Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.
This journal is © the Owner Societies 2023

Supporting Information

Finite temperature string by K-means clustering sampling with order parameter as collective variables for molecular crystal: application to polymorphic transformation between *β*-CL-20 and *ε*-CL-20

Fu-de Ren,[a] Ying-zhe Liu,[b] Ke-wei Ding,[b] Ling-ling Chang,[a] Duan-lin Cao,[a]

and Shubin Liu[c,d]

[a] *School of Chemical Engineering and Technology, North University of China, Taiyuan 030051, China*

[b] *Xi'an Modern Chemistry Research Institute, Xi'an 710065, China*

[c] *Research Computing Center, University of North Carolina, Chapel Hill, North Carolina 27599-3420, USA*

[d] *Depaertment of Chemistry, University of North Carolina, Chapel Hill, North Carolina 27599-3290, USA*

(1) Table S1 The structure, density, impact sensitivity, detonation velocity and detonation pressure of ε-CL-20 and β-CL-20

(2) Table S2 Average peak locations for the replicas by average-based sampling at 300 K

(3) Table S3 Values of the partition coefficient (PC) and partition entropy (PE)

(4) Fig. S1 Crystal structures of *β*-CL-20 and *ε*-CL-20

(5) Fig. S2 The distribution of (a) distance, (b) bond orientation, (c) relative orientation OPs for CL-20 at 300.0 K.

Table S1 The structure (Å), density (ρ, g/cm^3), impact sensitivity (h_{50}, cm), detonation velocity (D, m/s) and detonation pressure (P, GPa) of ε-CL-20 and β-CL-20[1,2]

Form	Structure	ρ	h_{50}	D	P
ε-CL-20	P21/n, Monoclinic	2.044	26.8	9660	45.6
	(a=8.852, b=12.556, c=13.386, α=γ=90.0°, β=106.82°)				
	V=1.4229 nm^3 [a]				
β-CL-20	$Pb2_1a$, Orthorhombic	1.985	24.2	9380	42.8
	(a=9.676, b=13.006, c=11.649, α=β=γ=90.0°)				
	V=1.4358 nm^3 [a]				

[a] The experimental values were obtained from Ref. 80 (D. C. Sorescu, B. M. Rice and D. L. Thompson, J. *Phys. Chem. B*, 1998, 102, 948–952)

Table S2 Average peak locations for the replicas by average-based sampling at 300 K

		1#			2#			3#			4#	
r(Å)	7.61	8.10	8.52	7.55	7.92	8.68	7.63	8.28	8.82	7.68	8.15	8.96
$1/\sigma^2$(Å^{-1})	10.23	21.56	28.62	55.18	22.65	16.18	19.50	17.51	28.22	27.13	24.02	31.68
		5#			6#			7#			8#	
r(Å)	7.98	8.35	8.67	7.92	8.23	8.91	7.55	8.45	8.78	7.58	8.25	9.01
$1/\sigma^2$(Å^{-1})	22.13	17.51	29.08	35.63	38.52	29.13	19.06	59.51	31.82	36.08	12.67	22.72
		9#			10#			11#			12#	
r(Å)	7.63	8.82	8.79	7.79	8.21	9.24	7.49	8.63	9.69	6.58	7.85	9.55
$1/\sigma^2$(Å^{-1})	26.18	31.02	18.63	18.23	28.62	19.37	21.63	43.55	18.92	22.63	41.18	24.01
		13#			14#			15#			16#	
r(Å)	7.56	7.71	9.56	7.59	8.05	9.23	7.69	7.60	9.49	7.59	8.69	9.40
$1/\sigma^2$(Å^{-1})	42.17	18.53	20.03	50.67	22.93	17.62	13.89	43.02	20.33	46.05	21.82	20.43
		17#			18#			19#			20#	
r(Å)	7.52	7.68	9.57	7.59	8.15	9.50	7.58	7.79	9.62	7.63	7.85	9.60
$1/\sigma^2$(Å^{-1})	62.17	25.03	20.22	18.02	55.17	15.86	21.97	28.50	31.29	33.18	22.67	29.85

Table S3 Values of the partition coefficient (PC) and partition entropy (PE)

	1#	2#	3#	4#	5#	6#	7#	8#	9#	10#
PC	0.81	0.72	0.77	0.79	0.63	0.76	0.82	0.70	0.75	0.80
PE	0.39	0.45	0.42	0.38	0.53	0.39	0.41	0.43	0.36	0.52
	11#	12#	13#	14#	15#	16#	17#	18#	19#	20#
PC	0.78	0.75	0.59	0.66	0.78	0.79	0.70	0.79	0.75	0.78
PE	0.41	0.45	0.62	0.33	0.40	0.39	0.51	0.38	0.45	0.45

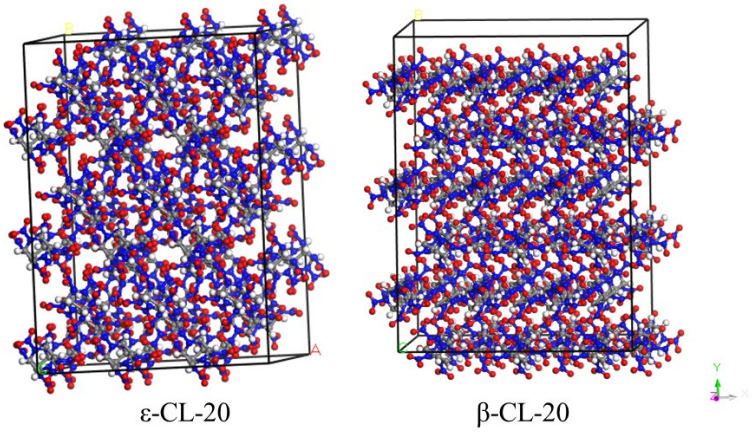
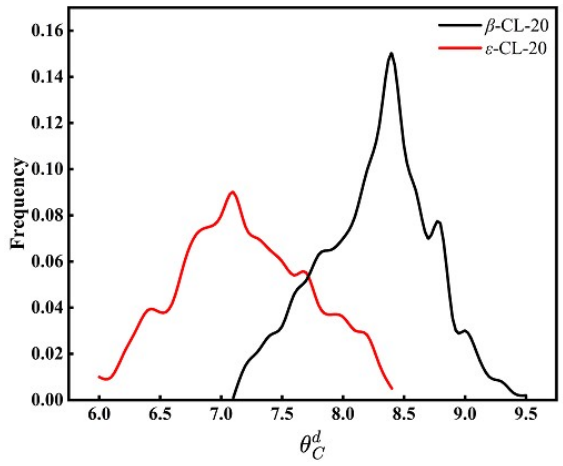
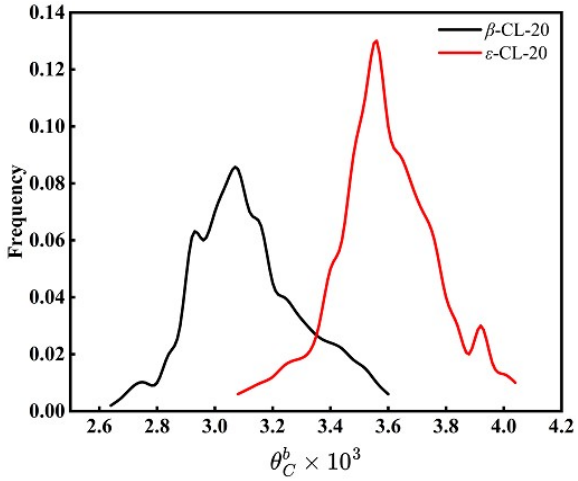


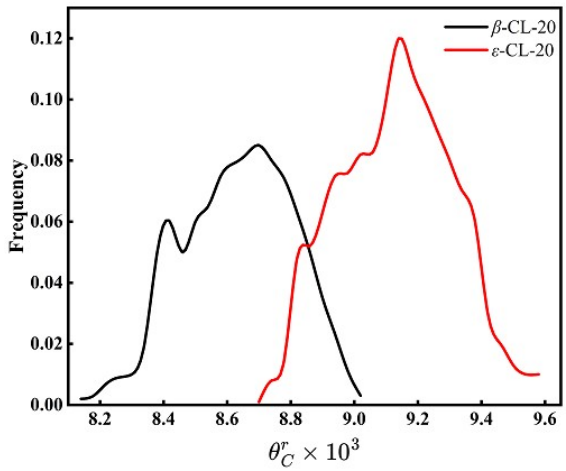
Fig. S1 Crystal structures of β-CL-20 and ε-CL-20



(a)



(b)



(c)

Fig. S2 The distribution of (a) distance, (b) bond orientation, (c) relative orientation OPs for CL-20 at 300.0 K.