Supplementary Material

Preparation, Crystal Structure and Solution-Mediated Phase Transformation of a Novel Solid-State Form of CL-20

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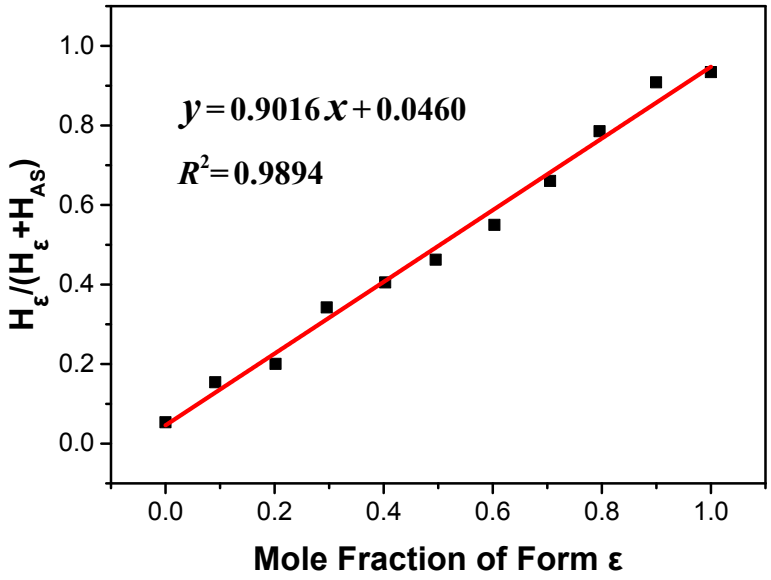

Fig. S1 Calibration curve of the Raman spectra. The H_ε and H_{AS} refer to the heights of the characteristic peak heights for form ε and acetonitrile solvate, respectively.

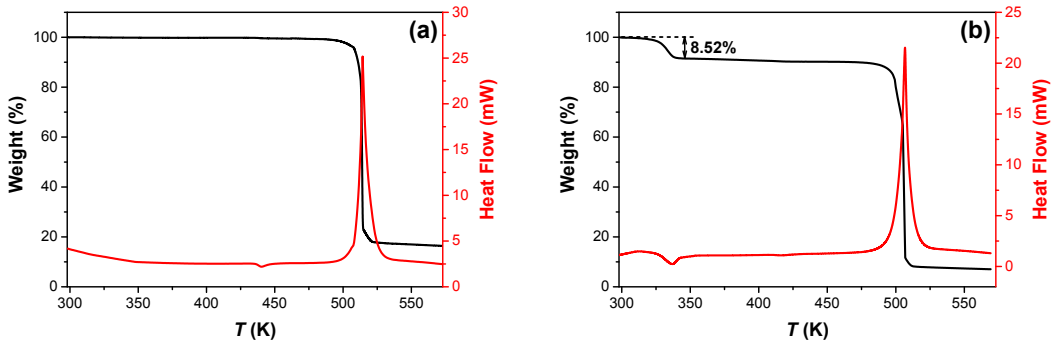

Fig. S2 The TGA/DSC curves of (a) form ε and (b) acetonitrile solvate.

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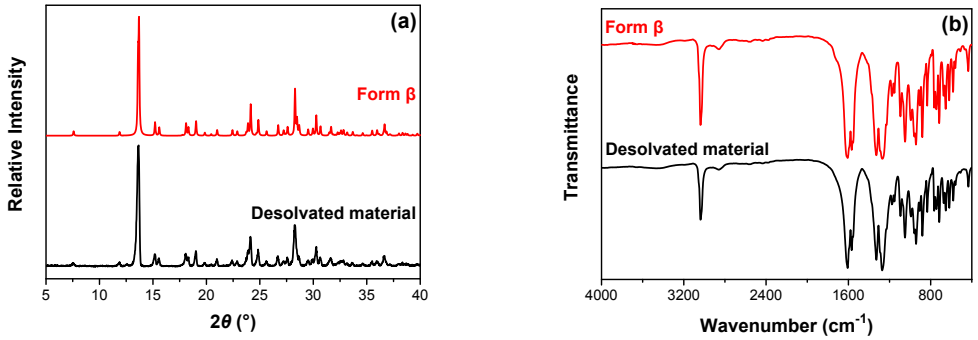

Fig. S3 The (a) PXRD patterns and (b) FTIR spectra of the desolvated material and form β.

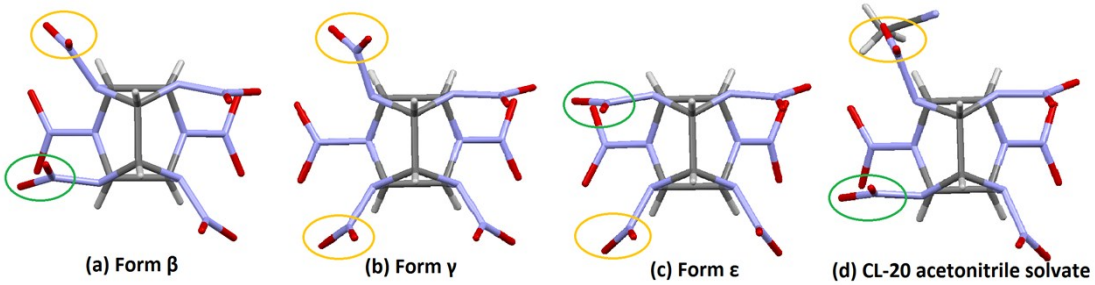

Fig. S4 Molecular conformations of (a) form β, (b) form γ, (c) form ε, and (d) acetonitrile solvate. Gray, white, red, and blue represent C, H, O, and N atoms, respectively. Orange and green circles represent the axial and equatorial orientations of NO_2 groups, respectively.

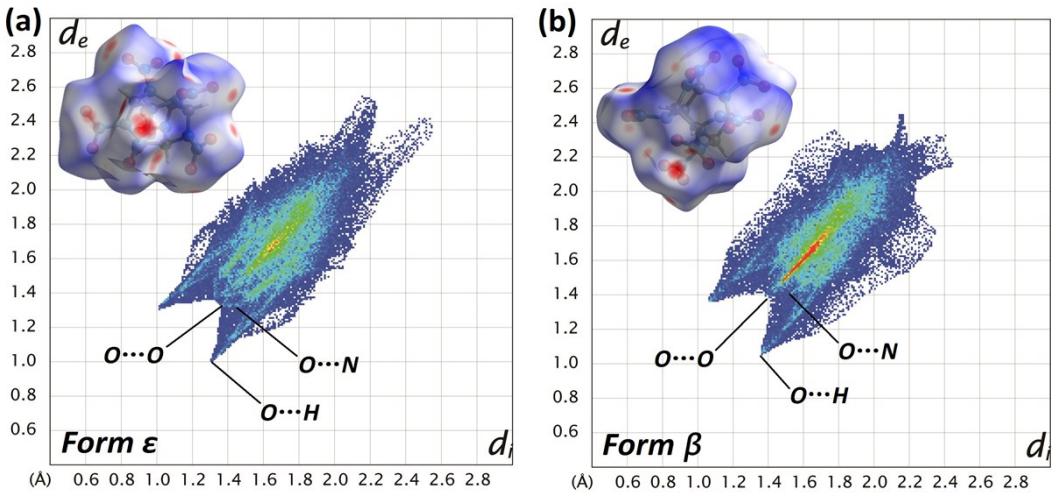

Fig. S5 The Hirshfeld surfaces mapped with d_{norm} and the 2D fingerprint plots for (a) form ε and (b) form β, respectively.

Table S1 Experimental mole fraction solubility data of acetonitrile solvate (x_{AS}) and form ε (x_ε) in acetonitrile-chloroform mixed solvents with different mole fractions of acetonitrile (x_A).

Mole Fraction of Acetonitrile	Acetonitrile Solvate			Form ε		
	x_{AS}	Average	Standard	x_ε	Average	Standard

x_A		value	Deviation		value	Deviation
	0.00120			0.00037		
0.150	0.00101	0.00110	0.00009	0.00041	0.00040	0.00003
	0.00108			0.00043		
	0.00126			0.00054		
0.175	0.00112	0.00120	0.00007	0.00052	0.00051	0.00002
	0.00123			0.00049		
	0.00138			0.00063		
0.200	0.00139	0.00135	0.00006	0.00065	0.00065	0.00003
	0.00129			0.00068		
	0.00144			0.00089		
0.225	0.00159	0.00152	0.00007	0.00087	0.00090	0.00004
	0.00152			0.00094		
	0.00183			0.00121		
0.250	0.00174	0.00179	0.00005	0.00124	0.00125	0.00004
	0.00180			0.00129		

Table S2 Experimental mole fraction solubility data of acetonitrile solvate (x_{AS}) and form ε (x_ε) in acetonitrile-chloroform mixed solvent (x_A=0.20) under different temperatures.

Temperature/K	Acetonitrile Solvate			Form ε		
	x_{AS}	Average value	Standard Deviation	x_ε	Average value	Standard Deviation
	0.00131			0.00063		
298.15	0.00121	0.00126	0.00005	0.00061	0.00060	0.00003
	0.00127			0.00057		
	0.00142			0.00063		
303.15	0.00143	0.00139	0.00006	0.00065	0.00065	0.00003
	0.00132			0.00068		
	0.00158			0.00067		
308.15	0.00152	0.00157	0.00005	0.00073	0.00071	0.00004
	0.00162			0.00075		
313.15	0.00172	0.00179	0.00008	0.00075	0.00079	0.00004
	0.00177			0.00079		

	0.00188			0.00082		
	0.00209			0.00095		
318.15	0.00221	0.00216	0.00007	0.00092	0.00093	0.00002
	0.00219			0.00091		

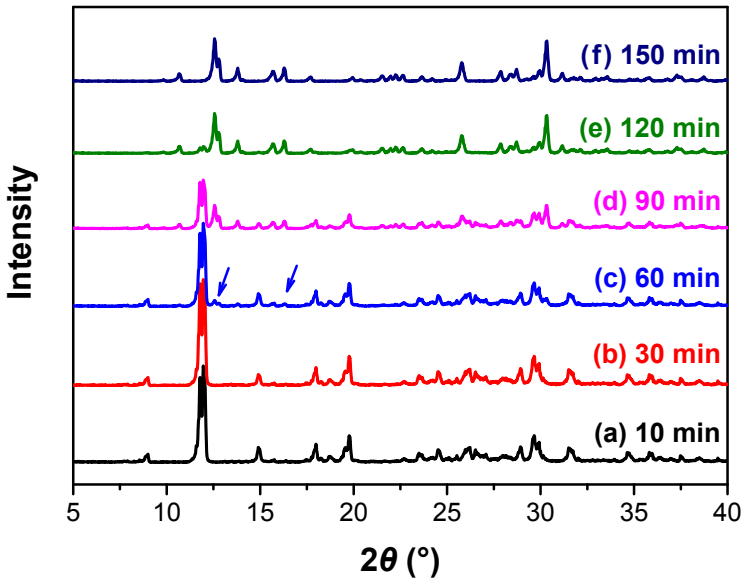

Fig. S6 Variation of the PXRD patterns during the SMPT process: (a) 10 min; (b) 30 min; (c) 60 min; (d) 90 min; (e) 120 min, and (f) 150 min.

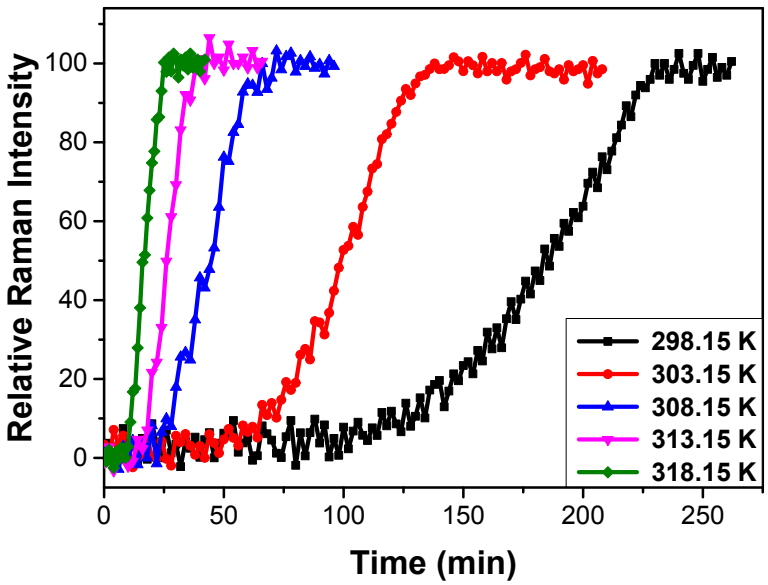

Fig. S7 Profiles of the SMPT process at different temperatures, in terms of the relative Raman intensity of form ε.

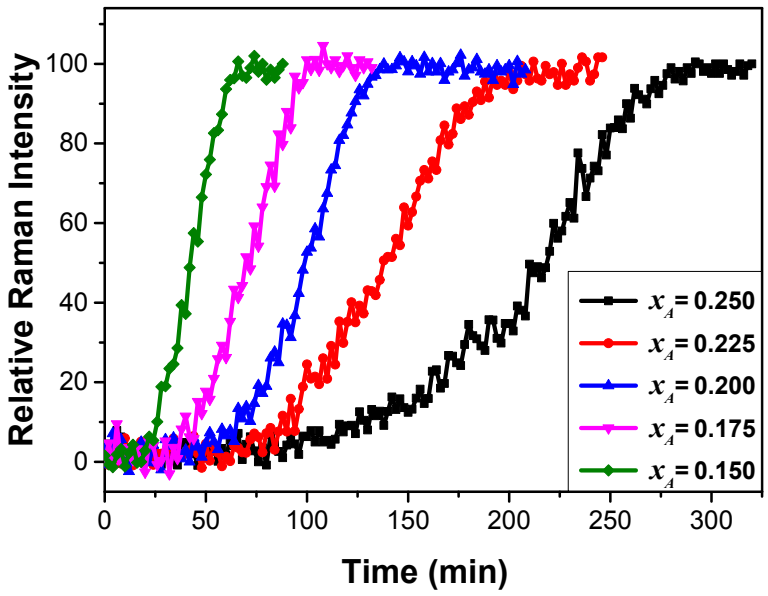

Fig. S8 Profiles of the SMPT process with different contents of acetonitrile, in terms of the relative Raman intensity of form ε.

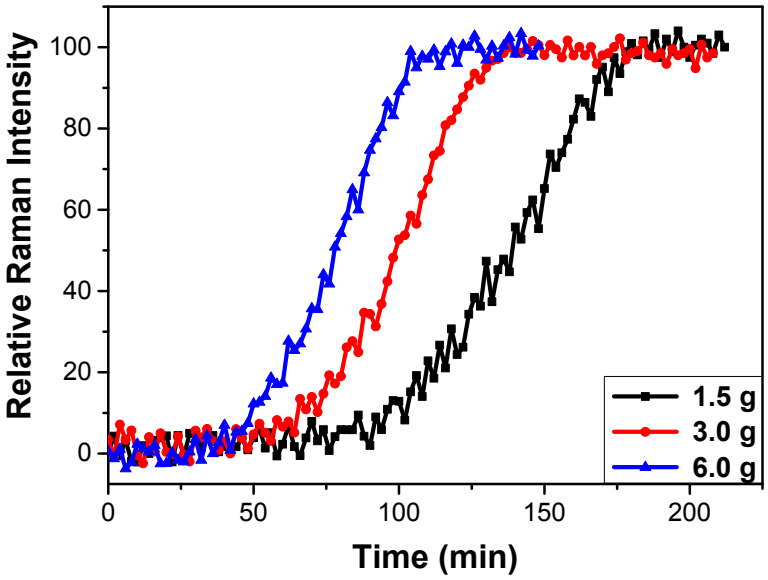

Fig. S9 Profiles of the SMPT process with different solid loadings, in terms of the relative Raman intensity of form ε.

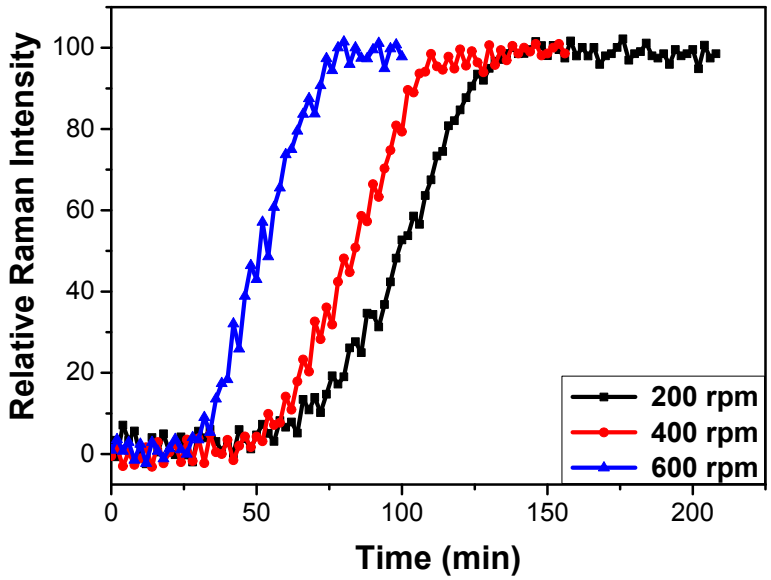

Fig. S10 Profiles of the SMPT process under different agitation rates, in terms of the relative Raman intensity of form ε.