

# IUCrJ

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**Supporting information for article:**

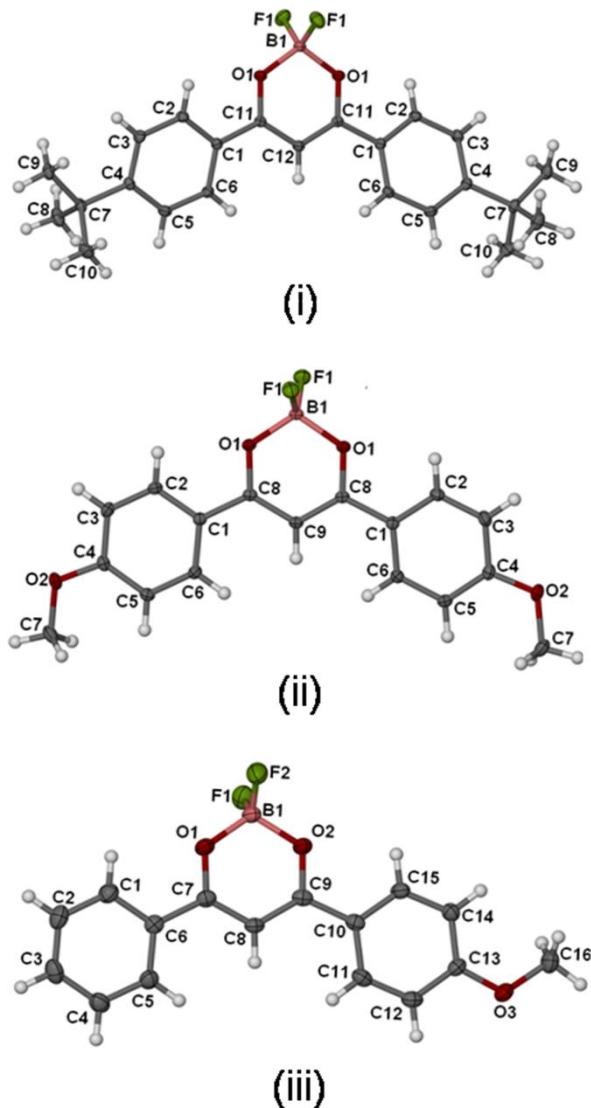
**Structure–mechanical property correlations in mechanochromic luminescent crystals of boron difluoride dibenzoylmethane derivatives**

**Gamidi Rama Krishna, Ramesh Devarapalli, Rajesh Prusty, Tiandong Liu, Cassandra L. Fraser, Upadrasta Ramamurty and Malla Reddy Chilla**

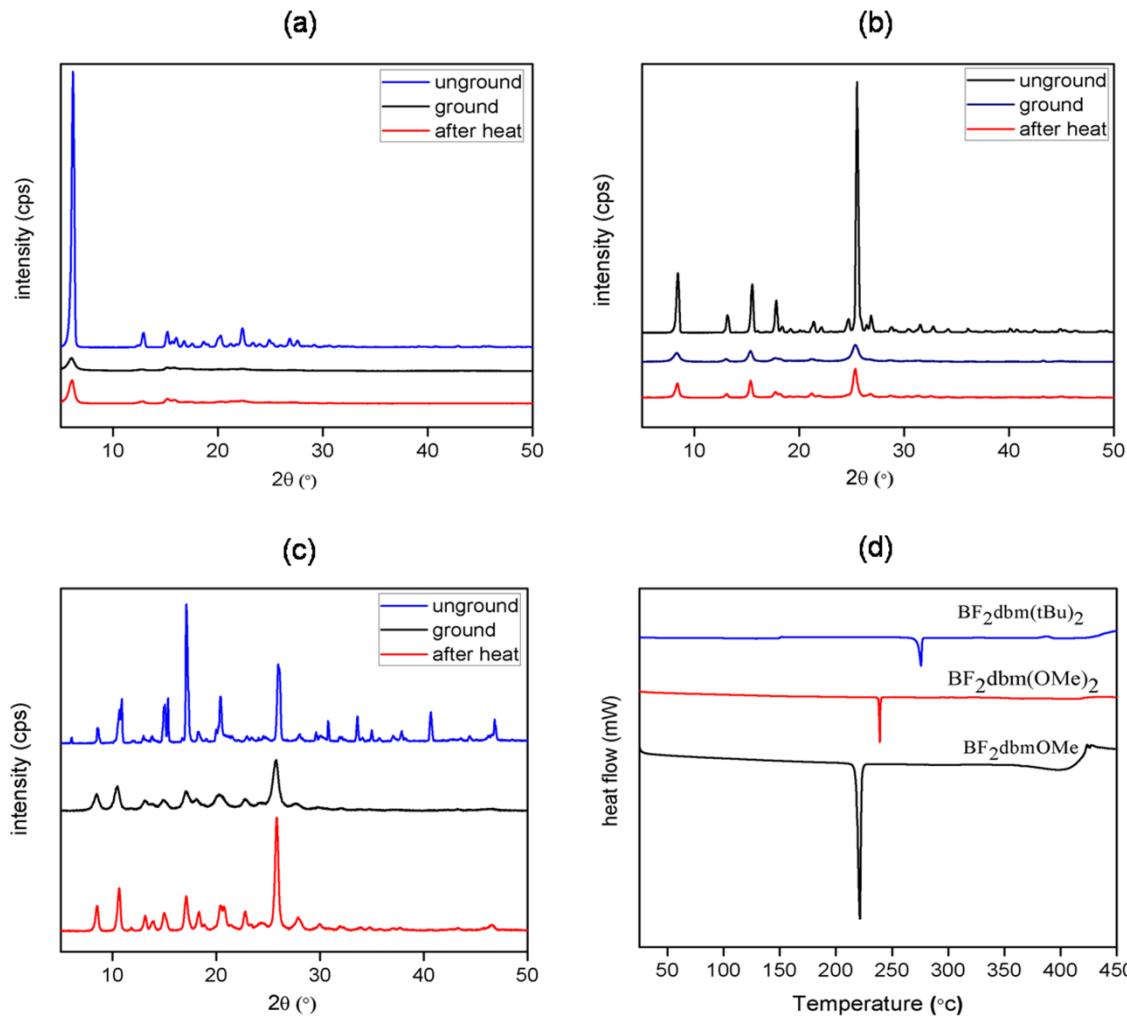
**Table S1** Crystallographic data and structure refinement parameters

	<b>BF<sub>2</sub>dbm(tBu)<sub>2</sub></b>	<b>BF<sub>2</sub>dbm(OMe)<sub>2</sub>*</b>	<b>BF<sub>2</sub>dbmOMe</b>
Formula	C <sub>23</sub> H <sub>27</sub> BF <sub>2</sub> O <sub>2</sub>	C <sub>17</sub> H <sub>15</sub> BF <sub>2</sub> O <sub>4</sub>	C <sub>16</sub> H <sub>13</sub> BF <sub>2</sub> O <sub>3</sub>
Crystal System	monoclinic	monoclinic	Triclinic
Space group	<i>C</i> 2/ <i>c</i>	<i>C</i> 2/ <i>c</i>	<i>P</i> -1
<i>a</i> [Å]	28.575(4)	21.1854(15)	8.0234(7)
<i>b</i> [Å]	7.0402(9)	7.0826(5)	9.0901(8)
<i>c</i> [Å]	10.3208(13)	10.0747(7)	10.7916(8)
$\alpha$ [°]	90	90	75.514(7)
$\beta$ [°]	102.920(3)	98.208(2)	80.766(7)
$\gamma$ [°]	90	90	69.797(8)
<i>V</i> [Å <sup>3</sup> ]	2023.7(5)	1496.20(18)	712.79(11)
<i>Z</i>	4	4	2
$\lambda$ [Å]	0.71073	0.71073	0.71073
$\rho_{\text{calcd}}$ [gcm <sup>-3</sup> ]	1.2611	1.474	1.407
<i>F</i> [000]	816.5	688.0	312.0
$\mu$ [mm <sup>-1</sup> ]	0.090	0.119	0.112
2 <i>θ</i> [°]	2.92 to 55.98	3.88 to 56	3.92 to 56.24
index ranges	$-41 \leq h \leq 41$ $-10 \leq k \leq 10$ $-7 \leq l \leq 15$	$-27 \leq h \leq 27$ $-9 \leq k \leq 9$ $-13 \leq l \leq 11$	$-10 \leq h \leq 10$ $-9 \leq k \leq 11$ $-14 \leq l \leq 12$
<i>T</i> [K]	100	100	100
<i>R</i> 1	0.0348	0.0327	0.0566
<i>wR</i> 2	0.0946	0.0924	0.1235
<i>R</i> <sub>merge</sub>	0.0413	0.0359	0.0779
Parameters	131	112	200
GOF	1.055	1.081	1.040
reflns total	21860	13225	4141
unique reflns	2442	1811	2991
obsd reflns	2124	1657	2092
ccdc/Refcode	1057664	905565/SANKUO02	1057663

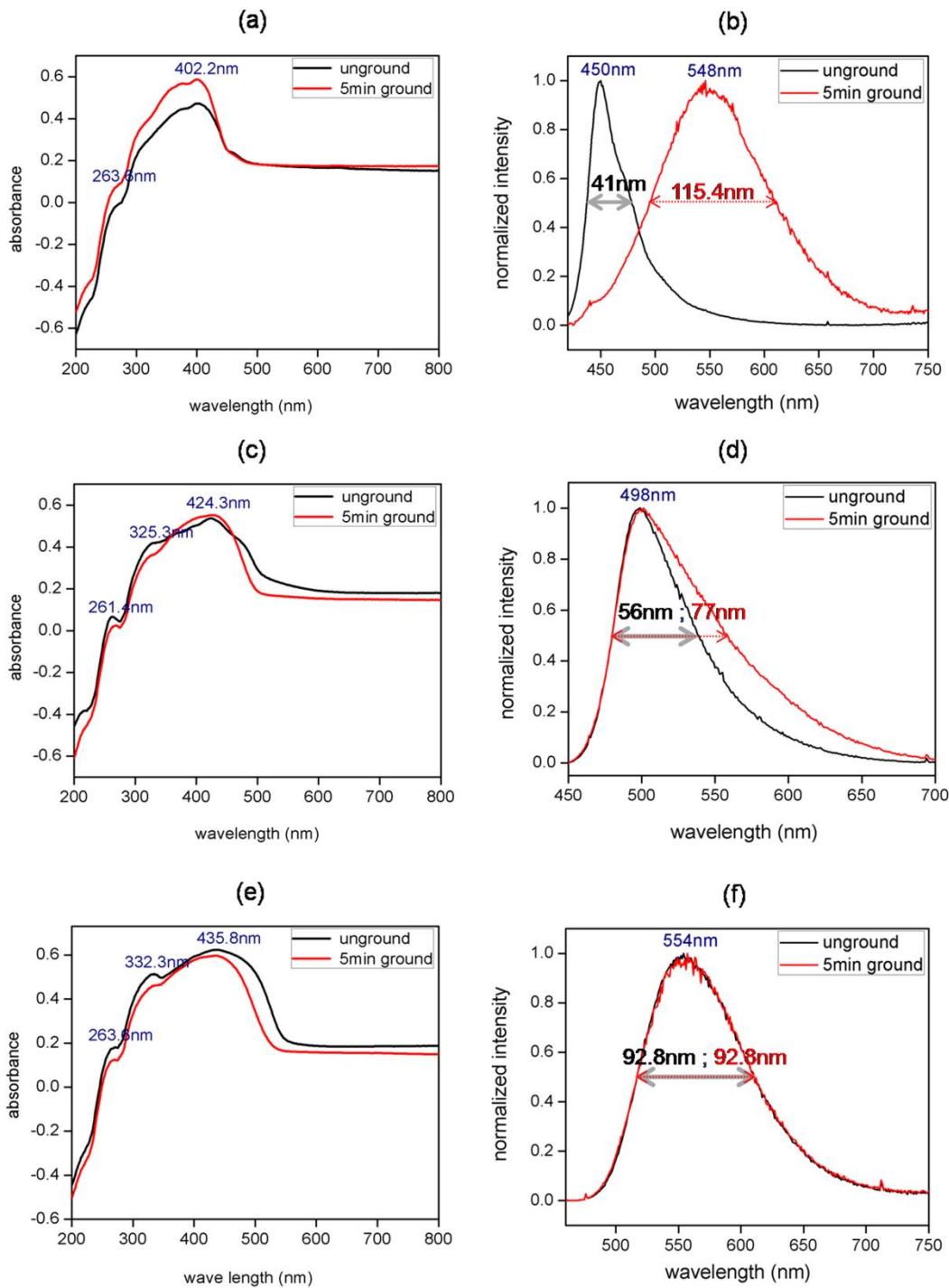
\* This is from our redetermined data. The REFCODE for the reported structure is SANKUO02 (Yoshii *et al.*, 2013. in the main text).



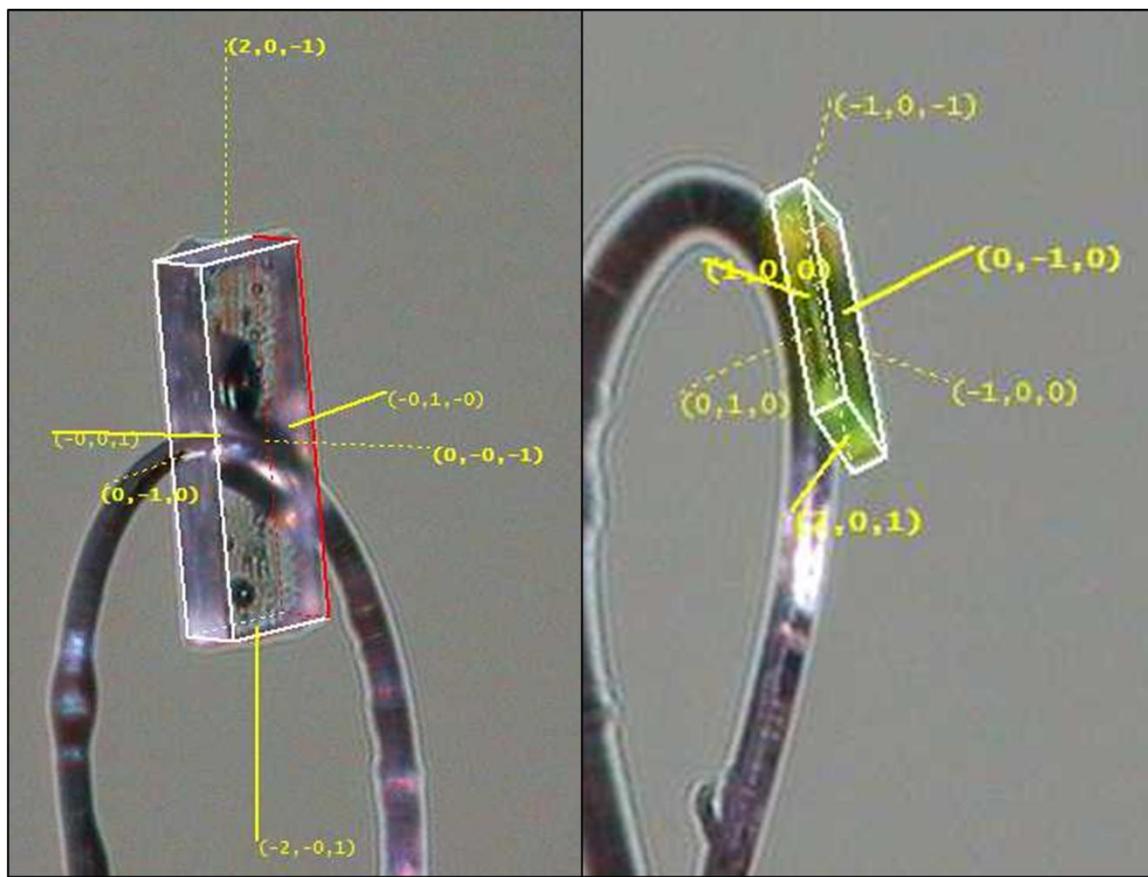
**Figure S1** ORTEP representation of (i)  $\text{BF}_2\text{dbm}(t\text{Bu})_2$ , (ii)  $\text{BF}_2\text{dbm}(\text{OMe})_2$ , and (iii)  $\text{BF}_2\text{dbmOMe}$  respectively. Displacement ellipsoids are drawn at the 50% probability level.



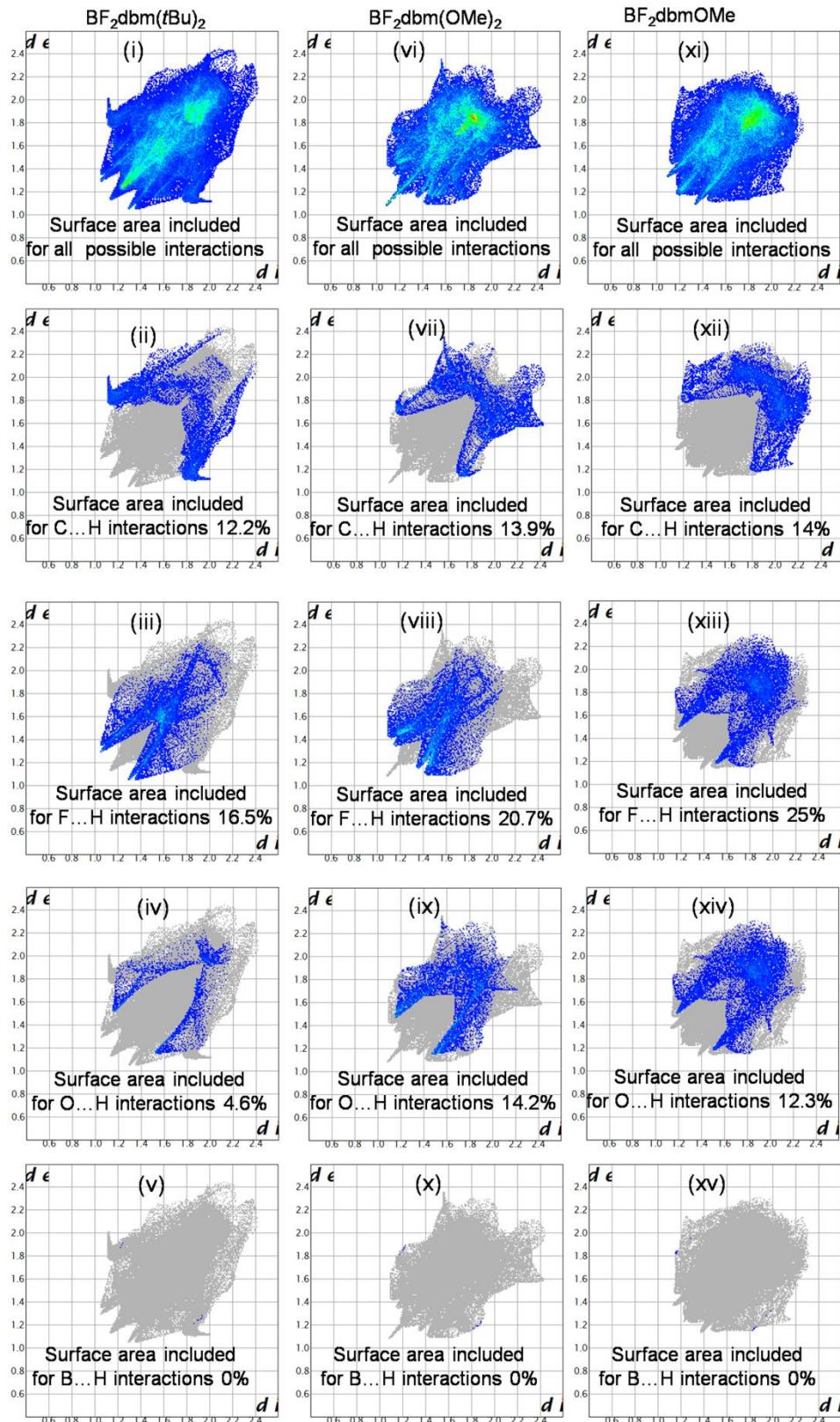
**Figure S2** (a), (b) and (c) shows the comparison of powder x-ray diffraction patterns of  $\text{BF}_2\text{dbm}(t\text{Bu})_2$ ,  $\text{BF}_2\text{dbm}(\text{OMe})_2$  and  $\text{BF}_2\text{dbmOMe}$  samples in various states respectively (before grinding (blue line), after 30min ball mill grinding (black line) and after heating the ground sample (red line)). (d) DSC curves of respective compounds.



**Figure S3** Solid state absorbance and emission spectra: (a), (b) corresponds to  $\text{BF}_2\text{dbm}(t\text{Bu})_2$ ; (c), (d) corresponds to  $\text{BF}_2\text{dbm}(\text{OMe})_2$ ; and (e), (f) corresponds to  $\text{BF}_2\text{dbm}\text{OMe}$  compounds respectively. Note: in all the graphs black color line represents unground sample and red color line represents 5min ground sample (using a mortar and pestle). All the emission spectra were recorded at the excitation of corresponding highest absorption maxima.



**Figure S4** Face index images of  $\text{BF}_2\text{dbm}(t\text{Bu})_2$ ,  $\text{BF}_2\text{dbm}(\text{OMe})_2$ .



**Figure S5** Hirshfeld fingerprint plots for various interactions of all three compounds.