Electronic Supplementary Material (ESI) for CrystEngComm

High pressure modification of organic NLO materials: large conformational re-arrangement of 4-aminobenzophenone.

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SUPPORTING INFORMATION

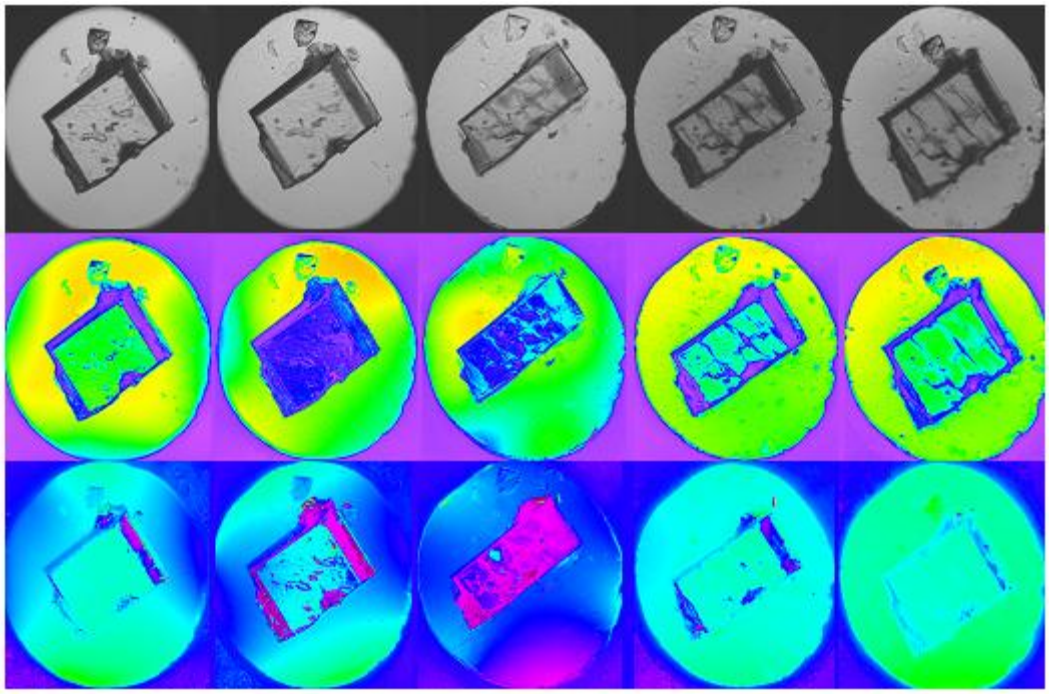

Figure S1: Polarized light micographs illustrating the transformation of **4-abp** as a function of Pressure. On the left, crystal at ambient pressure; the central Figures are taken at 1GPa and pictures on the right represent the crystal after returning to ambient conditions

Table S1 Experimental unit cell measurements from single crystal X-ray diffraction

Pressure (GPa)	a (Å)	b (Å)	c (Å)	β (°)	V (Å^3)
0.001	8.3080(5)	5.4673(4)	12.0570(13)	97.81(11)	542.57(8)
0.6	8.139(1)	5.2541(9)	11.853(4)	98.20(3)	501.7(2)
1	8.9533(18)	3.8650(8)	13.081(3)	90.47(3)	452.63(16)
2	9.047(5)	3.6626(2)	12.7481(15)	92.304(10)	422.07(6)
3.5	9.0624(6)	3.5605(2)	12.5539(17)	92.541(11)	404.68(7)
6.2	9.0721(17)	3.4383(6)	12.285(5)	92.72(3)	382.77(18)

Table S2 Unit cell parameters from PDFT calculations for the low pressure phase **4-ABP-RP** in the range 0-6 GPa.

Pressure (GPa)	a (Å)	b (Å)	c (Å)	β (°)	V (Å^3)
0.001	8.2108	5.1885	12.3578	98.7658	520.31
0.5	8.1506	5.1637	11.9846	98.5220	498.83
1	8.1073	5.0779	11.8682	98.2820	483.50
2	7.9955	5.0287	11.5679	99.2274	459.10
3	7.9087	4.9991	11.3610	99.7430	442.70
4	7.8261	4.9933	11.1816	100.6232	429.47
5	7.8014	4.7955	11.3510	99.1653	419.24
6	7.7334	4.8719	11.0832	100.4597	410.64

Table S3 Unit cell parameters from PDFT calculations for the high pressure phase **4-ABP-HP** in the range 0-6 GPa.

Pressure (GPa)	a (Å)	b (Å)	c (Å)	β (°)	V (Å^3)
0.001	8.6872	4.1310	14.4631	92.2349	518.64
0.5	8.7408	4.0239	13.7608	91.2111	483.88
1	8.8106	3.8995	13.3866	89.6735	459.92
2	8.8225	3.6691	13.4377	89.1346	434.94
3	8.8393	3.7122	12.8546	88.9931	421.74
4	8.8107	3.5801	12.9540	87.4422	408.21
5	8.7974	3.5292	12.8595	87.3254	398.82
6	8.7989	3.4997	12.7210	87.7885	391.43