

Solvent induced manipulation of Supramolecular Organic Frameworks

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Crystallographic data of frameworks

	1a	1b	2a	2b
Molecular formula	C ₅₂ H ₅₃ N ₄ O ₈	C ₅₆ H ₅₆ N ₄ O ₈	C ₁₃₄ H ₁₅₃ N ₁₁ O ₁₆	C ₁₂₃ H ₁₇₂ N ₁₀ O ₂₅
Formula weight	862.02	913.08	2173.76	2190.78
Crystal system	Monoclinic	Orthorhombic	Triclinic	Monoclinic
Space group	P2 ₁ /n	Iba1	P-1	P2 ₁ /n
Temp.(K)	173	100	173	100
a(Å)	11.31	27.03	14.17	17.69
b(Å)	14.44	18.31	16.37	20.02
c(Å)	27.01	19.17	26.37	34.76
α(°)	90	90	97.48	90
β(°)	94.70	90	95.91	98.45
γ(°)	90	90	102.92	90
V(Å ³)	4401.02	9493.32	5856.76	12186.09
Z	4	8	2	2

General procedure of growing crystals: In a 20 mL glass vial, 1mL 0.01M solution of R_sC in acetonitrile or ethanol was mixed with 2mL 0.01 M solution (in same solvent) of bpea molecule. The clear mixture was then sonicated for 5 minutes and allowed to stand for slow solvent evaporation. Crystals suitable for single-crystal X-ray diffraction were obtained over 4-7 days. Similar procedures were followed to grow the crystal for all the frameworks described in the article.