

Supplementary Information

Enhanced luminescence of single-benzene fluorescent molecules through halogen bond cocrystals

Fei Yu ^a, Xiunan Zhang ^a, Hongtu Zhao ^a, Zhicheng Jiang^{a,b}, Ting Wang^{a,b*}, Na
Wang^{a,b}, Xin Huang^{a,b}, Lina Zhou^{a,b}, Hongxun Hao ^{a,b,c*}

^a National Engineering Research Center of Industrial Crystallization Technology, School of Chemical Engineering and Technology, Tianjin University, Tianjin 300072, China

^b Collaborative Innovation Center of Chemical Science and Engineering (Tianjin), Tianjin, 300072, China

^c School of Chemical Engineering and Technology, Hainan University, Haikou 570208, China

Table S1. Some currently reported examples of halogen-bonded co-crystals¹⁻⁹

No.	Acceptor	Donner	Halogen bonds
1			I...O (3.11 Å) I...S (3.23 Å)
2			I...N (2.99 Å) I...S (3.17 Å)
3			I...N (2.821 Å, 2.846 Å) I...N (2.811)
4			I...N (2.932 Å, 2.902 Å, 2.934 Å, 2.927 Å)
5			I...N (2.95 Å, 2.81 Å)
6			I...N (3.000 Å, 2.84 Å)
7			I...N (2.988 Å, 2.907 Å) I...N (2.845 Å, 2.992 Å)
8			I...N (3.02 Å) Br...N (3.00 Å) Br...N (3.06 Å)
9			I...N (2.84 Å) Br...N (2.96 Å)
10			I...O (3.023 Å, 3.231 Å, 3.444 Å, 3.514 Å) I...O (3.498 Å, 3.225 Å)

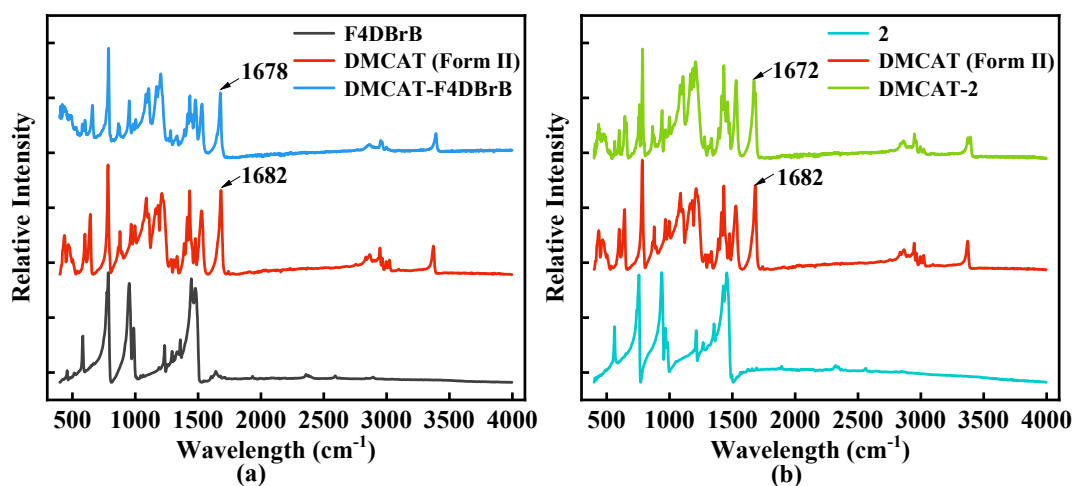
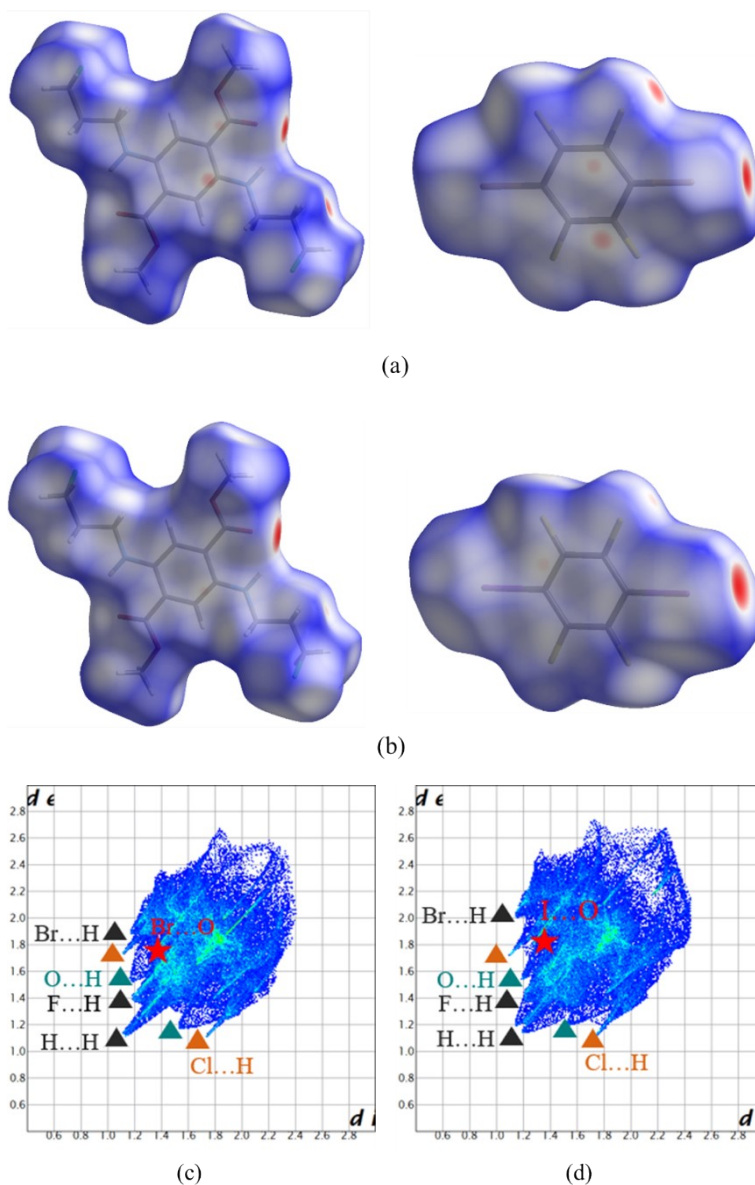


Figure S1. FT-IR spectra of (a) DMCAT-1 and (b) DMCAT-2, including corresponding co-formers and two polymorphs of DMCAT.



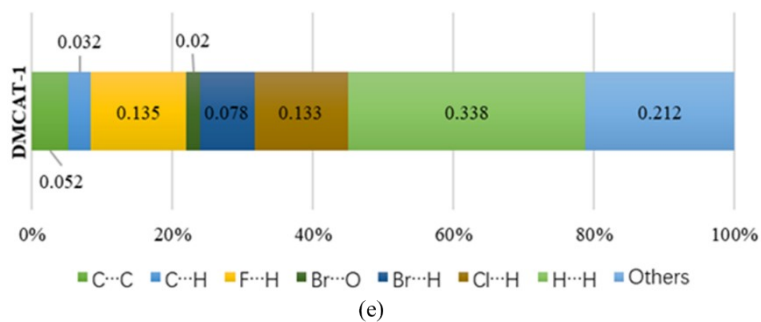
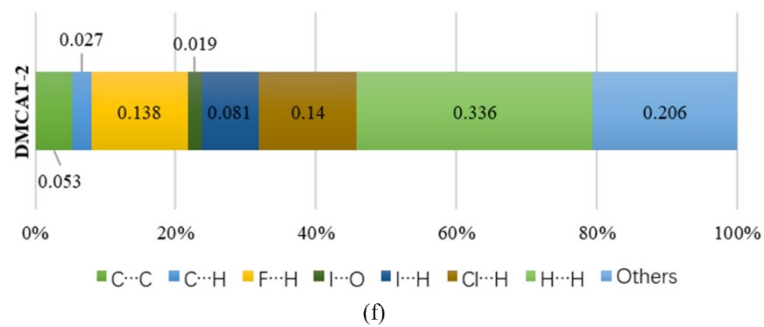
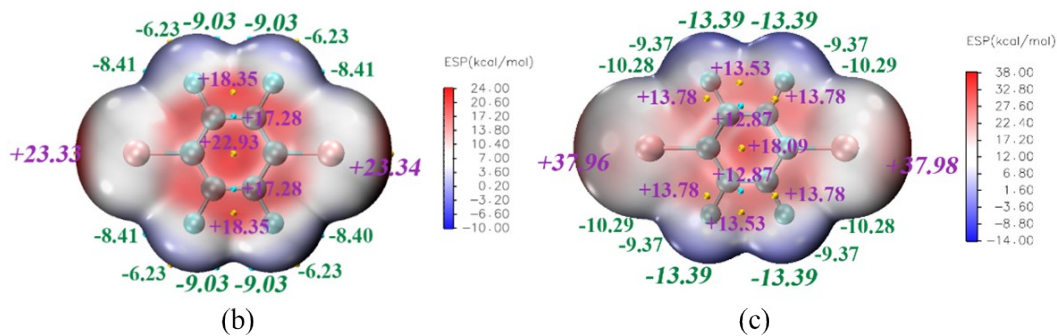
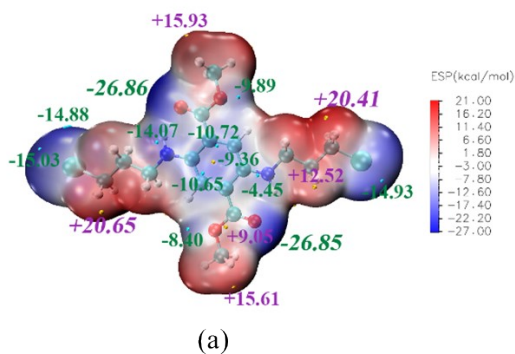


Figure S2. Hirshfeld surfaces for (a) DMCAT-1, (b) DMCAT-2; 2D fingerprint plots for (c) DMCAT-1, (d) DMCAT-2; Contributions to the Hirshfeld surface area in (e) DMCAT-1, (f) DMCAT-2.



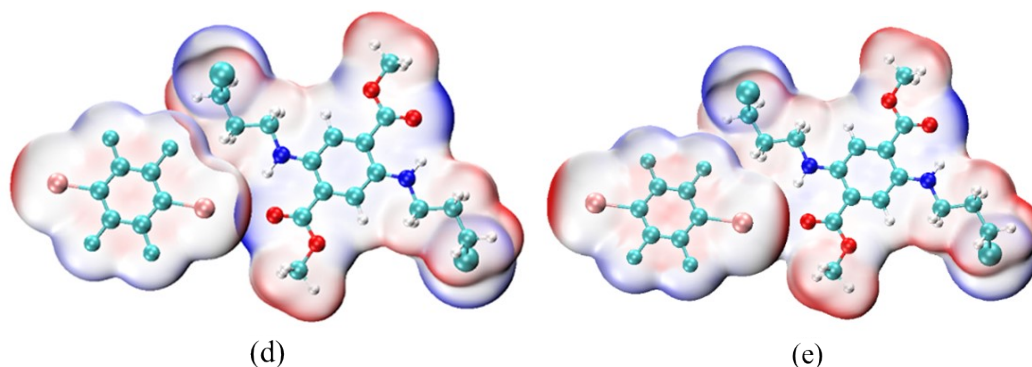


Figure S3. Molecular electrostatic potential maps of (a) DMCAT and (b) co-former 1 and (c) co-former 2. (The maxima and minima of the MEP points are indicated in purple and green italics, respectively.); Intermolecular van der Waals surface penetration map of (d) DMCAT-1 and (e) DMCAT-2.

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