Supporting Information

Theoretical investigation into polymorphic transformation between *β*-HMX and *δ*-HMX by finite temperature string

Xiu-mei Jia, Zhen-dong Xin, Yi-zheng Fu Hong-ji Duan

Table S1 Lattice parameters of *β*-HMX and *δ*-HMX

Table S2 Peaks in the pair distribution function for the reference structures of the *β*-HMX and *δ*-HMX crystals at 480 K with a cutoff of 10.0 Å.

Table S3 Average peak locations and concentrations parameters for the *β*-HMX and *δ*-HMX crystals at 480 K with a cutoff of 10.0 Å.

Table S4 Average peak locations for the replicas by average-based sampling at 480 K.

Table S5 Values of the partition coefficient (PC) and partition entropy (PE).

Table S6 Average peak locations and concentrations parameters for the β-HMX and δ-HMX crystals at 510 K, 450 K and 420 K.

Table S1 Lattice parameters of β-HMX and δ-HMX [20]

	Space group	***a*(Å)**	***b*(Å)**	***c*(Å)**	***β*(°)**	***Z***	***ρ*(g/cm^3)**
β-HMX	$P2_1/c$	6.54	11.05	8.70	124.4	2	1.905
δ-HMX	$P6_1$	7.71	7.71	32.55	90.0	6	1.80

Table S2 Peaks in the pair distribution function for the reference structures of the β-HMX and δ-HMX crystals at 480 K with a cutoff of 10.0 Å.

***β*-HMX**		
***r*(Å)**	ϕ_r **(°)**	ϕ_q **(°)**
6.62	53.18	32.18
7.51	27.01	57.22
7.88	62.37	65.18
***δ*-HMX**		
6.50	12.51	10.6
8.92	67.36	157.63
9.73	86.53	133.19

Table S3 Average peak locations and concentrations parameters for the β-HMX and δ-HMX crystals at 480 K with a cutoff of 10.0 Å.

β-HMX					
r(Å)	**$1/\sigma^2$ (Å^{-1})**	ϕ_r (°)	η_r^α	ϕ_q (°)	η_q^α
6.58	28.43	56.37	15.22	33.91	23.17
7.53	21.68	32.15	11.18	49.18	12.66
7.91	46.24	59.01	9.38	68.23	19.28
δ-HMX					
6.56	26.82	16.18	16.28	15.17	18.13
8.91	15.79	62.17	26.15	150.28	12.71
9.68	54.63	88.15	19.85	135.38	25.63

Table S4 Average peak locations for the replicas by average-based sampling at 480 K.

		1#			**2#**			**3#**			**4#**	
r(Å)	6.58	7.53	7.91	6.59	7.54	7.91	6.57	7.55	7.91	6.59	7.56	7.91
$1/\sigma^2$(Å^{-1})	28.43	21.68	46.24	55.18	22.65	16.18	19.50	17.51	28.22	27.13	24.02	31.68
		5#			**6#**			**7#**			**8#**	
r(Å)	6.58	7.57	7.91	6.60	7.60	7.93	6.56	7.63	7.95	6.59	7.78	7.96
$1/\sigma^2$(Å^{-1})	22.13	17.51	29.08	30.56	32.68	21.23	26.53	36.18	29.13	32.17	23.18	26.92
		9#			**10#**			**11#**			**12#**	
r(Å)	6.56	7.82	7.99	6.55	7.81	8.02	6.57	8.83	8.25	6.55	8.85	8.40
$1/\sigma^2$(Å^{-1})	23.98	25.18	27.11	13.78	22.40	11.37	25.39	35.69	22.18	29.16	32.40	39.26
		13#			**14#**			**15#**			**16#**	
r(Å)	6.58	8.86	8.62	6.57	8.87	8.92	6.56	8.90	9.08	6.55	8.89	9.23
$1/\sigma^2$(Å^{-1})	37.38	22.78	29.18	42.05	26.03	10.67	19.52	51.98	32.06	32.58	57.13	17.62
		17#			**18#**			**19#**			**20#**	
r(Å)	6.58	8.91	9.46	6.55	8.92	9.69	6.57	8.92	9.65	6.56	8.91	9.68
$1/\sigma^2$(Å^{-1})	19.56	28.67	26.53	12.31	42.28	26.23	45.18	33.21	39.17	26.82	15.79	54.63

Table S5 Values of the partition coefficient (PC) and partition entropy (PE).

	1#	**2#**	**3#**	**4#**	**5#**	**6#**	**7#**	**8#**	**9#**	**10#**
PC	0.79	0.81	0.76	0.76	0.82	0.53	0.83	0.81	0.81	0.76
PE	0.28	0.52	0.33	0.31	0.42	0.40	0.38	0.39	0.50	0.39
	11#	**12#**	**13#**	**14#**	**15#**	**16#**	**17#**	**18#**	**19#**	**20#**
PC	0.65	0.82	0.87	0.73	0.81	0.83	0.76	0.82	0.80	0.65
PE	0.28	0.43	0.55	0.50	0.35	0.32	0.28	0.45	0.51	0.29

Table S6 Average peak locations and concentrations parameters for the β-HMX and δ-HMX crystals at 510 K (in smooth), 450 K (in bold) and 420 K (in italic) with a cutoff of 10.0 Å.

β-HMX					
r(Å)	**$1/\sigma^2$ (Å^{-1})**	**ϕ_r (°)**	**η_r^α**	**ϕ_q (°)**	**η_q^α**
6.56 **6.52**	27.52 **28.79**	58.22 **69.18**	16.83 **18.19**	30.84 **35.68**	21.25 **25.18**
6.57	*26.18*	*67.25*	*26.13*	*30.63*	*22.30*
7.52 **7.58**	22.33 **20.12**	31.66 **38.27**	19.03 **10.35**	55.28 **47.62**	15.27 **16.27**
7.51	*17.96*	*39.26*	*5.37*	*50.19*	*17.27*
7.92 **7.86**	43.55 **42.18**	67.89 **52.18**	18.22 **11.17**	66.18 **87.27**	21.15 **13.05**
7.90	*45.03*	*51.76*	*5.32*	*61.17*	*17.65*
δ-HMX					
6.55 **6.57**	29.11 **27.10**	22.18 **11.03**	19.17 **16.52**	19.25 **11.63**	15.09 **24.16**
6.55	*29.15*	*10.52*	*11.10*	*18.49*	*17.23*
8.93 **8.94**	16.40 **18.13**	53.66 **63.86**	15.32 **23.27**	113.25 **111.33**	15.43 **13.16**
8.91	*17.63*	*67.19*	*29.19*	*125.89*	*18.03*
9.67 **9.69**	58.19 **50.33**	80.17 **80.28**	21.63 **17.92**	132.02 **128.19**	28.55 **20.32**
9.66	*50.17*	*82.95*	*11.63*	*116.67*	*26.71*