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Elastic Flexibility in an Optically Active Naphthalidenimine-Based Single Crystal

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PXRD

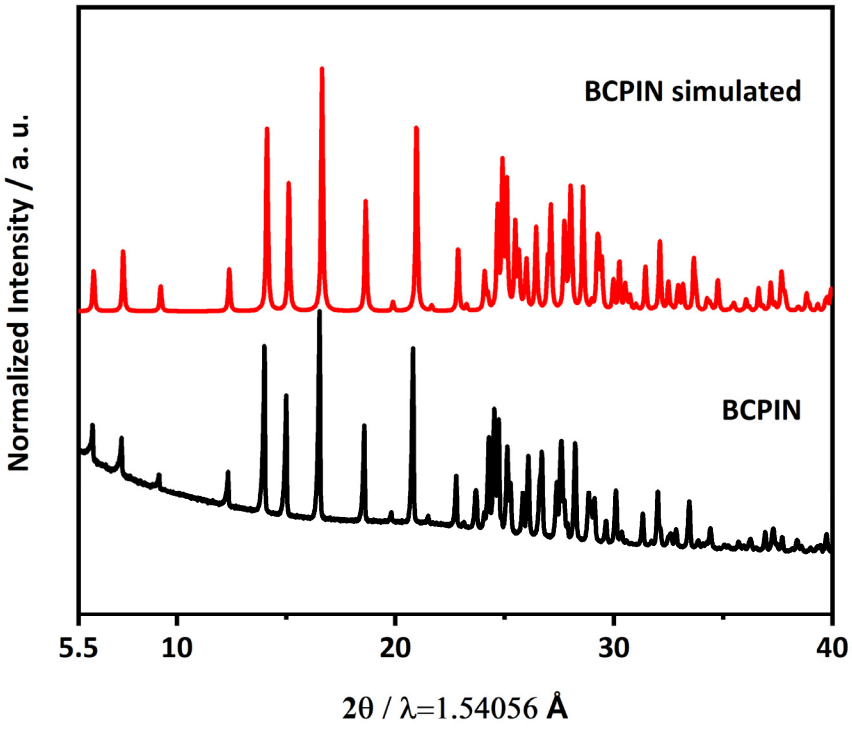


Figure S1. Experimental (black line) and simulated (red line) PXRD patterns of BCPIN.

DSC

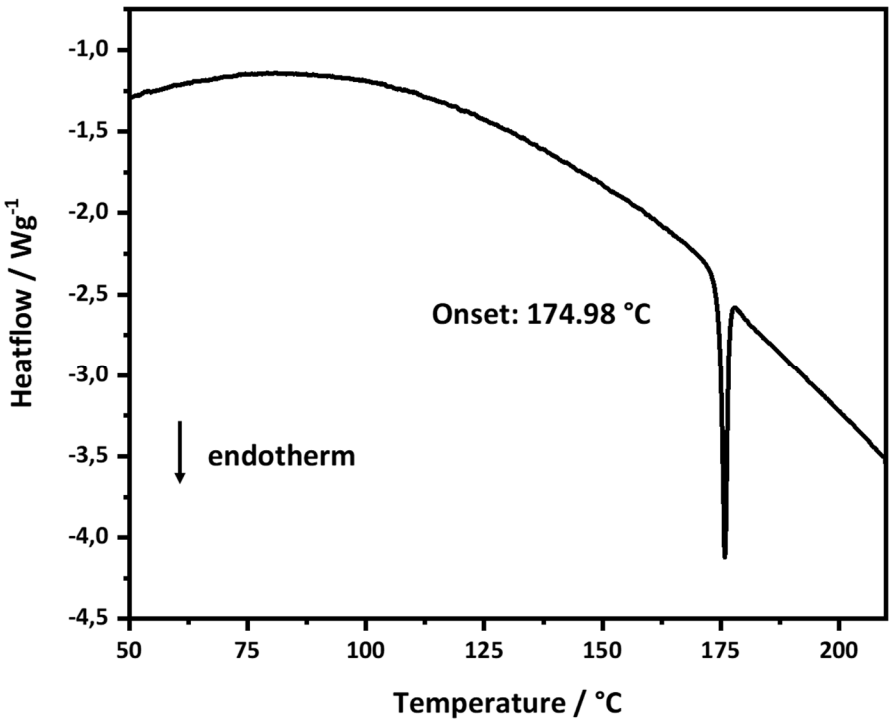


Figure S2. Differential scanning calorimetry measurement of BCPIN.

Face index of crystal

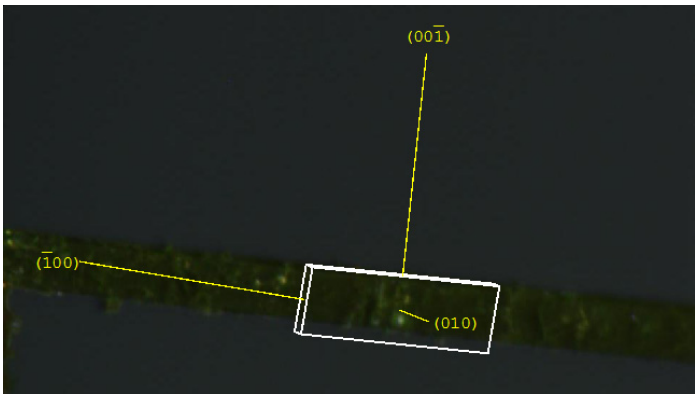


Figure S3. Face indexed image of pristine crystal of BCPIN.

Table related to SCXRD

Table S1. Crystallographic and structural refinement parameters of BCPIN.

Compound Name	**BCPIN**
Temperature/K	150
Formula	$C_{17}H_{11}BrClNO$
Formula Weight	360.63
Crystal System	Monoclinic
Space group	$P2_1/c$
a/Å	3.8281(2)
b/Å	28.5346(13)
c/Å	12.8657(8)
α/ ◦	90
β/ ◦	93.554(2)
γ/ ◦	90
V/Å^3	1402.66(13)
Z	4
*D*c/g cm−3	1.708
μ/mm−1	3.118
F(000)	720
θ range/ ◦	2.6-26.9
Reflections collected	15398
Unique reflections	3006
Reflections $I > 2\sigma(I)$	2536
Rint	0.052
Goodness of fit (F 2)	1.111
*R*1 ($I > 2\sigma$(I))	0.0381
*wR*2($I > 2\sigma$(I))	0.0510
CCDC No.	2117266

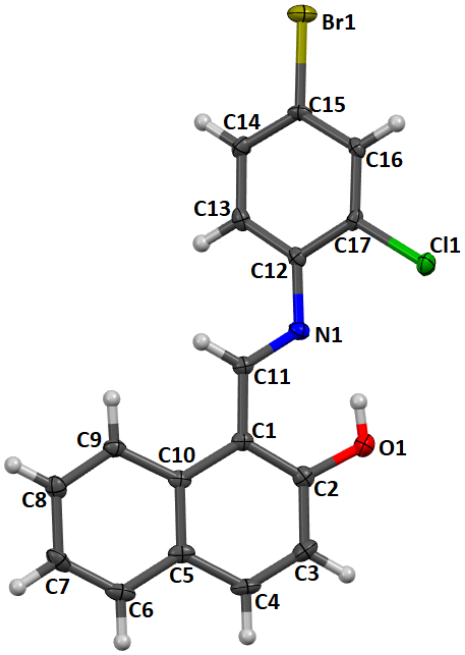


Figure S4. Thermal ellipsoid drawing of the asymmetric unit of BCPIN showing atom labels and 50% probability of ellipsoids.

Energy Framework Calculations

The energy frameworks calculations relating to intermolecular interactions of BCPIN were performed using the software suite Crystal-Explorer21[1] based on B3LYP/DGDZVP molecular wavefunctions calculated using .cif files. For calculations, the hydrogen atoms were normalized to standard neutron diffraction values. The energy frameworks constructed were based on the crystal symmetry and total interaction energy components of which included electrostatic, polarization, dispersion and exchange repulsion components scaled by 1.057, 0.740, 0.871 and 0.618, respectively. The interaction energies below 5 kJ.mol^{-1} are omitted for clarity and the cylinder thickness is proportional to the intermolecular interaction energies along the parallel vector passing through the cylinder.

A visualisation of the electrostatic, dispersion and total energy components is provided in Figure S4. The energy framework calculations indicate that the strongest interactions within the crystal lattice originate from the π···π stacking along the *a*-axis (-58.8 kJ.mol^{-1}). The chains (*c*-axis) are stabilized by a total interaction energy -53.4 kJ.mol^{-1}. The other inactions between the chains are with -31.8 kJ.mol^{-1} much weaker. Hence, overall intermolecular interactions in BCPIN are quasi-isotropic interactions (Table S2).

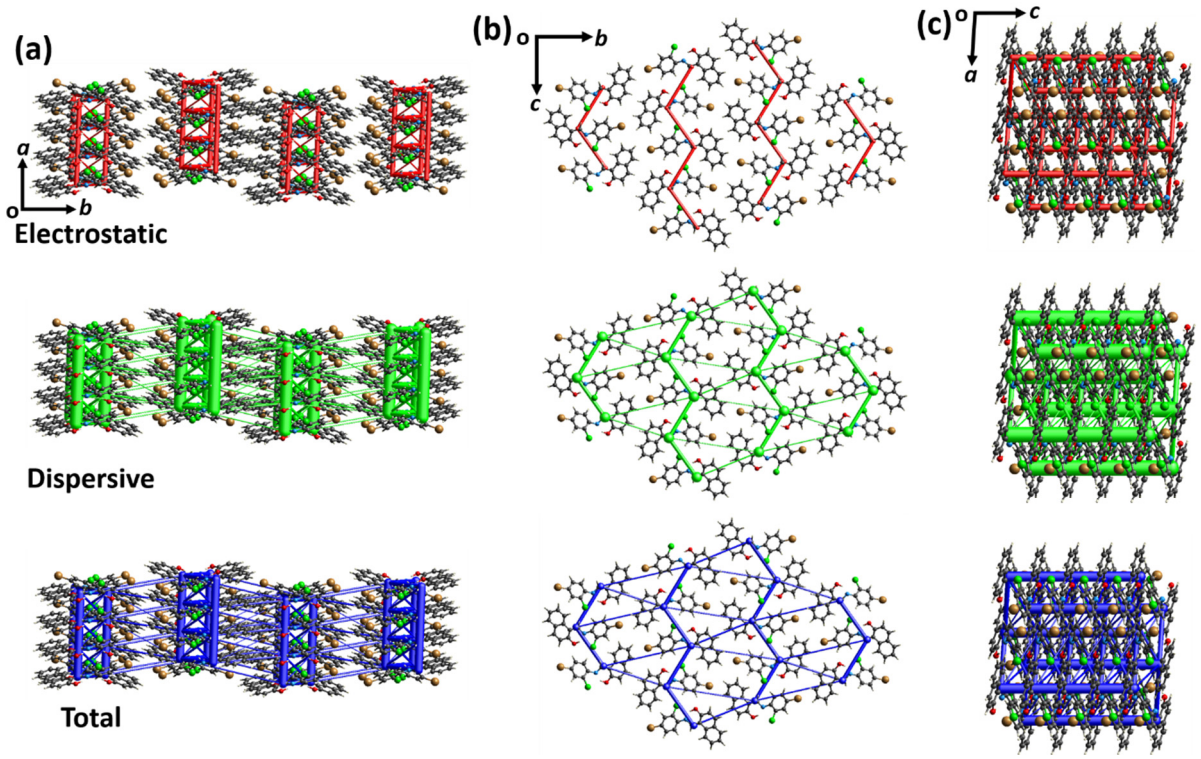
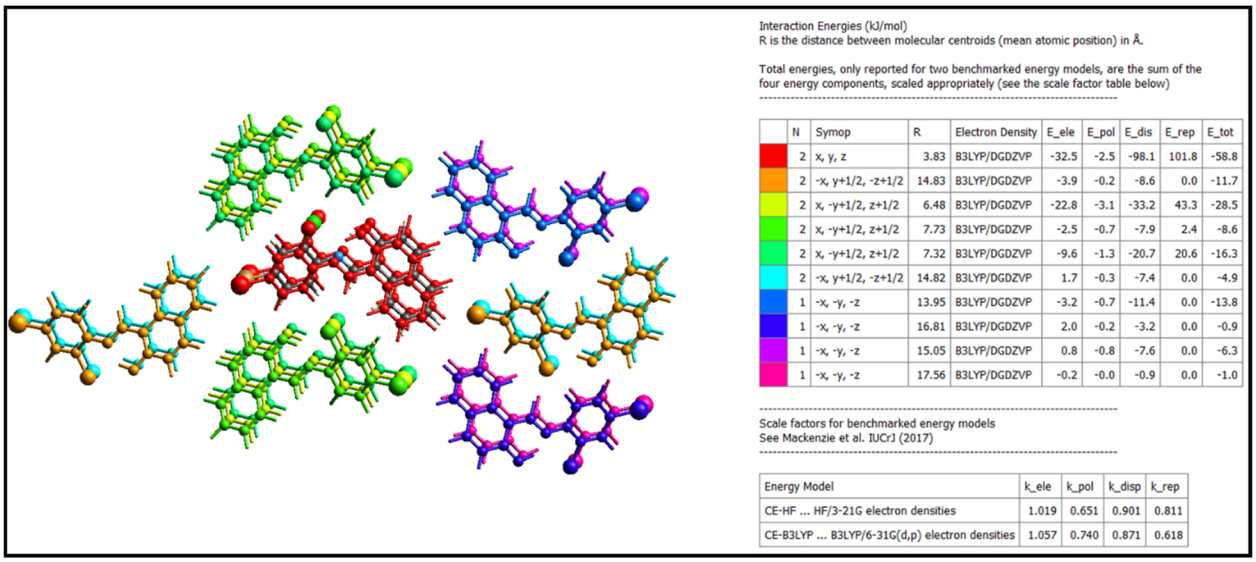


Figure S5. Visualization of energy frameworks showing electrostatic (red), dispersion (green) components and total interaction energy (blue) for BCPIN, in the (a) (001), (b) (100) and (c) (010) faces, respectively. The energy scale factor is 100 kJ.mol^{-1} and the energy threshold is 10 kJ.mol^{-1}.

Table S2. Molecular structure pairs and the interaction energies (kJ.mol^{-1}) obtained from energy frameworks calculation for BCPIN. Scale factors are in the lower table.



Interaction Energies (kJ/mol)
R is the distance between molecular centroids (mean atomic position) in Å.

Total energies, only reported for two benchmarked energy models, are the sum of the four energy components, scaled appropriately (see the scale factor table below)

N	Symop	R	Electron Density	E_ele	E_pol	E_dis	E_rep	E_tot
2	x, y, z	3.83	B3LYP/DGDZVP	-32.5	-2.5	-98.1	101.8	-58.8
2	-x, y+1/2, -z+1/2	14.83	B3LYP/DGDZVP	-3.9	-0.2	-8.6	0.0	-11.7
2	x, -y+1/2, z+1/2	6.48	B3LYP/DGDZVP	-22.8	-3.1	-33.2	43.3	-28.5
2	x, -y+1/2, z+1/2	7.73	B3LYP/DGDZVP	-2.5	-0.7	-7.9	2.4	-8.6
2	x, -y+1/2, z+1/2	7.32	B3LYP/DGDZVP	-9.6	-1.3	-20.7	20.6	-16.3
2	-x, y+1/2, -z+1/2	14.82	B3LYP/DGDZVP	1.7	-0.3	-7.4	0.0	-4.9
1	-x, -y, -z	13.95	B3LYP/DGDZVP	-3.2	-0.7	-11.4	0.0	-13.8
1	-x, -y, -z	16.81	B3LYP/DGDZVP	2.0	-0.2	-3.2	0.0	-0.9
1	-x, -y, -z	15.05	B3LYP/DGDZVP	0.8	-0.8	-7.6	0.0	-6.3
1	-x, -y, -z	17.56	B3LYP/DGDZVP	-0.2	-0.0	-0.9	0.0	-1.0

Scale factors for benchmarked energy models
See Mackenzie et al. IUCrJ (2017)

Energy Model	k_ele	k_pol	k_disp	k_rep
CE-HF ... HF/3-21G electron densities	1.019	0.651	0.901	0.811
CE-B3LYP ... B3LYP/6-31G(d,p) electron densities	1.057	0.740	0.871	0.618

Elastic Strain Calculation

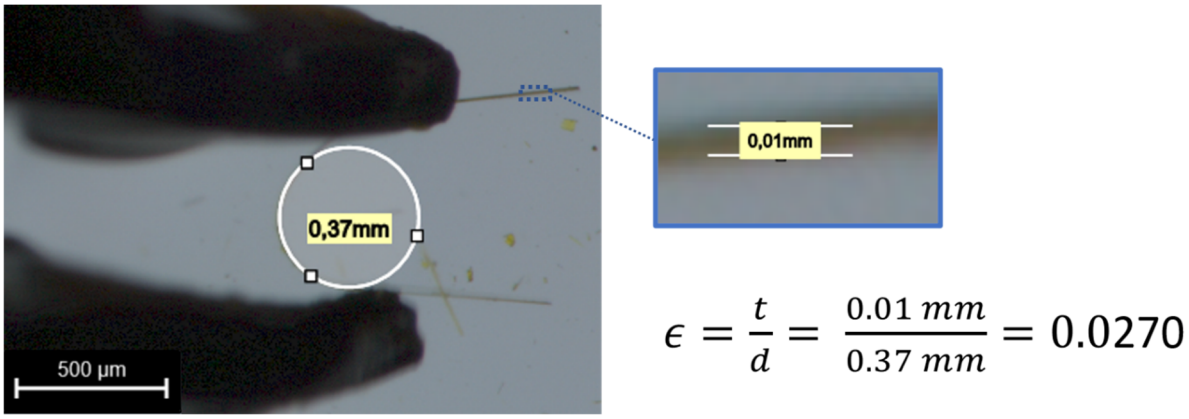


Figure S6. Microscopic image of bended BCPIN crystal. The elastic strain was calculated according to the Euler-Bernoulli equation $\varepsilon = \frac{t}{d}$ (t= beam thickness; d= diameter of curvature).[2] The observed elastic stress before breaking is 2.70 %.

References

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