Supporting Information

A novel multi-nitrogen 2,4,6,8,10,12-hexanitrohexaazaisowurtzitane based energetic cocrystal with 1-methyl-3,4,5- trinitropyrazole as a donor: experimental and theoretical investigations of intermolecular interactions

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Table and content

Computational details

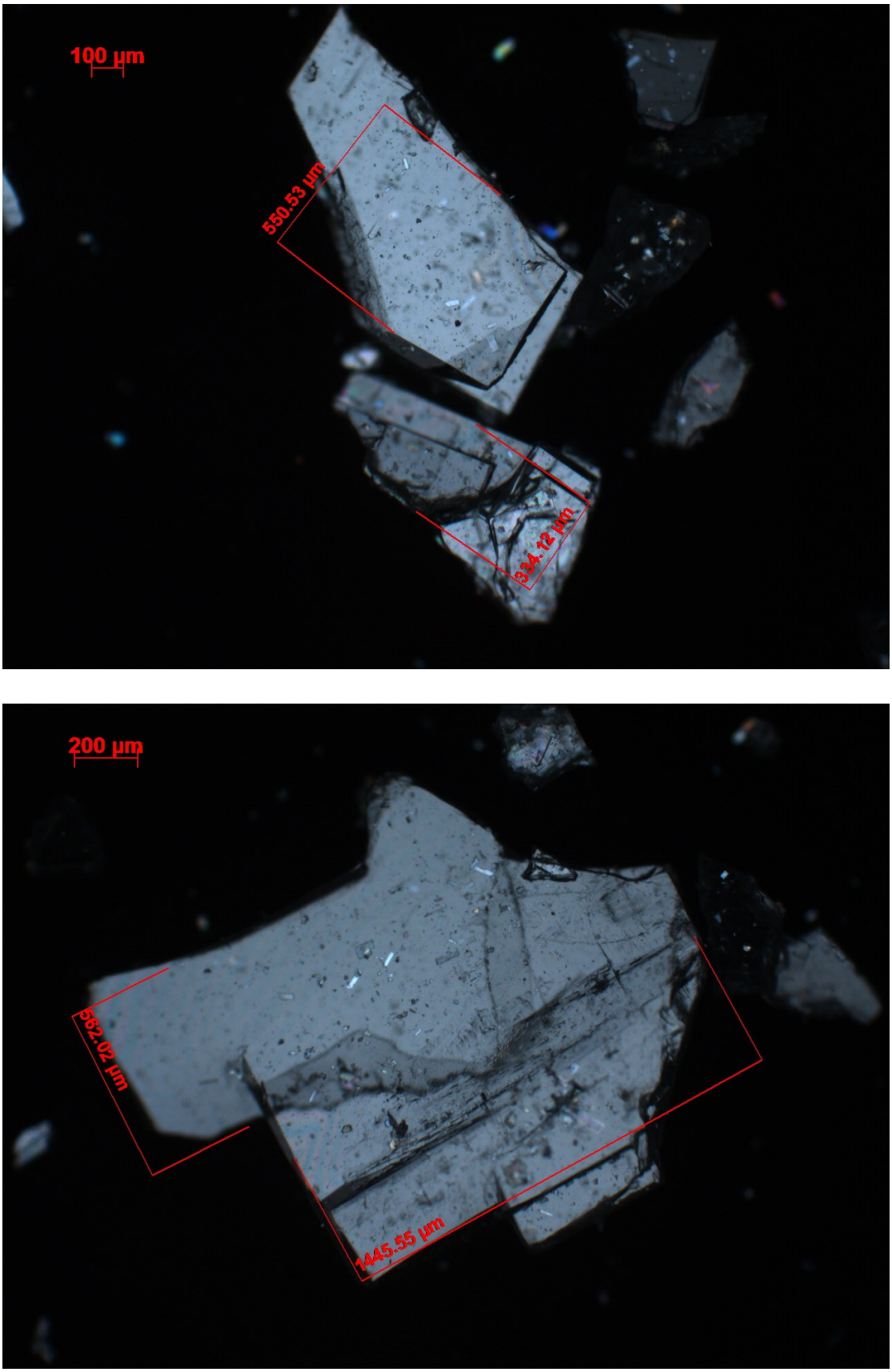


Figure S1 Polarizing microscope images of CL-20:MTNP

Table S1 Crystal data and structure refinement for MTNP and CL-20:MTNP.

	MTNP	CL-20:MTNP
Empirical formula	$C_4H_3N_5O_6$	$C_{10}H_9N_{17}O_{18}$
Formula weight	217.11	655.34
Temperature/K	293(2)	293(2)
Crystal dimensions/mm^3	0.15×0.14×0.11	0.22×0.14×0.13
Crystal description	yellow brick	colorless block
Crystal system	orthorhombic	monoclinic
Space group	$Pna2_1$	$P2_1$
a/Å	11.9211(5)	8.3515(3)
b/Å	8.3391(4)	11.4299(7)
c/Å	8.4760(4)	11.9398(6)
α/°	90	90
β/°	90	98.663(4)
γ/°	90	90
Volume/Å^3	842.61(7)	1126.73(10)
Z	4	2
ρ_{calc}g/cm^3	1.711	1.932
μ/mm^{-1}	0.162	0.184
F(000)	440.0	664.0
Radiation	MoKα (λ = 0.71073)	MoKα (λ = 0.71073)
2Θ range for data collection/°	3.42 to 24.99	6.90 to 58.10
Index ranges	-14 ≤ h ≤ 8, -9 ≤ k ≤ 7, -6 ≤ l ≤ 10	-11 ≤ h ≤ 11, -14 ≤ k ≤ 14, -15 ≤ l ≤ 13
Reflections collected	1828	10491
Data/restraints/parameters	1086/1/138	5168/1/408
Goodness-of-fit on F^2	1.054	1.044
Final R indexes [I>=2σ (I)]	R_1 = 0.0346, wR_2 = 0.0740	R_1 = 0.0487, wR_2 = 0.0855
Final R indexes [all data]	R_1 = 0.0390, wR_2 = 0.0787	R_1 = 0.0719, wR_2 = 0.0996
Largest diff. peak/hole / e Å^{-3}	0.15/-0.14	0.21/-0.20

Table S2 Fractional Atomic Coordinates (×10^4) and Equivalent Isotropic Displacement Parameters (Å^2×10^3) for MTNP. U_{eq} is defined as 1/3 of of the trace of the orthogonalised U_{IJ} tensor.

Atom	x	y	z	U(eq)
N1	6413(2)	2445(3)	5355(3)	45.1(6)
N2	7241(2)	3352(3)	4796(3)	48.2(7)

N3	7800(2)	6114(4)	4966(4)	51.9(7)
O4	4482(2)	1292(3)	6830(4)	70.8(8)
C5	7060(2)	4803(3)	5356(4)	37.9(7)
C6	6100(2)	4856(3)	6293(4)	40.1(7)
C7	5703(2)	3318(4)	6252(4)	40.2(7)
O8	7663(2)	7341(3)	5703(5)	86.4(11)
N9	5614(3)	6241(4)	7082(5)	62.7(9)
N10	4669(2)	2723(4)	6905(4)	52.2(7)
O11	8494(2)	5909(4)	3948(4)	73.6(8)
O12	4051(3)	3730(4)	7464(4)	87.7(11)
O13	5186(2)	7273(4)	6264(6)	108.8(15)
O14	5703(3)	6250(4)	8511(4)	98.3(12)
C15	6380(4)	738(4)	4925(6)	77.6(14)

Table S3 Anisotropic Displacement Parameters ($Å^2×10^3$) for MTNP. The Anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U_{11}+2hka^*b^*U_{12}+\ldots]$.

Atom	U11	U22	U33	U23	U13	U12
N1	47.0(14)	40.7(13)	47.6(15)	-3.7(13)	-3.1(15)	-1.1(12)
N2	44.7(15)	53.2(15)	46.7(15)	-5.5(14)	4.6(15)	-0.3(13)
N3	36.1(14)	57.4(17)	62.2(19)	8.7(16)	2.4(17)	-5.0(13)
O4	66.3(16)	62.3(15)	84(2)	19.1(16)	-10.4(16)	-25.0(13)
C5	35.1(14)	43.2(16)	35.5(16)	2.6(13)	-1.0(14)	1.3(12)
C6	39.4(15)	41.8(16)	39.2(16)	-0.1(15)	2.5(15)	1.0(13)
C7	38.8(15)	48.9(16)	32.8(14)	-0.7(14)	-3.7(14)	-4.9(13)
O8	73.1(17)	52.3(14)	134(3)	-13.8(19)	17(2)	-12.6(14)
N9	45.9(16)	53.5(19)	89(3)	-21.0(19)	19.2(19)	-3.3(14)
N10	47.6(15)	64.0(18)	45.1(16)	4.5(16)	0.2(15)	-14.0(14)
O11	58.2(16)	91(2)	71.2(18)	12.1(16)	23.3(16)	-13.6(15)
O12	64.9(18)	97(2)	102(3)	-22.3(18)	38.6(19)	-15.3(16)
O13	85(2)	72.4(19)	169(4)	-5(2)	1(3)	38.9(18)
O14	104(3)	108(3)	82(2)	-50(2)	34(2)	-23(2)
C15	90(3)	46(2)	97(3)	-23(2)	8(3)	-10(2)

Table S4 Bond Lengths for MTNP.

Atom	Atom	Length/Å	Atom	Atom	Length/Å

N1	N2	1.331(3)	C5	C6	1.394(4)
N1	C7	1.351(4)	C6	C7	1.368(4)
N1	C15	1.470(4)	C6	N9	1.455(4)
N2	C5	1.318(4)	C7	N10	1.439(4)
N3	C5	1.443(4)	N9	O13	1.217(5)
N3	O8	1.210(4)	N9	O14	1.216(5)
N3	O11	1.207(4)	N10	O12	1.213(4)
O4	N10	1.216(3)			

Table S5 Bond Angles for MTNP

Atom	Atom	Atom	Angle/°	Atom	Atom	Atom	Angle/°
N2	N1	C7	111.0(2)	C7	C6	C5	103.9(3)
N2	N1	C15	118.8(3)	C7	C6	N9	128.2(3)
C7	N1	C15	130.1(3)	N1	C7	C6	107.6(3)
C5	N2	N1	105.8(2)	N1	C7	N10	124.5(3)
O8	N3	C5	116.1(3)	C6	C7	N10	127.6(3)
O11	N3	C5	118.4(3)	O13	N9	C6	117.8(4)
O11	N3	O8	125.5(3)	O14	N9	C6	115.3(4)
N2	C5	N3	120.9(3)	O14	N9	O13	126.9(4)
N2	C5	C6	111.7(3)	O4	N10	C7	118.4(3)
C6	C5	N3	127.5(3)	O12	N10	O4	126.0(3)
C5	C6	N9	127.9(3)	O12	N10	C7	115.5(3)

Table S6 Torsion Angles for MTNP.

A	B	C	D	Angle/°	A	B	C	D	Angle/°
N1	N2	C5	N3	-179.2(3)	C6	C7	N10	O4	-176.0(3)
N1	N2	C5	C6	-0.2(3)	C6	C7	N10	O12	5.1(5)
N1	C7	N10	O4	10.2(5)	C7	N1	N2	C5	0.6(3)
N1	C7	N10	O12	-168.7(3)	C7	C6	N9	O13	-108.0(4)
N2	N1	C7	C6	-0.9(4)	C7	C6	N9	O14	73.3(5)
N2	N1	C7	N10	174.0(3)	O8	N3	C5	N2	-170.0(3)
N2	C5	C6	C7	-0.4(4)	O8	N3	C5	C6	11.1(5)
N2	C5	C6	N9	-178.4(3)	N9	C6	C7	N1	178.8(3)
N3	C5	C6	C7	178.6(3)	N9	C6	C7	N10	4.1(6)
N3	C5	C6	N9	0.6(5)	O11	N3	C5	N2	10.1(4)

C5	C6	C7	N1	0.7(3)	O11	N3	C5	C6	-168.8(3)
C5	C6	C7	N10	-173.9(3)	C15	N1	N2	C5	179.7(3)
C5	C6	N9	O13	69.5(4)	C15	N1	C7	C6	-179.8(4)
C5	C6	N9	O14	-109.1(4)	C15	N1	C7	N10	-5.0(5)

Table S7 Hydrogen Atom Coordinates (Å×10^4) and Isotropic Displacement Parameters (Å^2×10^3) for MTNP.

Atom	x	y	z	U(eq)
H15A	5705	520	4344	116
H15B	6393	96	5865	116
H15C	7019	483	4284	116

Table S8 Fractional Atomic Coordinates (×10^4) and Equivalent Isotropic Displacement Parameters (Å^2×10^3) for CL-20:MTNP. U_{eq} is defined as 1/3 of of the trace of the orthogonalised U_{IJ} tensor.

Atom	*x*	*y*	*z*	U(eq)
N1	2164(4)	5387(4)	4808(3)	34.7(8)
N0AA	-685(3)	5385(4)	6648(3)	32.9(8)
O3	1410(4)	5467(4)	3859(2)	53.6(9)
O0AA	3645(3)	5318(4)	5025(2)	49.4(9)
N1AA	-297(3)	5412(4)	5605(3)	31.8(8)
N2AA	4690(4)	4548(3)	2101(3)	29.9(9)
C3AA	1302(4)	5359(5)	5760(3)	28.4(8)
O9	1966(3)	4389(3)	1693(3)	46.9(9)
C10	1959(4)	5300(5)	6882(3)	30.5(9)
C11	6080(4)	6047(4)	3284(3)	27.9(9)
N12	7917(4)	7144(4)	291(3)	38.1(9)
N13	8347(4)	7394(4)	3728(3)	37.2(10)
O14	3784(4)	7603(3)	3620(3)	52.1(10)
O15	9426(4)	2938(3)	3239(3)	53.6(10)
O16	7696(4)	7725(4)	4520(3)	51.9(10)
O17	4222(4)	4227(4)	7458(4)	69.6(13)
O18	9544(4)	7817(3)	3422(3)	54.2(10)
N19	3167(4)	4072(4)	2315(4)	37.3(10)
N20	3598(4)	7186(4)	2670(4)	41.3(10)
O21	3265(4)	3350(4)	3064(3)	50.2(9)
O22	7168(3)	7141(4)	-659(3)	50.1(9)

C23	5927(4)	4688(4)	3111(3)	29.4(10)
O24	-617(4)	5214(5)	9013(3)	76.9(14)
N25	7720(4)	6388(3)	3163(3)	30.0(9)
O26	9187(4)	7623(4)	619(3)	60.9(11)
O27	1996(4)	5163(4)	9212(3)	61.8(12)
N28	663(4)	5241(4)	8654(3)	43.2(10)
N29	7442(4)	4233(4)	2879(3)	33.5(9)
N30	4912(3)	6541(4)	2375(3)	30.9(9)
N31	8155(5)	3294(4)	3493(3)	40.3(10)
O32	2447(4)	7303(4)	1933(3)	61.6(12)
N33	3655(4)	5206(5)	7392(3)	45.2(11)
O34	7461(4)	2923(4)	4234(3)	62.9(12)
O35	4374(4)	6096(4)	7672(4)	71.0(13)
C36	648(4)	5315(5)	7444(3)	30.3(9)
C37	4589(4)	5661(4)	1491(3)	31(1)
C40	-2399(4)	5433(6)	6783(4)	54.0(14)
C1	8139(4)	4736(4)	1964(3)	29.8(10)
N2	7047(4)	4663(3)	885(3)	31.7(8)
N3	7154(3)	6592(3)	1145(3)	29.1(8)
O4	7312(5)	2739(4)	815(4)	67.4(11)
C5	8269(4)	6097(4)	2115(3)	29(1)
N6	6509(5)	3580(4)	466(4)	45.1(10)
C7	5995(4)	5687(4)	732(3)	29.5(10)
O8	5289(4)	3600(4)	-245(3)	67.1(12)

Table S9 Anisotropic Displacement Parameters ($Å^2×10^3$) for CL-20:MTNP. The Anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U_{11}+2hka^*b^*U_{12}+\ldots]$.

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
N1	41.1(18)	34(2)	31.3(19)	-1(2)	11.4(14)	3.8(19)
N0AA	27.9(15)	33(2)	39.4(19)	0(2)	8.9(13)	1.6(17)
O3	70.7(18)	63(3)	27.2(16)	3(2)	8.4(14)	10(2)
O0AA	40.1(15)	61(2)	51.4(19)	-2(2)	20.2(12)	-0.1(19)
N1AA	32.7(15)	30(2)	31.6(18)	-1(2)	2.5(12)	0.4(18)
N2AA	26.7(16)	39(2)	25.6(19)	-2.0(17)	7.0(13)	-10.3(15)
C3AA	32.0(17)	26(2)	28(2)	-2(2)	8.6(14)	-1(2)
O9	26.7(14)	73(3)	41.0(19)	-6.7(19)	5.3(13)	-10.3(16)
C10	26.9(17)	34(2)	29(2)	-2(2)	0.8(14)	0(2)
C11	26.9(18)	35(3)	21(2)	4(2)	2.1(14)	0.7(18)

N12	38.0(19)	40(2)	37(2)	9(2)	7.5(16)	0.4(18)
N13	35(2)	31(2)	42(2)	-3(2)	-5.8(17)	1.7(17)
O14	59(2)	53(3)	49(2)	-5(2)	22.2(16)	15.1(18)
O15	41.1(18)	48(2)	74(3)	22(2)	15.8(16)	18.5(17)
O16	60(2)	50(3)	44(2)	-19(2)	5.7(16)	-3.4(18)
O17	56(2)	82(4)	67(3)	8(3)	-2.7(19)	32(2)
O18	39.8(18)	44(2)	79(3)	-13(2)	10.4(17)	-13.9(17)
N19	37(2)	39(3)	39(2)	-13(2)	17.3(17)	-11.6(17)
N20	36(2)	44(3)	47(3)	8(2)	14.7(17)	8.2(18)
O21	54.2(19)	47(2)	53(2)	4(2)	20.6(15)	-15.7(17)
O22	54.0(18)	64(3)	31.2(19)	12.7(19)	3.6(14)	-3.2(18)
C23	27.6(19)	35(3)	27(2)	2(2)	6.6(15)	-2.3(18)
O24	75(2)	110(4)	55(2)	18(3)	39.5(17)	28(3)
N25	29.8(17)	32(2)	25.8(18)	-2.5(17)	-2.3(13)	-3.1(15)
O26	47.5(18)	73(3)	61(2)	20(2)	2.7(15)	-27.9(19)
O27	67(2)	83(4)	33.0(18)	4(2)	-1.5(15)	-7(2)
N28	56(2)	39(3)	39(2)	0(2)	18.6(17)	6(2)
N29	31.8(16)	32(2)	39(2)	15.1(19)	14.3(15)	9.7(16)
N30	23.5(15)	37(2)	32(2)	0.1(18)	4.2(13)	4.4(15)
N31	45(2)	31(2)	46(3)	10(2)	10.0(17)	4.3(18)
O32	34.6(17)	84(3)	64(2)	11(2)	2.4(16)	27.5(18)
N33	32.5(18)	67(4)	35(2)	-6(2)	2.8(15)	8(2)
O34	71(2)	63(3)	61(3)	35(2)	30.9(19)	18(2)
O35	38.4(19)	92(4)	81(3)	-31(3)	4.4(17)	-20(2)
C36	35.4(19)	30(2)	27(2)	-1(2)	7.4(14)	2(2)
C37	23.7(17)	43(3)	26(2)	-1(2)	2.8(14)	0.0(18)
C40	29(2)	58(4)	78(4)	7(4)	18(2)	6(3)
C1	25.6(19)	31(3)	34(2)	3(2)	8.8(16)	1.4(17)
N2	34.8(17)	33(2)	28.8(19)	-3.7(18)	10.0(14)	-3.8(16)
N3	26.3(15)	33(2)	27.9(19)	8.2(17)	4.4(13)	-2.3(15)
O4	98(3)	35(3)	73(3)	-8(2)	25(2)	1(2)
C5	24.6(18)	32(3)	29(2)	3(2)	-0.8(15)	2.0(17)
N6	59(3)	39(3)	43(3)	-14(2)	22.7(19)	-11(2)
C7	28.9(18)	36(3)	23(2)	2.5(19)	5.3(14)	-3.6(17)
O8	76(2)	73(3)	49(2)	-14(2)	-0.3(18)	-29(2)

Table S10 Bond Lengths for CL-20:MTNP.

Atom	Atom	Length/Å	Atom	Atom	Length/Å
N1	O3	1.214(4)	O15	N31	1.217(5)

N1	O0AA	1.227(4)	O17	N33	1.213(6)
N1	C3AA	1.435(4)	N19	O21	1.211(5)
N0AA	N1AA	1.333(4)	N20	N30	1.409(5)
N0AA	C36	1.353(4)	N20	O32	1.209(5)
N0AA	C40	1.466(4)	C23	N29	1.433(5)
N1AA	C3AA	1.322(4)	O24	N28	1.211(4)
N2AA	N19	1.441(4)	N25	C5	1.434(5)
N2AA	C23	1.474(5)	O27	N28	1.212(4)
N2AA	C37	1.462(6)	N28	C36	1.445(5)
C3AA	C10	1.371(5)	N29	N31	1.383(5)
O9	N19	1.211(5)	N29	C1	1.433(5)
C10	N33	1.459(4)	N30	C37	1.455(6)
C10	C36	1.368(5)	N31	O34	1.205(5)
C11	C23	1.569(6)	N33	O35	1.204(6)
C11	N25	1.452(5)	C37	C7	1.587(5)
C11	N30	1.459(5)	C1	N2	1.465(5)
N12	O22	1.211(4)	C1	C5	1.568(6)
N12	O26	1.205(5)	N2	N6	1.385(6)
N12	N3	1.428(5)	N2	C7	1.457(6)
N13	O16	1.220(5)	N3	C5	1.485(5)
N13	O18	1.215(5)	N3	C7	1.452(5)
N13	N25	1.394(5)	O4	N6	1.210(6)
O14	N20	1.218(5)	N6	O8	1.223(5)

Table S11 Bond Angles for CL-20:MTNP.

Atom	Atom	Atom	Angle/°	Atom	Atom	Atom	Angle/°
O3	N1	O0AA	124.5(3)	O24	N28	C36	118.8(3)
O3	N1	C3AA	119.3(3)	O27	N28	C36	115.0(3)
O0AA	N1	C3AA	116.2(3)	C23	N29	C1	118.2(4)
N1AA	N0AA	C36	111.6(3)	N31	N29	C23	120.1(4)
N1AA	N0AA	C40	118.7(3)	N31	N29	C1	121.6(3)
C36	N0AA	C40	129.7(3)	N20	N30	C11	118.4(3)
C3AA	N1AA	N0AA	104.5(3)	N20	N30	C37	118.5(3)
N19	N2AA	C23	115.2(3)	C37	N30	C11	107.6(3)
N19	N2AA	C37	115.5(3)	O15	N31	N29	116.7(4)
C37	N2AA	C23	107.1(3)	O34	N31	O15	126.9(4)
N1AA	C3AA	N1	120.3(3)	O34	N31	N29	116.4(4)
N1AA	C3AA	C10	112.7(3)	O17	N33	C10	116.1(5)
C10	C3AA	N1	126.9(3)	O35	N33	C10	117.8(5)

C3AA	C10	N33	129.2(3)	O35	N33	O17	126.0(4)
C36	C10	C3AA	104.3(3)	N0AA	C36	C10	106.9(3)
C36	C10	N33	126.5(3)	N0AA	C36	N28	126.0(3)
N25	C11	C23	108.2(3)	C10	C36	N28	127.1(3)
N25	C11	N30	111.0(3)	N2AA	C37	C7	108.0(3)
N30	C11	C23	104.7(3)	N30	C37	N2AA	104.4(3)
O22	N12	N3	116.4(3)	N30	C37	C7	109.2(3)
O26	N12	O22	127.7(4)	N29	C1	N2	112.2(3)
O26	N12	N3	115.7(4)	N29	C1	C5	109.8(4)
O16	N13	N25	116.9(4)	N2	C1	C5	100.4(3)
O18	N13	O16	126.3(4)	N6	N2	C1	119.6(4)
O18	N13	N25	116.6(4)	N6	N2	C7	121.1(3)
O9	N19	N2AA	116.8(4)	C7	N2	C1	110.3(3)
O9	N19	O21	127.9(4)	N12	N3	C5	115.5(3)
O21	N19	N2AA	115.2(4)	N12	N3	C7	114.8(3)
O14	N20	N30	116.2(3)	C7	N3	C5	107.5(3)
O32	N20	O14	127.6(4)	N25	C5	C1	107.8(4)
O32	N20	N30	116.1(4)	N25	C5	N3	110.3(3)
N2AA	C23	C11	104.4(3)	N3	C5	C1	105.3(3)
N29	C23	N2AA	109.5(3)	O4	N6	N2	117.0(4)
N29	C23	C11	109.1(4)	O4	N6	O8	127.9(5)
N13	N25	C11	117.7(3)	O8	N6	N2	115.1(5)
N13	N25	C5	117.9(4)	N2	C7	C37	113.4(3)
C5	N25	C11	117.0(3)	N3	C7	C37	109.4(3)
O24	N28	O27	126.1(4)	N3	C7	N2	99.9(3)

Table S12 Torsion Angles for CL-20:MTNP.

A	B	C	D	Angle/°	A	B	C	D	Angle/°
N1	C3AA	C10	N33	-2.7(9)	C23	N29	C1	N2	-57.5(5)
N1	C3AA	C10	C36	179.1(5)	C23	N29	C1	C5	53.3(5)
N0AA	N1AA	C3AA	N1	-179.0(5)	O24	N28	C36	N0AA	1.5(8)
N0AA	N1AA	C3AA	C10	-0.1(6)	O24	N28	C36	C10	-176.8(6)
O3	N1	C3AA	N1AA	0.5(8)	N25	C11	C23	N2AA	-117.6(3)
O3	N1	C3AA	C10	-178.3(5)	N25	C11	C23	N29	-0.7(5)
O0AA	N1	C3AA	N1AA	-179.0(5)	N25	C11	N30	N20	-127.1(4)
O0AA	N1	C3AA	C10	2.2(8)	N25	C11	N30	C37	95.2(4)
N1AA	N0AA	C36	C10	0.2(6)	O26	N12	N3	C5	-32.6(6)
N1AA	N0AA	C36	N28	-178.4(5)	O26	N12	N3	C7	-158.5(4)
N1AA	C3AA	C10	N33	178.4(6)	O27	N28	C36	N0AA	178.7(5)

N1AA	C3AA	C10	C36	0.2(6)	O27	N28	C36	C10	0.3(8)
N2AA	C23	N29	N31	-117.3(4)	N29	C1	N2	N6	-58.8(5)
N2AA	C23	N29	C1	59.4(5)	N29	C1	N2	C7	88.6(4)
N2AA	C37	C7	N2	-3.3(4)	N29	C1	C5	N25	3.0(4)
N2AA	C37	C7	N3	-113.9(4)	N29	C1	C5	N3	-114.7(3)
C3AA	C10	N33	O17	-83.9(7)	N30	C11	C23	N2AA	0.8(5)
C3AA	C10	N33	O35	93.8(6)	N30	C11	C23	N29	117.7(3)
C3AA	C10	C36	N0AA	-0.2(6)	N30	C11	N25	N13	92.4(4)
C3AA	C10	C36	N28	178.3(5)	N30	C11	N25	C5	-56.8(5)
C11	C23	N29	N31	129.0(4)	N30	C37	C7	N2	109.7(4)
C11	C23	N29	C1	-54.2(5)	N30	C37	C7	N3	-0.9(5)
C11	N25	C5	C1	-58.5(5)	N31	N29	C1	N2	119.2(4)
C11	N25	C5	N3	56.0(5)	N31	N29	C1	C5	-130.0(4)
C11	N30	C37	N2AA	34.1(3)	O32	N20	N30	C11	-160.4(4)
C11	N30	C37	C7	-81.2(4)	O32	N20	N30	C37	-27.3(6)
N12	N3	C5	N25	135.7(4)	N33	C10	C36	N0AA	-178.6(5)
N12	N3	C5	C1	-108.3(4)	N33	C10	C36	N28	0.0(9)
N12	N3	C7	C37	-147.8(3)	C36	N0AA	N1AA	C3AA	-0.1(6)
N12	N3	C7	N2	93.0(4)	C36	C10	N33	O17	94.0(6)
N13	N25	C5	C1	152.3(3)	C36	C10	N33	O35	-88.3(7)
N13	N25	C5	N3	-93.2(4)	C37	N2AA	N19	O9	23.2(5)
O14	N20	N30	C11	22.7(6)	C37	N2AA	N19	O21	-160.6(4)
O14	N20	N30	C37	155.8(4)	C37	N2AA	C23	C11	19.8(4)
O16	N13	N25	C11	20.3(5)	C37	N2AA	C23	N29	-96.9(4)
O16	N13	N25	C5	169.3(4)	C40	N0AA	N1AA	C3AA	179.8(5)
O18	N13	N25	C11	-163.6(4)	C40	N0AA	C36	C10	-179.7(6)
O18	N13	N25	C5	-14.7(5)	C40	N0AA	C36	N28	1.7(9)
N19	N2AA	C23	C11	-110.2(4)	C1	N29	N31	O15	2.1(7)
N19	N2AA	C23	N29	133.2(4)	C1	N29	N31	O34	-178.9(4)
N19	N2AA	C37	N30	96.4(3)	C1	N2	N6	O4	-21.5(6)
N19	N2AA	C37	C7	-147.4(3)	C1	N2	N6	O8	160.5(4)
N20	N30	C37	N2AA	-103.6(4)	C1	N2	C7	C37	-75.0(4)
N20	N30	C37	C7	141.1(4)	C1	N2	C7	N3	41.3(3)
O22	N12	N3	C5	152.0(4)	N2	C1	C5	N25	121.3(3)
O22	N12	N3	C7	26.0(5)	N2	C1	C5	N3	3.6(4)
C23	N2AA	N19	O9	148.9(4)	C5	C1	N2	N6	-175.4(3)
C23	N2AA	N19	O21	-34.9(5)	C5	C1	N2	C7	-27.9(4)
C23	N2AA	C37	N30	-33.4(3)	C5	N3	C7	C37	82.2(4)
C23	N2AA	C37	C7	82.8(4)	C5	N3	C7	N2	-37.1(3)
C23	C11	N25	N13	-153.3(3)	N6	N2	C7	C37	72.0(5)

C23	C11	N25	C5	57.5(5)	N6	N2	C7	N3	-171.7(4)
C23	C11	N30	N20	116.4(4)	C7	N2	N6	O4	-165.5(4)
C23	C11	N30	C37	-21.3(4)	C7	N2	N6	O8	16.5(6)
C23	N29	N31	O15	178.8(4)	C7	N3	C5	N25	-94.7(4)
C23	N29	N31	O34	-2.2(7)	C7	N3	C5	C1	21.3(4)

Table S13 Hydrogen Atom Coordinates (Å×10^4) and Isotropic Displacement Parameters (Å^2×10^3) for CL-20:MTNP.

Atom	*x*	*y*	*z*	U(eq)
H11	5823	6275	4028	33
H23	5592	4307	3774	35
H37	3522	5771	1034	37
H40A	-2699	6229	6902	81
H40B	-2572	4967	7423	81
H40C	-3049	5135	6112	81
H1	9196	4388	1907	36
H5	9382	6366	2111	35
H7	5560	5806	-68	35

Computational details

Hirshfeld analysis

All the surfaces and fingerprint plots of the crystals were obtained by using the CrystalExplore3.0 program. Hirshfeld surface is a powerful tool to geometrically explore the inter- and intra- molecular interactions in the crystals. Hirshfeld surfaces of crystal are in terms of the electron distribution. The normalized contact distance (d_{norm}) is determined by d_i and d_e, which represent the distances from the surface to the nearest atom interior and exterior to the surface respectively and vdW radii of the atoms. d_{norm} can also be illustrated by the following eqn:[1]

$$d_{norm} = \frac{d_i - r_i^{vdW}}{r_i^{vdW}} + \frac{d_e - r_e^{vdW}}{r_e^{vdW}} \quad (1)$$

For any symmetrically dependent molecule in any crystal, the fingerprint is unique. Through the locations of (d_i, d_e) prints and their relative frequencies discernible on the surfaces and 2D fingerprint plots, the distances and intensities of these contact-interactions can be ascertained.

NCI and RDG analysis

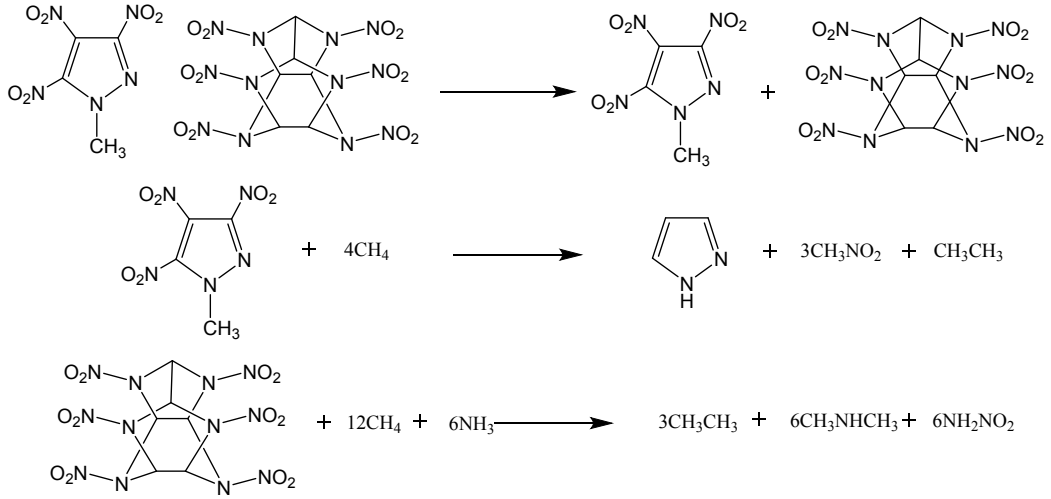
Reduced density gradient (RDG) is useful for analyzing non-covalent interactions (NCI), which could also provide valuable information to further explain the origin of the transformation in molecular structures, crystal

packing and thermodynamic stability. According to the NCI theory,[2] when a weak inter- or intra-molecular interaction appears, the RDG between the interacting atoms will have a massive change and produce density critical points (CP) between those fragments. The RDG can be represented as the following eqn:

$$RDG = \frac{1}{2(3\pi^2)^{1/3}} \frac{|\nabla\rho|}{\rho^{4/3}} \quad (2)$$

Heat of formation

The isodesmic reaction used for the prediction of gas-phase heats of formation (HOFs) of CL-20, MTNP and CL-20:MTNP are shown in Scheme S1. Table S14 lists the experimental EOF of the small molecules used in the isodesmic reactions.



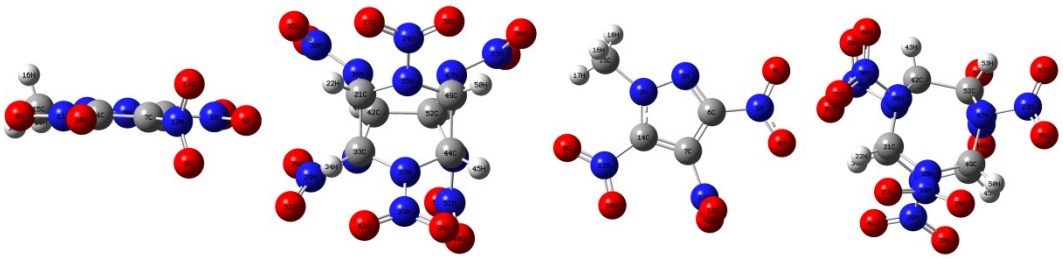
Scheme S1 Isodesmic reactions used to obtain the HOF of MTNP, CL-20 and CL-20:MTNP at 298K

Table S14 Experimental gas-phase heats of formation for small molecules at 298K[3-5]

Comp.	$\Delta_f H_{gas}$ /kJ mol^{-1}
CH_4	-74.6
NH_3	-46.1
CH_3NO_2	-74.5
CH_3CH_3	-84.0
CH_3NHCH_3	-18.8
NH_2NO_2	-3.9
Pyrazole	179.4

BSSE correction calculation

Interaction energies of CL-20:MTNP were obtained from BSSE correction calculations of the optimized cocrystal conformation employing the meta-hybrid M06-2X functional,[6] aug-cc-pVDZ basis set,[7] and Grimme's dispersion-correction D3 (zero-damping) to give accurate results and also for better comparison.[8]



Results calculated by M06-2X/aug-cc-pVDZ:

Counterpoise corrected energy = -2669.600918807972

BSSE energy = 0.002043871546

Results calculated by M06-2X-D3/aug-cc-pVDZ:

Counterpoise corrected energy = -2669.606870923233

BSSE energy = 0.002043871229

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