Electronic Supplementary Information

How does the combination of the nitro group and fluorine atoms affect the (co)crystallization behaviour of arylenediamines?

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Table S1 Crystallographic data and structure refinement parameters

	A·cr	**A_2·cr**	**B·cr**	**B_2·cr**	**C·cr**
CCDC number	2253808	2253806	2253809	2253807	2253810
Crystal data					
Chemical formula	$C_{18}H_{28}F_3N_3O_8$	$C_{24}H_{32}F_6N_6O_{10}$	$C_{18}H_{29}F_2N_3O_8$	$C_{24}H_{34}F_4N_6O_{10}$	$C_{18}H_{30}FN_3O_8$
M_r	471.43	678.55	453.44	642.57	435.45
Crystal system, space group	Triclinic, $P\bar{1}$	Triclinic, $P\bar{1}$	Triclinic, $P\bar{1}$	Triclinic, $P\bar{1}$	Monoclinic, *Cc*
Temperature (K)	296	296	296	170	296
a, *b*, *c* (Å)	8.0036 (7), 9.2934 (7), 15.7077 (12)	11.6265 (4), 11.6941 (6), 12.1146 (6)	7.9046 (8), 9.2505 (8), 15.7606 (16)	11.4494 (6), 11.7343 (6), 12.2027 (6)	14.0576 (5), 11.0469 (3), 15.0431 (6)
α, β, γ (°)	80.801 (4), 81.339 (4), 78.770 (4)	73.313 (2), 77.928 (1), 80.047 (1)	79.769 (3), 84.623 (3), 78.313 (4)	73.603 (2), 77.788 (2), 79.850 (2)	90, 111.343 (2), 90
V (Å^3)	1122.60 (16)	1531.64 (12)	1108.61 (19)	1525.26 (14)	2175.87 (13)
Z	2	2	2	2	4
Radiation type	Mo $K\alpha$	Mo $K\alpha$	Mo $K\alpha$	Mo $K\alpha$	Mo $K\alpha$
μ (mm^{-1})	0.12	0.14	0.12	0.12	0.11
Crystal size (mm)	0.36 × 0.34 × 0.16	0.62 × 0.26 × 0.10	0.68 × 0.38 × 0.23	0.51 × 0.14 × 0.07	0.64 × 0.23 × 0.17
Data collection					
Diffractometer	Bruker APEX-II	Bruker APEX-II	Bruker APEX-II	Bruker APEX-II	Bruker APEX-II
Absorption correction	SADABS-2008/1	SADABS-2008/1	SADABS-2008/1	SADABS-2008/1	SADABS-2008/1
No. of measured, independent and observed reflections	30056, 5213, 3990 [$I > 2\sigma(I)$]	41112, 6787, 4918 [$I > 2\sigma(I)$]	29238, 4929, 3734 [$I > 2\sigma(I)$]	36075, 6654, 4559 [$I > 2\sigma(I)$]	20815, 4900, 4074 [$I > 2\sigma(I)$]
R_{int}	0.046	0.035	0.056	0.051	0.040
$(\sin\theta/\lambda)_{max}$ (Å^{-1})	0.653	0.643	0.644	0.640	0.660
Refinement					
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.094, 0.332, 1.01	0.044, 0.145, 1.01	0.064, 0.199, 1.03	0.041, 0.135, 0.97	0.035, 0.087, 1.01
No. of reflections	5213	6787	4929	6654	4900
No. of parameters	302	431	296	429	287
No. of restraints	4	4	4	8	6
H-atom treatment	H atoms treated by a mixture of independent and constrained refinement	H atoms treated by a mixture of independent and constrained refinement	H atoms treated by a mixture of independent and constrained refinement	H atoms treated by a mixture of independent and constrained refinement	H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.43, -0.36	0.85, -0.32	0.46, -0.36	0.60, -0.16	0.13, -0.17
Absolute structure parameter	–	–	–	–	0.7 (3)

Table S1 Crystallographic data and structure refinement parameters (continued)

	D·cr	**A**	**B**	**C**
CCDC number	2253811	2253812	2253813	2253814
Crystal data				
Chemical formula	$C_{18}H_{31}N_3O_8$	$C_6H_4F_3N_3O_2$	$C_6H_5F_2N_3O_2$	$C_6H_6FN_3O_2$
M_r	417.46	207.12	189.13	171.14
Crystal system, space group	Monoclinic, *Cc*	Orthorhombic, *Pna*2_1	Monoclinic, *Pc*	Monoclinic, *P*2_1/*n*
Temperature (K)	296	296	296	296
a, *b*, *c* (Å)	13.7751 (10), 11.1808 (6), 14.7876 (11)	7.1452 (4), 13.5660 (8), 7.7555 (5)	7.6215 (4), 3.6750 (2), 13.2829 (7)	4.5277 (2), 11.3347 (6), 13.8350 (7)
α, β, γ (°)	90, 109.477 (3), 90	90, 90, 90	90, 104.936 (2), 90	90, 93.8990 (17), 90
V (Å^3)	2147.2 (3)	751.75 (8)	359.47 (3)	708.37 (6)
Z	4	4	2	4
Radiation type	Mo *K*α	Mo *K*α	Mo *K*α	Mo *K*α
μ (mm^{-1})	0.10	0.19	0.17	0.14
Crystal size (mm)	0.64 × 0.28 × 0.24	0.54 × 0.19 × 0.12	0.42 × 0.27 × 0.19	0.49 × 0.43 × 0.14
Data collection				
Diffractometer	Bruker APEX-II	Bruker APEX-II	Bruker APEX-II	Bruker APEX-II
Absorption correction	SADABS-2008/1	SADABS-2008/1	SADABS-2008/1	SADABS-2008/1
No. of measured, independent and observed reflections	5827, 3403, 3035 [$I > 2\sigma(I)$]	13714, 1823, 1521 [$I > 2\sigma(I)$]	4750, 1592, 1487 [$I > 2\sigma(I)$]	7480, 1571, 1337 [$I > 2\sigma(I)$]
R_{int}	0.047	0.031	0.017	0.049
$(\sin\theta/\lambda)_{max}$ (Å^{-1})	0.650	0.662	0.642	0.643
Refinement				
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.040, 0.115, 0.99	0.033, 0.105, 1.05	0.026, 0.079, 1.03	0.041, 0.123, 1.05
No. of reflections	3403	1823	1592	1571
No. of parameters	278	143	134	125
No. of restraints	6	1	2	4
H-atom treatment	H atoms treated by a mixture of independent and constrained refinement	All H-atom parameters refined	H atoms treated by a mixture of independent and constrained refinement	H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.22, -0.19	0.24, -0.16	0.17, -0.15	0.32, -0.24
Absolute structure parameter	-0.7 (9)	0.1 (2)	-0.4 (2)	–

Computer programs: *SHELXT* 2014/5 (Sheldrick, 2014), *SHELXL2018*/3 (Sheldrick, 2018), *SADABS*-2008/1.

Table S2 Hydrogen bonding in the co-crystals and homocrystals

Sample code	Interaction D-H···A	$l_{D\text{-}H}$ (Å)	$l_{H\cdots A}$ (Å)	$l_{D\cdots A}$ (Å)	Angle D-H···A (deg)	Symmetry code for acceptor
A·cr	N(1)-H(1A)···O(6)	0.90(5)	2.34(5)	3.121(5)	145(4)	1-x,1-y,-z
	N(1)-H(1A)···O(7)	0.90(5)	2.49(6)	3.052(7)	122(5)	1-x,1-y,-z
	N(1)-H(1B)···O(6)	0.90(4)	2.31(4)	3.190(5)	165(5)	
	N(2)-H(2B)···O(3)	0.90(4)	2.30(4)	3.186(6)	168(4)	1-x,1-y,1-z
	C(12)-H(12A)···F(2)	0.97	2.51	3.260(5)	134	1-x,1-y,1-z
A_2·cr	N(1)-H(1B)···O(4)	0.895(19)	2.34(2)	3.215(3)	166(2)	1-x,2-y,-z
	N(2)-H(2A)···O(7)	0.882(19)	2.208(19)	3.055(2)	161(2)	
	N(2)-H(2B)···O(9)	0.89(2)	2.222(19)	3.082(2)	164(2)	
	N(4)-H(4B)···O(1)	0.86	2.44	3.124(3)	136	-x,2-y,-z
	N(5)-H(5A)···O(10)	0.86	2.28	3.096(2)	159	
	N(5)-H(5B)···O(8)	0.86	2.29	3.129(2)	166	
	C(15)-H(15B)···F(1)	0.97	2.52	3.279(3)	135	
	C(16)-H(16A)···O(1)	0.97	2.52	3.462(3)	165	1+x,y,z
	C(23)-H(23A)···O(3)	0.97	2.52	3.492(3)	175	-1+x,y,z
	C(24)-H(24B)···F(4)	0.97	2.52	3.283(3)	136	
B·cr	N(1)-H(1A)···O(3)	0.87(3)	2.42(3)	3.167(3)	144(2)	
	N(1)-H(1A)···O(5)	0.87(3)	2.50(3)	3.091(3)	126(3)	1-x,1-y,2-z
	N(1)-H(1B)···O(3)	0.88(2)	2.30(2)	3.164(3)	167(2)	1-x,1-y,2-z
	N(1)-H(1B)···O(4)	0.88(2)	2.59(2)	3.166(3)	123.6(18)	1-x,1-y,2-z
	N(2)-H(2A)···O(6)	0.87(3)	2.43(3)	3.267(3)	162(3)	1-x,1-y,1-z
	C(13)-H(13A)···F(2)	0.97	2.49	3.260(3)	136	
B_2·cr	N(1)-H(1B)···O(4)	0.888(19)	2.277(19)	3.138(3)	163.3(19)	1+x,y,z
	N(2)-H(2A)···O(10)	0.882(19)	2.243(19)	3.088(2)	160(2)	
	N(2)-H(2B)···O(8)	0.89(2)	2.252(19)	3.104(2)	162(2)	
	N(4)-H(4B)···O(1)	0.88(2)	2.35(2)	3.123(2)	146.4(19)	
	N(5)-H(5A)···O(7)	0.88(2)	2.32(2)	3.130(2)	153(2)	1-x,1-y,1-z
	N(5)-H(5B)···O(9)	0.865(19)	2.292(19)	3.125(2)	162(2)	1-x,1-y,1-z
	C(15)-H(15B)···F(3)	0.99	2.50	3.269(3)	135	1-x,1-y,1-z
	C(16) -H(16A)···O(3)	0.99	2.42	3.401(3)	174	-x,1-y,1-z
	C(23) -H(23A)···O(1)	0.99	2.45	3.399(3)	161	1+x,y,z
	C(24)-H(24B)···F(1)	0.99	2.49	3.272(3)	135	

Table S2 Hydrogen bonding in the co-crystals and homocrystals (continued)

Sample code	Interaction D-H···A	$l_{D\text{-}H}$ (Å)	$l_{H\ldots A}$ (Å)	$l_{D\ldots A}$ (Å)	Angle D-H···A (deg)	Symmetry code for acceptor
C·cr	N(1)-H(1B)···O(5)	0.889(15)	2.340(16)	3.209(3)	166(3)	
	N(2)-H(2A)···O(8)	0.91(2)	2.23(2)	3.110(3)	164(4)	x,-y,-1/2+z
	N(2)-H(2B)···O(6)	0.89(3)	2.35(3)	3.140(4)	148(3)	x,-y,-1/2+z
	C(11)-H(11B)···F(1)	0.97	2.40	3.274(3)	149	
	C(17)-H(17A)···O(2)	0.99	2.42	3.297(4)	150	x,-y,1/2+z
D·cr	N(1)-H(1B)···O(6)	0.87(2)	2.50(3)	3.335(3)	159(4)	x,1-y,-1/2+z
	N(2)-H(2A)···O(3)	0.90(3)	2.19(2)	3.081(3)	172(4)	
	N(2)-H(2B)···O(5)	0.88(3)	2.26(4)	3.091(4)	157(3)	
	C(18)-H(18A)···O(2)	0.97	2.46	3.344(4)	151	x,1-y,1/2+z
A	N(2)-H(2A)···F(3)	0.86(4)	2.55(4)	3.183(3)	132(4)	3/2-x,1/2+y,-1/2+z
	N(2)-H(2A)···O(2)	0.86(4)	2.29(4)	3.107(4)	159(3)	3/2-x,1/2+y,-1/2+z
	N(2)-H(2B)···O(1)	0.92(5)	2.10(5)	2.997(4)	166(4)	1/2+x,1/2-y,-1+z
B	N(1)-H(1B)···O(1)	0.92(4)	2.17(4)	3.063(3)	164(3)	x,-y,-1/2+z
	N(2)-H(2A)···O(2)	0.90(4)	2.35(4)	3.072(3)	138(4)	-1+x,-y,-1/2+z
	N(2)-H(2B)···O(1)	0.87(5)	2.37(4)	3.014(3)	132(3)	-1+x,1-y,-1/2+z
C	N(1)-H(1A)···N(2)	0.892(17)	2.513(18)	3.1829(18)	132.3(14)	3/2-x,-1/2+y,3/2-z
	N(1)-H(1B)···O(1)	0.886(16)	2.277(16)	3.1380(17)	163.8(17)	1/2+x,1/2-y,1/2+z
	N(2)-H(2A)···O(2)	0.890(17)	2.285(17)	3.1658(17)	170.6(17)	-1/2+x,1/2-y,1/2+z
	N(2)-H(2B)···N(1)	0.885(19)	2.400(19)	3.2730(19)	169.2(16)	1/2-x,1/2+y,3/2-z
	C(3)-H(3)···O(1)	0.93	2.59	3.3635(18)	141	1/2+x,1/2-y,1/2+z
	C(6)-H(6)···F(1)	0.93	2.48	3.4013(16)	169	-x,1-y,1-z
D[a]	N(1)-H(11)···N(3)	0.86	2.41	3.2595(18)	171	-1/2-x,1/2+y,1/2-z
	N(1)-H(12)···O(1)	0.86	2.25	3.0210(17)	149	-1/2+x,3/2-y,1/2+z
	N(3)-H(31)···O(2)	0.86	2.16	2.9641(16)	155	1/2+x,3/2-y,1/2+z
	N(3)-H(32)···N(1)	0.86	1.62	3.2811(1)	135	1/2-x,-1/2+y,1/2-z
	C(2)-H(2)···O(2)	0.93	2.55	3.3205(19)	140	1/2+x,3/2-y,1/2+z

[a] Data from the work C. Glidewell, D. Cannon, A. Quesada, J. N. Low, S. A. McWilliam, J. M. S. Skakle, J. L. Wardell, *Acta Crystallogr., Sect. C: Cryst. Struct. Commun.,* 2001, **C57,** 455-458; CCDC **163928**.

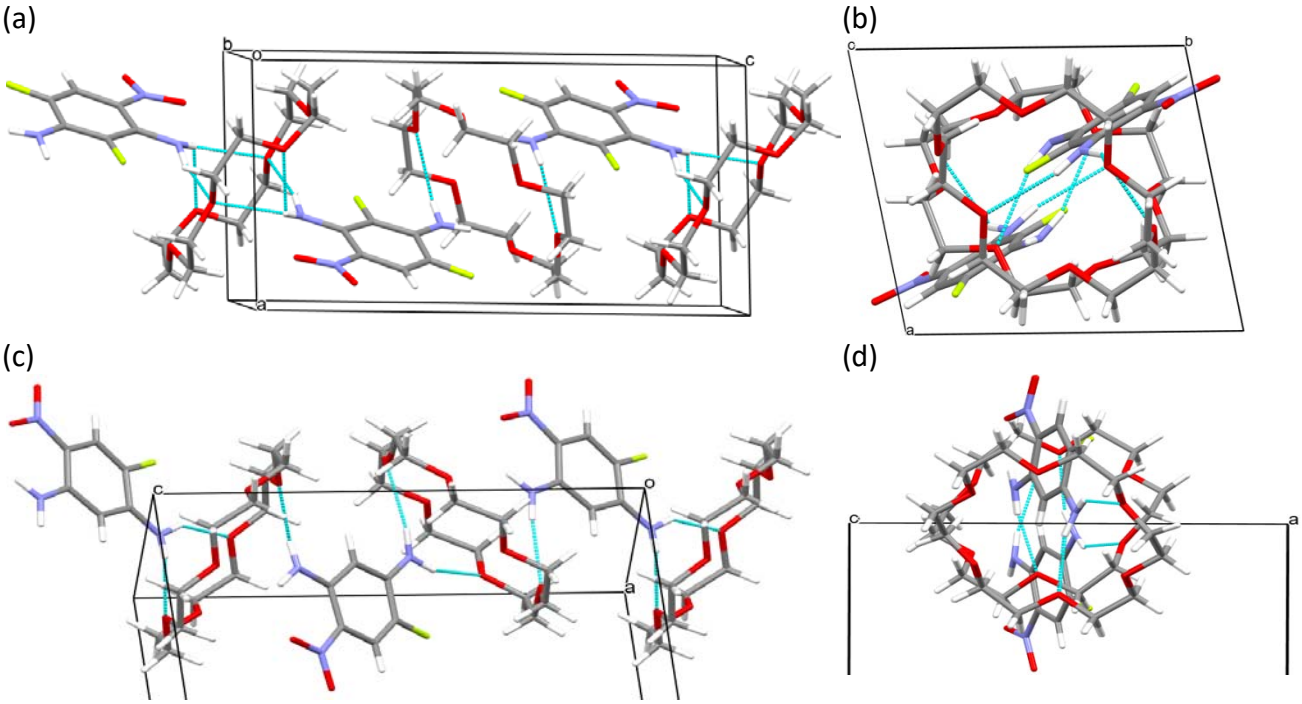


Fig. S1 1D assembly in the co-crystals, top and cross-section view: **B·cr** (a, b), **C·cr** (c, d).

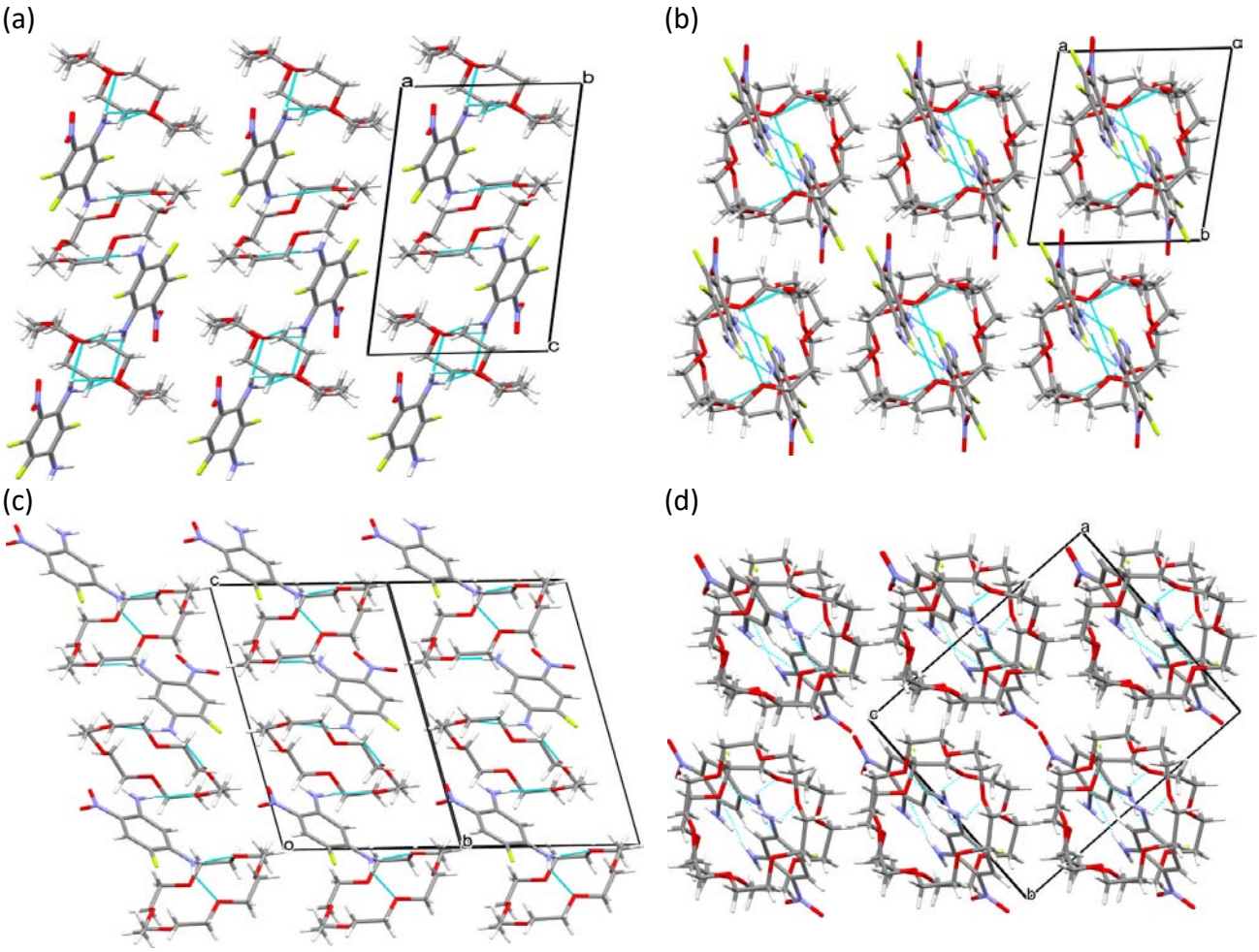


Fig. S2 Packing of the rods in co-crystals, top view on the layer and cross-section view: **A·cr** (a, b), **C·cr** (c, d).

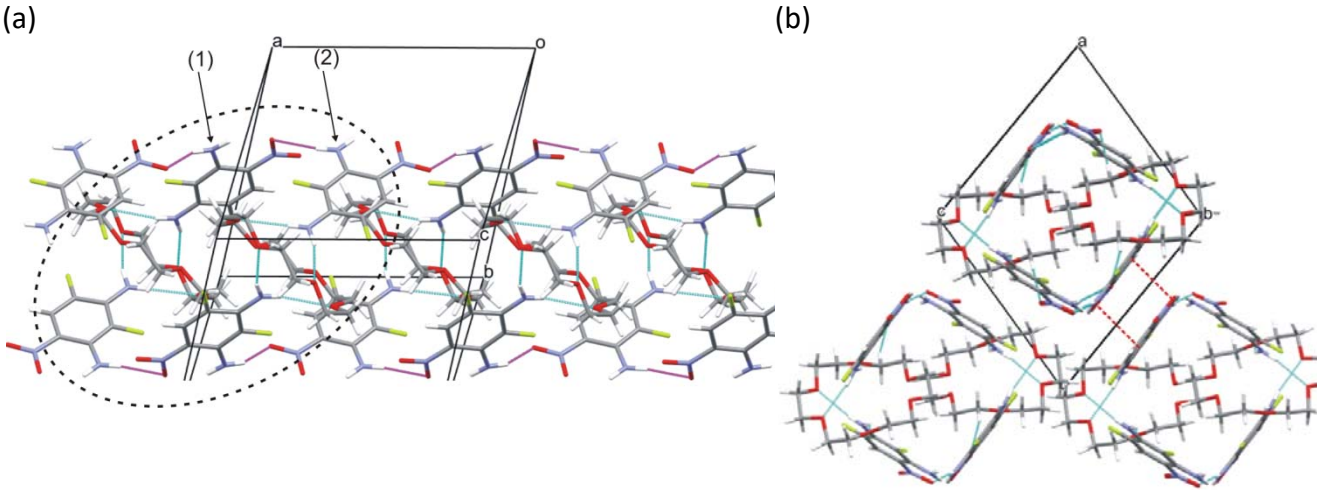


Fig. S3 Crystal packing in **B_2·cr**: H-bonded 1D assembly (a): N–H···O_{cr} (turquoise), N–H···O_{nitro} (magenta), unit (6 molecules) is framed; p···π interactions between assemblies (b).

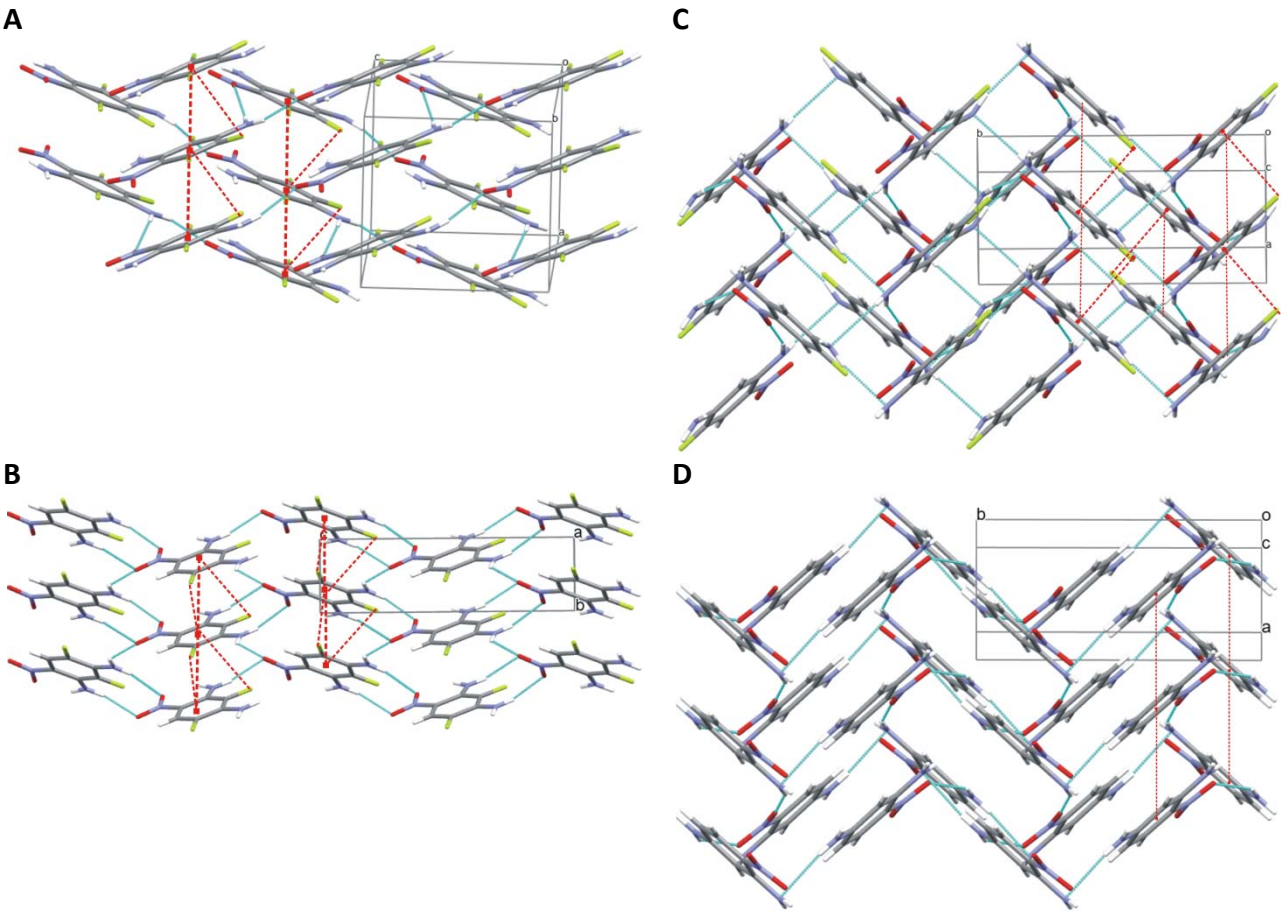


Fig. S4 Molecular packing of diaminonitrobenzenes **A** – **D** in the crystals, side view on the p···π electron bonded stacks.

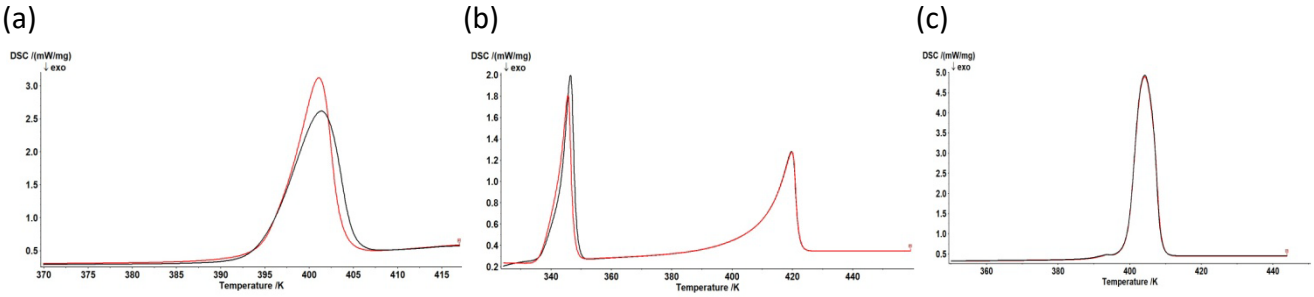


Fig. S5 DSC curves of the co-crystals, the first (black) and second (red) heating runs: **B_2·cr** (a); **A·cr** (b); **D·cr** (c).

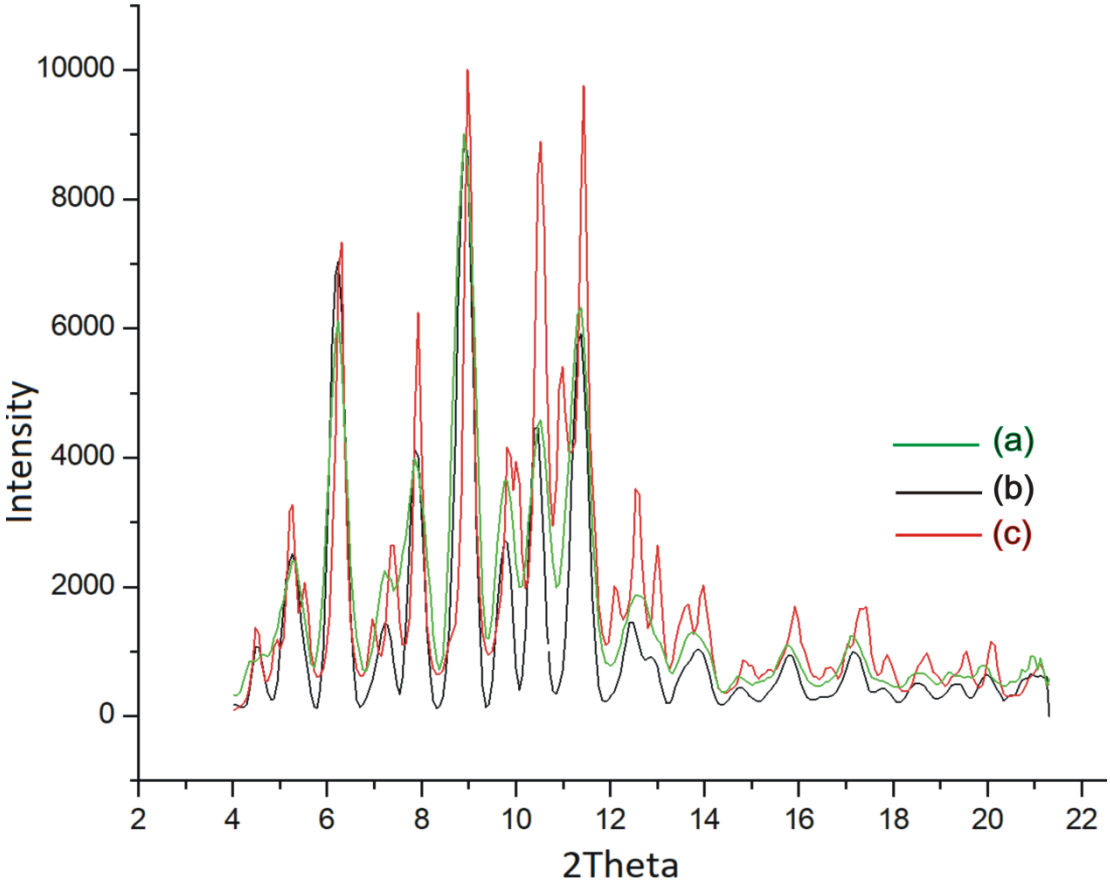


Fig. S6 PXRD patterns of **A·cr**: bulky precipitate crystallized from *t*-BuOMe (experimental, a), crystallized from the melt (experimental, b), simulated from SC-XRD data using MERCURY software with peak shape 0.3 (calculated, c).

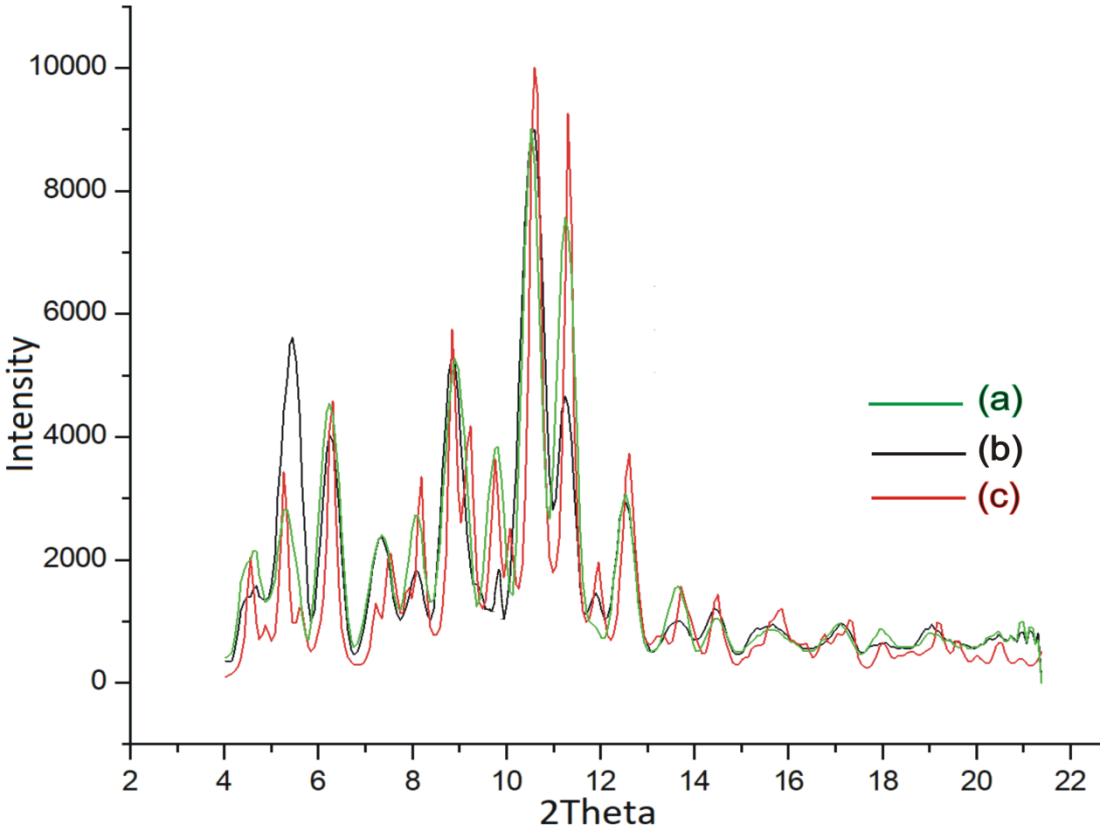


Fig. S7 PXRD patterns of **B·cr**: bulky precipitate crystallized from *t*-BuOMe (experimental, a), crystallized from the melt (experimental, b), simulated from SC-XRD data using MERCURY software with peak shape 0.3 (calculated, c).

Table S3 Enthalpies of co-crystals, homocrystals, and isolated molecules. Level of theory: DFT/GGA-PBE/ USPP in QUANTUM ESPRESSO

Code	Final enthalpy (Ry)	Z	H/Z (Ry)[a]	$H(Y_x{\cdot}cr_{1-x})$[b](Ry)
1:1 co-crystals				
A·cr	-1407,99039845	2	-703,99519922	-351,99759961
B·cr	-1313,20407953	2	-656,60203976	-328,30101988
C·cr	-2436,81011652	4	-609,20252913	-304,60126456
D·cr	-2247,12475905	4	-561,78118976	-280,89059488
2:1 co-crystals				
A_2·cr	-2096,52758610	2	-1048,26379305	-349,42126435
B_2·cr	-1906,96370388	2	-953,48185194	-317,82728398
Homocrystals				
A	-1376,96147914	4	-344,24036978	-344,24036978
B	-593,70367933	2	-296,85183967	-296,85183967
C	-997,77559239	4	-249,44389810	-249,44389810
D	-808,06295742	4	-202,01573936	-202,01573936
cr	-1438,90959346	4	-359,72739836	-359,72739836
Isolated molecules				
A	-344,21390406			
B	-296,82691698			
C	-249,40658711			
D	-201,98518814			
cr	-359,73061909			

[a] Z is the number of molecules in a cell.

[b] $H(Y_x{\cdot}cr_{1-x})$ is the enthalpy of a co-crystal normalized per unit, where Y – diamine, x – molar fraction of the diamine in the co-crystal (1/2 in 1:1 co-crystals and 2/3 in 2:1 co-crystals).

Table S4 Energies of individual molecules, H-bonded and p···π dimers in co-crystals and homocrystals.[a] Level of theory: DFT/B3LYP/ M6-31G (TM)+*

Crystal	Molecule/dimer	*E* (Ha)	*E* (kJ mol^{-1})
1:1 co-crystals			
A·cr	A	-845,1848988	-2218441,322
	cr1	-923,0044119	-2422701,980
	cr2	-923,0088610	-2422713,658
	A···cr1 (*ortho*-N-H···Ocr)	-1768,2057666	-4641186,496
	A···cr2 (*para*-N-H···O_{cr})	-1768,2135690	-4641206,976
B·cr	B	-745,9656389	-1958010,609
	cr1	-923,0038250	-2422700,440
	cr2	-923,0088048	-2422713,511
	B···cr1 (*ortho*-N-H···O_{cr})	-1668,9847970	-4380751,295
	B···cr2 (*para*-N-H···O_{cr})	-1668,9924264	-4380771,321
C·cr	C	-646,7286414	-1697533,338
	cr	-923,0101844	-2422717,132
	C···cr (*ortho*-N-H···O_{cr})	-1569,7534317	-4120288,808
	C···cr (*para*-N-H···O_{cr})	-1569,7595820	-4120304,951
D·cr	D	-547,4910547	-1437054,520
	cr	-923,0107357	-2422718,579
	D···cr (*ortho*-N-H···O_{cr})	-1470,5152328	-3859808,383
	D···cr (*para*-N-H···O_{cr})	-1470,5206950	-3859822,720
2:1 co-crystals			
A_2·cr	A1	-845,1853395	-2218442,479
	A2	-845,1855136	-2218442,936
	cr	-923,0094343	-2422715,163
	A1···cr (*para*-N-H···O_{cr})	-1768,2175976	-4641217,550
	A2···cr (*para*-N-H···O_{cr})	-1768,2173117	-4641216,800
	A1…A2 (*ortho*-N-H···O_{nitro})	-1690,3771100	-4436901,838
	A2…A1 (*ortho*-N-H···O_{nitro})	-1690,3777999	-4436903,649
	A1…A1 (N-O···π)	-1690,3732623	-4436891,739
	A2…A2 (C-F···π)	-1690,3760518	-4436899,061
B_2·cr	B1	-745,9658098	-1958011,058
	B2	-745,9660216	-1958011,614
	cr	-923,0098700	-2422716,307
	B1···cr (*para*-N-H···O_{cr})	-1668,9964419	-4380781,861
	B2···cr (*para*-N-H···O_{cr})	-1668,9966955	-4380782,526
	B1…B2 (*ortho*-N-H···O_{nitro})	-1491,9384600	-3916040,070
	B2…B1 (*ortho*-N-H···O_{nitro})	-1491,9381708	-3916039,311
	B1…B1 (N-O···π)	-1491,9316240	-3916022,127

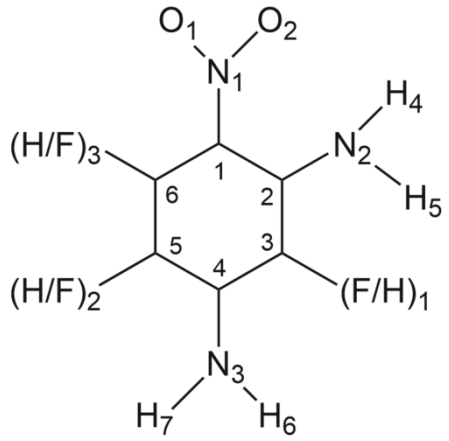
[a] Intermolecular interaction energies Δ*E* (Table 6) were calculated by subtracting the energy of the two molecules from the dimer energy.

Table S4 Energies of individual molecules, H-bonded and p···π dimers in co-crystals and homocrystals.[a] Level of theory: DFT/B3LYP/ M6-31G (TM)+* (continued)

Crystal	Molecule/dimer	*E* (Ha)	*E* (kJ mol^{-1})
Homocrystals			
A	A	-845,1860657	-2218444,385
	para-N-H···O_{nitro}	-1690,3844557	-4436921,119
	para-N-H···F	-1690,3793020	-4436907,592
	π...π	-1690,3711746	-4436886,259
B	B	-745,9654640	-1958010,150
	ortho-N-H···O_{nitro}	-1491,9368756	-3916035,911
	para-N-H···O_{nitro}	-1491,9386834	-3916040,656
	para-N-H···O_{nitro}	-1491,9372784	-3916036,968
	C-F···π	-1491,9231670	-3915999,929
C	C	-646,7284995	-1697532,965
	ortho-N-H···O_{nitro}	-1293,4632510	-3395082,340
	para-N-H···O_{nitro}	-1293,4671870	-3395092,673
	ortho -N-H···N_{amino}	-1293,4611950	-3395076,945
	para-N-H···N_{amino}	-1293,4648510	-3395086,540
	C-F···π	-1293,4522250	-3395053,400
D	D	-547,4900608	-1437051,912
	ortho-N-H···O_{nitro}	-1094,9846199	-2874115,630
	para-N-H···O_{nitro}	-1094,9884760	-2874125,752
	ortho -N-H···N_{amino}	-1094,9859252	-2874119,056
	para-N-H···N_{amino}	-1094,9859445	-2874119,107
	C-N_{amino}···π	-1094,9749154	-2874090,158

[a] Intermolecular interaction energies Δ*E* (Table 6) were calculated by subtracting the energy of the two molecules from the dimer energy.

Table S5 ESP atomic charges for atoms of diaminonitrobenzenes in the gas phase (*q*, in units of elementary charge). The structure shows the atom numbering scheme. Level of theory: DFT/B3LYP/ M6-31G (TM)+*.



code	A	B	C	D
$q(C_1)$	-0,216	-0,143	-0,131	-0,172
$q(C_2)$	0,127	0,227	0,355	0,420
$q(C_3)$	0,101	0,081	-0,421	-0,462
$q(C_4)$	0,101	0,136	0,294	0,453
$q(C_5)$	0,113	0,229	0,207	-0,312
$q(C_6)$	0,105	-0,354	-0,315	-0,124
$q(N_1)$	0,776	0,762	0,726	0,712
$q(N_2)$	-0,677	-0,801	-0,822	-0,853
$q(N_3)$	-0,682	-0,750	-0,789	-0,824
$q(O_1)$	-0,398	-0,430	-0,422	-0,424
$q(O_2)$	-0,479	-0,482	-0,473	-0,470
$q(F/H_1)$	-0,117	-0,130	0,199	0,187
$q(F/H_2)$	-0,122	-0,153	-0,161	0,162
$q(F/H_3)$	-0,080	0,228	0,214	0,165
$q(H_4)$	0,397	0,430	0,418	0,422
$q(H_5)$	0,340	0,384	0,376	0,385
$q(H_6)$	0,350	0,382	0,375	0,368
$q(H_7)$	0,361	0,382	0,370	0,367