STRUCTURAL SCIENCE
CRYSTAL ENGINEERING
MATERIALS

Volume 78 (2022)

Supporting information for article:

A novel energetic cocrystal composed of CL-20 and 1-methyl-2,4,5-trinitroimidazole with high energy and low sensitivity

Pengbao Lian, Luyao Zhang, Hongping Su, Jun Chen, Lizhen Chen and Jianlong Wang

S1. Single crystal X-ray diffraction

The single crystal structure, bond lengths, and bond angles were listed in Figure S1, and Tables S1, S2 respectively.

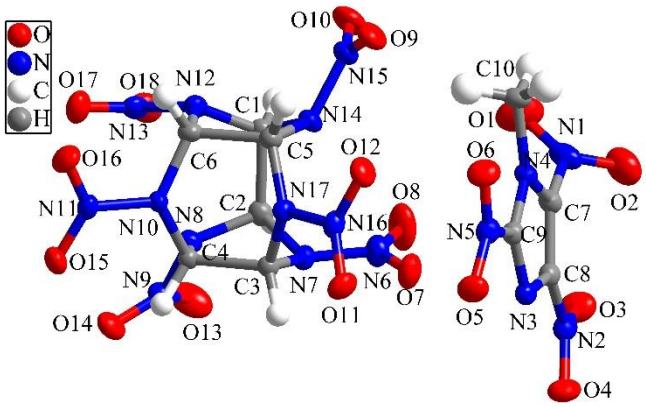

Figure S1 OPTEP diagram for cocrystal **1** with 50% probability ellipsoids.

Table S1 Bond Lengths (Å) for cocrystal **1**

Bond	Value (Å)	Bond	Value (Å)
O5-N5	1.227(2)	N17-C5	1.432(2)
O11-N16	1.213(2)	N4-C9	1.363(2)
O15-N11	1.218(2)	N4-C7	1.365(3)
O4-N2	1.224(2)	N4-C10	1.484(3)
O12-N16	1.222(2)	N5-C9	1.451(2)
O6-N5	1.222(2)	O3-N2	1.224(2)
O14-N9	1.213(2)	O17-N13	1.224(2)
N7-N6	1.385(2)	N14-N15	1.440(2)
N7-C3	1.472(2)	N14-C5	1.491(3)
N7-C2	1.474(3)	N14-C1	1.457(3)
O7-N6	1.228(2)	O10-N15	1.215(2)
N10-N11	1.401(2)	N2-C8	1.446(3)
N10-C4	1.433(3)	N12-N13	1.396(2)
N10-C6	1.439(3)	N12-C6	1.484(3)
O18-N13	1.214(2)	N12-C1	1.467(3)
O16-N11	1.216(2)	O13-N9	1.209(2)
N8-N9	1.428(2)	O8-N6	1.215(2)
N8-C4	1.485(2)	N1-O2	1.222(3)
N8-C2	1.453(3)	N1-O1	1.209(3)
N3-C9	1.305(3)	N1-C7	1.472(3)
N3-C8	1.341(2)	C3-C4	1.573(3)
O9-N15	1.218(3)	C8-C7	1.378(3)
N17-N16	1.411(2)	C6-C5	1.574(3)
N17-C3	1.448(3)	C2-C1	1.585(3)

Table S2 Bond Angles (º) for cocrystal **1**

Bond	Value (Å)	Bond	Value (Å)
N6-N7-C3	119.30(16)	O18-N13-N12	116.41(18)
N6-N7-C2	119.08(16)	O17-N13-N12	116.00(17)
C3-N7-C2	110.18(15)	O9-N15-N14	115.65(17)
N11-N10-C4	119.10(16)	O10-N15-O9	127.30(19)
N11-N10-C6	119.36(16)	O10-N15-N14	116.93(18)
C4-N10-C6	117.98(16)	O2-N1-C7	114.6(2)
N9-N8-C4	115.68(15)	O1-N1-O2	128.9(2)
N9-N8-C2	117.08(16)	O1-N1-C7	116.44(19)
C2-N8-C4	108.01(15)	O7-N6-N7	116.32(17)
C9-N3-C8	103.65(16)	O8-N6-N7	116.25(18)
N16-N17-C3	118.63(15)	O8-N6-O7	127.40(19)
N16-N17-C5	119.22(16)	N7-C3-C4	100.38(14)
C5-N17-C3	117.83(15)	N17-C3-N7	113.96(16)
C9-N4-C7	103.97(16)	N17-C3-C4	108.55(15)
C9-N4-C10	129.39(17)	N3-C9-N4	114.81(17)
C7-N4-C10	126.64(16)	N3-C9-N5	120.85(17)
O5-N5-C9	115.75(17)	N4-C9-N5	124.34(18)
O6-N5-O5	126.02(17)	N10-C4-N8	110.50(15)
O6-N5-C9	118.24(16)	N10-C4-C3	107.47(15)
N15-N14-C5	114.12(16)	N8-C4-C3	105.65(15)
N15-N14-C1	114.96(16)	N3-C8-N2	120.25(17)
C1-N14-C5	107.78(15)	N3-C8-C7	111.28(18)
O15-N11-N10	116.56(17)	C7-C8-N2	128.24(18)
O16-N11-O15	126.93(18)	N10-C6-N12	113.93(17)
O16-N11-N10	116.47(17)	N10-C6-C5	108.44(16)
O4-N2-O3	124.82(18)	N12-C6-C5	100.47(15)
O4-N2-C8	117.83(17)	N4-C7-N1	122.39(18)

O3-N2-C8	117.34(17)	N4-C7-C8	106.28(17)
O11-N16-O12	126.60(17)	C8-C7-N1	131.10(19)
O11-N16-N17	117.07(17)	N7-C2-C1	113.06(16)
O12-N16-N17	116.26(16)	N8-C2-N7	99.98(15)
N13-N12-C6	119.12(16)	N8-C2-C1	108.44(16)
N13-N12-C1	116.95(17)	N17-C5-N14	110.69(16)
C1-N12-C6	109.90(15)	N17-C5-C6	107.70(16)
O14-N9-N8	115.24(17)	N14-C5-C6	105.44(15)
O13-N9-O14	127.74(19)	N14-C1-N12	100.18(16)
O13-N9-N8	116.94(17)	N14-C1-C2	109.05(16)
O18-N13-O17	127.58(18)	N12-C1-C2	113.05(16)