Supplementary Information for:

Synthesis, growth and characterization of 4-bromo-4'nitro benzylideneaniline (BNBA): A new second-order nonlinear optical material with a (3+1) dimensional incommensurately modulated structure

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Content:

Refinement details of the (3+1) dimensional incommensurately modulated structure at 173 K.

The experimental data allows two interpretations. The first one describes all diffraction reflections in an orthorhombic unit cell (a = 19.715, b = 16.253, c = 7.440 Å) within (3+2)-dimensional superspace group $Fd2d$(-α0γ, α0γ)s0s with two **q**-vectors describing the satellites. However, a group of the 0kl reflections with $k + l = 2n$ violate the gliding d plane (Fig. S1). The second one considers the monoclinic (3+1)-dimensional subgroup, $A2$(α0γ)0, with one **q**-vector and twinning by a mirror plane normal to the c axis. Lattice constants of the monoclinic unit cell, a = 10.5217(10), b = 16.2535(16), c = 7.4403(7) Å, β = 110.709(7)°, can be obtained from the orthorhombic one by the matrix transformation (½ 0 ½ / 010 / 001). Both versions have been tested for the refinement of the starting model, which has been obtained as an average structure using only the main reflections. The refinement in the orthorhombic cell results in higher R-factors and negative tensor of ADP parameters for all non-H atoms. A reliable solution of the incommensurately modulated structure (twinned by a mirror plane normal to the c axis) has been reached with twin coefficients 0.50(1) and 0.48(1); the Flack-factor is equal to 0.01(1). Details of the structure refinement are listed in Table S1.

The refined model consists of rigid BNBA molecules (Fig. 6 in the main text), which are located on two independent positions (a and b) within the unit cell and connected by the approximate vector 0.5**a** 0.25**b** 0.5**c**. Each molecular position, has been defined by crenel function [Ref. 24 in the main text] with parameters x_4^0 = 0.75 and Δx_4 = 0.5 for a and x_4^0 = 0.25 and Δx_4 = 0.5 for b. In both positions, the modulation affects the displacements and rotations of the molecules relatively the fixed point and the unit cell axes, respectively. The refined positions and ADP parameters are listed in Table S2 and S3 for all atoms of the rigid BNBA molecule. Positional parameters and the amplitudes of the modulations are shown in Table S4 for both the a and b positions of the rigid molecule. The average, minimal and maximal values of interatomic distances occurring between each atomic pair in the incommensurately modulated structure are listed in Table S5. For the distance calculation, the limited maximal value was derived from atomic radii expanded by 3.7%. The angles between closest atoms in BNBA molecule are given in Table S6.

Discussion of the C-H…O and C-H…Br interactions in the (3+1) dimensional incommensurately modulated structure at 173 K.

According to (3+1)-dimension symmetry, the molecules have a freedom to tilt and to shift according to the wave of the structure modulation (Table S4). The displacements and rotations are imposed by C-H…O and C-H…Br interactions occurring between molecules (Fig. 5 and 7 in the main text). These interactions do not exhibit periodicity in the 3-dimentional bulk of the crystal, only the [010] direction is periodic (Fig. 5 in the main text). In such a structure, a distance between any two atoms varies according to the modulation wave, and it is possible to define the minimum, maximum and average value of a selected distance. These characteristics are listed in Table S7 for the selected C-H-O and C-H-Br atomic combinations, which can be regarded as candidates for C-H…O and C-H…Br interactions. The minimal distance shorter than 2.7 Å for H-O and 3.7 Å for H-Br and the minimal angle over 130° for both C-H-O and C-H-Br were used as selection criteria. A percentage of presence is indicated for each the combination with the given characteristics. For example, 80% presence is indicated for C6a-H6a-O1b (the second line in Table S7). It means that 80% of the C6a-H6a-O1b combination has the indicated distances and angles, while 20% of the combination do not match one or both the criteria. The most probable C-H…O and C-H…Br interactions can be recognized in the atomic combinations underlined by bold font in the Table S7; they are illustrated in Figure S2.

Room temperature X-ray analysis of BNBA

A room temperature (293 K) data set was collected using synchrotron radiation (details are given in Table S1). Here no satellite reflections were observed in the diffraction images, however, diffuse scattering pointed to a partially disordered crystal structure. The powder XRD pattern taken at room temperature (Fig. 8 in the main text) also confirms the high level of diffuse scattering. This 290 K structure has been successfully refined using the average structural model obtained for the incommensurately modulated structure at 173 K (Table S2). This model corresponds to split atomic positions for all atoms (Figure S2, Table S8), and implies that the short-range ordering at room temperature is identical to that at 173 K. The recorded powder X-ray diffraction pattern of BNBA (Fig. 8) is similar to that calculated using the room temperature single crystal CIF file if a strong preferred orientation along [-102] is applied (Fig. S4). This direction is normal to the structural layers (Fig. 5 in the main text and Fig. S2) and contains the C-H...A interactions, which justify the observed texture.

Table S1. Single crystal X-ray experiments and crystal structure refinement

Chemical formula	$C_{13}H_9BrN_2O_2$	$C_{13}H_9BrN_2O_2$
Structural formula	Br-Car-(CH)4-Car-N=CH-Car-(CH)4-Car-NO_2	Br-Car-(CH)4-Car-N=CH-Car-(CH)4-Car-NO_2
Mol wt.	305.1	305.1
System	Monoclinic	Monoclinic
Group of symmetry	*A*2(α0γ)0	*A*2
Unit cell parameters	*a* = 10.5217(10), *b* = 16.2535(16), *c* = 7.4403(7) Å, β = 110.709(7); V = 1190.2(2) $Å^3$	*a* = 10.6408(09), *b* = 16.2706(10), *c* = 7.5669(7) Å, β = 110.783(8); V = 1224.8(2) $Å^3$
q-vector	0.0658(1)***a**** -0.2658(1)***c****	none
Z	4	4
d_{dif}, g/cm^3	1.7023	1.6542
Absorption coefficient, mm^{-1}	3.448	3.207
T, K	173	290 K
Radiation; λ, Å	Mo (*K*α); 0.71073	Synchrotron; 0.7
Diffractometer	STOE	MAR Research
Detector	IPDS	MAR345 IP detector
No. measured reflections	18324	9117
Θmin - Θmax, deg.	2.07 - 25.61	2.02 – 26.26
Limits of indexes	-12 ≤ *h* ≤12, -19 ≤ *k* ≤ 19, -9 ≤ *l* ≤ 9, -1 ≤ *m* ≤ 1	-13 ≤ *h* ≤13, -20 ≤ *k* ≤ 20, -9 ≤ *l* ≤ 9
Absorption correction	Numerical	SADABS
*R*int, %	6.84	3.31
No. unique reflections: observed / total	4686 / 6701	1555 / 2557

No. main reflections: observed / total	1898 / 2228	1555 / 2557
No. satellite reflections: observed / total	2788 / 4473	none
Observation criteria	I>3s(I)	I>3s(I)
No. refined parameters	194	169
GOFobs; GOFall	2.01; 1.76	1.66; 1.31
Weighting scheme	$w = 1/(\sigma^2 (F)+0.0001F^2)$	$w = 1/(\sigma^2 (F)+0.0001F^2)$
R_{obs}; Rw_{obs}; R_{all}; Rw_{all} (%):		2.96; 3.02; 4.88; 3.12
main reflections	3.04; 3.06; 3.66; 3.13	
satellites	7.01; 6.76; 11.22; 7.18	
altogether	4.73; 4.48; 7.18; 4.71	
Residual electron density ρ_{max} and ρ_{min} e.Å^{-3}	0.32 ; -0.30	0.28; -0.16
Isotropic extinction: B-C type 1 Gaussian (Becker & Coppens, 1974)	0.35(9)	0.005(2)
Absolute structure Flack-factor	0.01(1)	0.01(1)
Number of twins; twin operator(s); mass coefficients	2; mirror m-plane, normal to c axes 0.504(3); 0.496(3)	2; mirror m-plane, normal to c axes; 0.419(8); 0.582(8)
Constrains	All H atoms	All H atoms

Table S2. Positional parameters of atoms in the rigid BNBA molecule[a] at 173 K

Atom	x	y	z	Ueq
Br1	-0.5	0.5	-0.5	0.0428(4)
C1	-0.4892(6)	0.6163(2)	-0.5011(5)	0.0367(16)
C2	-0.6000(8)	0.6626(4)	-0.5953(8)	0.040(2)
C3	-0.5914(6)	0.7488(3)	-0.5957(7)	0.045(2)
C4	-0.4696(8)	0.7873(4)	-0.4997(8)	0.042(3)
C5	-0.3582(7)	0.7390(3)	-0.4048(9)	0.044(2)
C6	-0.3655(6)	0.6527(3)	-0.4034(8)	0.037(2)
N1	-0.4421(6)	0.8739(3)	-0.4847(8)	0.045(2)
C7	-0.5380(6)	0.9235(4)	-0.5207(8)	0.048(2)
C8	-0.5151(7)	1.0129(3)	-0.5082(8)	0.047(3)
C9	-0.6250(8)	1.0635(3)	-0.5458(12)	0.053(2)
C10	-0.6113(8)	1.1489(3)	-0.5368(12)	0.049(2)
C11	-0.4826(10)	1.1817(3)	-0.4884(10)	0.040(2)
C12	-0.3693(9)	1.1334(3)	-0.4495(11)	0.049(3)
C13	-0.3892(7)	1.0468(3)	-0.4608(10)	0.049(2)
N2	-0.4715(8)	1.2717(3)	-0.4801(11)	0.053(2)
O1	-0.3557(7)	1.2999(2)	-0.4367(13)	0.065(2)
O2	-0.5731(7)	1.3122(3)	-0.5152(13)	0.066(2)
H2	-0.6852	0.6362	-0.6626	0.048272
H3	-0.6705	0.7809	-0.663	0.054155
H5	-0.2729	0.7652	-0.3375	0.052295
H6	-0.2869	0.6201	-0.3365	0.044485
H7	-0.6292	0.9029	-0.5575	0.057709
H9	-0.7139	1.0397	-0.5792	0.063398
H10	-0.6893	1.1839	-0.5635	0.058438
H12	-0.2803	1.157	-0.4159	0.059395
H13	-0.3118	1.0113	-0.4345	0.05877

[a]H atoms are numbering after the corresponding linked C atoms

Table S3. ADP harmonic parameters of atoms in the rigid BNBA molecule at 173 K

Atom	U11	U22	U33	U12	U13	U23
Br1	0.0604(8)	0.0268(2)	0.0441(7)	0.0018(8)	0.0222(7)	0.0019(4)
C1	0.048(3)	0.0331(17)	0.032(2)	-0.005(3)	0.018(3)	-0.001(2)
C2	0.035(4)	0.035(3)	0.048(3)	-0.008(3)	0.012(3)	-0.012(2)
C3	0.057(4)	0.027(3)	0.049(3)	0.008(3)	0.015(3)	0.004(2)
C4	0.051(5)	0.034(3)	0.036(3)	-0.007(3)	0.011(3)	-0.005(2)
C5	0.056(4)	0.023(3)	0.052(3)	-0.003(3)	0.020(3)	0.002(2)
C6	0.035(4)	0.037(3)	0.034(3)	0.005(3)	0.007(3)	-0.002(2)
N1	0.054(4)	0.032(2)	0.048(2)	0.008(3)	0.014(3)	0.003(2)
C7	0.044(4)	0.051(4)	0.053(3)	-0.003(3)	0.023(3)	-0.001(3)
C8	0.083(4)	0.019(4)	0.031(3)	0.012(3)	0.009(4)	0.003(2)
C9	0.072(4)	0.031(2)	0.057(4)	-0.003(3)	0.024(3)	-0.004(2)
C10	0.062(4)	0.026(2)	0.057(3)	-0.001(2)	0.019(3)	-0.005(2)
C11	0.049(4)	0.033(3)	0.040(2)	-0.001(3)	0.020(3)	-0.006(2)
C12	0.048(4)	0.048(4)	0.048(4)	-0.010(3)	0.011(3)	-0.009(2)
C13	0.064(4)	0.042(3)	0.043(3)	0.024(3)	0.022(3)	0.008(2)
N2	0.063(4)	0.045(3)	0.057(3)	-0.005(3)	0.030(3)	-0.010(2)
O1	0.060(3)	0.035(3)	0.106(4)	-0.020(2)	0.037(3)	-0.014(2)
O2	0.058(3)	0.038(3)	0.101(3)	0.007(2)	0.029(3)	-0.007(2)

Table S4. Positional parameters of the rigid BNBA molecule (173 K) relative to reference point (-0.5, 0.9, -0.5). s and c define the amplitudes of the sinus and cosine wave of the corresponding parameter modulation

Position	Wave	Rotation around the *a* axis, ϕ°	Rotation around the *b* axis, χ°	Rotation around the *c* axis, ψ°	x displacement	y displacement	z displacement
a		0	0	0	1.0076(3)	-1.8	0.9968(4)
	s	0.00032(12)	0.01323(18)	-0.00042(14)	-0.0039(6)	-0.01139(10)	0.0016(9)
	c	-0.0018(3)	0.0027(9)	-0.0025(4)	-0.0030(13)	-0.0044(9)	0.002(2)
b		-179.17(7)	42.1(4)	0.60(8)	0.5234(5)	-2.04868(16)	0.5134(8)
	s	0.00098(17)	-0.01005(18)	-0.0020(2)	-0.0108(9)	0.01719(11)	-0.0063(12)
	c	-0.0003(3)	0.0009(10)	0.0042(4)	0.0150(15)	-0.0033(6)	0.002(2)

Table S5. Interatomic distances in BNBA incommensurately modulated structure at 173 K

Atom-Atom	Average distance, Å	Minimal distance, Å	Maximal distance, Å
Br1a-C1a	1.894(12)	1.894(11)	1.89(2)
Br1a-C2a	2.844(15)	2.841(8)	2.85(2)
Br1a-C6a	2.827(16)	2.822(9)	2.85(3)
Br1a-O2a^i^	3.145(14)	3.08(2)	3.172(7)
Br1a-H2a	2.924(18)	2.914(9)	2.95(3)
Br1a-H6a	2.91(2)	2.897(10)	2.95(3)
Br1a-H5b^ii^	2.88(5)	2.87(5)	2.89(5)
C1a-C2a	1.364(19)	1.356(12)	1.38(3)
C1a-C3a	2.402(15)	2.399(8)	2.41(2)
C1a-C4a	2.787(14)	2.787(12)	2.79(2)
C1a-C5a	2.391(16)	2.385(10)	2.41(2)
C1a-C6a	1.39(2)	1.380(13)	1.42(3)
C1a-H2a	2.03(2)	2.012(13)	2.07(3)
C1a-H6a	2.06(2)	2.047(13)	2.11(4)
C2a-C3a	1.403(15)	1.403(13)	1.40(2)
C2a-C4a	2.414(17)	2.409(11)	2.44(2)
C2a-C5a	2.75(2)	2.732(14)	2.80(3)
C2a-C6a	2.40(2)	2.379(15)	2.45(3)
C2a-H2a	0.97(2)	0.960(13)	0.99(3)
C2a-H3a	2.060(15)	2.058(8)	2.07(2)
C3a-C4a	1.385(18)	1.377(13)	1.41(3)
C3a-C5a	2.38(2)	2.366(13)	2.44(3)
C3a-C6a	2.795(19)	2.780(12)	2.83(3)
C3a-N1a	2.530(16)	2.523(10)	2.56(2)
C3a-C7a	2.912(15)	2.910(10)	2.92(2)
C3a-H2a	2.058(16)	2.055(9)	2.07(3)
C3a-H3a	0.965(19)	0.960(10)	0.98(3)
C3a-H7a	2.569(14)	2.568(7)	2.57(2)
C3a-H9b^iii^	3.02(3)	2.86(5)	3.07(2)
C4a-C5a	1.387(18)	1.380(12)	1.41(3)
C4a-C6a	2.442(16)	2.438(9)	2.45(2)
C4a-N1a	1.434(15)	1.433(10)	1.44(2)
C4a-C7a	2.318(15)	2.316(10)	2.32(2)

C4a-H3a	2.05(2)	2.034(13)	2.10(3)
C4a-H5a	2.04(2)	2.026(13)	2.08(3)
C4a-H7a	2.463(16)	2.455(10)	2.48(2)
C4a-H9b^ii^	2.92(4)	2.90(4)	2.94(4)
C5a-C6a	1.404(14)	1.404(14)	1.40(2)
C5a-N1a	2.363(15)	2.360(8)	2.37(2)
C5a-H5a	0.97(2)	0.960(12)	0.99(3)
C5a-H6a	2.072(16)	2.070(7)	2.08(2)
C5a-H6b^iv^	3.26(2)	2.98(4)	3.43(3)
C5a-H9b^ii^	2.76(5)	2.72(5)	2.80(5)
C5a-H13b^iii^	3.05(3)	3.02(2)	3.10(5)
C6a-H5a	2.051(16)	2.048(9)	2.06(3)
C6a-H6a	0.97(2)	0.960(11)	0.98(3)
C6a-H10a^iii^	3.13(4)	2.94(5)	3.33(4)
C6a-H12a^v^	3.25(3)	2.99(5)	3.36(3)
N1a-C7a	1.251(17)	1.245(12)	1.27(2)
N1a-C8a	2.374(15)	2.372(9)	2.38(2)
N1a-C13a	2.859(14)	2.858(10)	2.86(2)
N1a-H3a	2.765(18)	2.750(10)	2.81(3)
N1a-H5a	2.482(18)	2.473(9)	2.51(3)
N1a-H7a	1.921(17)	1.907(12)	1.96(3)
N1a-H13a	2.582(15)	2.577(9)	2.60(2)
N1a-H6b^iv^	3.34(3)	2.86(4)	3.55(3)
N1a-H9b^ii^	3.03(4)	3.02(4)	3.05(4)
N1a-H10b^ii^	3.11(4)	3.09(4)	3.13(4)
C7a-C8a	1.470(15)	1.470(11)	1.47(2)
C7a-C9a	2.437(16)	2.434(10)	2.44(2)
C7a-C13a	2.491(16)	2.484(11)	2.51(2)
C7a-H3a	2.725(16)	2.719(9)	2.75(2)
C7a-H7a	0.967(17)	0.960(12)	0.99(3)
C7a-H9a	2.580(17)	2.571(10)	2.60(3)
C7a-H13a	2.666(18)	2.651(11)	2.71(3)
C7a-H10b^iii^	3.18(3)	3.02(4)	3.25(4)
C8a-C9a	1.372(19)	1.365(13)	1.39(3)
C8a-C10a	2.414(16)	2.410(10)	2.42(2)
C8a-C11a	2.764(14)	2.763(11)	2.77(2)

C8a-C12a	2.436(17)	2.430(12)	2.46(3)
C8a-C13a	1.370(19)	1.361(14)	1.40(3)
C8a-H7a	2.116(15)	2.111(9)	2.13(2)
C8a-H9a	2.03(2)	2.016(13)	2.07(3)
C8a-H13a	2.027(19)	2.011(13)	2.07(3)
C9a-C10a	1.396(14)	1.396(11)	1.40(2)
C9a-C11a	2.388(18)	2.381(13)	2.41(3)
C9a-C12a	2.79(2)	2.771(16)	2.85(3)
C9a-C13a	2.37(2)	2.349(16)	2.42(3)
C9a-H7a	2.611(14)	2.611(13)	2.61(2)
C9a-H9a	0.97(2)	0.960(13)	0.99(3)
C9a-H10a	2.063(15)	2.061(8)	2.07(2)
C9a-O1b^ii^	3.13(5)	3.10(5)	3.16(5)
C9a-O2b^iii^	3.24(3)	3.04(4)	3.32(4)
C9a-H5b^vi^	2.99(5)	2.97(4)	2.99(5)
C10a-C11a	1.39(2)	1.379(18)	1.42(3)
C10a-C12a	2.43(2)	2.408(17)	2.48(4)
C10a-C13a	2.77(2)	2.758(14)	2.81(3)
C10a-N2a	2.432(18)	2.426(12)	2.45(3)
C10a-O2a	2.680(14)	2.680(10)	2.68(2)
C10a-H9a	2.048(16)	2.044(9)	2.06(3)
C10a-H10a	0.96(2)	0.960(13)	0.98(3)
C10a-H7b^vii^	3.02(2)	2.973(18)	3.16(3)
C11a-C12a	1.38(2)	1.371(16)	1.40(3)
C11a-C13a	2.386(16)	2.383(10)	2.39(2)
C11a-N2a	1.467(14)	1.467(12)	1.47(2)
C11a-O1a	2.299(19)	2.293(13)	2.32(3)
C11a-O2a	2.307(17)	2.304(10)	2.31(2)
C11a-H10a	2.06(2)	2.046(17)	2.11(4)
C11a-H12a	2.06(2)	2.043(17)	2.10(4)
C12a-C13a	1.421(15)	1.421(11)	1.42(2)
C12a-N2a	2.472(17)	2.469(10)	2.48(3)
C12a-O1a	2.712(14)	2.711(13)	2.71(2)
C12a-H6a^viii^	3.13(4)	2.95(5)	3.20(3)
C12a-H12a	0.97(2)	0.960(15)	0.99(4)
C12a-H13a	2.067(15)	2.066(8)	2.07(2)

C12a-H7b	3.09(3)	3.08(3)	3.12(3)
C13a-H12a	2.093(17)	2.088(10)	2.11(3)
C13a-H13a	0.965(18)	0.960(11)	0.98(3)
C13a-H5b^iv^	2.91(3)	2.57(5)	3.08(3)
N2a-O1a	1.24(3)	1.233(18)	1.27(4)
N2a-O2a	1.21(2)	1.202(16)	1.23(4)
N2a-H10a	2.60(2)	2.582(14)	2.64(3)
N2a-H12a	2.67(2)	2.660(12)	2.70(3)
N2a-H9b	2.80(3)	2.79(3)	2.81(3)
O1a-O2a	2.18(3)	2.160(19)	2.23(4)
O1a-H12a	2.445(15)	2.443(7)	2.45(2)
O1a-C6b^x^	3.41(3)	3.06(4)	3.54(2)
O1a-C9b	2.88(4)	2.84(3)	2.93(4)
O1a-H2b^viii^	2.46(5)	2.44(5)	2.49(5)
O1a-H6b^x^	2.51(4)	2.21(5)	2.62(2)
O1a-H9b	2.16(5)	2.12(4)	2.22(5)
O1a-H10b	3.02(3)	2.86(3)	3.20(3)
O1a-H12b^iv^	2.83(3)	2.73(3)	3.01(4)
O1a-H13b^iv^	2.61(3)	2.48(3)	2.66(3)
O2a-H10a	2.383(17)	2.379(10)	2.40(3)
O2a-H2b^x^	2.67(3)	2.54(2)	3.03(5)
O2a-H6b^viii^	2.49(5)	2.46(5)	2.52(5)
O2a-H9b^vii^	2.61(3)	2.59(2)	2.68(4)
H2a-H3a	2.358(13)	2.357(12)	2.36(2)
H2a-N1b^ii^	3.01(5)	2.98(5)	3.04(5)
H2a-O1b^xi^	2.73(3)	2.72(3)	2.74(3)
H2a-O2b^xii^	2.62(2)	2.55(3)	2.72(4)
H2a-H3b^iii^	2.80(3)	2.71(5)	2.83(2)
H2a-H5b^ii^	2.71(5)	2.66(5)	2.76(5)
H2a-H7b^iii^	2.91(3)	2.66(5)	3.01(3)
H3a-H7a	2.122(15)	2.120(6)	2.13(2)
H3a-C9b^iii^	3.14(3)	2.83(5)	3.25(3)
H3a-C13b^ii^	3.04(5)	3.01(5)	3.08(5)
H3a-H2b^vii^	2.86(3)	2.811(16)	2.99(4)
H3a-H6b^vi^	2.68(4)	2.67(4)	2.70(4)
H3a-H9b^iii^	2.83(4)	2.67(6)	2.89(2)

H3a-H13b^ii^	2.80(6)	2.75(6)	2.85(6)
H5a-H6a	2.363(14)	2.363(12)	2.36(2)
H5a-Br1b^iv^	3.26(2)	2.97(3)	3.37(2)
H5a-C6b^iv^	3.08(2)	2.92(3)	3.19(3)
H5a-C9b^ii^	3.08(5)	3.04(5)	3.11(6)
H5a-C13b^iii^	3.07(3)	2.86(5)	3.32(5)
H5a-H2b	2.92(4)	2.77(4)	3.09(4)
H5a-H6b^iv^	2.49(3)	2.40(5)	2.58(4)
H5a-H9b^ii^	2.69(7)	2.65(7)	2.74(7)
H5a-H13b^iii^	2.69(4)	2.56(6)	2.86(6)
H6a-H9a^iii^	3.18(5)	3.02(5)	3.36(5)
H6a-H10a^iii^	3.12(5)	2.87(5)	3.38(5)
H6a-H12a^v^	2.94(4)	2.78(5)	2.99(3)
H6a-O1b^xiii^	2.48(3)	2.41(4)	2.57(3)
H6a-O2b^i^	2.61(4)	2.61(4)	2.62(4)
H6a-H3b^ii^	2.65(5)	2.62(5)	2.68(5)
H6a-H5b^iii^	2.72(3)	2.57(6)	2.79(5)
H6a-H7b^ii^	3.07(5)	3.04(5)	3.11(5)
H7a-H9a	2.381(14)	2.379(5)	2.39(2)
H7a-C10b^iii^	2.98(3)	2.86(4)	3.02(2)
H7a-C12b^ii^	3.08(4)	3.05(4)	3.10(4)
H7a-H2b^vii^	3.00(3)	2.930(19)	3.15(4)
H7a-H6b^vi^	2.96(4)	2.95(5)	2.98(4)
H7a-H9b^iii^	3.07(3)	2.90(4)	3.23(4)
H7a-H10b^iii^	2.58(3)	2.47(5)	2.63(2)
H7a-H12b^ii^	2.61(5)	2.57(5)	2.65(5)
H9a-H10a	2.358(13)	2.357(9)	2.36(2)
H9a-C3b^vii^	3.10(3)	2.97(3)	3.45(4)
H9a-C4b^vi^	3.13(3)	3.09(3)	3.16(3)
H9a-C5b^vi^	2.71(4)	2.70(4)	2.71(4)
H9a-N2b^ii^	3.06(4)	3.04(4)	3.08(4)
H9a-N2b^iii^	3.25(3)	2.94(4)	3.45(5)
H9a-O1b^ii^	2.26(5)	2.22(5)	2.29(5)
H9a-O2b^iii^	2.56(4)	2.17(5)	2.75(5)
H9a-H3b^vii^	2.93(3)	2.83(4)	3.18(5)
H9a-H5b^vi^	2.48(6)	2.43(5)	2.54(6)

H9a-H7b^vii^	3.13(2)	3.02(3)	3.35(4)
H9a-H10b^iii^	2.72(3)	2.70(4)	2.73(3)
H9a-H12b^ii^	2.89(4)	2.85(4)	2.94(4)
H10a-Br1b^viii^	3.07(4)	3.02(4)	3.12(4)
H10a-C7b^vii^	3.24(2)	3.09(2)	3.57(3)
H10a-H7b^vii^	2.66(3)	2.54(3)	2.93(4)
H10a-H9b^vii^	2.77(3)	2.71(4)	2.84(4)
H10a-H13b^vi^	2.62(4)	2.55(4)	2.70(4)
H12a-H13a	2.389(13)	2.388(9)	2.39(2)
H12a-N1b^iv^	3.13(2)	3.03(3)	3.164(16)
H12a-O1b^iii^	2.97(3)	2.89(5)	3.00(3)
H12a-O2b^ii^	3.08(5)	3.07(5)	3.09(5)
H12a-H7b	2.68(4)	2.62(4)	2.76(4)
H12a-H9b	2.84(4)	2.63(4)	3.07(4)
H12a-H13b^iv^	2.59(2)	2.55(3)	2.70(4)
H13a-C5b^iv^	2.87(3)	2.73(4)	2.92(2)
H13a-O1b^iii^	2.71(4)	2.68(2)	2.78(5)
H13a-O2b^ii^	3.04(5)	3.02(5)	3.06(5)
H13a-H3b	3.06(5)	2.98(5)	3.17(5)
H13a-H5b^iv^	2.47(3)	2.30(6)	2.57(5)
H13a-H10b^ii^	2.49(5)	2.47(5)	2.51(5)
H13a-H12b^iii^	2.78(3)	2.69(5)	2.82(2)
Br1b-C1b	1.894(10)	1.894(8)	1.897(15)
Br1b-C2b	2.843(16)	2.841(12)	2.85(2)
Br1b-C6b	2.825(17)	2.822(12)	2.84(2)
Br1b-H2b	2.92(2)	2.915(14)	2.94(3)
Br1b-H6b	2.90(2)	2.897(16)	2.92(3)
C1b-C2b	1.36(3)	1.356(19)	1.37(3)
C1b-C3b	2.401(16)	2.399(12)	2.41(2)
C1b-C4b	2.787(12)	2.787(9)	2.791(16)
C1b-C5b	2.389(18)	2.385(13)	2.40(2)
C1b-C6b	1.39(3)	1.380(19)	1.40(3)
C1b-H2b	2.02(3)	2.01(2)	2.04(4)
C1b-H6b	2.06(3)	2.05(2)	2.08(4)
C2b-C3b	1.404(13)	1.403(11)	1.406(17)
C2b-C4b	2.413(18)	2.409(14)	2.42(2)

C2b-C5b	2.74(3)	2.733(19)	2.77(3)
C2b-C6b	2.39(3)	2.38(2)	2.42(4)
C2b-H2b	0.96(3)	0.960(18)	0.97(4)
C2b-H3b	2.060(16)	2.058(11)	2.07(2)
C3b-C4b	1.38(2)	1.377(18)	1.39(3)
C3b-C5b	2.38(3)	2.37(2)	2.40(3)
C3b-C6b	2.79(3)	2.781(18)	2.81(3)
C3b-N1b	2.528(17)	2.523(13)	2.54(2)
C3b-C7b	2.911(14)	2.911(11)	2.914(18)
C3b-H2b	2.058(17)	2.055(11)	2.06(2)
C3b-H3b	0.96(3)	0.960(15)	0.97(3)
C3b-H7b	2.568(12)	2.568(11)	2.570(18)
C4b-C5b	1.38(2)	1.380(18)	1.40(3)
C4b-C6b	2.440(17)	2.438(13)	2.45(2)
C4b-N1b	1.434(13)	1.434(10)	1.436(17)
C4b-C7b	2.317(14)	2.316(11)	2.320(18)
C4b-H3b	2.04(3)	2.034(18)	2.07(3)
C4b-H5b	2.03(3)	2.026(18)	2.06(4)
C4b-H7b	2.459(16)	2.455(11)	2.47(2)
C5b-C6b	1.404(13)	1.404(11)	1.406(17)
C5b-N1b	2.362(15)	2.361(12)	2.37(2)
C5b-H5b	0.96(3)	0.960(17)	0.97(3)
C5b-H6b	2.071(17)	2.070(11)	2.08(2)
C6b-H5b	2.050(17)	2.048(11)	2.06(2)
C6b-H6b	0.96(3)	0.960(17)	0.97(4)
C6b-H12b^ii^	3.31(4)	3.03(6)	3.48(5)
N1b-C7b	1.248(17)	1.245(13)	1.26(2)
N1b-C8b	2.373(13)	2.372(11)	2.376(18)
N1b-C13b	2.859(13)	2.858(10)	2.864(17)
N1b-H3b	2.76(2)	2.750(15)	2.78(3)
N1b-H5b	2.48(2)	2.473(13)	2.49(3)
N1b-H7b	1.915(19)	1.907(14)	1.93(2)
N1b-H13b	2.581(14)	2.577(10)	2.593(19)
C7b-C8b	1.470(13)	1.470(11)	1.472(17)
C7b-C9b	2.435(15)	2.434(11)	2.439(19)
C7b-C13b	2.489(16)	2.484(13)	2.50(2)

C7b-H3b	2.722(18)	2.719(12)	2.73(2)
C7b-H7b	0.964(19)	0.960(14)	0.97(2)
C7b-H9b	2.576(17)	2.571(12)	2.59(2)
C7b-H13b	2.661(19)	2.652(13)	2.69(2)
C8b-C9b	1.369(19)	1.365(15)	1.38(2)
C8b-C10b	2.412(15)	2.411(11)	2.416(19)
C8b-C11b	2.764(13)	2.764(10)	2.768(17)
C8b-C12b	2.435(17)	2.430(13)	2.45(2)
C8b-C13b	1.37(2)	1.361(16)	1.38(2)
C8b-H7b	2.115(14)	2.112(10)	2.125(19)
C8b-H9b	2.02(2)	2.016(15)	2.04(3)
C8b-H13b	2.02(2)	2.011(15)	2.04(3)
C9b-C10b	1.396(13)	1.396(10)	1.398(17)
C9b-C11b	2.386(18)	2.381(14)	2.40(2)
C9b-C12b	2.78(2)	2.771(18)	2.81(3)
C9b-C13b	2.36(2)	2.350(18)	2.38(3)
C9b-H7b	2.611(11)	2.611(10)	2.613(16)
C9b-H9b	0.96(2)	0.960(15)	0.97(3)
C9b-H10b	2.062(14)	2.061(9)	2.06(2)
C10b-C11b	1.38(2)	1.379(19)	1.40(3)
C10b-C12b	2.42(3)	2.408(19)	2.44(3)
C10b-C13b	2.76(2)	2.758(15)	2.78(3)
C10b-N2b	2.431(18)	2.426(14)	2.44(2)
C10b-O2b	2.681(12)	2.680(10)	2.685(17)
C10b-H9b	2.047(16)	2.044(11)	2.06(2)
C10b-H10b	0.96(2)	0.960(15)	0.97(3)
C11b-C12b	1.37(2)	1.371(18)	1.38(3)
C11b-C13b	2.384(15)	2.383(11)	2.39(2)
C11b-N2b	1.467(12)	1.467(10)	1.469(17)
C11b-O1b	2.297(19)	2.294(14)	2.31(2)
C11b-O2b	2.305(16)	2.304(12)	2.31(2)
C11b-H10b	2.05(3)	2.046(19)	2.08(3)
C11b-H12b	2.05(3)	2.043(19)	2.07(3)
C12b-C13b	1.421(13)	1.421(10)	1.423(17)
C12b-N2b	2.470(16)	2.469(12)	2.47(2)
C12b-O1b	2.712(13)	2.711(11)	2.715(17)

C12b-H2b^xiv^	3.18(5)	3.03(5)	3.32(5)
C12b-H12b	0.96(2)	0.960(17)	0.97(3)
C12b-H13b	2.067(13)	2.066(10)	2.069(19)
C13b-H12b	2.092(16)	2.089(11)	2.10(2)
N2b-O1b	1.24(3)	1.23(2)	1.25(3)
N2b-O2b	1.21(2)	1.202(19)	1.21(3)
N2b-H10b	2.59(2)	2.582(17)	2.61(3)
N2b-H12b	2.67(2)	2.660(14)	2.68(3)
O1b-O2b	2.17(3)	2.16(2)	2.19(4)
O1b-H3b^xiv^	3.20(5)	3.05(5)	3.34(5)
O1b-H12b	2.444(14)	2.443(10)	2.45(2)
O2b-H3b^viii^	3.25(4)	3.10(4)	3.37(5)
O2b-H10b	2.382(16)	2.379(11)	2.39(2)
H2b-H3b	2.358(11)	2.358(9)	2.361(17)
H2b-H12b^xv^	3.05(6)	2.89(6)	3.21(6)
H3b-H7b	2.121(16)	2.120(9)	2.12(2)
H5b-H6b	2.363(12)	2.363(9)	2.367(18)
H6b-H10b^iii^	3.22(6)	3.02(6)	3.43(6)
H6b-H12b^ii^	3.01(5)	2.85(6)	3.14(6)
H7b-H9b	2.380(12)	2.379(7)	2.383(19)
H9b-H10b	2.358(11)	2.357(8)	2.361(17)
H12b-H13b	2.389(11)	2.389(8)	2.392(17)

(i) x+1,y,z
(ii) x,y+1/2,z+1/2
(iii) -x,y+1/2,-z+1/2
(iv) -x,y+1,-z+1
(v) x,y-1/2,z+1/2
(vi) x,y+1,z
(vii) -x,y+2,-z+1
(viii) x-1,y+1/2,z+1/2
(ix) -x-1,y+3/2,-z+1/2
(x) -x-1,y+1/2,-z+1/2
(xi) x+1,y+1,z
(xii) -x+1,y+2,-z+1
(xiii) -x+1,y+1,-z+1
(xiv) -x-1,y-1/2,-z+1/2
(xv) -x,y-1/2,-z+1/2

Table S6. Angles between closest non-H atoms in BNBA molecule

Br1-C1-C2	120.7(10)	119.9(14)	121.0(7)
Br1-C1-C6	118.1(9)	117.8(12)	118.2(6)
C2-C1-C6	121.2(9)	120.8(5)	122.2(13)
C1-C2-C3	120.5(12)	119.7(17)	120.7(9)
C2-C3-C4	119.9(12)	119.6(15)	120.1(8)
C3-C4-C5	118.6(9)	118.2(6)	119.7(13)
C3-C4-N1	127.6(10)	127.4(13)	127.7(8)
C5-C4-N1	113.8(10)	112.8(14)	114.1(8)
C4-C5-C6	122.0(12)	121.2(17)	122.3(8)
C1-C6-C5	117.7(12)	117.4(16)	117.9(7)
C4-N1-C7	119.3(11)	118.3(15)	119.6(9)
N1-C7-C8	121.3(11)	120.4(15)	121.6(9)
C7-C8-C9	118.0(11)	117.1(14)	118.3(9)
C7-C8-C13	122.6(10)	122.3(12)	122.7(8)
C9-C8-C13	119.4(9)	119.1(6)	120.5(14)
C8-C9-C10	121.4(13)	120.5(18)	121.6(10)
C9-C10-C11	118.1(13)	117.8(16)	118.2(9)
C10-C11-C12	122.6(10)	122.2(6)	123.6(14)
C10-C11-N2	116.8(13)	116.5(15)	116.9(10)
C12-C11-N2	120.6(14)	119.8(19)	120.9(11)
C11-C12-C13	116.9(13)	116.0(19)	117.2(10)
C8-C13-C12	121.6(12)	121.4(14)	121.7(9)
C11-N2-O2	118.8(15)	118(2)	119.0(11)
C11-N2-O1	115.9(14);	115.6(17);	116.0(10)
O1-N2-O2	125.4(11)	125.0(7)	126.4(16)

Table S7. Characterization of candidates for the C-H…O and C-H…Br interactions aperiodically appear between BNBA molecules at 173 K

Bond	H-A distance (Å): interval and <average> values	D-H-A angle (degree): interval and <average> values	Percent of presence
C2a-H2a-O2b(i)	2.55(3) - 2.72(4) <2.62(2)>	138(4) - 173(3) <161(2)>	80%
C6a-H6a-O1b(ii)	2.41(4) - 2.57(3) <2.48(3)>	157(3) - 173(3) <165(2)>	80%

C6a-H6a-O2b(iii)	2.61(4) - 2.62(4) <2.61(4)>	144(4) - 152(3) <148(4)>	20%
C2b-H2b-O1a(v)	2.44(5) - 2.49(4) <2.47(5)>	163(3) - 166(3) <164(3)>	6%
C6b-H6b-O1a(iv)	2.20(5) - 2.62(2) <2.50(4)>	145(4) - 164(4) <157(3)>	94%
C2b-H2b-O2a(iv)	2.54(5) - 2.99(5) <2.63(5)>	154(4) - 173(4) <163(3)>	94%
C6b-H6b-O2a(v)	2.47(5) - 2.53(5) <2.50(5)>	147(4) - 150(4) <148(4)>	6%
C3a-H3a-Br1b(vi)	3.146(17) - 3.45(3) <3.25(2)>	130(2) - 140.7(12) <136.6(11)>	80%
C5a-H5a-Br1b	3.39(4) - 3.60(3) <3.48(3)>	135(3) - 139(2) <137(3)>	20%
C5a-H5a-Br1b(vii)	2.97(3) - 3.37(2) <3.26(2)>	134(2) - 150.1(17) <144.7(11)>	80%
C10a-H10a-Br1b(x)	3.02(4) - 3.12(4) <3.07(4)>	161(2) - 162(2) <161(2)>	6%
C10a-H10a-Br1b(viii)	3.26(2) - 3.76(4) <3.41(3)>	142(3) - 157.9(19) <151(2)>	94%
C12a-H12a-Br1b(x)	3.61(4) - 3.68(4) <3.65(4)>	144(4) - 145(4) <144(4)>	6%
C12a-H12a-Br1b(viii)	3.27(4) - 4.01(3) <3.82(3)>	144(4) - 173(2) <159(2)>	94%
C3b-H3b-Br1a(ix)	3.48(4) - 3.49(4) <3.48(4)>	138.5(13) - 139.0(13) <138.8(13)>	6%
C3b-H3b-Br1a(viii)	3.16(4) - 3.41(4) <3.26(3)>	137.1(9) - 141(2) <138.0(13)>	94%
C5b-H5b-Br1a(ix)	2.87(5) - 2.88(5) <2.88(5)>	131(3) - 133(3) <132(3)>	6%
C5b-H5b-Br1a(viii)	3.29(5) - 3.50(5) <3.38(3)>	134(3) - 148.7(11) <145.0(15)>	94%
C10b-H10b-Br1a(xi)	3.47(3) - 3.52(3) <3.49(3)>	162.0(18) - 169(2) <165(2)>	20%
C10b-H10b-Br1a(xii)	3.22(3) - 3.45(3) <3.32(2)>	144(3) - 157(3) <151(2)>	80%

(i) -x+1,y+2,-z+1	(v) x,y-1/2,z+1/2	(ix) x-1,y-1/2,z+1/2
(ii) -x+1,y+1,-z+1	(vi) -x,y+2,-z+1	(x) x-1,y+1/2,z+1/2
(iii) x+1,y,z	(vii) -x,y+1,-z+1	(xi) x-1,y,z
(iv) -x,y+1/2,-z+1/2	(viii) -x-1,y+1/2,-z+1/2	(xii) -x-1,y+2,-z+1

Table S8. Positional parameters of atoms in the rigid BNBA molecule at 290 K

Atom	Occupancy	x	y	z	Ueq
Br1a	0.5	0.5175(4)	-0.5	0.4965(8)	0.0726(8)
C1a	0.5	0.4973(4)	-0.61648(18)	0.4912(9)	0.0619(17)
C2a	0.5	0.6087(5)	-0.6670(2)	0.5840(9)	0.060(3)
C3a	0.5	0.5939(5)	-0.7510(2)	0.5800(10)	0.060(3)
C4a	0.5	0.4682(6)	-0.78610(19)	0.4838(11)	0.045(3)
C5a	0.5	0.3588(5)	-0.7362(2)	0.3929(10)	0.056(2)
C6a	0.5	0.3739(5)	-0.6511(2)	0.3969(10)	0.077(4)
N1a	0.5	0.4525(6)	-0.8731(3)	0.4798(12)	0.086(4)
C7a	0.5	0.5555(6)	-0.9196(3)	0.5208(10)	0.074(3)
C8a	0.5	0.5385(6)	-1.0115(2)	0.5088(10)	0.062(4)
C9a	0.5	0.6490(6)	-1.0615(2)	0.5478(10)	0.080(3)
C10a	0.5	0.6332(6)	-1.1469(2)	0.5366(10)	0.061(3)
C11a	0.5	0.5054(7)	-1.18137(19)	0.4858(11)	0.0460(18)
C12a	0.5	0.3940(6)	-1.1311(2)	0.4464(10)	0.098(4)
C13a	0.5	0.4097(6)	-1.0462(2)	0.4576(10)	0.075(4)
N2a	0.5	0.4896(8)	-1.2678(2)	0.4745(12)	0.071(3)
O1a	0.5	0.3780(9)	-1.2979(3)	0.4301(13)	0.102(3)
O2a	0.5	0.5877(10)	-1.3120(3)	0.5092(13)	0.111(4)
H2a	0.5	0.6950(4)	-0.6427	0.6499(8)	0.0726
H3a	0.5	0.6698(4)	-0.7856	0.6432(8)	0.0719
H5a	0.5	0.2725(4)	-0.7603	0.3269(8)	0.0674
H6a	0.5	0.2980(4)	-0.6167	0.3338(8)	0.0926
H7a	0.5	0.6438(4)	-0.896	0.5594(8)	0.0892
H9a	0.5	0.7481(4)	-1.0348	0.5871(8)	0.0958
H10a	0.5	0.7106(4)	-1.1818	0.5639(8)	0.0734
H12a	0.5	0.3059(4)	-1.1548	0.4114(8)	0.1173
H13a	0.5	0.3324(4)	-1.0112	0.4303(8)	0.0901
Br1b	0.5	0.0207(5)	-0.74910(9)	0.0083(9)	0.0725(12)
C1b	0.5	-0.0003(6)	-0.8656(2)	-0.0038(9)	0.062(2)
C2b	0.5	0.1101(6)	-0.9165(3)	0.0115(10)	0.061(4)
C3b	0.5	0.0947(6)	-1.0005(2)	0.0027(11)	0.060(3)
C4b	0.5	-0.0305(7)	-1.0351(2)	-0.0213(12)	0.045(4)
C5b	0.5	-0.1388(6)	-0.9848(2)	-0.0364(11)	0.056(3)
C6b	0.5	-0.1232(6)	-0.8998(2)	-0.0275(10)	0.077(5)
N1b	0.5	-0.0467(7)	-1.1222(3)	-0.0308(13)	0.086(6)
C7b	0.5	0.0561(7)	-1.1688(3)	0.0283(11)	0.075(4)
C8b	0.5	0.0386(7)	-1.2607(2)	0.0257(11)	0.062(6)
C9b	0.5	0.1491(7)	-1.3108(3)	0.0943(11)	0.080(4)
C10b	0.5	0.1329(7)	-1.3962(2)	0.0919(12)	0.062(3)
C11b	0.5	0.0047(8)	-1.4304(2)	0.0200(12)	0.046(2)
C12b	0.5	-0.1067(7)	-1.3799(3)	-0.0491(12)	0.098(6)
C13b	0.5	-0.0906(7)	-1.2951(3)	-0.0468(11)	0.075(5)
N2b	0.5	-0.0115(9)	-1.5167(2)	0.0177(14)	0.071(4)
O1b	0.5	-0.1235(10)	-1.5466(3)	-0.0450(16)	0.102(4)
O2b	0.5	0.0866(10)	-1.5611(3)	0.0785(16)	0.110(5)

H2b	0.5	0.1960(5)	-0.89257(9)	0.0281(9)	0.0726
H3b	0.5	0.1698(5)	-1.03534(9)	0.0129(9)	0.0719
H5b	0.5	-0.2248(5)	-1.00865(9)	-0.0531(9)	0.0674
H6b	0.5	-0.1984(5)	-0.86503(9)	-0.0380(9)	0.0926
H7b	0.5	0.1447(5)	-1.14540(9)	0.0745(9)	0.0892
H9b	0.5	0.2485(5)	-1.28436(9)	0.1501(9)	0.0958
H10b	0.5	0.2103(5)	-1.43123(9)	0.1399(9)	0.0734
H12b	0.5	-0.1951(5)	-1.40349(9)	-0.0987(9)	0.1173
H13b	0.5	-0.1679(5)	-1.26000(9)	-0.0947(9)	0.0901

Table S9. ADP harmonic parameters of atoms in the rigid BNBA molecule at 290 K

Atom	U11	U22	U33	U12	U13	U23
Br1a	0.0928(19)	0.04205(15)	0.0903(7)	-0.0014(11)	0.0415(12)	-0.0006(10)
C1a	0.087(3)	0.0388(15)	0.067(2)	0.00(3)	0.036(3)	-0.001(18)
C2a	0.035(4)	0.049(3)	0.084(6)	0.001(3)	0.005(4)	-0.002(3)
C3a	0.025(4)	0.034(3)	0.100(4)	-0.027(3)	-0.004(3)	-0.010(3)
C4a	0.029(6)	0.030(2)	0.068(4)	0.014(2)	0.006(5)	-0.001(4)
C5a	0.023(3)	0.042(3)	0.084(3)	0.014(3)	-0.004(2)	0.010(2)
C6a	0.075(6)	0.058(4)	0.085(7)	0.021(4)	0.013(5)	0.006(4)
N1a	0.135(9)	0.037(2)	0.089(4)	0.008(3)	0.042(6)	-0.011(4)
C7a	0.094(5)	0.039(3)	0.094(4)	-0.022(3)	0.038(5)	-0.003(4)
C8a	0.064(9)	0.062(5)	0.049(3)	-0.029(4)	0.008(6)	0.008(5)
C9a	0.095(5)	0.040(3)	0.118(5)	-0.011(3)	0.055(4)	-0.010(3)
C10a	0.078(4)	0.028(2)	0.084(5)	-0.007(3)	0.037(3)	-0.012(2)
C11a	0.044(3)	0.035(2)	0.063(3)	0.007(6)	0.024(2)	0.008(4)
C12a	0.103(6)	0.083(7)	0.109(7)	-0.048(5)	0.040(5)	0.004(5)
C13a	0.100(7)	0.047(6)	0.075(5)	0.010(5)	0.027(5)	-0.003(4)
N2a	0.069(4)	0.065(3)	0.076(4)	0.008(6)	0.022(4)	-0.004(3)
O1a	0.079(5)	0.043(3)	0.162(6)	-0.002(3)	0.015(4)	0.019(3)
O2a	0.085(5)	0.077(5)	0.156(6)	-0.006(4)	0.025(5)	-0.019(4)
Br1b	0.0923(19)	0.04206(16)	0.078(2)	-0.0017(11)	0.0240(18)	0.0000(12)
C1b	0.087(3)	0.0388(15)	0.059(4)	0.00(3)	0.025(3)	0.00(3)
C2b	0.036(4)	0.049(3)	0.096(9)	0.001(3)	0.022(5)	0.002(4)
C3b	0.026(4)	0.034(3)	0.120(7)	-0.026(3)	0.025(4)	-0.007(4)
C4b	0.029(6)	0.030(2)	0.074(8)	0.015(2)	0.015(6)	0.011(4)
C5b	0.024(3)	0.042(3)	0.103(5)	0.014(3)	0.022(3)	0.001(3)
C6b	0.076(6)	0.058(4)	0.104(10)	0.021(4)	0.041(7)	0.008(5)
N1b	0.136(9)	0.037(2)	0.096(10)	0.008(3)	0.053(9)	0.017(4)
C7b	0.094(6)	0.039(3)	0.088(8)	-0.023(3)	0.029(6)	-0.012(4)
C8b	0.065(9)	0.062(5)	0.070(10)	-0.029(4)	0.038(9)	-0.028(6)
C9b	0.094(5)	0.041(3)	0.089(8)	-0.011(3)	0.012(6)	0.003(4)
C10b	0.078(4)	0.029(2)	0.071(7)	-0.007(3)	0.018(4)	0.008(3)
C11b	0.043(3)	0.035(2)	0.052(5)	0.007(7)	0.007(3)	-0.003(6)
C12b	0.103(6)	0.083(7)	0.105(11)	-0.049(5)	0.034(7)	-0.037(6)
C13b	0.100(7)	0.047(6)	0.086(9)	0.010(5)	0.043(7)	0.010(5)
N2b	0.069(5)	0.065(3)	0.079(7)	0.008(6)	0.027(5)	0.010(5)
O1b	0.080(5)	0.043(3)	0.183(9)	-0.002(3)	0.045(6)	-0.019(4)
O2b	0.085(5)	0.077(5)	0.164(10)	-0.006(4)	0.038(6)	0.016(5)

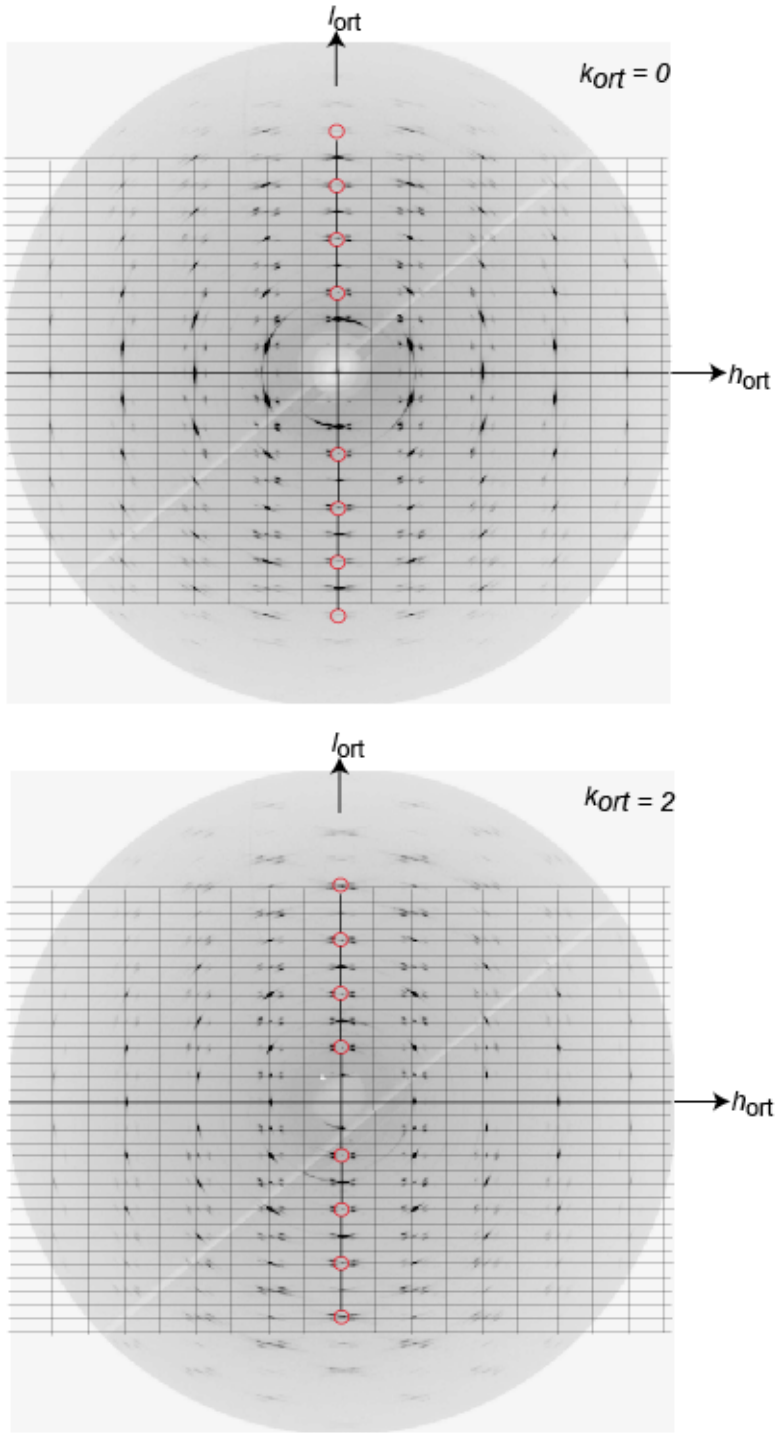


Figure S1. The *h*0*l* and *h*2*l* experimental pattern of the reciprocal space of BNBA at 173 K. The *h* and *l* axes and gridding correspond to orthorhombic set. Red circles underline reflections violating *Fd*2*d* group symmetry.

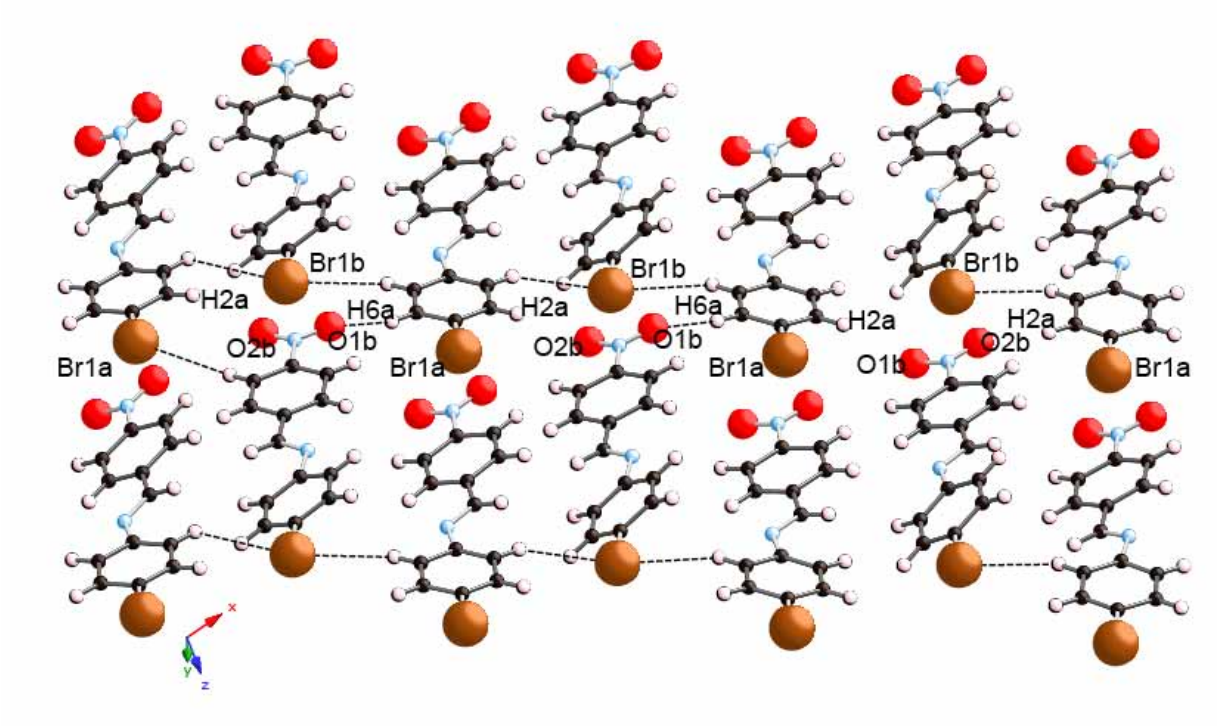


Figure S2. The most probable C-H…O and C-H…Br interactions in a portion of the representative layer of the incommensurately modulated BNBA structure

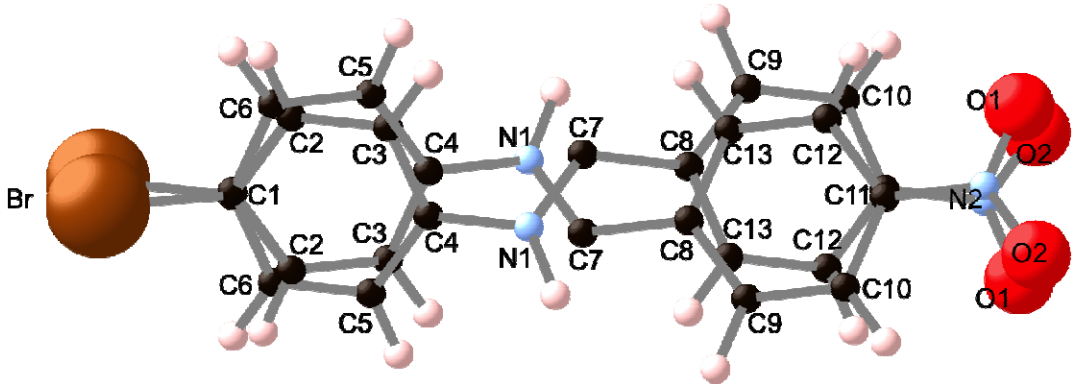
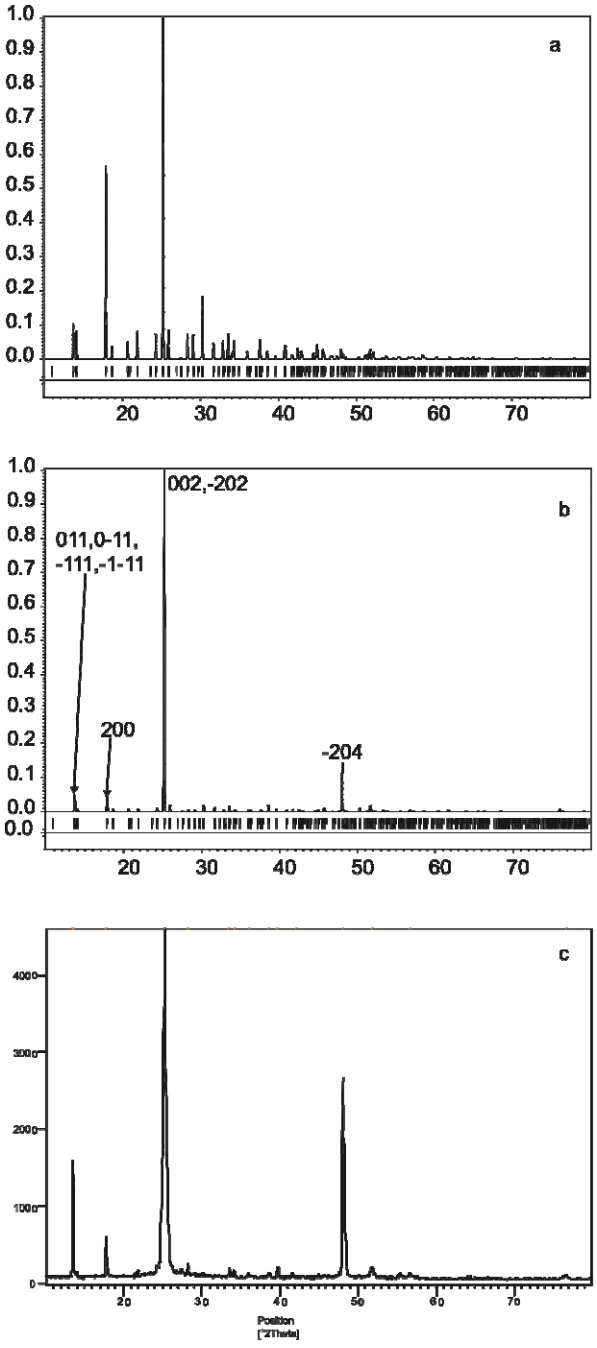


Figure S3. Split BNBA molecule in partially disordered structure of BNBA at 290 K



1. **Figure S4.** The powder X-ray diffraction patterns of BNBA at room temperature.
    a. the XRD pattern simulated without any specific parameters
    b. the XRD pattern simulated with application of the [-102] preferable orientation
    c. the experimental PXRD pattern