Electronic Supplementary Material (ESI) for CrystEngComm.

Supporting Information

Preparation of CL-20/DNDAP cocrystal by a rapid and continuous spray drying method: an alternative to cocrystal formation

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1. Crystal morphology

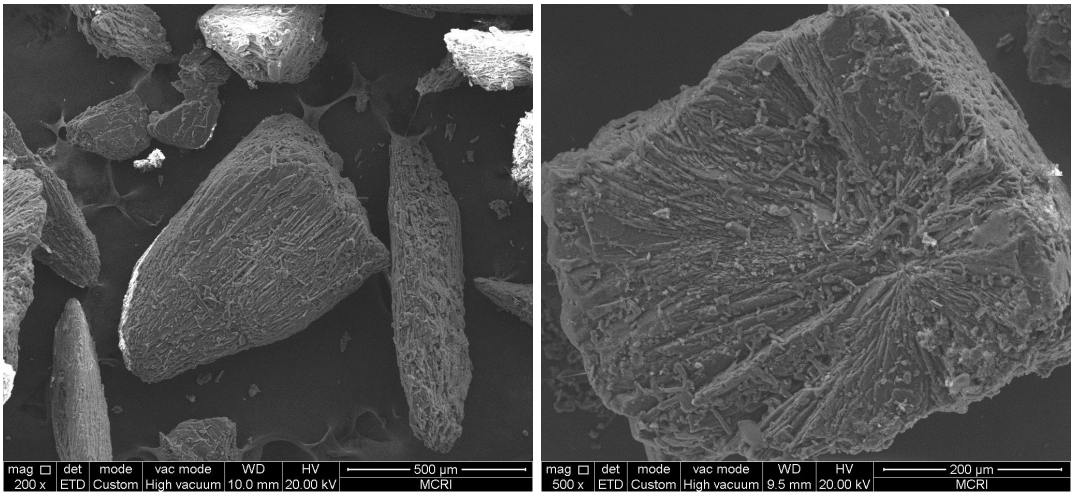


Fig. S1 SEM images of cocrystal 1a

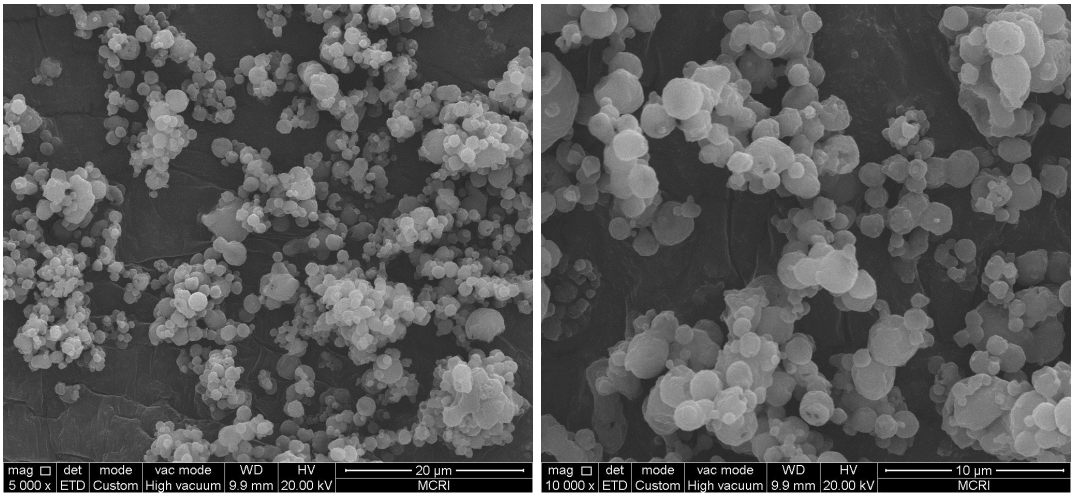


Fig. S2 SEM images of cocrystal 1b

2. X-ray crystallography

The CL-20/DNDAP cocrystal was obtained from the solution in methyl acetate at room temperature. The X-ray structure, crystal data, bond lengths, bond angles and dihedral angles of the data collection and refinement are given in Fig S3, Table S1, S2, S3 and S4. The geometrical parameters of the most significant hydrogen bonds are listed in Table S5.

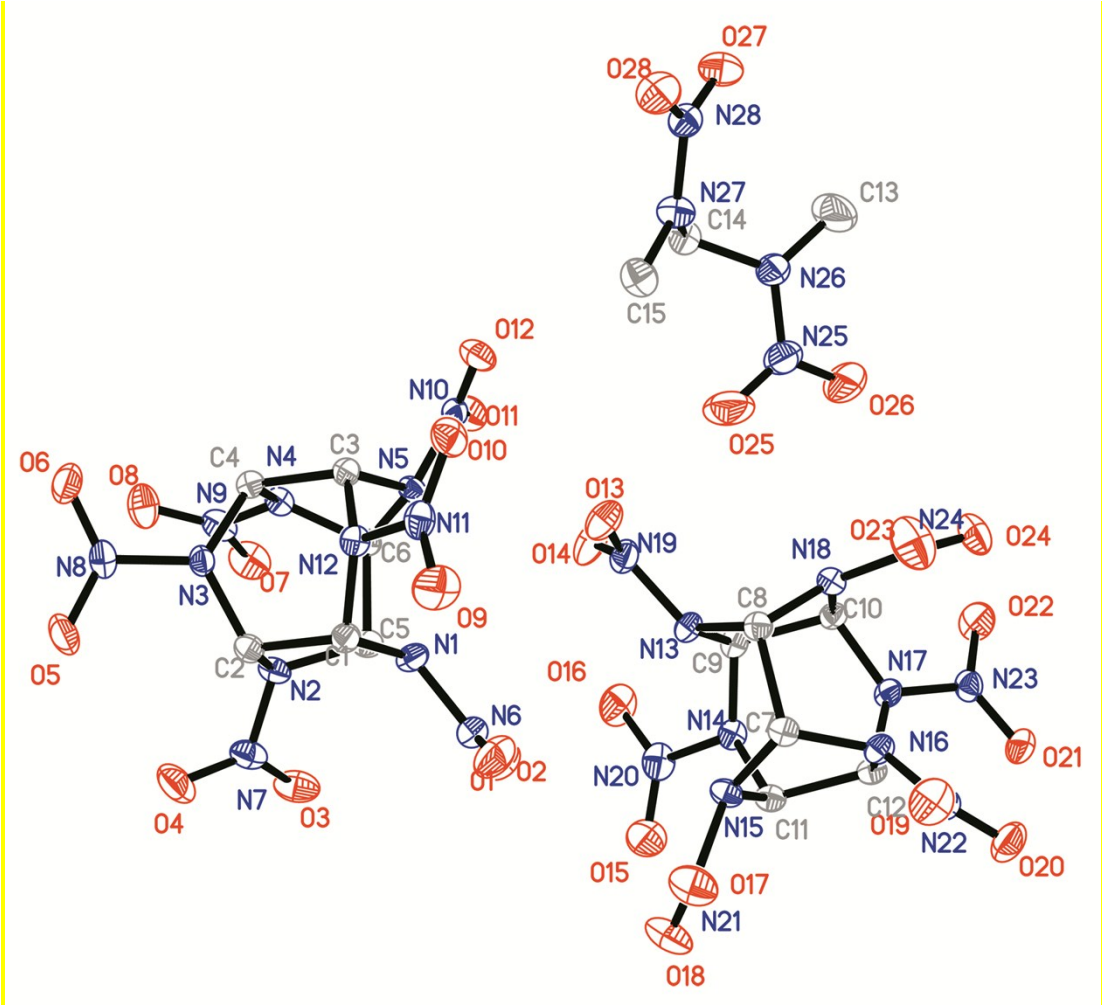


Fig. S3 X-ray structure of CL-20/DNDAP cocrystal with thermal ellipsoids at 50%.

Table S1 Crystal data and structure refinement for CL-20/DNDAP cocrystal

CL-20/DNDAP cocrystal	
Empirical formula	$C_{15}H_{20}N_{28}O_{28}$
Formula weight	1040.59
Temperature/K	296(2)
Crystal system	Monoclinic
Wavelength/Å	0.71073
space group	$P2_1/c$
Unit cell dimensions/Å, º	a = 13.022(2), α = 90
	b = 22.619(4), β = 104.648(3)
	c = 12.962(2), γ = 90
Cell volume/Å^3	3693.7(12)
Z	4
ρ_{cal}/g cm^{-3}	1.871
μ/mm^{-1}	0.178
F(000)	2120
Crystal size/mm	0.37 × 0.29 × 0.18
Crystal description	colorless block
2θ range for data collection/°	1.62 to 25.10
Limiting indices	$-15 \le h \le 14$, $-27 \le k \le 23$, $-8 \le l \le 15$
Reflections collected	17990
Max. and min. transmission	0.9688 and 0.9375
Data/restraints/parameters	6571/0/643
Goodness-of-fit on F^2	1.013
Final R indexes [$I \ge 2\sigma$]	R_1 = 0.0382, wR_2 = 0.0922
R indexes [all data]	R_1 = 0.0539, wR_2 = 0.1024
Extinction coefficient	0.0007(2)
Largest diff. peak and hole/e Å^{-3}	0.242 and –0.216

Table S2 Bond Lengths (Å) for CL-20/DNDAP cocrystal

N(1)-N(6)	1.412(3)	N(15)-C(11)	1.484(2)
N(1)-C(5)	1.462(3)	N(16)-N(22)	1.423(2)
N(1)-C(1)	1.470(3)	N(16)-C(7)	1.465(3)
N(2)-N(7)	1.422(2)	N(16)-C(12)	1.474(2)
N(2)-C(5)	1.464(3)	N(17)-N(23)	1.401(2)
N(2)-C(2)	1.474(2)	N(17)-C(10)	1.444(2)
N(3)-N(8)	1.412(2)	N(17)-C(12)	1.446(2)
N(3)-C(2)	1.445(3)	N(18)-N(24)	1.365(2)
N(3)-C(4)	1.447(2)	N(18)-C(8)	1.464(2)
N(4)-N(9)	1.392(2)	N(18)-C(10)	1.472(2)
N(4)-C(6)	1.465(3)	N(19)-O(14)	1.216(2)
N(4)-C(4)	1.478(2)	N(19)-O(13)	1.214(2)
N(5)-N(10)	1.431(2)	N(20)-O(15)	1.205(3)
N(5)-C(6)	1.456(2)	N(20)-O(16)	1.223(3)
N(5)-C(3)	1.495(2)	N(21)-O(18)	1.210(2)
N(6)-O(2)	1.211(3)	N(21)-O(17)	1.218(2)
N(6)-O(1)	1.223(2)	N(22)-O(20)	1.210(2)
N(7)-O(4)	1.213(3)	N(22)-O(19)	1.218(2)
N(7)-O(3)	1.211(2)	N(23)-O(21)	1.205(2)
N(8)-O(5)	1.215(2)	N(23)-O(22)	1.221(2)
N(8)-O(6)	1.210(2)	N(24)-O(23)	1.215(2)
N(9)-O(8)	1.216(3)	N(24)-O(24)	1.230(2)
N(9)-O(7)	1.225(2)	N(25)-O(25)	1.225(3)
N(10)-O(11)	1.214(2)	N(25)-O(26)	1.230(3)
N(10)-O(12)	1.213(2)	N(25)-N(26)	1.350(3)
N(11)-O(10)	1.213(2)	N(26)-C(13)	1.449(3)
N(11)-O(9)	1.215(2)	N(26)-C(14)	1.464(3)
N(11)-N(12)	1.420(2)	N(27)-N(28)	1.344(2)
N(12)-C(3)	1.447(2)	N(27)-C(14)	1.453(3)
N(12)-C(1)	1.450(2)	N(27)-C(15)	1.462(3)
N(13)-N(19)	1.417(2)	N(28)-O(27)	1.235(2)
N(13)-C(8)	1.455(3)	N(28)-O(28)	1.236(2)
N(13)-C(9)	1.483(2)	C(1)-C(2)	1.579(3)
N(14)-N(20)	1.420(2)	C(3)-C(4)	1.570(3)
N(14)-C(9)	1.444(3)	C(5)-C(6)	1.591(3)
N(14)-C(11)	1.451(2)	C(7)-C(8)	1.595(3)
N(15)-N(21)	1.421(2)	C(9)-C(10)	1.567(3)
N(15)-C(7)	1.459(2)	C(11)-C(12)	1.578(3)

Table S3 Bond Angles (º) for CL-20/DNDAP cocrystal

N(6)-N(1)-C(5)	119.49(17)	O(18)-N(21)-N(15)	116.45(18)
N(6)-N(1)-C(1)	118.75(16)	O(17)-N(21)-N(15)	116.76(17)
C(5)-N(1)-C(1)	107.92(16)	O(20)-N(22)-O(19)	127.77(19)
N(7)-N(2)-C(5)	117.48(17)	O(20)-N(22)-N(16)	116.38(18)
N(7)-N(2)-C(2)	117.16(15)	O(19)-N(22)-N(16)	115.65(18)
C(5)-N(2)-C(2)	107.47(15)	O(21)-N(23)-O(22)	127.15(18)
N(8)-N(3)-C(2)	119.21(16)	O(21)-N(23)-N(17)	116.59(17)
N(8)-N(3)-C(4)	118.76(16)	O(22)-N(23)-N(17)	116.22(17)
C(2)-N(3)-C(4)	116.74(15)	O(23)-N(24)-O(24)	126.7(2)
N(9)-N(4)-C(6)	119.30(16)	O(23)-N(24)-N(18)	116.88(19)
N(9)-N(4)-C(4)	120.34(16)	O(24)-N(24)-N(18)	116.44(18)
C(6)-N(4)-C(4)	109.96(15)	O(25)-N(25)-O(26)	123.5(2)
N(10)-N(5)-C(6)	114.78(15)	O(25)-N(25)-N(26)	117.8(2)
N(10)-N(5)-C(3)	114.89(14)	O(26)-N(25)-N(26)	118.7(2)
C(6)-N(5)-C(3)	107.46(15)	N(25)-N(26)-C(13)	117.1(2)
O(2)-N(6)-O(1)	127.5(2)	N(25)-N(26)-C(14)	117.59(19)
O(2)-N(6)-N(1)	116.44(19)	C(13)-N(26)-C(14)	121.5(2)
O(1)-N(6)-N(1)	115.8(2)	N(28)-N(27)-C(14)	118.48(17)
O(4)-N(7)-O(3)	127.3(2)	N(28)-N(27)-C(15)	118.31(18)
O(4)-N(7)-N(2)	115.60(19)	C(14)-N(27)-C(15)	122.24(18)
O(3)-N(7)-N(2)	116.95(19)	O(27)-N(28)-O(28)	123.98(19)
O(5)-N(8)-O(6)	127.65(18)	O(27)-N(28)-N(27)	118.70(18)
O(5)-N(8)-N(3)	115.85(18)	O(28)-N(28)-N(27)	117.30(18)
O(6)-N(8)-N(3)	116.40(17)	N(12)-C(1)-N(1)	110.66(15)
O(8)-N(9)-O(7)	127.55(19)	N(12)-C(1)-C(2)	108.39(15)
O(8)-N(9)-N(4)	117.04(18)	N(1)-C(1)-C(2)	104.04(15)
O(7)-N(9)-N(4)	115.4(2)	N(3)-C(2)-N(2)	111.06(15)
O(11)-N(10)-O(12)	126.79(17)	N(3)-C(2)-C(1)	107.89(15)
O(11)-N(10)-N(5)	117.28(16)	N(2)-C(2)-C(1)	104.77(15)
O(12)-N(10)-N(5)	115.75(16)	N(12)-C(3)-N(5)	111.37(15)
O(10)-N(11)-O(9)	127.45(19)	N(12)-C(3)-C(4)	107.81(15)
O(10)-N(11)-N(12)	116.86(17)	N(5)-C(3)-C(4)	105.01(15)
O(9)-N(11)-N(12)	115.59(18)	N(3)-C(4)-N(4)	114.11(15)
N(11)-N(12)-C(3)	117.02(16)	N(3)-C(4)-C(3)	108.89(15)
N(11)-N(12)-C(1)	117.60(16)	N(4)-C(4)-C(3)	100.57(14)
C(3)-N(12)-C(1)	116.89(15)	N(1)-C(5)-N(2)	104.40(15)
N(19)-N(13)-C(8)	116.70(15)	N(1)-C(5)-C(6)	109.78(16)
N(19)-N(13)-C(9)	116.09(15)	N(2)-C(5)-C(6)	107.28(16)
C(8)-N(13)-C(9)	107.81(15)	N(5)-C(6)-N(4)	99.53(14)
N(20)-N(14)-C(9)	116.18(17)	N(5)-C(6)-C(5)	109.67(16)
N(20)-N(14)-C(11)	116.69(16)	N(4)-C(6)-C(5)	113.64(16)
C(9)-N(14)-C(11)	116.53(15)	N(15)-C(7)-N(16)	104.32(15)
N(21)-N(15)-C(7)	117.15(15)	N(15)-C(7)-C(8)	108.83(15)

N(21)-N(15)-C(11)	117.44(15)	N(16)-C(7)-C(8)	107.72(14)
C(7)-N(15)-C(11)	107.59(15)	N(13)-C(8)-N(18)	99.63(14)
N(22)-N(16)-C(7)	117.94(15)	N(13)-C(8)-C(7)	109.76(15)
N(22)-N(16)-C(12)	118.67(16)	N(18)-C(8)-C(7)	112.51(16)
C(7)-N(16)-C(12)	108.12(15)	N(14)-C(9)-N(13)	110.17(15)
N(23)-N(17)-C(10)	120.64(16)	N(14)-C(9)-C(10)	108.20(16)
N(23)-N(17)-C(12)	119.36(16)	N(13)-C(9)-C(10)	105.76(15)
C(10)-N(17)-C(12)	117.11(15)	N(17)-C(10)-N(18)	113.82(15)
N(24)-N(18)-C(8)	120.96(16)	N(17)-C(10)-C(9)	108.85(15)
N(24)-N(18)-C(10)	120.53(16)	N(18)-C(10)-C(9)	100.14(14)
C(8)-N(18)-C(10)	110.72(15)	N(14)-C(11)-N(15)	111.56(16)
O(14)-N(19)-O(13)	127.13(19)	N(14)-C(11)-C(12)	108.24(15)
O(14)-N(19)-N(13)	115.76(17)	N(15)-C(11)-C(12)	104.17(15)
O(13)-N(19)-N(13)	116.87(17)	N(17)-C(12)-N(16)	110.13(15)
O(15)-N(20)-O(16)	127.3(2)	N(17)-C(12)-C(11)	108.24(15)
O(15)-N(20)-N(14)	116.8(2)	N(16)-C(12)-C(11)	104.42(15)
O(16)-N(20)-N(14)	115.91(19)	N(27)-C(14)-N(26)	114.55(18)
O(18)-N(21)-O(17)	126.68(19)	O(18)-N(21)-N(15)	116.45(18)

Table S4 Torsion Angles (º) for CL-20/DNDAP cocrystal

C(5)-N(1)-N(6)-O(2)	-163.12(19)	N(9)-N(4)-C(4)-C(3)	172.72(16)
C(1)-N(1)-N(6)-O(2)	-27.6(3)	C(6)-N(4)-C(4)-C(3)	28.05(18)
C(5)-N(1)-N(6)-O(1)	21.7(3)	N(12)-C(3)-C(4)-N(3)	-1.7(2)
C(1)-N(1)-N(6)-O(1)	157.22(19)	N(5)-C(3)-C(4)-N(3)	117.19(16)
C(5)-N(2)-N(7)-O(4)	166.31(19)	N(12)-C(3)-C(4)-N(4)	-121.85(15)
C(2)-N(2)-N(7)-O(4)	36.0(3)	N(5)-C(3)-C(4)-N(4)	-3.01(18)
C(5)-N(2)-N(7)-O(3)	-17.2(3)	N(6)-N(1)-C(5)-N(2)	106.17(19)
C(2)-N(2)-N(7)-O(3)	-147.49(19)	C(1)-N(1)-C(5)-N(2)	-33.62(19)
C(2)-N(3)-N(8)-O(5)	6.4(3)	N(6)-N(1)-C(5)-C(6)	-139.10(17)
C(4)-N(3)-N(8)-O(5)	159.92(17)	C(1)-N(1)-C(5)-C(6)	81.11(18)
C(2)-N(3)-N(8)-O(6)	-176.82(17)	N(7)-N(2)-C(5)-N(1)	-102.08(18)
C(4)-N(3)-N(8)-O(6)	-23.3(3)	C(2)-N(2)-C(5)-N(1)	32.60(19)
C(6)-N(4)-N(9)-O(8)	164.22(18)	N(7)-N(2)-C(5)-C(6)	141.44(16)
C(4)-N(4)-N(9)-O(8)	22.8(3)	C(2)-N(2)-C(5)-C(6)	-83.88(18)
C(6)-N(4)-N(9)-O(7)	-17.4(2)	N(10)-N(5)-C(6)-N(4)	-90.75(17)
C(4)-N(4)-N(9)-O(7)	-158.82(17)	C(3)-N(5)-C(6)-N(4)	38.37(17)
C(6)-N(5)-N(10)-O(11)	-20.1(2)	N(10)-N(5)-C(6)-C(5)	149.79(15)
C(3)-N(5)-N(10)-O(11)	-145.45(17)	C(3)-N(5)-C(6)-C(5)	-81.09(18)
C(6)-N(5)-N(10)-O(12)	164.50(17)	N(9)-N(4)-C(6)-N(5)	172.83(15)
C(3)-N(5)-N(10)-O(12)	39.2(2)	C(4)-N(4)-C(6)-N(5)	-42.09(18)
O(10)-N(11)-N(12)-C(3)	12.0(2)	N(9)-N(4)-C(6)-C(5)	-70.7(2)
O(9)-N(11)-N(12)-C(3)	-171.48(18)	C(4)-N(4)-C(6)-C(5)	74.40(19)
O(10)-N(11)-N(12)-C(1)	159.12(17)	N(1)-C(5)-C(6)-N(5)	1.2(2)
O(9)-N(11)-N(12)-C(1)	-24.4(2)	N(2)-C(5)-C(6)-N(5)	114.05(17)
C(8)-N(13)-N(19)-O(14)	156.87(18)	N(1)-C(5)-C(6)-N(4)	-109.22(18)
C(9)-N(13)-N(19)-O(14)	28.0(2)	N(2)-C(5)-C(6)-N(4)	3.7(2)
C(8)-N(13)-N(19)-O(13)	-28.4(2)	N(21)-N(15)-C(7)-N(16)	101.27(18)
C(9)-N(13)-N(19)-O(13)	-157.26(17)	C(11)-N(15)-C(7)-N(16)	-33.63(18)
C(9)-N(14)-N(20)-O(15)	-163.70(19)	N(21)-N(15)-C(7)-C(8)	-143.96(16)
C(11)-N(14)-N(20)-O(15)	-20.2(3)	C(11)-N(15)-C(7)-C(8)	81.13(18)
C(9)-N(14)-N(20)-O(16)	18.9(3)	N(22)-N(16)-C(7)-N(15)	-105.68(17)
C(11)-N(14)-N(20)-O(16)	162.40(18)	C(12)-N(16)-C(7)-N(15)	32.48(18)
C(7)-N(15)-N(21)-O(18)	-163.28(19)	N(22)-N(16)-C(7)-C(8)	138.77(16)
C(11)-N(15)-N(21)-O(18)	-32.8(3)	C(12)-N(16)-C(7)-C(8)	-83.07(17)
C(7)-N(15)-N(21)-O(17)	20.3(3)	N(19)-N(13)-C(8)-N(18)	-96.34(17)
C(11)-N(15)-N(21)-O(17)	150.71(19)	C(9)-N(13)-C(8)-N(18)	36.40(18)
C(7)-N(16)-N(22)-O(20)	157.54(18)	N(19)-N(13)-C(8)-C(7)	145.39(16)
C(12)-N(16)-N(22)-O(20)	23.8(2)	C(9)-N(13)-C(8)-C(7)	-81.87(18)
C(7)-N(16)-N(22)-O(19)	-27.1(2)	N(24)-N(18)-C(8)-N(13)	170.16(16)
C(12)-N(16)-N(22)-O(19)	-160.88(17)	C(10)-N(18)-C(8)-N(13)	-40.50(18)
C(10)-N(17)-N(23)-O(21)	162.55(18)	N(24)-N(18)-C(8)-C(7)	-73.6(2)
C(12)-N(17)-N(23)-O(21)	2.3(3)	C(10)-N(18)-C(8)-C(7)	75.70(18)

C(10)-N(17)-N(23)-O(22)	-19.6(3)	N(15)-C(7)-C(8)-N(13)	-0.5(2)
C(12)-N(17)-N(23)-O(22)	-179.83(19)	N(16)-C(7)-C(8)-N(13)	112.05(16)
C(8)-N(18)-N(24)-O(23)	-16.2(3)	N(15)-C(7)-C(8)-N(18)	-110.45(17)
C(10)-N(18)-N(24)-O(23)	-162.58(19)	N(16)-C(7)-C(8)-N(18)	2.1(2)
C(8)-N(18)-N(24)-O(24)	164.96(18)	N(20)-N(14)-C(9)-N(13)	87.02(19)
C(10)-N(18)-N(24)-O(24)	18.6(3)	C(11)-N(14)-C(9)-N(13)	-56.6(2)
O(25)-N(25)-N(26)-C(13)	-177.1(3)	N(20)-N(14)-C(9)-C(10)	-157.81(15)
O(26)-N(25)-N(26)-C(13)	3.5(4)	C(11)-N(14)-C(9)-C(10)	58.6(2)
O(25)-N(25)-N(26)-C(14)	-18.8(3)	N(19)-N(13)-C(9)-N(14)	-131.44(17)
O(26)-N(25)-N(26)-C(14)	161.9(2)	C(8)-N(13)-C(9)-N(14)	95.49(18)
C(14)-N(27)-N(28)-O(27)	-15.8(3)	N(19)-N(13)-C(9)-C(10)	111.85(17)
C(15)-N(27)-N(28)-O(27)	175.3(2)	C(8)-N(13)-C(9)-C(10)	-21.21(19)
C(14)-N(27)-N(28)-O(28)	165.92(19)	N(23)-N(17)-C(10)-N(18)	-106.02(19)
C(15)-N(27)-N(28)-O(28)	-3.1(3)	C(12)-N(17)-C(10)-N(18)	54.6(2)
N(11)-N(12)-C(1)-N(1)	-90.31(19)	N(23)-N(17)-C(10)-C(9)	143.25(17)
C(3)-N(12)-C(1)-N(1)	56.8(2)	C(12)-N(17)-C(10)-C(9)	-56.1(2)
N(11)-N(12)-C(1)-C(2)	156.20(15)	N(24)-N(18)-C(10)-N(17)	60.9(2)
C(3)-N(12)-C(1)-C(2)	-56.7(2)	C(8)-N(18)-C(10)-N(17)	-88.61(19)
N(6)-N(1)-C(1)-N(12)	124.87(18)	N(24)-N(18)-C(10)-C(9)	176.83(16)
C(5)-N(1)-C(1)-N(12)	-94.99(18)	C(8)-N(18)-C(10)-C(9)	27.34(18)
N(6)-N(1)-C(1)-C(2)	-118.90(18)	N(14)-C(9)-C(10)-N(17)	-1.7(2)
C(5)-N(1)-C(1)-C(2)	21.23(19)	N(13)-C(9)-C(10)-N(17)	116.29(16)
N(8)-N(3)-C(2)-N(2)	98.06(19)	N(14)-C(9)-C(10)-N(18)	-121.37(15)
C(4)-N(3)-C(2)-N(2)	-56.0(2)	N(13)-C(9)-C(10)-N(18)	-3.34(18)
N(8)-N(3)-C(2)-C(1)	-147.65(16)	N(20)-N(14)-C(11)-N(15)	-86.76(19)
C(4)-N(3)-C(2)-C(1)	58.3(2)	C(9)-N(14)-C(11)-N(15)	56.6(2)
N(7)-N(2)-C(2)-N(3)	-128.14(18)	N(20)-N(14)-C(11)-C(12)	159.19(16)
C(5)-N(2)-C(2)-N(3)	97.02(18)	C(9)-N(14)-C(11)-C(12)	-57.4(2)
N(7)-N(2)-C(2)-C(1)	115.64(18)	N(21)-N(15)-C(11)-N(14)	130.49(17)
C(5)-N(2)-C(2)-C(1)	-19.21(19)	C(7)-N(15)-C(11)-N(14)	-94.76(18)
N(12)-C(1)-C(2)-N(3)	-1.8(2)	N(21)-N(15)-C(11)-C(12)	-112.97(18)
N(1)-C(1)-C(2)-N(3)	-119.56(16)	C(7)-N(15)-C(11)-C(12)	21.78(19)
N(12)-C(1)-C(2)-N(2)	116.65(16)	N(23)-N(17)-C(12)-N(16)	104.32(19)
N(1)-C(1)-C(2)-N(2)	-1.16(18)	C(10)-N(17)-C(12)-N(16)	-56.6(2)
N(11)-N(12)-C(3)-N(5)	91.07(19)	N(23)-N(17)-C(12)-C(11)	-142.10(17)
C(1)-N(12)-C(3)-N(5)	-56.2(2)	C(10)-N(17)-C(12)-C(11)	57.0(2)
N(11)-N(12)-C(3)-C(4)	-154.24(15)	N(22)-N(16)-C(12)-N(17)	-124.80(17)
C(1)-N(12)-C(3)-C(4)	58.5(2)	C(7)-N(16)-C(12)-N(17)	97.39(17)
N(10)-N(5)-C(3)-N(12)	-137.07(16)	N(22)-N(16)-C(12)-C(11)	119.20(17)
C(6)-N(5)-C(3)-N(12)	93.86(18)	C(7)-N(16)-C(12)-C(11)	-18.61(18)
N(10)-N(5)-C(3)-C(4)	106.51(17)	N(14)-C(11)-C(12)-N(17)	-0.4(2)
C(6)-N(5)-C(3)-C(4)	-22.56(19)	N(15)-C(11)-C(12)-N(17)	-119.19(16)
N(8)-N(3)-C(4)-N(4)	-99.5(2)	N(14)-C(11)-C(12)-N(16)	116.96(16)

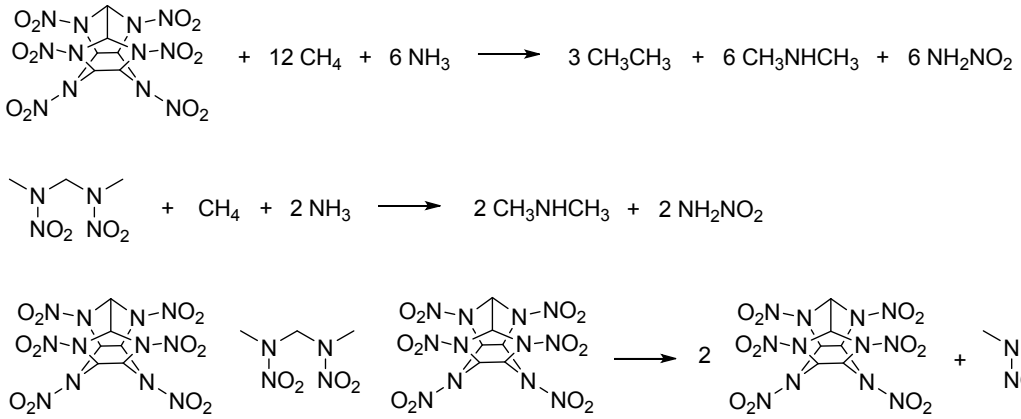
C(2)-N(3)-C(4)-N(4)	54.7(2)	N(15)-C(11)-C(12)-N(16)	-1.87(18)
N(8)-N(3)-C(4)-C(3)	149.09(16)	N(28)-N(27)-C(14)-N(26)	96.6(2)
C(2)-N(3)-C(4)-C(3)	-56.8(2)	C(15)-N(27)-C(14)-N(26)	-94.9(2)
N(9)-N(4)-C(4)-N(3)	56.3(2)	N(25)-N(26)-C(14)-N(27)	102.4(2)
C(6)-N(4)-C(4)-N(3)	-88.33(19)	C(13)-N(26)-C(14)-N(27)	-100.3(3)

Table S5 Bond lengths and angles of intermolecular hydrogen bonds found in CL-20/DNDAP cocrystal.

Interaction	H···O bond length (Å)	Bond angles (°)
C(8)-H(15)···O(28)	2.448	123.39
C(7)-H(23)···O(28)	2.478	121.85
C(15)-H(27c)···O(6)	2.554	142.37
C(13)-H(25b)···O(1)	2.559	146.96
C(13)-H(25a)···O(21)	2.578	154.1
C(15)-H(27a)···O(10)	2.667	136.69
C(14)-H(26a)···O(3)	2.675	166.73
C(15)-H(27b)···O(13)	2.684	158.51
C(6)-H(11)···O(26)	2.721	138.65
C(14)-H(26b)···O(12)	2.745	143.51
C(15)-H(27a)···O(13)	2.764	153.19
C(10)-H(17)···O(26)	2.885	135.18
C(5)-H(2)···O(26)	2.950	128.14
C(13)-H(25a)···O(18)	3.084	133.28
C(13)-H(25c)···O(3)	3.084	125.68
C(15)-H(27a)···O(9)	3.094	116.78
C(14)-H(26a)···O(4)	3.100	141.14
C(15)-H(27c)···O(10)	3.106	114.69
C(14)-H(26a)···O(15)	3.113	127.46
C(13)-H(25c)···O(16)	3.194	111.5

3. Computational details

Computations were performed with the Gaussian 09 (Revision B. 01) suite of programs.[1] The isodesmic reaction used for the prediction of gas-phase heats of formation (HOF) of CL-20, DNDAP and CL-20/DNDAP cocrystal are shown in Scheme S1. The experimental HOF of the reference compounds used in the isodesmic reactions are listed in Table S6



Scheme S1 Isodesmic reactions used to obtain the HOFs of CL-20/DNDAP cocrystal and co-formers at 298K

Table S6 experimental gas-phase heats of formation for reference compounds at 298 K[2,3]

Compd.	$\Delta H_{f,gas}$ /kJ mol^{-1}
CH_4	–74.6
NH_3	–46.1
CH_3CH_3	–84.0
CH_3NHCH_3	–18.8
NH_2NO_2	–3.9

Furthermore, the solid-state HOF ($\Delta H_{f,solid}$) can be calculated by Eq. (1):[4]

$$\Delta H_{f,solid} = \Delta H_{f,gas} - \Delta H_{sub} = \Delta H_{f,gas} - 188 \times T_m \quad (1)$$

where T_m represents the melting point of the cocrystal.

The detonation velocity (D) and detonation pressure (P) were evaluated by the empirical Kamlet–Jacobs (K–J) equations as shown in Eq. (2) – (3).[5]

$$D = 1.01\left(N\overline{M}^{1/2}Q^{1/2}\right)^{1/2}(1+1.30\rho) \quad (2)$$

$$P = 1.558\rho^2 N\overline{M}^{1/2}Q^{1/2} \quad (3)$$

where D is the predicted detonation velocity (m s^{-1}), P is the detonation pressure (GPa). N is the amount (mol^{-1}) of gaseous products per gram of explosive, $\overline{M}$ is the

average molecular weight of the gaseous products, Q is the heat of detonation (cal g^{-1}) derived from HOFs of the products and reactants, and ρ is the density of explosive (g cm^{-3}).

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