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SUPPORTING INFORMATION

Stress and Light Sensitive Dual Mechanical Property of Acylhydrazone Crystal

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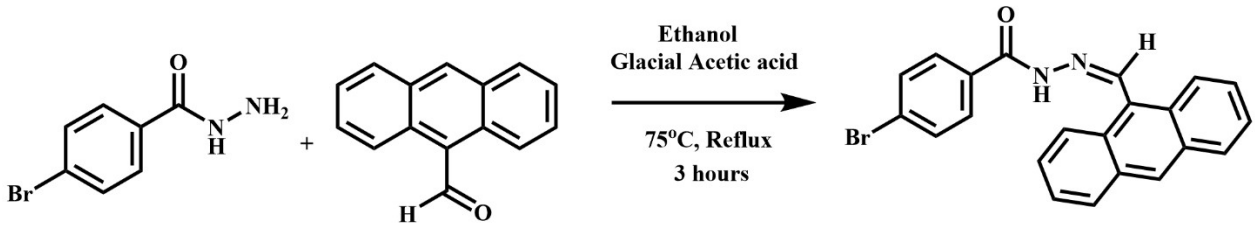


Fig. S1. Synthesis scheme of **BrAc** Crystal.

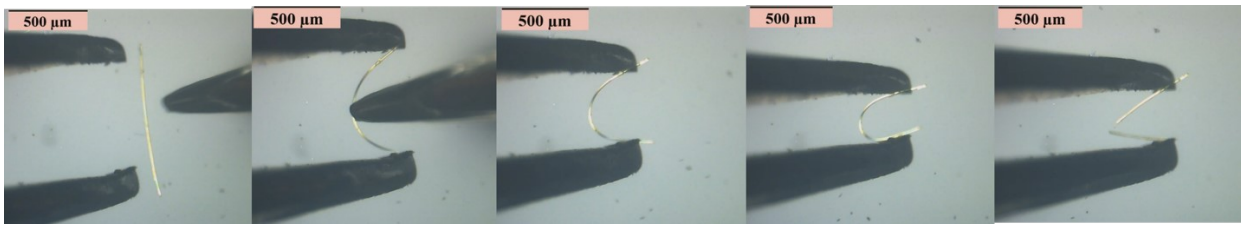


Fig. S2. Stepwise three point bending images of **BrAc** Crystal.

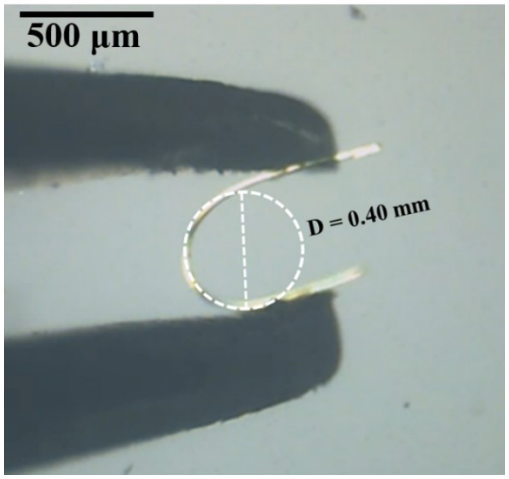


Fig. S3. Elastic strain representation of **BrAc** Crystal.

R= $\frac{D}{2}$ = **0.175mm**, (where D is the diameter of the semi-circle formed and so radius is $\frac{D}{2}$)

For a beam with thickness t,

$\varepsilon(\%) = \frac{t}{2R} = \frac{0.014}{0.40}$ x 100 = **3.5%**

Where ‘ε (%)’ is the elastic strain of the crystal,‘t’ is the thickness of the crystal and ‘R’ is the radius of the semi-circle formed by bending the crystal.

Table S1: Crystallographic information table.

Compound	**Crystal BrAc**
Formula	$C_{22}H_{15}Br\ N_2O_2$
Molecular weight	403.27
T/K	150
Crystal system	Monoclinic
Space group	$P2_1/c$
a/Å	4.3315 (4)
b/Å	18.5293(17)
c/Å	21.324(2)
α/°	90
β/°	93.751(4)
γ/°	90
Volume/Å^3	1707.8(3)
Z	4
ρ, Mg.cm^{-3}	1.568
μ /mm^{-1}	2.420
Reflections collected	64457
Independent Reflections	3620
R_{int}	0.0793
GOF	1.038
Final R[I>2σ]	0.0425
R_1/ wR_2	0.1149
CCDC Number.	2245738

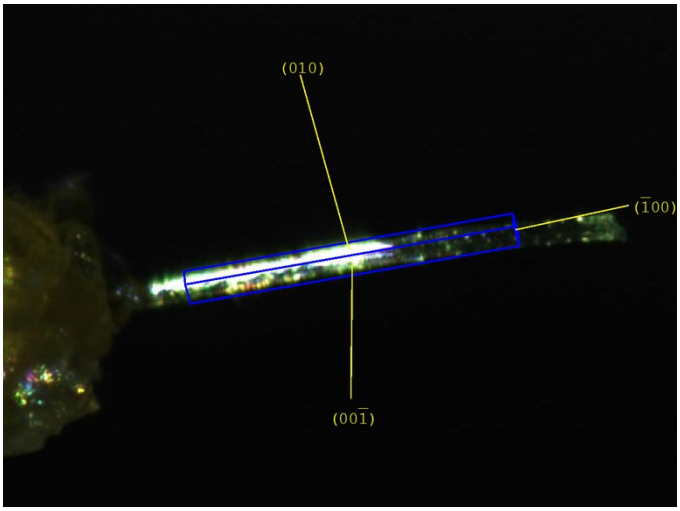
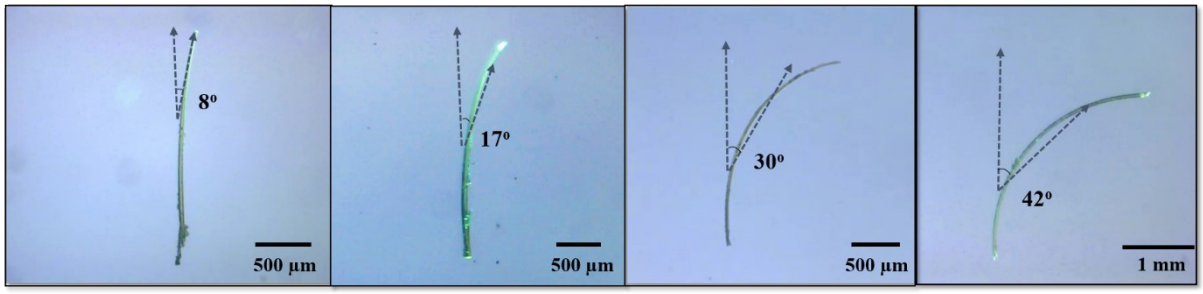
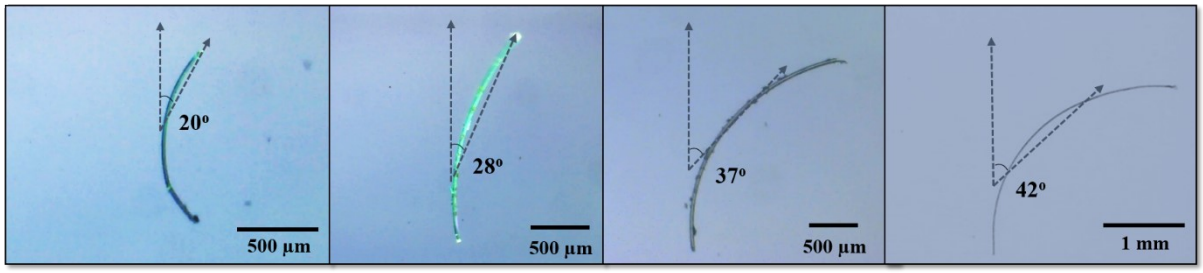


Fig. S4. Face indexing image of **BrAc** Crystal.



Length - 2.1 mm	Length - 2.6 mm	Length - 2.5 mm	Length - 2.9 mm
Width - 0.065mm	Width - 0.05mm	Width - 0.039mm	Width - 0.025mm
Thickness -0.055 mm	Thickness -0.045 mm	Thickness -0.033 mm	Thickness -0.021 mm

Fig. S5. Light induced bending of **BrAc** crystals arranged in order of increasing thickness.



Length - 1.2 mm	Length - 1.8 mm	Length - 2.4 mm	Length – 3.3 mm
Width - 0.035mm	Width - 0.045mm	Width - 0.040mm	Width - 0.035 mm
Thickness -0.32 mm	Thickness -0.042 mm	Thickness -0.036 mm	Thickness -0.025 mm

Fig. S6. Light induced bending of **BrAc** crystals arranged in order of increasing length.

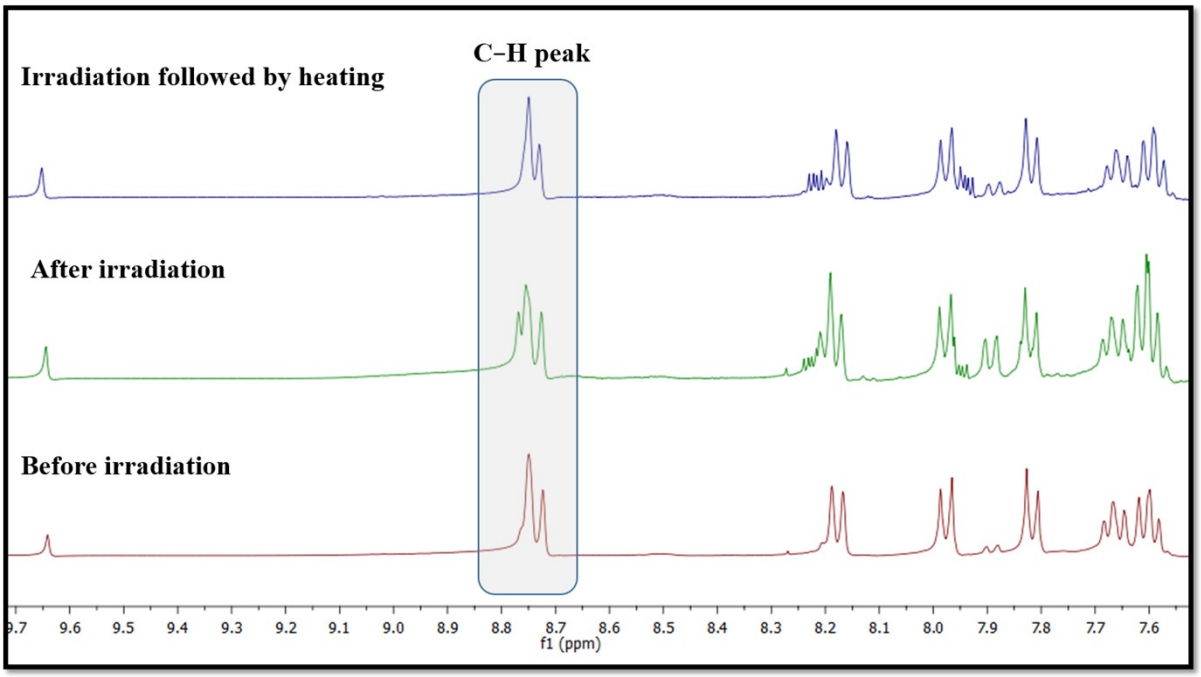


Fig. S7. ^{1}H NMR comparison for Z and E isomers of **BrAc** Crystal.

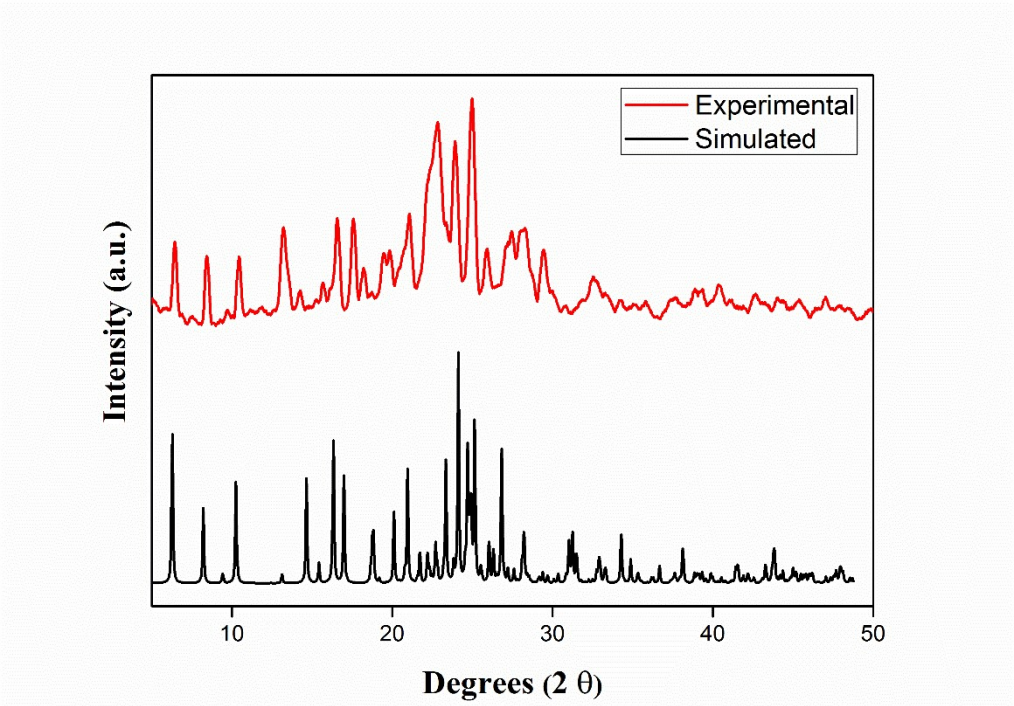


Fig. S8. PXRD comparison of simulated pattern and experimental pattern for **BrAc** Crystal.

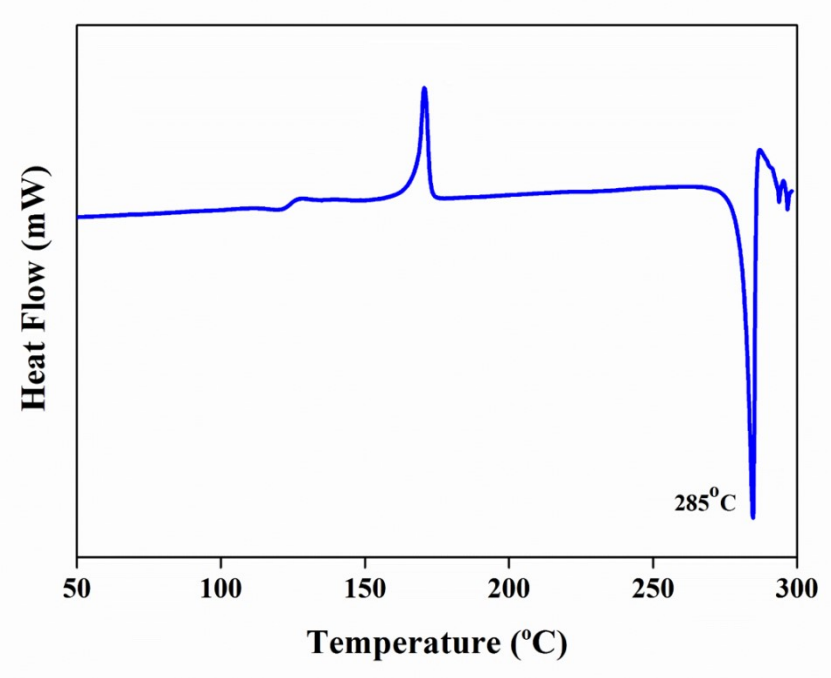


Fig. S9. DSC heating graph of **BrAc** crystal beyond melting point.

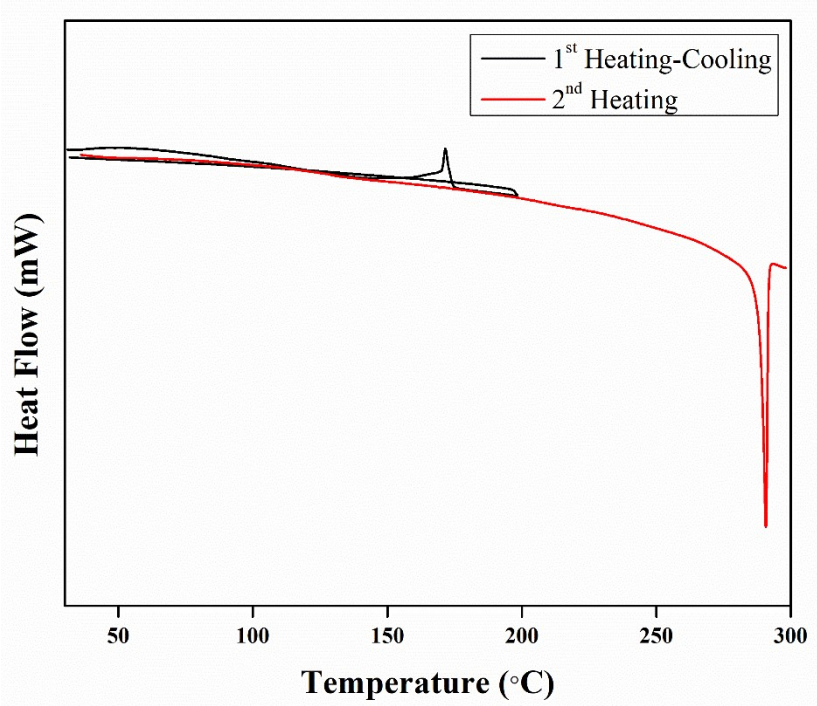


Fig. S10. DSC heating-cooling graph of **BrAc** crystal.

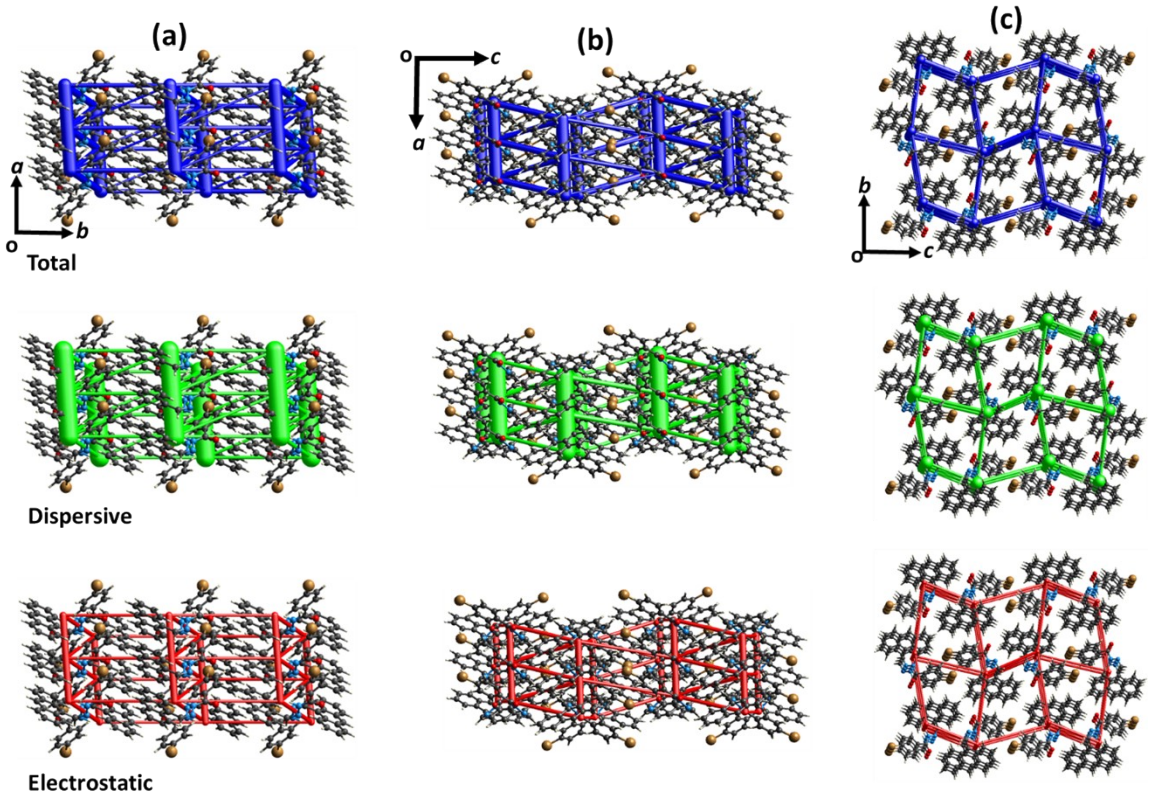
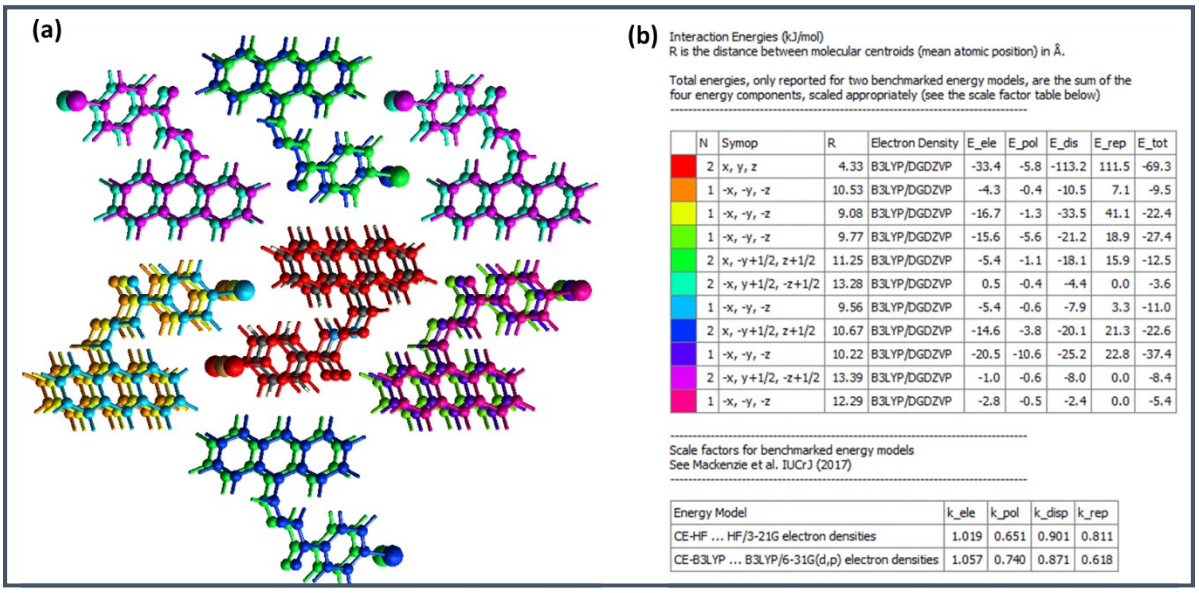


Fig. S11. Visualization of energy frameworks showing total interaction energy (top, blue), dispersion (middle, green) and electrostatic (below, red) components **BrAc**, in the (a) (001), (b) (010) and (c) (100) faces, respectively. The energy threshold is 10 kJ.mol^{-1}.

Table S2 Molecular structure pairs and the interaction energies (kJ.mol^{-1}) obtained from energy frameworks calculation for **BrAc**. 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	4.33	B3LYP/DGDZVP	-33.4	-5.8	-113.2	111.5	-69.3
1	-x, -y, -z	10.53	B3LYP/DGDZVP	-4.3	-0.4	-10.5	7.1	-9.5
1	-x, -y, -z	9.08	B3LYP/DGDZVP	-16.7	-1.3	-33.5	41.1	-22.4
1	-x, -y, -z	9.77	B3LYP/DGDZVP	-15.6	-5.6	-21.2	18.9	-27.4
2	x, -y+1/2, z+1/2	11.25	B3LYP/DGDZVP	-5.4	-1.1	-18.1	15.9	-12.5
2	-x, y+1/2, -z+1/2	13.28	B3LYP/DGDZVP	0.5	-0.4	-4.4	0.0	-3.6
1	-x, -y, -z	9.56	B3LYP/DGDZVP	-5.4	-0.6	-7.9	3.3	-11.0
2	x, -y+1/2, z+1/2	10.67	B3LYP/DGDZVP	-14.6	-3.8	-20.1	21.3	-22.6
1	-x, -y, -z	10.22	B3LYP/DGDZVP	-20.5	-10.6	-25.2	22.8	-37.4
2	-x, y+1/2, -z+1/2	13.39	B3LYP/DGDZVP	-1.0	-0.6	-8.0	0.0	-8.4
1	-x, -y, -z	12.29	B3LYP/DGDZVP	-2.8	-0.5	-2.4	0.0	-5.4

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

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