

*Electronic Supplementary Information (ESI)***Table S1.** Crystal Data Collection and Structure Refinement Parameters of FXT H1

Parameters	Form H1
Chemical formula	C ₁₆ H ₁₆ N ₂ O ₃ S
Formula mass	316.37
Crystal system	Triclinic
Space group	P $\bar{1}$
<i>a</i> /Å	7.216(5)
<i>b</i> /Å	15.347(5)
<i>c</i> /Å	15.682(5)
α (°)	90.282(5)
β (°)	96.179(5)
γ (°)	99.574(5)
<i>V</i> (Å ³)	1702.1(14)
<i>Z</i>	4
<i>D_c</i> (g cm ⁻³)	1.235
μ (mm ⁻¹)	0.203
<i>F</i> (000)	664
<i>T</i> (K)	150
λ (Mo K α)(Å)	0.71073
$\theta_{\min}$ (°)	2.6
$\theta_{\max}$ (°)	28.3
Total data	56211
Unique data	8443
<i>R</i> _{int}	0.039
Data [<i>I</i> >2 σ (<i>I</i>)]	6869
^a <i>R</i> ₁	0.0429
^b <i>wR</i> ₂	0.1205
<i>S</i>	1.03

$$^aR_1 = \sum \|F_o\| - \|F_c\| / \sum \|F_o\|, \quad ^b wR_2 = [\sum w(F_o^2 - F_c^2)^2 / \sum w(F_o^2)^2]^{1/2}$$

Table S2. Selected bond lengths and angles of Form H1

Band lengths (Å)		Band angles (°)	
S1 -C2	1.7266(19)	C2 -S1-C5	88.79(7)
S1-C5	1.723(2)	C9-O3-C13	119.00(12)
C9-C10	1.406(2)	N2 -C12-C10	178.62(16)
C10-C11	1.399(2)	O3-C13 -C14	107.35(13)
C13 -C14	1.511(3)	C3-N1-C5	111.09(13)
O1-C1	1.309(2)	C15-C14 -C16	113.6(2)
C14-C15	1.512(4)	O1-C1-C2	113.33(13)
O2-C1	1.235(2)	O1-C1-O2	123.73(15)
C14-C16	1.517(4)	O2 -C1-C2	122.94(14)
O5-C11	1.340(2)	C1-C2-C3	129.67(13)
O3-C13	1.452(2)	S1-C2-C3	110.47(11)
N1-C5	1.315(2)	S1-C2-C1	119.83(11)
N2-C12	1.146(2)	C2-C3-C4	127.48(13)
C1-C2	1.462(2)	N1-C3-C2	114.44(13)
C3-C4	1.496(2)	N1-C3-C4	118.09(13)
C5 -C6	1.468(2)	S1-C5-N1	115.22(11)
C6 -C7	1.396(2)	N1-C5-C6	122.64(14)
C6 -C11	1.395(2)	S1-C5-C6	122.14(11)
C7-C8	1.381(3)	C5-C6-C7	122.51(14)
C8-C9	1.399(2)	C7-C6-C11	118.46(13)
C2-C3	1.378(2)	C5-C6-C11	119.02(13)
N1-C3	1.370(2)	C6-C7-C8	121.80(14)
		C6-C11-C10	120.18(13)
		C11-C10-C12	119.89(13)
		C9-C10-C11	121.10(13)
		C9-C10-C12	119.01(13)
		C13-C14-C15	111.05(17)
		C13 -C14-C16	110.98(18)
		O3-C9-C8	126.08(14)
		C7-C8-C9	120.06(14)

Table S3. Hydrogen bonding interactions (Å) in Form H1

D–H···A	H···A	D···A	D–H···A
O1 -- H1 ... O2 ⁱ	1.8100	2.624 (2)	173.00
C4 -- H4A ... O2	2.3500	3.063 (3)	131.00

Symmetry codes: (i) 2-x, -y, -z

Table S4. Heckel Analysis of Form Q and Form H1

P (MPa)	Form Q		Form H1	
	ln (1/ε)	(Std dev)	ln (1/ε)	(Std dev)
4.6	2.437982	0.02451	1.979106	0.089988
9.2	2.551898	0.011319	2.144051	0.047671
13.8	2.675198	0.008275	2.25147	0.02455
18.4	2.756478	0.042889	2.340856	0.04526
23.0	2.966443	0.034041	2.377522	0.012521
27.6	3.035011	0.077207	2.484921	0.046234
32.2	3.435809	0.067492	2.818027	0.093878
36.8	3.486324	0.035157	2.977136	0.094611

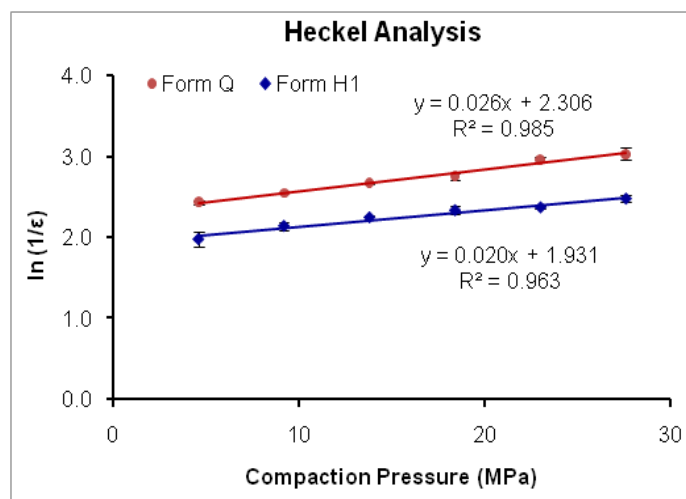


Figure S1. Plot showing linear portion of the Heckel curves ($R^2 > 0.96$ for both the forms)

Nano-indentation Experiment

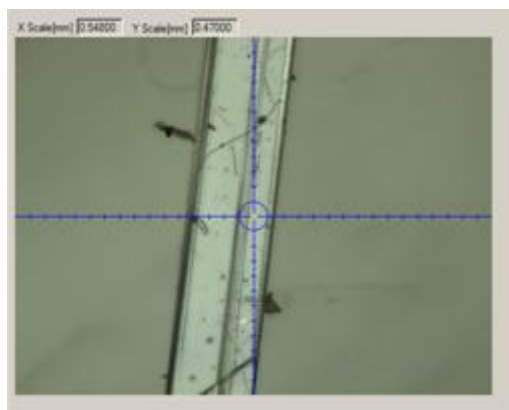


Figure S2. Crystal image through optical microscope for choosing indent location

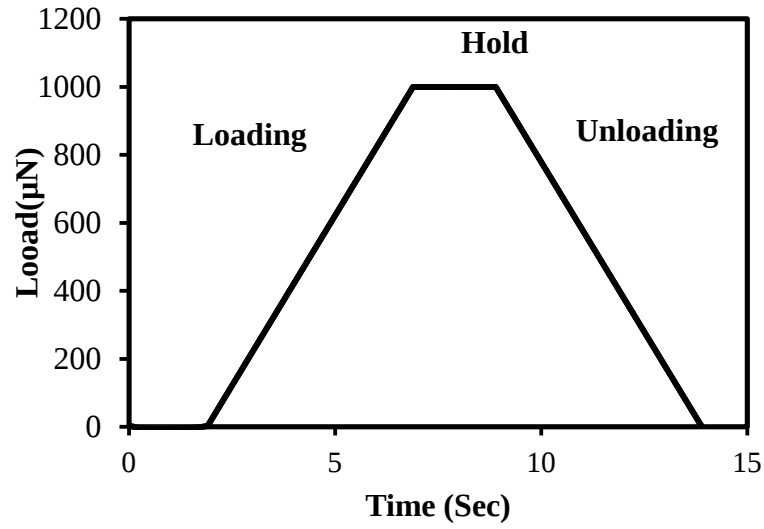


Figure S3. Load-time curve represents the loading function for quasi static indentations

The hardness and the reduced modulus were automatically computed using the Oliver and Pharr method. The reduced modulus E_r is related to the young's modulus E_s of testing material through the following relationship:

$$\frac{1}{E_r} = \frac{(1 - \nu_i^2)}{E_i} + \frac{(1 - \nu_s^2)}{E_s} \quad \text{Equation ... (1)}$$

Where E_i , E_s and ν_i , ν_s are the elastic modulus and Poisson's ratio for the indenter and the substrate materials, respectively. Reduced modulus was calculated by taking the value of elastic modulus and Poisson's ratio to be 1141.00 GPa and 0.07 respectively (for diamond indenter tip).

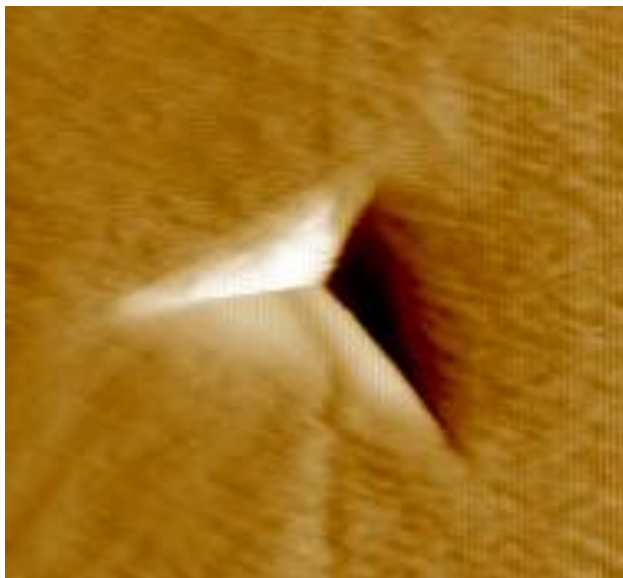


Figure S4 Indentation impression of FXT Q