Electronic Supplementary Material (ESI) for CrystEngComm.

Self-reversible thermofluorochromism of D-A-D triphenylamine derivatives and effect of molecular conformation and packing

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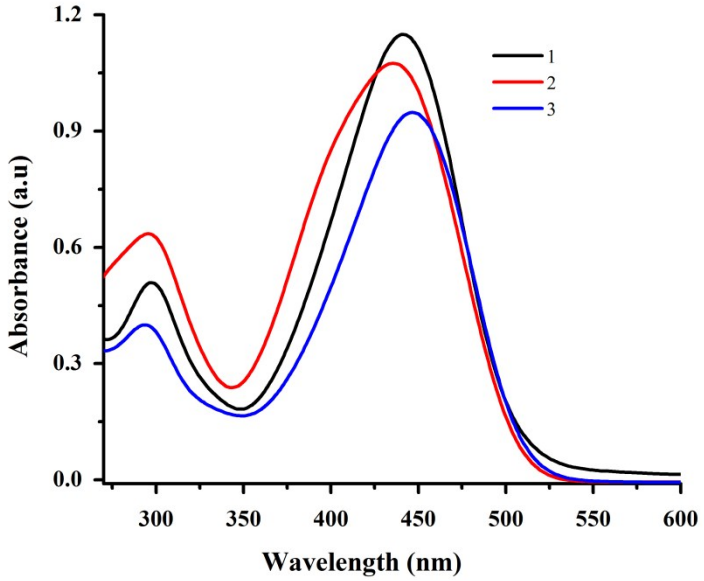

Figure S1. Absorption spectra of 1, 2 and 3 in CH_3CN.

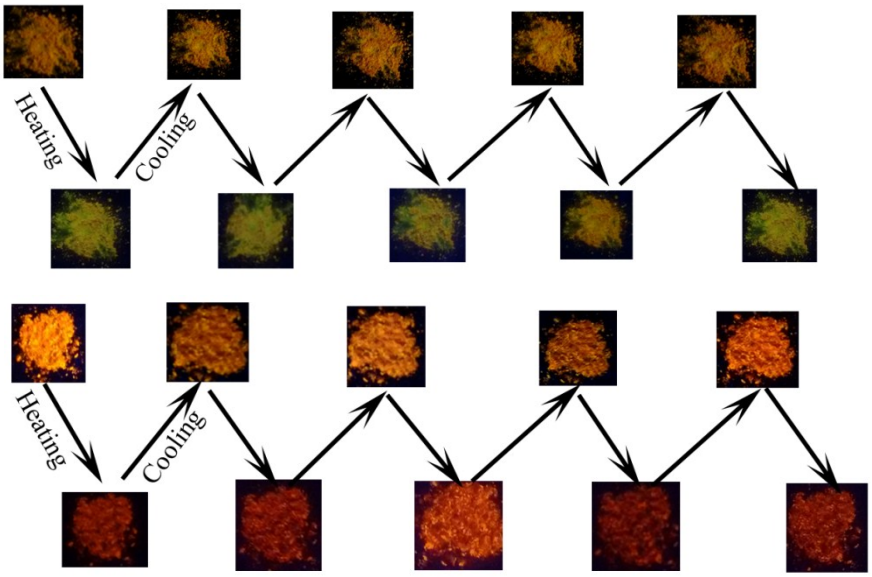

Figure S2. Heating and cooling cycle studies of **1** and **2**.

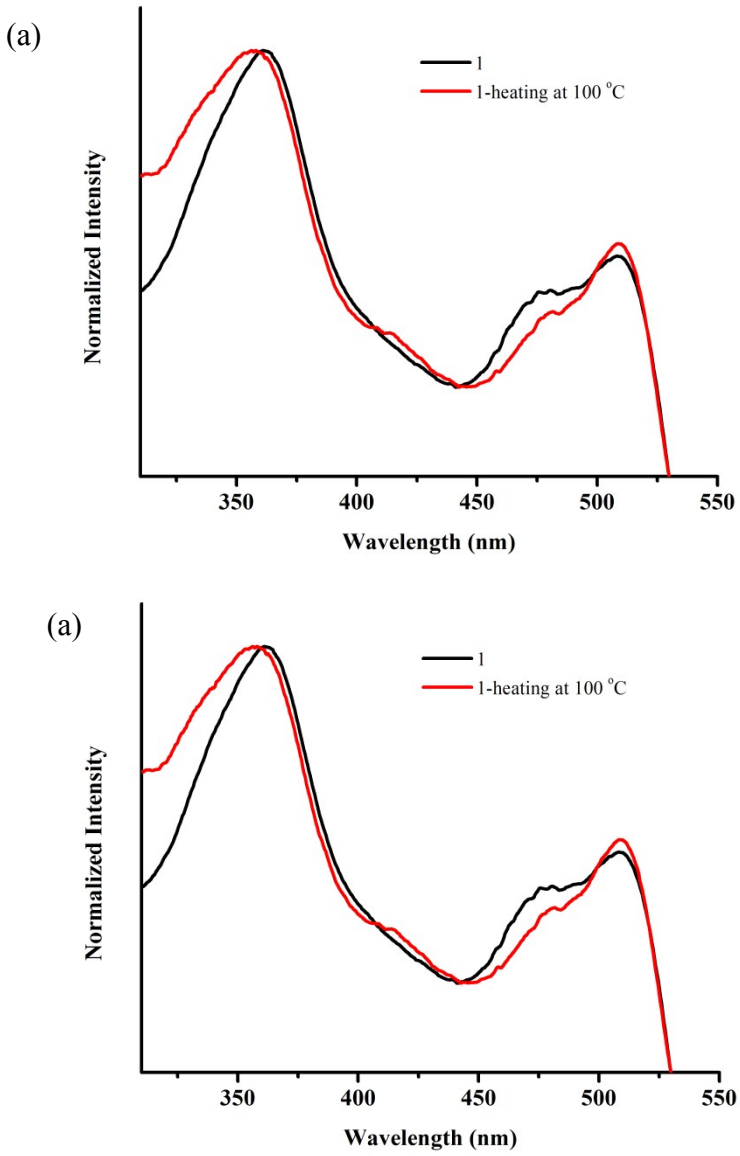

Figure S3. Excitation spectra of (a) 1 and (b) 2 before and after heating.

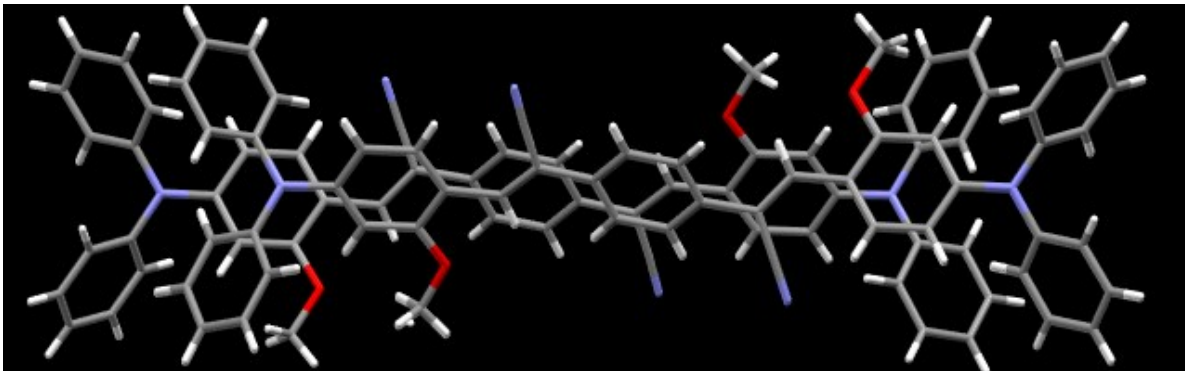

Figure S4. ABAB pattern of 2 in the crystal lattice. C (grey), N (blue), O (red), H (white).

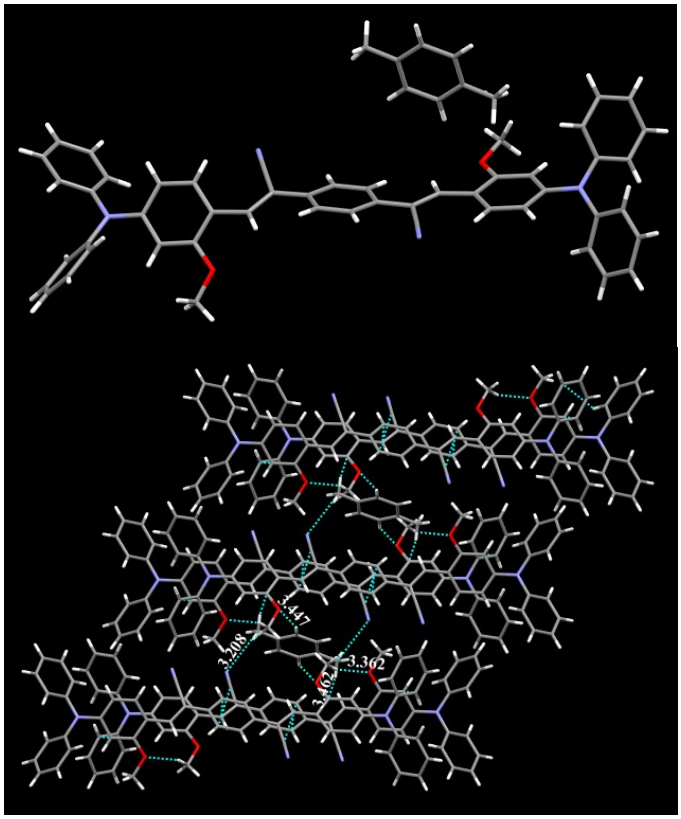

Figure S5. Inclusion of toluene in the crystal lattice of 2 and different intermolecular interactions involved in the crystal lattice.

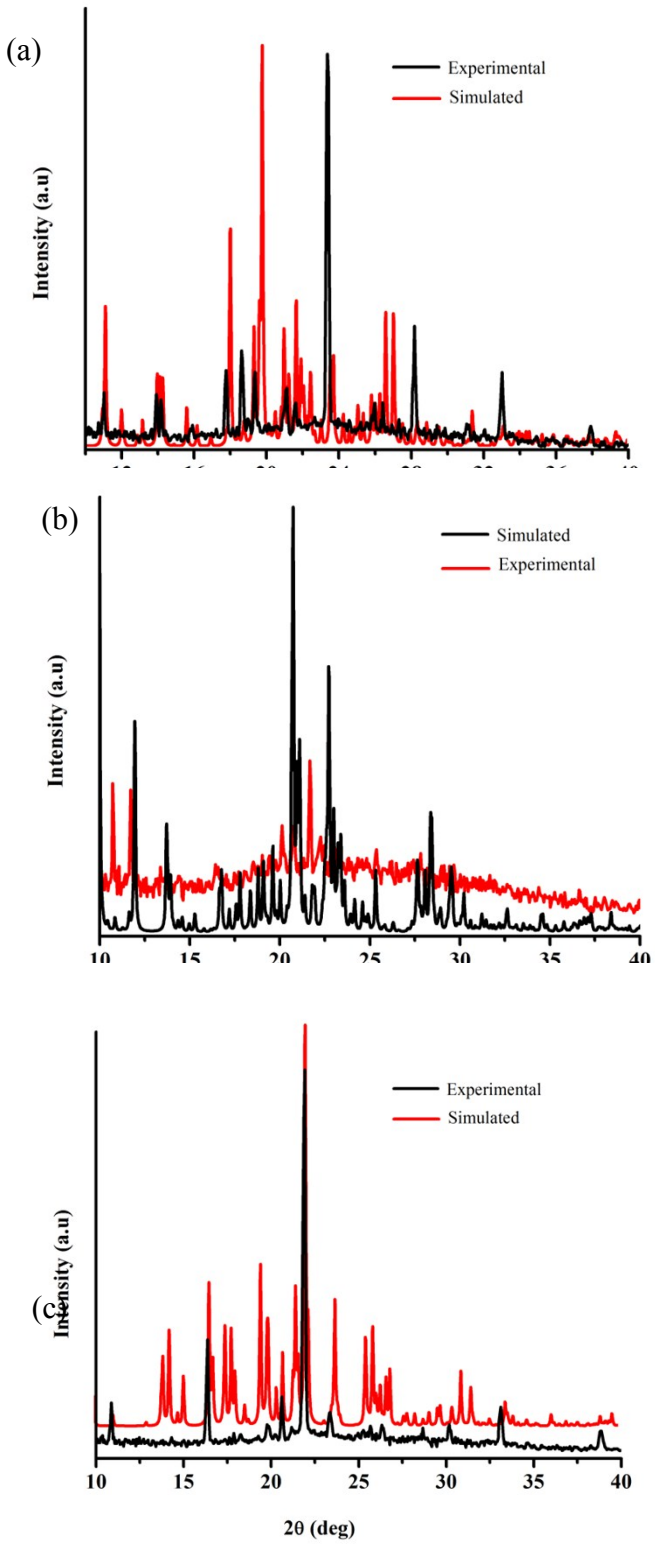

Figure S6. PXRD pattern of experimental and simulated (a) 1, (b) 2 and (c) 3..

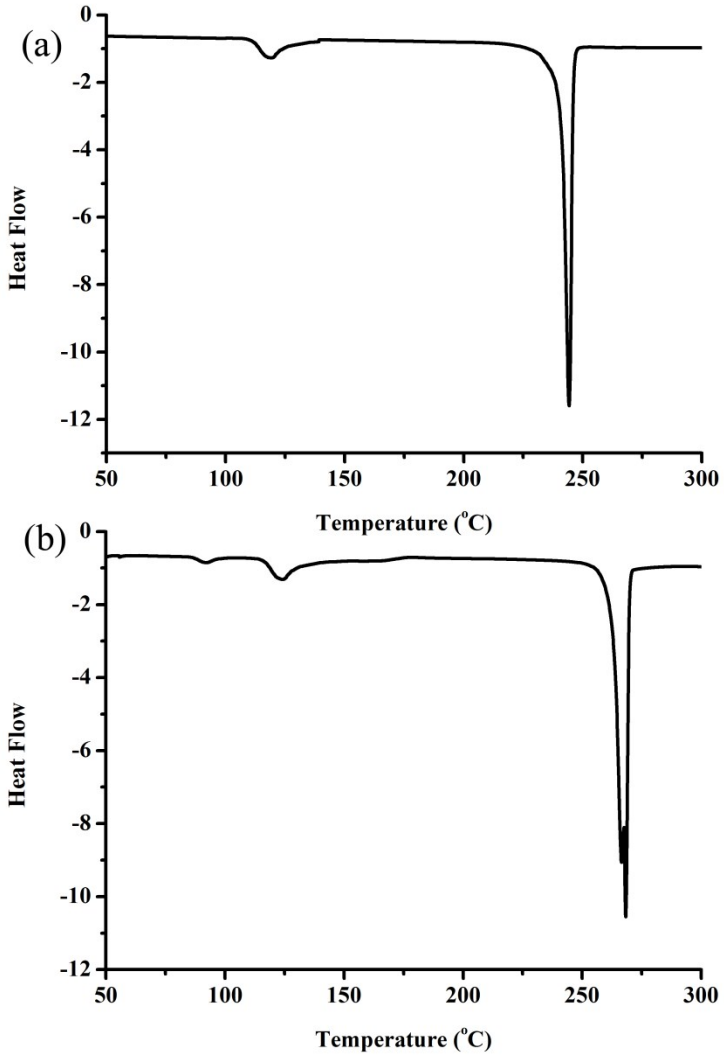

Figure S7. DSC of (a) **1** and (b) **2**.

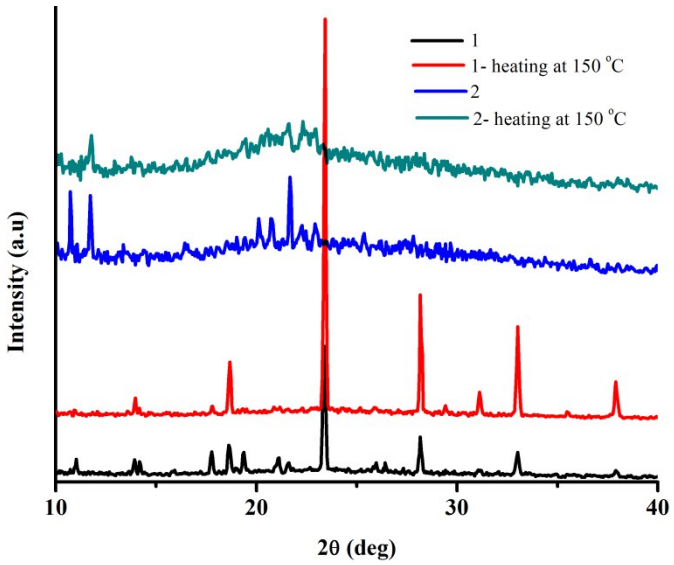

Figure S8. PXRD pattern of 1 and 2 before and after heating.

Table S1. HOMO-LUMO energy level of 1-3.

	HOMO (eV)	LUMO (eV)	Band gap (eV)
1	-5.336	-2.498	2.838
2	-5.173	-2.302	2.871
3	-5.172	-2.340	2.832