Supporting information

Influence of molecular width on the thermal expansion in solids

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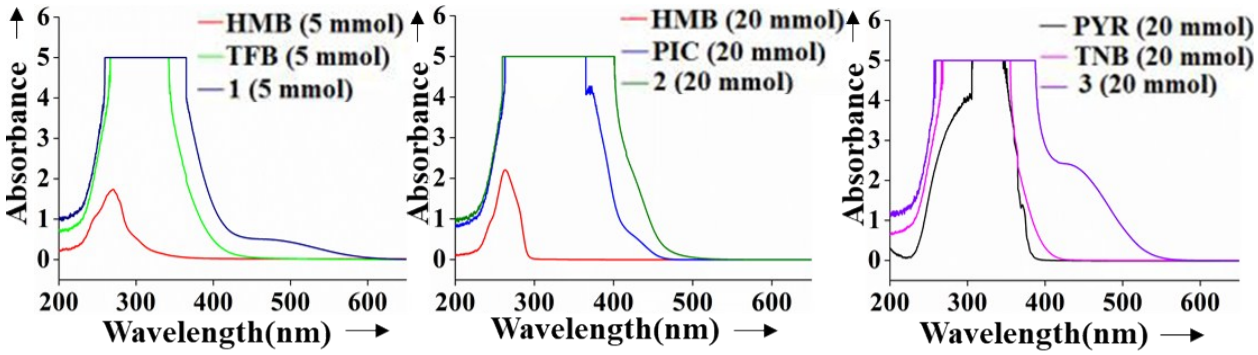
Contents:

(a)



(b)

Fig. S1 (a) Colours and (b) UV-vis spectra of the three charge transfer complexes (**1**–**3**) and their individual components (HMB: hexamethylbenzene, PYR: pyrene, TFB: tetrafluoro-1,4-benzoquinone, PIC: picric acid and TNB: 1,3,5-trinitrobenzene).

Table S1. Crystallographic details of **1** (1:1 hexamethylbenzene/tetrafluro-1,4-benzoquinone co-crystal) and **3** (1:1 pyrine/trinitrobenzene co-crystal) at two different temperatures for each.

Identification code	1-190k	1-298K	3-118	3-298k
Empirical formula	$C_{18}H_{18}F_4O_2$	$C_{18}H_{18}F_4O_2$	$C_{22}H_{13}N_3O_6$	$C_{22}H_{13}N_3O_6$
Formula weight	342.32	342.32	415.35	415.35
Temperature/K	190(2)	298(2)	118(2)	298(2)
Crystal system	trigonal	trigonal	triclinic	triclinic
Space group	$R\bar{3}m$	$R\bar{3}m$	$P\bar{1}$	$P\bar{1}$
a/Å	14.5418(12)	14.6259(12)	6.6469(4)	6.7752(5)
b/Å	14.5418(12)	14.6259(12)	8.4809(6)	8.5522(9)
c/Å	6.6076(8)	6.7359(6)	16.2117(12)	16.3550(15)
α/°	90	90	93.121(6)	93.041(8)
β/°	90	90	95.577(6)	95.628(7)
γ/°	120	120	101.583(6)	101.281(7)
Volume/Å^3	1210.1(2)	1247.9(2)	888.46(11)	922.34(14)
Z	3	3	2	2
ρ_{calc}g/cm^3	1.409	1.367	1.553	1.496
μ/mm^{-1}	0.121	0.118	0.116	0.112
F(000)	534.0	534.0	428.0	428.0
Crystal size/mm^3	0.8 × 0.25 × 0.18	0.8 × 0.25 × 0.18	0.6 × 0.2 × 0.15	0.6 × 0.2 × 0.15
Radiation	MoKα (λ = 0.71073)	MoKα (λ = 0.71073)	MoKα (λ = 0.71073)	MoKα (λ = 0.71073)
2Θ range for data collection/°	8.942 to 57.606	8.834 to 58.526	7.32 to 58.3	7.58 to 58.4
Index ranges	-15 ≤ h ≤ 16, -19 ≤ k ≤ 18, -4 ≤ l ≤ 8	-18 ≤ h ≤ 18, -19 ≤ k ≤ 19, -9 ≤ l ≤ 8	-9 ≤ h ≤ 8, -11 ≤ k ≤ 10, -21 ≤ l ≤ 22	-9 ≤ h ≤ 9, -11 ≤ k ≤ 11, -21 ≤ l ≤ 21
Reflections collected	1388	3935	9229	9322
Independent reflections	364 [R_{int} = 0.0171, R_{sigma} = 0.0161]	399 [R_{int} = 0.0315, R_{sigma} = 0.0132]	4009 [R_{int} = 0.0277, R_{sigma} = 0.0404]	4259 [R_{int} = 0.0318, R_{sigma} = 0.0522]
Data/restraints/parameters	364/0/33	399/0/33	4009/0/280	4259/0/281
Goodness-of-fit on F^2	1.085	1.042	1.061	1.009
Final R indexes [I>=2σ (I)]	R_1 = 0.0440, wR_2 = 0.1050	R_1 = 0.0530, wR_2 = 0.1293	R_1 = 0.0441, wR_2 = 0.1039	R_1 = 0.0571, wR_2 = 0.1273
Final R indexes [all data]	R_1 = 0.0622, wR_2 = 0.1166	R_1 = 0.0834, wR_2 = 0.1561	R_1 = 0.0614, wR_2 = 0.1159	R_1 = 0.1238, wR_2 = 0.1656
CCDC no.	1954373	1954374	1954375	1954376