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Supporting information for article:

**Design, preparation, characterization and formation
mechanism of a novel kinetic CL-20 based cocrystal**

**Shanhu Sun, Haobin Zhang, Jinjiang Xu, Hongfan Wang, Zhihui Yu,
Chunhua Zhu and Jie Sun**

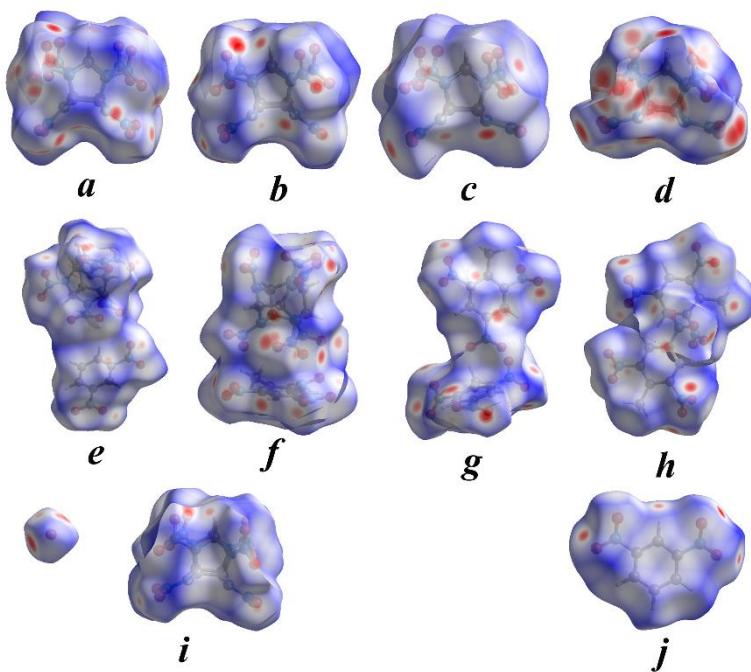


Figure S1 Hirshfeld surface for CL-20-based cocrystals and its coformers. a) ε -CL-20, b) β -CL-20, c) γ -CL-20, d) ζ -CL-20, e) CL-20/DNB, f) CL-20/TNT, g) monolinic-TNT, h) orthorhombic-TNT, i) α -CL-20, and j) DNB.

Table S1 Summary of the various interactions contributions to the Hirshfeld surface area in CL-20-based cocrystals and its pure coformers.

Interactions	Compound									
	ϵ -CL-20	α -CL-20	β -CL-20	γ -CL-20	ζ -CL-20	CL-20/DNB	CL-20/TNT	DNB	m-TNT	o-TNT
C…C	0	0	0	0	0	1.0	0	8.8	0	0
C…O	0.1	0	0	0	0.6	5.2	4.2	3.6	18.6	18.4
C…H	0	0	0	0	0	4.3	1.9	7.7	3.0	2.6
C…N	0	0	0	0	0	0.2	0	1.0	0.2	0.2
H…H	1.6	1.3	2.2	0.5	0.6	1.9	2.4	2.9	8.9	8.3
H…O	36.8	31.6	37.3	35.3	35.0	39.4	44.1	58.2	43.6	45.9
H…N	0.8	0.6	0.9	0.9	3.3	2.0	2.5	2.4	0.2	0
O…O	41.4	48.6	40.3	44.2	36.1	32.8	32.8	9.3	18.3	17.7
O…N	19.2	17.6	16.9	18.9	24.5	13.1	12.1	6.1	7.2	6.7
N…N	0.1	0.3	2.4	0.2	0	0	0	0	0	0



Figure S2 The microtopographies of crystals of (a) raw CL-20, (b) CL-20/TNP cocrystal and (c) TNP.