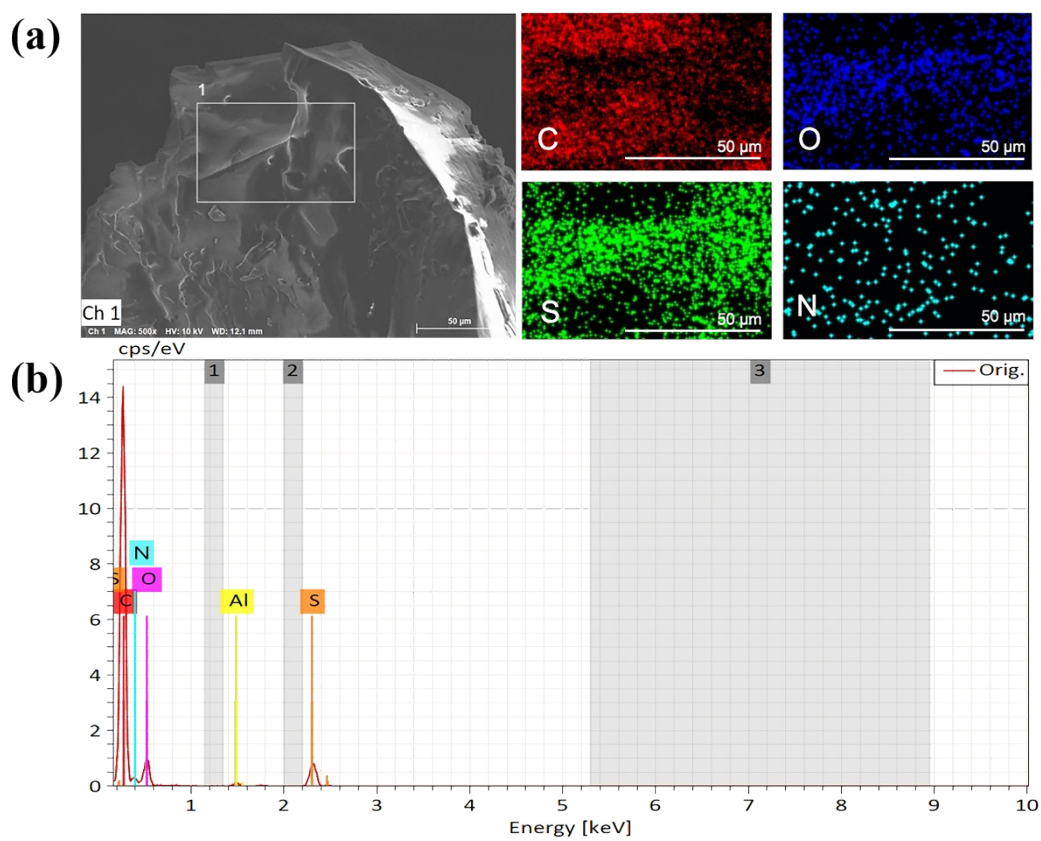


Fig. S1. (a) Scanning electron microscope (SEM) image and the corresponding EDS mappings of the gray box area for PTCs:THT; (b) The EDS spectra recorded from the gray box area.

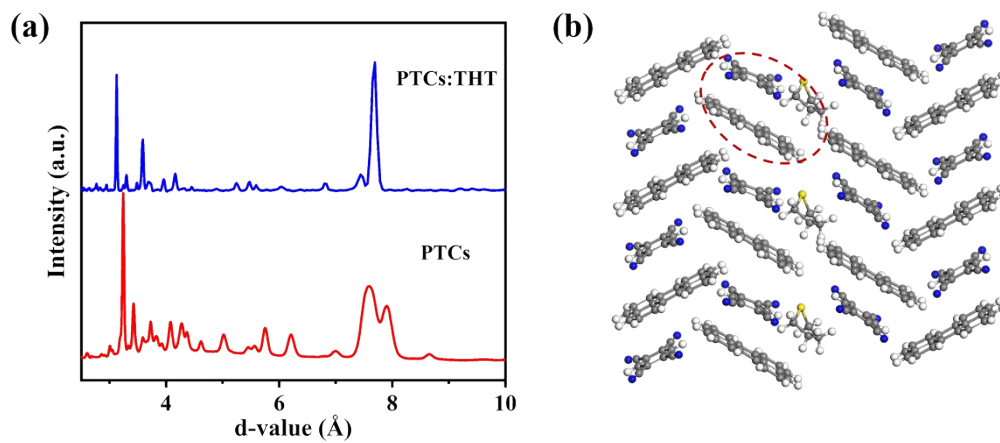


Fig. S2. (a) The XRD patterns of PTCs:THT and PTCs; (b) The sketch map for the molecular packing of PTCs:THT.

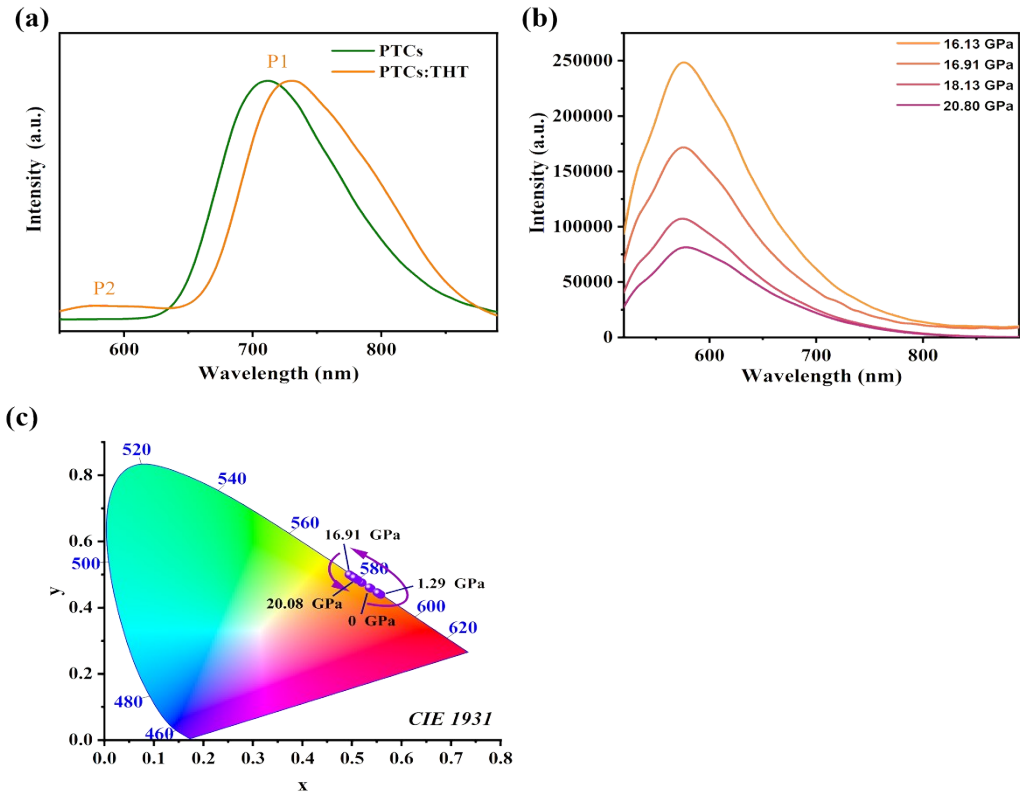


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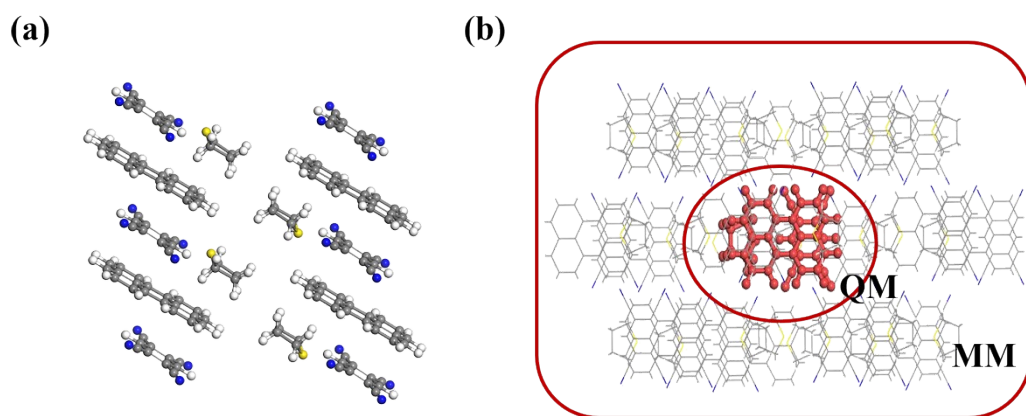


Fig. S4. The sketch map for molecular packing (a) and QM/MM model (b) of PTC-THT.

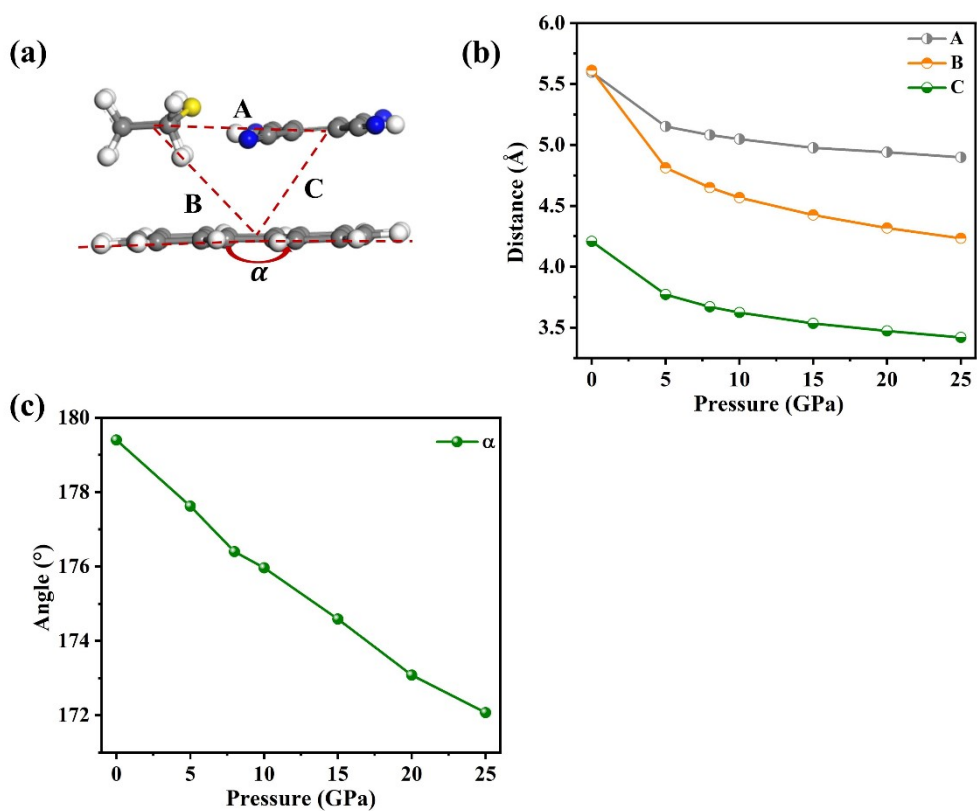


Fig. S5. (a) The definition of parameters A, B, C and α for describing molecular configurations of PTC-THT (parameters A, B and C represent the distances indicated by the dashed lines, while angle α represents the degree of distortion of perylene); the plotted curves for the change of (b) A, B, C and (c) angle α for PTC-THT as pressure increases.

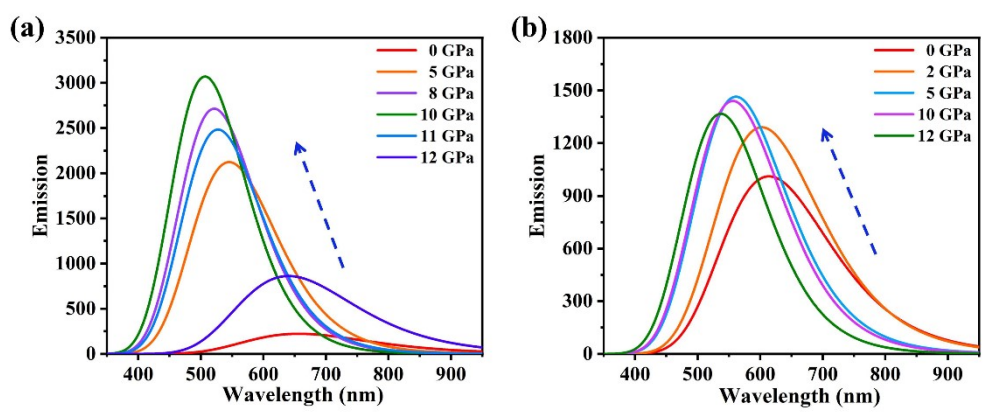


Fig. S6. The calculated luminescence spectra of (a) PTC-THP and (b) PTC-THF at different pressures.

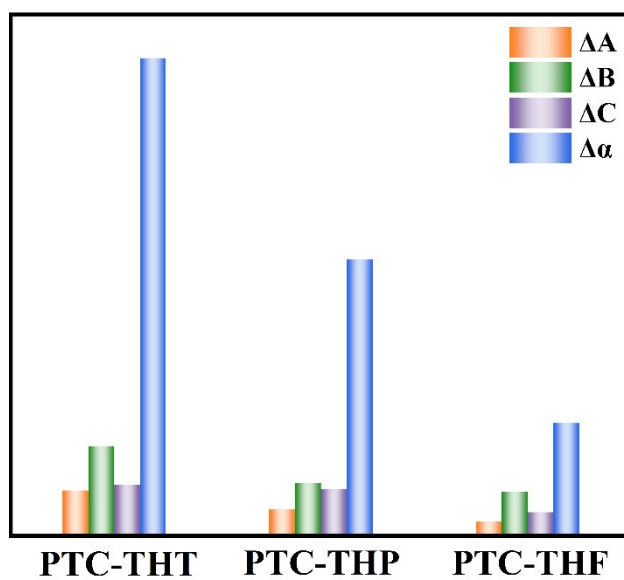


Fig. S7. The changes of A, B, C and α (defined in Fig. S5) for describing molecular configurations of PTC-THT, PTC-THP and PTC-THF in the range from ambient pressure to the pressure where the corresponding luminescence gets the strongest.

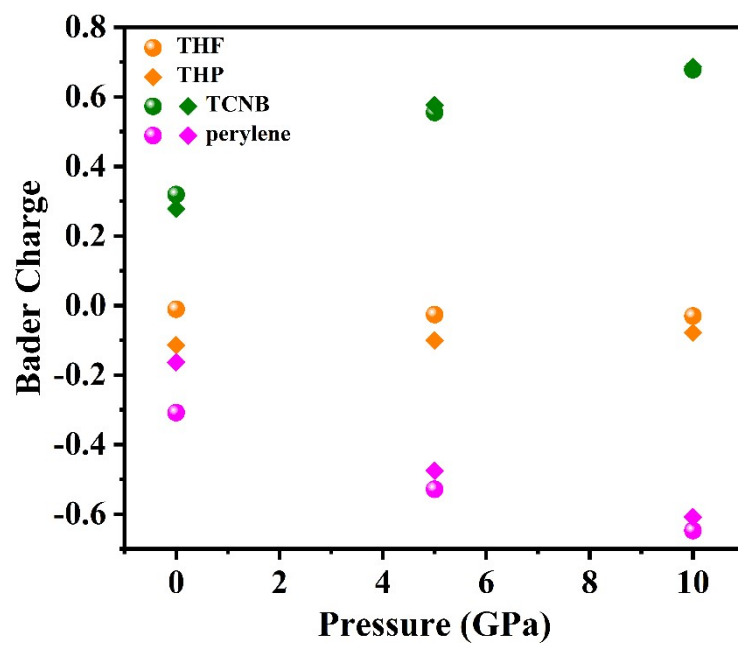


Fig. S8. The calculated Bader Charge of PTC-THP and PTC-THF at high pressures.