Supplementary Information

for

Effects of Vacancy Defects on the Structural Stability and Thermal Decomposition of CL-20/MTNP Cocrystal: A Reactive Molecular Dynamic Study

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Table S1. Model compositions and vacancy concentrations for the perfect and defective CL-20/MTNP cocrystals.

Models	Atoms	Cl-20 Molecules	MTNP Molecules	Vacancy Parentage (%)
VD-0	3888	72	72	0
VD-4.17	3726	69	69	4.17
VD-6.94	3618	67	67	6.94
VD-972	3510	65	65	9.72

Table S2. Comparison of selected bond lengths (Å) and bond angles (°) of CL-20 and MTNP molecules in the perfect and defective CL-20/MTNP cocrystal. The defective structure represents molecules located adjacent to the vacancy site. For consistency, structural parameters were extracted from identical crystallographic positions before and after defect introduction after full geometry optimization.

			ReaxFF-lg	
	Coordinates	Experimental [13]	Perfect	Defective
CL-20 bond length	O19–N18	1.212	1.286	1.288
	O20–N18	1.212	1.279	1.290
	O21–N21	1.223	1.284	1.271
	O22–N21	1.222	1.287	1.282
	O23–N23	1.220	1.289	1.284
	O24–N23	1.222	1.304	1.272
	O25–N25	1.216	1.299	1.288
	O26–N25	1.213	1.276	1.275
	O27–N27	1.222	1.275	1.297
	O28–N27	1.222	1.289	1.266
	N18–N19	1.441	1.481	1.544
	N19–C11	1.481	1.563	1.483
	N19–C16	1.468	1.501	1.664
	N20–C11	1.437	1.277	1.520
	N20–C12	1.445	1.524	1.556
	N22–N23	1.383	1.496	1.519
	N22–C13	1.471	1.531	1.546
	N24–N25	1.433	1.482	1.595
	N24–C13	1.459	1.501	1.468
	N24–C14	1.483	1.277	1.447
	N26–C14	1.444	1.503	1.528
	N26–C15	1.451	1.581	1.537
	N28–N29	1.410	1.524	1.549
	N28–C15	1.467	1.528	1.510
	N28–C16	1.457	1.597	1.511
	C11–C15	1.575	1.537	1.537
	C11–H10	1.000	1.110	1.126
	C12–C14	1.578	1.554	1.465
	C13–H12	1.000	1.164	1.251
	C14–H13	1.000	1.119	1.077
	C15–H14	1.000	1.157	1.109
	C16–H15	1.000	1.158	1.118
MTNP bond length	O13 – N13	1.222	1.281	1.289
	O17 – N17	1.219	1.317	1.274
	O18 – N17	1.218	1.287	1.294
	N13 – O14	1.223	1.262	1.280
	N17 – C9	1.452	1.299	1.317
	C7 – N14	1.353	1.456	1.457

	C7 – C9	1.374	1.497	1.307
	C8 – N15	1.330	1.460	1.550
	C8 – N16	1.440	1.581	1.507
	C8 – C9	1.391	1.313	1.441
	N14 – N15	1.339	1.463	1.473
	N14 – C10	1.467	1.474	1.510
	C10 – H7	0.979	1.147	1.102
	C10 – H8	0.980	1.102	1.126
	C10 – H9	0.980	1.097	1.112
CL-20 angle	O19 – N18 – O20	127.875	122.96	120.117
	O21 – N21 – O22	126.753	120.811	119.119
	O23 – N23 – C24	127.209	122.735	124.534
	O29 – N29 – O30	126.990	122.219	123.021
	O25 – N25 – O26	127.759	125.686	122.663
	O27 – N27 – O28	126.488	122.582	121.051
	N28 – C16 – N19	104.312	106.155	105.601
	N18 – N19 – C11	114.730	111.097	110.564
	N25 – N24 – C14	115.405	112.563	113.634
	C16 – N19 – C11	106.923	104.125	102.360
	C16 – N28 – C15	107.998	103.051	105.672
	C15 – C11 – H10	111.046	111.897	114.466
	C16 – C13 – H12	111.195	114.289	113.031
	H11 – C12 – C14	111.638	109.532	110.098
	H14 – C15 – N26	111.145	107.601	109.245
MTNP angle	O16 – N16 – O15	125.165	127.163	124.094
	O14 – N13 – O13	126.382	122.682	124.773
	O17 – N17 – C18	126.386	122.947	125.960
	N15 – N14 – C7	111.141	108.744	105.580
	N15 – N14 – C10	118.981	115.829	117.663
	C10 – N14 – C7	125.909	126.420	123.868
	C9 – C7 – N13	125.909	123.097	122.831
	C7 – C9 – N17	127.956	125.005	128.011
	O9 – C8 – N16	126.476	121.985	121.111
	H8 – C10 – H7	109.497	107.485	106.830

Table S3. Compression of initiation step reactions involved in the decomposition of the perfect and defective CL-20/MTNP cocrystals models within first 10 ps.

Decomposition initiation Reactions	Time (ps)				Temperature (K)
	VD-0	VD-4.97	VD-6.94	VD-9.72	
$C_6H_6N_{12}O_{12} \rightarrow C_6H_6N_{11}O_{10} + NO_2$	0.40 ~ 2.15	0.40 ~ 2.15	0.35 ~ 2.90	0.40 ~ 1.95	2000
	0.40 ~ 1.10	0.45 ~ 1.15	0.40 ~ 1.00	0.35 ~ 0.90	2500
	0.35 ~ 0.95	0.35 ~ 0.95	0.40 ~ 0.75	0.35 ~ 0.95	3000
	0.35 ~ 1.00	0.40 ~ 0.75	0.40 ~ 0.75	0.35 ~ 0.70	3500
$C_4H_3N_5O_6 \rightarrow C_4H_3N_4O_4 + NO_2$	0.70 ~ 8.15	1.10 ~ 8.00	0.85 ~ 9.65	0.60 ~ 8.50	2000
	0.65 ~ 7.45	0.55 ~ 8.60	0.55 ~ 4.20	0.45 ~ 5.20	2500
	0.60 ~ 3.15	0.60 ~ 4.15	0.50 ~ 2.40	0.50 ~ 1.90	3000
	0.60 ~ 1.70	0.55 ~ 1.45	0.50 ~ 1.70	0.55 ~ 1.55	3500

Table S4. Compression of primary decomposition reactions with highest frequencies of the perfect and defective CL-20/MTNP cocrystals models within first 10 ps. The frequencies of the forward and reverse reactions are separated with the "/" symbol

Temperature (K)	Decomposition Reactions	VD-0		VD-4.17		VD-6.94		VD-9.72	
		Net Flux	Frequency	Net Flux	Frequency	Net Flux	Frequency	Net Flux	Frequency
2000	$C_6H_6N_{12}O_{12} \rightarrow C_6H_6N_{11}O_{10} + NO_2$	51	83/-32	47	78/-31	47	76/-29	45	71/-26
	$C_6H_6N_{11}O_{10} \rightarrow C_6H_6N_{10}O_8 + NO_2$	22	56/-34	17	45/-28	18	43/-25	15	38/-23
	$C_6H_6N_{10}O_8 \rightarrow C_6H_6N_9O_6 + NO_2$	19	38/-19	7	11/-4	8	28/-20	9	27/-18
	$C_6H_6N_9O_6 \rightarrow C_6H_6N_8O_4 + NO_2$	9	19/-10	6	10/-4	7	16/-9	3	7/-4
	$C_6H_6N_8O_4 \rightarrow C_6H_6N_7O_2 + NO_2$	7	9/-2	3	5/-2	5	6/-1	4	4/0
	$C_6H_6N_7O_2 \rightarrow C_6H_6N_6 + NO_2$	5	5/0	3	3/0	3	3/0	2	2/0
	$C_4H_3N_5O_6 \rightarrow C_4H_3N_4O_4 + NO_2$	12	15/-3	8	12/-4	7	11/-4	3	3/0
	$C_4H_3N_4O_4 \rightarrow C_4H_3N_3O_2 + NO_2$	8	8/0	5	5/0	4	5/-1	3	3/0
2500	$C_6H_6N_{12}O_{12} \rightarrow C_6H_6N_{11}O_{10} + NO_2$	50	63/-13	47	64/-17	31	60/-29	47	61/-14
	$C_6H_6N_{11}O_{10} \rightarrow C_6H_6N_{10}O_8 + NO_2$	28	42/-14	24	37/-13	14	27/-13	22	41/-19
	$C_6H_6N_{10}O_8 \rightarrow C_6H_6N_9O_6 + NO_2$	18	32/-14	11	18/-7	11	17/-6	11	30/-19
	$C_6H_6N_9O_6 \rightarrow C_6H_6N_8O_4 + NO_2$	10	14/-4	11	16/-5	6	13/-7	10	13/-3
	$C_6H_6N_8O_4 \rightarrow C_6H_6N_7O_2 + NO_2$	5	7/-2	3	6/-3	4	6/-2	2	4/-2
	$C_6H_6N_7O_2 \rightarrow C_6H_6N_6 + NO_2$	3	3/0	2	2/0	2	4/-2	2	2/0
	$C_4H_3N_5O_6 \rightarrow C_4H_3N_4O_4 + NO_2$	8	17/-9	7	7/0	7	12/-5	6	19/-13
	$C_4H_3N_4O_4 \rightarrow C_4H_3N_3O_2 + NO_2$	3	4/-1	2	3/-1	3	3/0	3	5/-2
3000	$C_6H_6N_{12}O_{12} \rightarrow C_6H_6N_{11}O_{10} + NO_2$	42	54/-12	42	56/-14	50	64/-14	43	53/-10
	$C_6H_6N_{11}O_{10} \rightarrow C_6H_6N_{10}O_8 + NO_2$	16	28/-12	14	21/-7	17	27/-10	14	26/-12
	$C_6H_6N_{10}O_8 \rightarrow C_6H_6N_9O_6 + NO_2$	9	20/-11	9	18/-9	7	11/-4	6	13/-7
	$C_6H_6N_9O_6 \rightarrow C_6H_6N_8O_4 + NO_2$	7	9/-2	7	9/-2	6	8/-6	6	8/-2
	$C_6H_6N_8O_4 \rightarrow C_6H_6N_7O_2 + NO_2$	3	5/-2	2	4/-2	3	8/-5	2	3/-1
	$C_6H_6N_7O_2 \rightarrow C_6H_6N_6 + NO_2$	3	4/-1	2	2/0	2	2/0	1	1/0
	$C_6H_6N_6 \rightarrow CH_2N_3 + C_5H_4N_3$	1	1/0	1	1/0	1	1/0	1	1/0
	$C_4H_3N_5O_6 \rightarrow C_4H_3N_4O_4 + NO_2$	6	15/-9	5	12/-7	5	12/-7	6	12/-6
	$C_4H_3N_4O_4 \rightarrow C_4H_3N_3O_2 + NO_2$	2	3/-1	2	2/0	1	2/-1	1	1/0
3500	$C_6H_6N_{12}O_{12} \rightarrow C_6H_6N_{11}O_{10} + NO_2$	43	51/-10	40	49/-9	46	53/-7	45	56/-11
	$C_6H_6N_{11}O_{10} \rightarrow C_6H_6N_{10}O_8 + NO_2$	11	18/-7	11	13/-2	25	26/-1	11	17/-6
	$C_6H_6N_{10}O_8 \rightarrow C_6H_6N_9O_6 + NO_2$	10	10/-0	10	10/-0	8	8/-0	6	6/-0
	$C_6H_6N_9O_6 \rightarrow C_6H_6N_8O_4 + NO_2$	7	9/-2	3	6/-3	2	5/-3	2	4/-2
	$C_6H_6N_8O_4 \rightarrow C_6H_6N_7O_2 + NO_2$	2	3/-1	2	4/-2	3	3/-0	3	3/0
	$C_6H_6N_7O_2 \rightarrow C_6H_6N_6 + NO_2$	1	1/-0	2	4/-2	2	3/-1	1	1/0
	$C_6H_6N_6 \rightarrow CH_2N_3 + C_5H_4N_3$	1	1/0	1	1/0	1	1/0	1	1/0
	$C_4H_3N_5O_6 \rightarrow C_4H_3N_4O_4 + NO_2$	9	15/-6	1	10/-9	9	14/-5	9	15/-6
	$C_4H_3N_4O_4 \rightarrow C_4H_3N_3O_2 + NO_2$	3	4/-1	3	4/-1	1	2/-1	1	3/-2
	$C_4H_3N_3O_2 \rightarrow C_4H_3N_2 + NO_2$	2	3/-1	1	2/-1	1	1/0	1	1/0
	$C_4H_3N_2 \rightarrow C_3O + CH_3N_2$	2	2/-1	1	1/0	1	1/0	1	1/0

Table S5. Summary of the onset time (t_0, ps), peak formation time (t_{max}, ps), and corresponding molecular populations (N_0 and N_{max}) of the initial species during the decomposition of the perfect and defective CL-20/MTNP cocrystal models.

	NO		NO_2		NO_3		HNO		HNO_2		HNO_3		
Models	$t_0(N_0)$	$t_{max}(N_{max})$	$t_0(N_0)$	$t_{max}(N_{max})$	$t_0(N_0)$	$t_{max}(N_{max})$	$t_0(N_0)$	$t_{max}(N_{max})$	$t_0(N_0)$	$t_{max}(N_{max})$	$t_0(N_0)$	$t_{max}(N_{max})$	Temperature
0	1.30(1)	10.30(19)	0.50(1)	2.40(129)	1.50(2)	10.00(49)	2.60(1)	72.60(28)	0.90(1)	27.10(36)	1.70(1)	43.70(55)	
4.17	1.10(1)	15.20(22)	0.50(2)	6.30(140)	1.60(1)	9.60(54)	3.60(1)	116.20(28)	1.30(1)	66.50(31)	2.40(1)	21.80(51)	2000 K
6.94	1.60(1)	12.50(20)	0.50(1)	4.80(135)	1.70(2)	10.80(46)	2.40(1)	72.70(30)	0.80(1)	46.60(37)	2.20(1)	37.70(45)	
9.72	1.20(1)	17.80(20)	0.60(7)	5.80(148)	1.20(2)	10.50(48)	2.70(1)	50.60(27)	0.90(1)	62.70(34)	2.90(1)	37.80(47)	
0	0.80(1)	12.40(35)	0.50(2)	1.40(151)	0.90(3)	4.90(33)	1.50(1)	17.30(35)	1.20(1)	8.30(37)	1.50(1)	11.60(32)	
4.17	0.90(1)	5.70(34)	0.50(1)	2.00(170)	0.80(1)	5.10(36)	1.30(1)	28.20(37)	0.90(1)	13.30(40)	0.90(1)	7.80(38)	2500 K
6.94	0.80(1)	3.40(33)	0.50(2)	1.90(181)	0.90(1)	6.50(30)	1.60(1)	22.40(33)	0.90(1)	8.30(41)	1.30(1)	7.40(32)	
9.72	0.80(1)	10.60(36)	0.60(20)	3.80(171)	0.70(1)	7.00(35)	1.70(1)	21.30(34)	1.00(1)	12.30(42)	1.10(1)	9.00(27)	
0	0.80(2)	5.30(52)	0.50(4)	1.20(207)	0.80(3)	3.60(24)	1.30(2)	4.90(36)	0.90(1)	6.40(42)	1.10(2)	4.60(26)	
4.17	0.90(8)	7.50(54)	0.50(4)	1.30(198)	0.70(1)	2.500(29)	1.10(1)	9.20(47)	0.80(2)	7.60(36)	1.10(1)	4.60(28)	3000 K
6.94	0.80(2)	3.90(48)	0.50(3)	1.30(197)	0.70(1)	2.60(26)	1.00(2)	10.10(44)	0.70(1)	4.50(35)	090(1)	5.40(22)	
9.72	0.80(1)	2.40(59)	0.50(2)	1.10(185)	0.80(2)	2.30(25)	0.90(1)	8.20(45)	0.80(2)	4.20(34)	0.80(1)	3.70(21)	
0	0.80(9)	2.10(72)	0.50(4)	1.00(189)	0.70(4)	1.20(17)	1.00(4)	5.30(39)	0.80(6)	2.80(40)	0.90(3)	1.90(21)	
4.17	0.80(9)	1.80(67)	0.50(2)	1.00(205)	0.80(2)	1.10(15)	0.80(2)	5.00(46)	0.80(1)	4.10(35)	1.10(2)	2.60(14)	3500 K
6.94	0.80(6)	2.60(77)	0.50(4)	1.00(184)	0.70(1)	1.80(19)	0.80(1)	3.90(41)	0.80(1)	4.10(32)	0.90(1)	2.00(12)	
9.72	0.80(9)	2.40(73)	0.50(2)	1.10(193)	0.70(1)	1.60(17)	0.80(2)	5.70(44)	0.80(4)	3.20(37)	0.90(2)	4.60(19)	

Table S6. Summary of the onset time (t_0, ps), peak formation time (t_{max}, ps), and corresponding molecular populations (N_0 and N_{max}) of the final species during the decomposition of the perfect and defective CL-20/MTNP cocrystal models.

	H_2		N_2		CO_2		H_2O		
Models	$t_0(N_0)$	$t_{max}(N_{max})$	$t_0(N_0)$	$t_{max}(N_{max})$	$t_0(N_0)$	$t_{max}(N_{max})$	$t_0(N_0$	$t_{max}(N_{max})$	Temperature
0	78.80(1)	88.90(3)	1.20(1)	191.30(475)	12.90(1)	194.20(252)	2.00(1)	196.20(195)	2000 K
4.17	27.00(1)	31.10(2)	1.00(1)	197.90(428)	12.70(1)	196.40(249)	3.20(1)	199.60(175)	
6.94	4.80(1)	26.40(3)	1.60(1)	196.90(421)	12.90(2)	189.70(233)	5.10(1)	197.20(178)	
9.72	107.60(1)	121.20(2)	0.80(1)	199.10(404)	9.60(1)	197.50(237)	3.50(1)	198.40(167)	
0	3.10(1)	197.00(36)	1.00(3)	165.60(538)	3.10(1)	179.50(319)	2.60(2)	97.30(189)	2500 K
4.17	9.80(1)	187.10(31)	0.80(2)	187.30(521)	5.10(1)	192.50(306)	1.90(1)	80.30(194)	
6.94	8.00(1)	195.80(28)	0.70(1)	188.50(507)	2.80(1)	175.70(315)	2.60(1)	72.20(191)	
9.72	2.40(1)	173.00(33)	0.80(1)	174.20(484)	3.10(1)	175.20(313)	2.10(1)	97.30(178)	
0	5.10(2)	146.60(45)	0.80(1)	171.80(547)	2.70(1)	124.80(295)	1.30(1)	197.60(187)	3000 K
4.17	2.20(1)	185.30(52)	0.80(2)	199.60(531)	2.10(1)	109.70(301)	0.80(1)	113.70(177)	
6.94	2.50(1)	158.00(54)	0.80(2)	189.30(511)	2.50(1)	126.30(307)	0.90(1)	38.50(169)	
9.72	1.20(1)	197.30(61)	0.90(6)	179.20(506)	2.40(1)	178.60(302)	1.00(1)	38.90(180)	
0	1.20(1)	191.10(52)	0.80(3)	146.20(527)	1.60(1)	60.20(265)	1.00(1)	52.50(169)	3500 K
4.17	1.20(1)	152.90(65)	0.80(5)	155.10(514)	1.20(1)	110.40(282)	0.90(2)	181.70(173)	
6.94	1.10(1)	74.30(61)	0.80(2)	133.70(501)	1.60(2)	180.30(277)	1.20(1)	183.30(169)	
9.72	1.30(1)	131.40(61)	0.80(1)	173.80(490)	2.000(1)	53.700(268)	1.00(1)	177.90(170)	

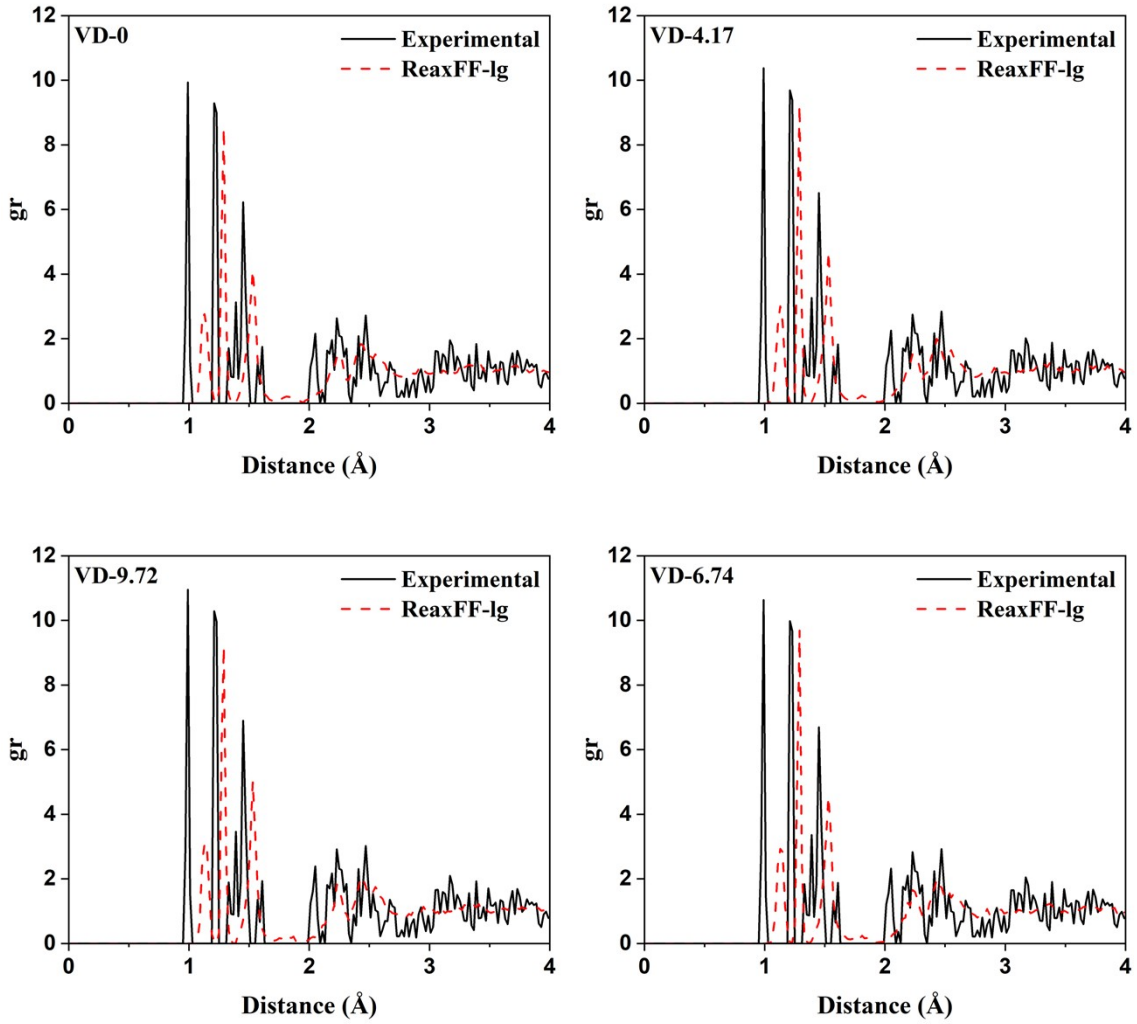

Figure S1. Comparison of the radial distribution functions (RDFs) for the perfect and defective CL-20/MTNP cocrystal models with the experimental structure and the corresponding ReaxFF/lg-optimized models.

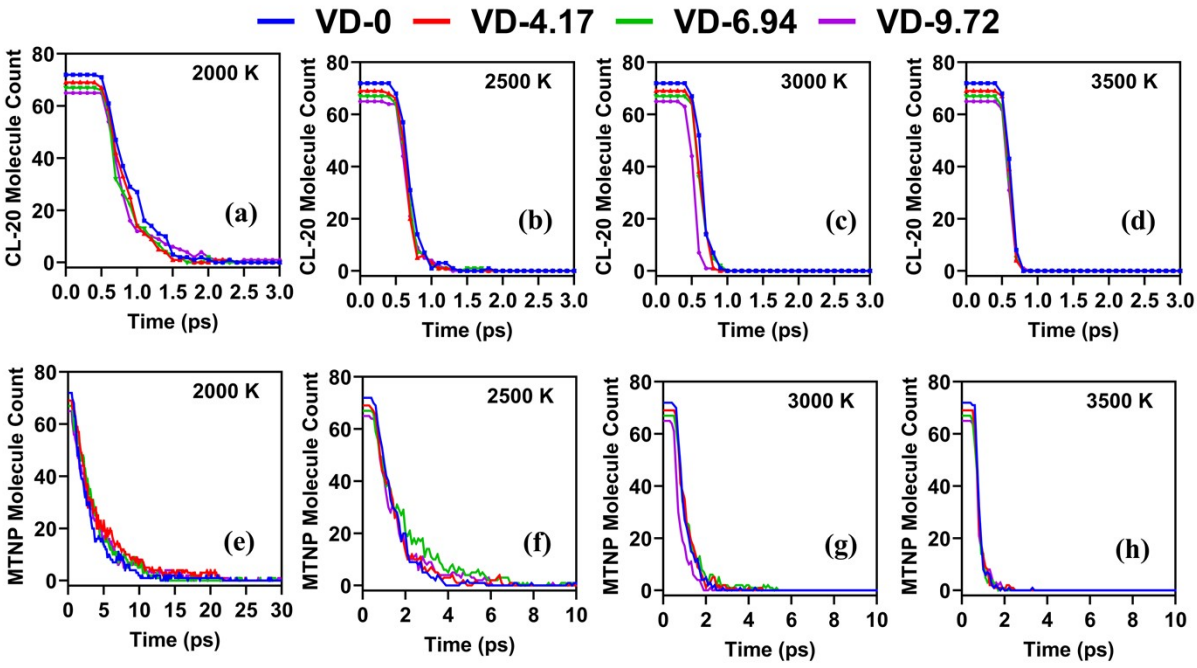

Figure S2. Decay of intact CL-20 and MTNP molecules in perfect and defective CL-20/MTNP cocrystal models at various temperatures.

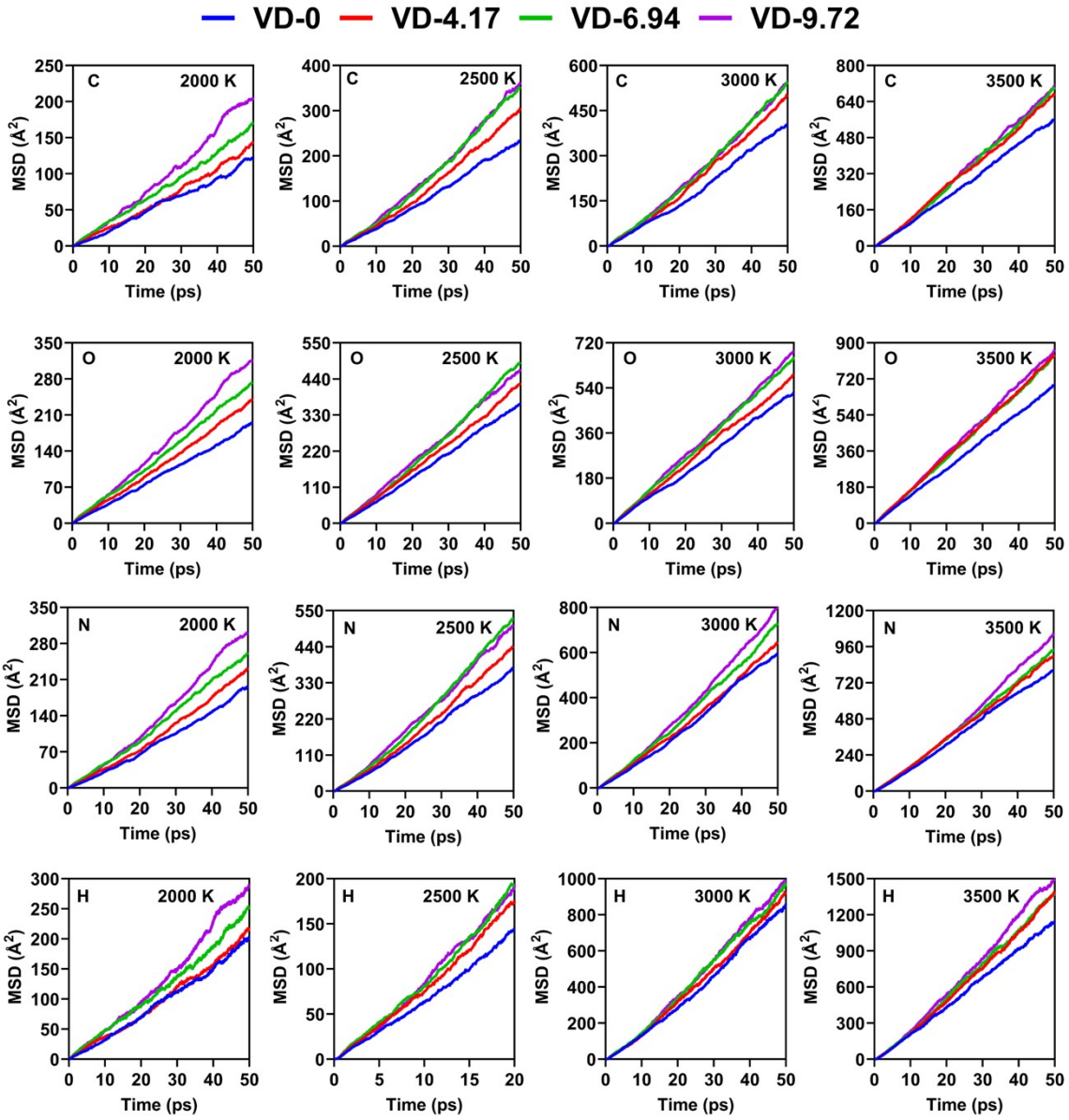

Figure S3. Comparison of the mean square displacement (MSD) curves of H, N, O, and C atoms for the perfect and defective CL-20/MTNP cocrystal models at 2000–3500 K.

Force Field Parameters

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Reactive MD-force field: nitramines (RDX/HMX/TATB/PETN)+lg
 39       ! Number of general parameters
  50.0000 !Overcoordination parameter
   9.4514 !Overcoordination parameter
  29.8953 !Valency angle conjugation parameter
 216.5421 !Triple bond stabilisation parameter
  12.2245 !Triple bond stabilisation parameter
   0.0000 !C2-correction
   1.0701 !Undercoordination parameter
   7.5000 !Triple bond stabilisation parameter
  11.9083 !Undercoordination parameter
  13.3822 !Undercoordination parameter
 -10.9834 !Triple bond stabilization energy
   0.0000 !Lower Taper-radius
  10.0000 !Upper Taper-radius
   2.8793 !Not used
  33.8667 !Valency undercoordination
   3.3976 !Valency angle/lone pair parameter
   1.0563 !Valency angle
   2.0384 !Valency angle parameter
   6.1431 !Not used
   6.9290 !Double bond/angle parameter
   0.0283 !Double bond/angle parameter: overcoord
   0.0570 !Double bond/angle parameter: overcoord
  -2.4837 !Not used
   5.8374 !Torsion/BO parameter
  10.0000 !Torsion overcoordination
   1.8820 !Torsion overcoordination
```

-1.2327 !Conjugation 0 (not used)
2.1861 !Conjugation
1.5591 !vdWaals shielding
0.0100 !Cutoff for bond order (*100)
4.8414 !Valency angle conjugation parameter
3.5857 !Overcoordination parameter
38.6472 !Overcoordination parameter
2.1533 !Valency/lone pair parameter
0.5000 !Not used
1.0000 !Scale factor (d) in dispersion
5.0000 !Molecular energy (not used)
0.0000 !Molecular energy (not used)
6.9784 !Valency angle conjugation parameter
7 ! Nr of atoms; cov.r; valency;a.m;Rvdw;Evdw;gammaEEM;cov.r2;#
alfa;gammavdW;valency;Eunder;Eover;chiEEM;etaEEM;n.u.
cov r3;Elp;Heat inc.;n.u.;n.u.;n.u.;n.u.
ov/un;val1;n.u.;val3,vval4
C 1.3742 4.0000 12.0000 1.9684 0.1723 0.8712 1.2385 4.0000
8.7696 100.0000 4.0000 31.0823 79.5548 5.7254 6.9235 0.0000
1.2104 0.0000 183.8108 5.7419 33.3951 11.9957 0.8563 0.0000
-2.8983 4.7820 1.0564 4.0000 2.9663 1.6737 0.1421 14.0707
0.0001 1.9255
H 0.6867 1.0000 1.0080 1.3525 0.0616 0.8910 -0.1000 1.0000
9.1506 100.0000 1.0000 0.0000 121.1250 3.8446 10.0839 1.0000
-0.1000 0.0000 58.4369 3.8461 3.2540 1.0000 1.0698 0.0000
-15.7683 2.1504 1.0338 1.0000 2.8793 1.2669 0.0139 12.4538
0.0001 1.4430
O 1.3142 2.0000 15.9990 1.9741 0.0880 0.8712 1.1139 6.0000
9.9926 100.0000 4.0000 29.5271 116.0768 8.5000 7.1412 2.0000
0.9909 14.7235 69.2921 9.1371 1.6258 0.1863 0.9745 0.0000

-3.5965 2.5000 1.0493 4.0000 2.9225 1.7221 0.1670 13.9991
623.8417 1.7500
N 1.2456 3.0000 14.0000 2.0437 0.1035 0.8712 1.1911 5.0000
9.8823 100.0000 4.0000 32.4758 100.0000 6.8453 6.8349 2.0000
1.0636 0.0276 127.9672 2.2169 2.8632 2.4419 0.9745 0.0000
-4.0959 2.0047 1.0183 4.0000 2.8793 1.5967 0.1649 13.9888
1240.001 1.8300
S 1.9647 2.0000 32.0600 2.0783 0.2176 1.0336 1.5386 6.0000
9.9676 5.0812 4.0000 35.1648 112.1416 6.5000 8.2545 2.0000
1.4703 9.4922 70.0338 8.5146 28.0801 8.5010 0.9745 0.0000
-10.0773 2.7466 1.0338 6.2998 2.8793 1.8000 0.0000 14.0000
180.0000 2.0783
Si 2.0276 4.0000 28.0600 2.2042 0.1322 0.8218 1.5758 4.0000
11.9413 2.0618 4.0000 11.8211 136.4845 1.8038 7.3852 0.0000
-1.0000 0.0000 126.5331 6.4918 8.5961 0.2368 0.8563 0.0000
-3.8112 3.1873 1.0338 4.0000 2.5791 0.0000 0.0000 0.0000
180.0000 2.2042
X -0.1000 2.0000 1.0080 2.0000 0.0000 1.0000 -0.1000 6.0000
10.0000 2.5000 4.0000 0.0000 0.0000 8.5000 1.5000 0.0000
-0.1000 0.0000 -2.3700 8.7410 13.3640 0.6690 0.9745 0.0000
-11.0000 2.7466 1.0338 4.0000 2.8793 0.0000 0.0000 0.0000
180.0000 2.0000
18 ! Nr of bonds; Edis1;LPpen;n.u.;pbe1;pbo5;13corr;pbo6
pbe2;pbo3;pbo4;Etrip;pbo1;pbo2;ovcorr
1 1 141.9346 113.4487 67.6027 0.1554 -0.3045 1.0000 30.4515 0.4283
0.0801 -0.2113 8.5395 1.0000 -0.0933 6.6967 1.0000 0.0000
1 2 163.6889 0.0000 0.0000 -0.4525 0.0000 1.0000 6.0000 0.5921
12.1053 1.0000 0.0000 1.0000 -0.0097 8.6351 0.0000 0.0000
2 2 169.8421 0.0000 0.0000 -0.3591 0.0000 1.0000 6.0000 0.7503
9.3119 1.0000 0.0000 1.0000 -0.0169 5.9406 0.0000 0.0000

1 3 159.7219 116.8921 77.9315 -0.4324 -0.1742 1.0000 15.0019 0.5160
1.2934 -0.3079 7.0252 1.0000 -0.1543 4.5116 0.0000 0.0000
3 3 108.9631 158.3501 42.0558 0.1226 -0.1324 1.0000 28.5716 0.2545
1.0000 -0.2656 8.6489 1.0000 -0.1000 6.8482 1.0000 0.0000
1 4 128.9104 171.2945 100.5836 -0.1306 -0.4948 1.0000 26.7458 0.4489
0.3746 -0.3549 7.0000 1.0000 -0.1248 4.9232 1.0000 0.0000
3 4 85.0402 118.8680 75.7263 0.7080 -0.1062 1.0000 16.6913 0.2407
0.3535 -0.1906 8.4054 1.0000 -0.1154 5.6575 1.0000 0.0000
4 4 160.6599 73.3721 154.2849 -0.7107 -0.1462 1.0000 12.0000 0.6826
0.9330 -0.1434 10.6712 1.0000 -0.0890 4.6486 1.0000 0.0000
2 3 219.7016 0.0000 0.0000 -0.6643 0.0000 1.0000 6.0000 0.9854
5.1146 1.0000 0.0000 1.0000 -0.0532 5.1189 0.0000 0.0000
2 4 208.0443 0.0000 0.0000 -0.3923 0.0000 1.0000 6.0000 0.3221
10.5505 1.0000 0.0000 1.0000 -0.0690 6.2949 0.0000 0.0000
1 5 128.7959 56.4134 39.0716 0.0688 -0.4463 1.0000 31.1766 0.4530
0.1955 -0.3587 6.2148 1.0000 -0.0770 6.6386 1.0000 0.0000
2 5 128.6090 0.0000 0.0000 -0.5555 0.0000 1.0000 6.0000 0.4721
10.8735 1.0000 0.0000 1.0000 -0.0242 9.1937 1.0000 0.0000
3 5 0.0000 0.0000 0.0000 0.5563 -0.4038 1.0000 49.5611 0.6000
0.4259 -0.4577 12.7569 1.0000 -0.1100 7.1145 1.0000 0.0000
4 5 0.0000 0.0000 0.0000 0.4438 -0.2034 1.0000 40.3399 0.6000
0.3296 -0.3153 9.1227 1.0000 -0.1805 5.6864 1.0000 0.0000
5 5 96.1871 93.7006 68.6860 0.0955 -0.4781 1.0000 17.8574 0.6000
0.2723 -0.2373 9.7875 1.0000 -0.0950 6.4757 1.0000 0.0000
6 6 109.1904 70.8314 30.0000 0.2765 -0.3000 1.0000 16.0000 0.1583
0.2804 -0.1994 8.1117 1.0000 -0.0675 8.2993 0.0000 0.0000
2 6 137.1002 0.0000 0.0000 -0.1902 0.0000 1.0000 6.0000 0.4256
17.7186 1.0000 0.0000 1.0000 -0.0377 6.4281 0.0000 0.0000
3 6 191.1743 52.0733 43.3991 -0.2584 -0.3000 1.0000 36.0000 0.8764
1.0248 -0.3658 4.2151 1.0000 -0.5004 4.2605 1.0000 0.0000

```
10    ! Nr of off-diagonal terms; Ediss;Ro;gamma;rsigma;rpi;rpi2
 1  2   0.0464   1.8296   9.9214   1.0029  -1.0000  -1.0000   0.0000
 2  3   0.0403   1.6913  10.4801   0.8774  -1.0000  -1.0000   0.0000
 2  4   0.0524   1.7325  10.1306   0.9982  -1.0000  -1.0000 294.9500
 1  3   0.1028   1.9277   9.1521   1.3399   1.1104   1.1609 631.8500
 1  4   0.2070   1.7366   9.5916   1.2960   1.2008   1.1262 650.0000
 3  4   0.0491   1.7025  10.6101   1.3036   1.1276   1.0173 880.0000
 2  6   0.0470   1.6738  11.6877   1.1931  -1.0000  -1.0000   0.0000
 3  6   0.1263   1.8163  10.6833   1.6266   1.2052  -1.0000   0.0000
 1  5   0.1408   1.8161   9.9393   1.7986   1.3021   1.4031   0.0000
 2  5   0.0895   1.6239  10.0104   1.4640  -1.0000  -1.0000   0.0000
62    ! Nr of angles;at1;at2;at3;Thetao,o;ka;kb;pv1;pv2
 1  1  1  74.0317  32.2712   0.9501   0.0000   0.1780  10.5736   1.0400
 1  1  2  70.6558  14.3658   5.3224   0.0000   0.0058   0.0000   1.0400
 2  1  2  76.7339  14.4217   3.3631   0.0000   0.0127   0.0000   1.0400
 1  2  2   0.0000   0.0000   6.0000   0.0000   0.0000   0.0000   1.0400
 1  2  1   0.0000   3.4110   7.7350   0.0000   0.0000   0.0000   1.0400
 2  2  2   0.0000  27.9213   5.8635   0.0000   0.0000   0.0000   1.0400
 1  1  3  65.1700   8.0170   7.5000   0.0000   0.2028  10.0000   1.0400
 3  1  3  71.7582  26.7070   6.0466   0.0000   0.2000   0.0000   1.8525
 1  1  4  65.4228  43.9870   1.5602   0.0000   0.2000  10.0000   1.8525
 3  1  4  73.7046  23.8131   3.9811   0.0000   0.2000   0.0000   1.8525
 4  1  4  65.6602  40.5852   1.8122   0.0000   0.2000   0.0000   1.8525
 2  1  3  56.4426  17.6020   5.3044   0.0000   0.9699   0.0000   1.1272
 2  1  4  71.0777   9.1462   3.4142   0.0000   0.9110   0.0000   1.0400
 1  2  4   0.0000   0.0019   6.3000   0.0000   0.0000   0.0000   1.0400
 1  3  1  72.1018  38.4720   1.3926   0.0000   0.4785   0.0000   1.2984
 1  3  3  89.9987  44.9806   0.5818   0.0000   0.7472   0.0000   1.2639
 1  3  4  70.3281  12.9371   7.5000   0.0000   0.7472   0.0000   1.2639
 3  3  3  84.2807  24.1938   2.1695 -10.0000   0.7472   0.0000   1.2639
```

3	3	4	84.2585	44.1039	0.9185	0.0000	0.7472	0.0000	1.2639
4	3	4	74.2312	25.7005	4.3943	0.0000	0.7472	0.0000	1.2639
1	3	2	89.0416	36.9460	0.4569	0.0000	2.7636	0.0000	2.0494
2	3	3	81.1709	4.2886	6.5904	0.0000	3.0000	0.0000	1.2618
2	3	4	75.9203	44.9675	0.8889	0.0000	3.0000	0.0000	1.2618
2	3	2	82.2020	12.7165	3.9296	0.0000	0.2765	0.0000	1.0470
1	4	1	68.3788	18.3716	1.8893	0.0000	2.4132	0.0000	1.3993
1	4	3	86.5585	37.6814	1.1611	0.0000	1.7325	0.0000	1.0440
1	4	4	74.4818	12.0954	7.5000	0.0000	1.7325	0.0000	1.0440
3	4	3	78.5850	44.3389	1.3239	-26.2246	1.7325	40.0000	1.0440
3	4	4	77.6245	32.0866	1.8889	-0.9193	1.7325	0.0000	1.0440
4	4	4	66.4718	15.9087	7.5000	0.0000	1.7325	0.0000	1.0440
1	4	2	90.0000	33.6636	1.1051	0.0000	0.2638	0.0000	1.1376
2	4	3	83.8493	44.9000	1.3580	0.0000	0.5355	0.0000	2.5279
2	4	4	78.7452	24.2010	3.7481	0.0000	0.5355	0.0000	2.5279
2	4	2	55.8679	14.2331	2.9225	0.0000	0.2000	0.0000	2.9932
1	2	3	0.0000	0.0019	6.0000	0.0000	0.0000	0.0000	1.0400
1	2	4	0.0000	0.0019	6.0000	0.0000	0.0000	0.0000	1.0400
1	2	5	0.0000	0.0019	6.0000	0.0000	0.0000	0.0000	1.0400
3	2	3	0.0000	0.0019	6.0000	0.0000	0.0000	0.0000	1.0400
3	2	4	0.0000	0.0019	6.0000	0.0000	0.0000	0.0000	1.0400
4	2	4	0.0000	0.0019	6.0000	0.0000	0.0000	0.0000	1.0400
2	2	3	0.0000	0.0019	6.0000	0.0000	0.0000	0.0000	1.0400
2	2	4	0.0000	0.0019	6.0000	0.0000	0.0000	0.0000	1.0400
1	1	5	74.4180	33.4273	1.7018	0.1463	0.5000	0.0000	1.6178
1	5	1	79.7037	28.2036	1.7073	0.1463	0.5000	0.0000	1.6453
2	1	5	63.3289	29.4225	2.1326	0.0000	0.5000	0.0000	3.0000
1	5	2	85.9449	38.3109	1.2492	0.0000	0.5000	0.0000	1.1000
1	5	5	85.6645	40.0000	2.9274	0.1463	0.5000	0.0000	1.3830
2	5	2	83.8555	5.1317	0.4377	0.0000	0.5000	0.0000	3.0000

```
 2  5  5  97.0064  32.1121   2.0242   0.0000   0.5000   0.0000   2.8568
 6  6  6  69.3456  21.7361   1.4283   0.0000  -0.2101   0.0000   1.3241
 2  6  6  75.6168  21.5317   1.0435   0.0000   2.5179   0.0000   1.0400
 2  6  2  78.3939  20.9772   0.8630   0.0000   2.8421   0.0000   1.0400
 3  6  6  70.3016  15.4081   1.3267   0.0000   2.1459   0.0000   1.0400
 2  6  3  73.8232  16.6592   3.7425   0.0000   0.8613   0.0000   1.0400
 3  6  3  90.0344   7.7656   1.7264   0.0000   0.7689   0.0000   1.0400
 6  3  6  22.1715   3.6615   0.3160   0.0000   4.1125   0.0000   1.0400
 2  3  6  83.7634   5.6693   2.7780   0.0000   1.6982   0.0000   1.0400
 3  3  6  73.4663  25.0761   0.9143   0.0000   2.2466   0.0000   1.0400
 2  2  6   0.0000  47.1300   6.0000   0.0000   1.6371   0.0000   1.0400
 6  2  6   0.0000  31.5209   6.0000   0.0000   1.6371   0.0000   1.0400
 3  2  6   0.0000  31.0427   4.5625   0.0000   1.6371   0.0000   1.0400
 2  2  5   0.0000   0.0019   6.0000   0.0000   0.0000   0.0000   1.0400
31    ! Nr of torsions;at1;at2;at3;at4;;V1;V2;V3;V2(BO);vconj;n.u;n
 1  1  1  1   0.0000  48.4194   0.3163  -8.6506  -1.7255   0.0000   0.0000
 1  1  1  2   0.0000  63.3484   0.2210  -8.8401  -1.8081   0.0000   0.0000
 2  1  1  2   0.0000  45.2741   0.4171  -6.9800  -1.2359   0.0000   0.0000
 0  1  2  0   0.0000   0.0000   0.0000   0.0000   0.0000   0.0000   0.0000
 0  2  2  0   0.0000   0.0000   0.0000   0.0000   0.0000   0.0000   0.0000
 0  1  3  0   1.7254  86.0769   0.3440  -4.2330  -2.0000   0.0000   0.0000
 0  2  3  0   0.0000   0.1000   0.0200  -2.5415   0.0000   0.0000   0.0000
 0  3  3  0   1.2314 116.5137   0.5599  -4.1412   0.0000   0.0000   0.0000
 0  1  4  0  -1.3258 149.8644   0.4790  -7.1541  -2.0000   0.0000   0.0000
 0  2  4  0   0.0000   0.1000   0.0200  -2.5415   0.0000   0.0000   0.0000
 0  3  4  0   1.3168  57.0732   0.2679  -4.1516  -2.0000   0.0000   0.0000
 0  4  4  0   2.0000  75.3685  -0.7852  -9.0000  -2.0000   0.0000   0.0000
 0  1  1  0   0.0930  18.6070  -1.3191  -9.0000  -1.0000   0.0000   0.0000
 4  1  4  4  -2.0000  20.6655  -1.5000  -9.0000  -2.0000   0.0000   0.0000
 0  1  5  0   4.0885  78.7058   0.1174  -2.1639   0.0000   0.0000   0.0000
```

0 5 5 0 -0.0170 -56.0786 0.6132 -2.2092 0.0000 0.0000 0.0000

0 2 5 0 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000

0 6 6 0 0.0000 0.0000 0.1200 -2.4426 0.0000 0.0000 0.0000

0 2 6 0 0.0000 0.0000 0.1200 -2.4847 0.0000 0.0000 0.0000

0 3 6 0 0.0000 0.0000 0.1200 -2.4703 0.0000 0.0000 0.0000

1 1 3 3 1.2707 21.6200 1.5000 -9.0000 -2.0000 0.0000 0.0000

1 3 3 1 -1.8804 79.9255 -1.5000 -4.1940 -2.0000 0.0000 0.0000

3 1 3 3 -2.0000 22.5092 1.5000 -8.9500 -2.0000 0.0000 0.0000

1 4 4 3 0.1040 70.1152 0.5284 -3.5026 -2.0000 0.0000 0.0000

1 1 3 4 1.2181 119.6186 -1.5000 -7.0635 -2.0000 0.0000 0.0000

2 1 3 4 -2.0000 156.6604 1.1004 -7.3729 -2.0000 0.0000 0.0000

1 3 4 3 2.0000 96.6281 -1.5000 -3.8076 -2.0000 0.0000 0.0000

1 1 4 2 -2.0000 147.2445 -1.5000 -7.0142 -2.0000 0.0000 0.0000

1 1 4 3 -2.0000 47.8326 -1.5000 -9.0000 -2.0000 0.0000 0.0000

2 3 4 3 -0.2997 152.9040 -1.5000 -4.4564 -2.0000 0.0000 0.0000

2 4 4 3 0.1040 70.1152 0.5284 -3.5026 -2.0000 0.0000 0.0000

9 ! Nr of hydrogen bonds;at1;at2;at3;Rhb;Dehb;vhb1

3 2 3 2.1845 -2.3549 3.0582 19.1627

3 2 4 1.6658 -3.8907 3.0582 19.1627

4 2 3 1.8738 -3.5421 3.0582 19.1627

4 2 4 1.8075 -4.1846 3.0582 19.1627

3 2 5 2.6644 -3.0000 3.0000 3.0000

4 2 5 4.0476 -3.0000 3.0000 3.0000

5 2 3 2.1126 -4.5790 3.0000 3.0000

5 2 4 2.2066 -5.7038 3.0000 3.0000

5 2 5 1.9461 -4.0000 3.0000 3.0000