

## Supplementary Materials

## A new polymorph of 5-bromo ortho vanillin: Synthesis, characterization, crystal engineering, Hirshfeld surface, calculation of interaction energy, and energy frameworks

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Table S1. Bond lengths for similar reported compound 2.

Atom	Atom	Length (Å)	Atom	Atom	Length (Å)
Br1	C1	1.894(10)	C4	C5	1.399(14)
O2	C4	1.331(11)	C1	C6	1.394(15)
O3	C5	1.352(12)	C1	C2	1.351(14)
O3	C7	1.447(14)	C3	C2	1.410(13)
O1	C8	1.220(14)	C3	C8	1.454(14)
C4	C3	1.404(13)	C6	C5	1.399(15)

Table S2. Bond angles for similar reported compound 2.

Atom	Atom	Atom	Angle (°)	Atom	Atom	Atom	Angle (°)
C5	O3	C7	118.1(9)	C4	C3	C8	120.2(9)
O2	C4	C3	121.4(9)	C2	C3	C8	119.7(10)
O2	C4	C5	119.4(9)	C1	C6	C5	119.2(9)
C5	C4	C3	119.2(9)	C1	C2	C3	119.5(10)
C6	C1	Br1	117.9(8)	O3	C5	C4	115.7(9)
C2	C1	Br1	120.2(8)	O3	C5	C6	124.3(9)
C2	C1	C6	122.0(9)	C4	C5	C6	120.1(9)
C4	C3	C2	120.0(9)	O1	C8	C3	124.5(11)

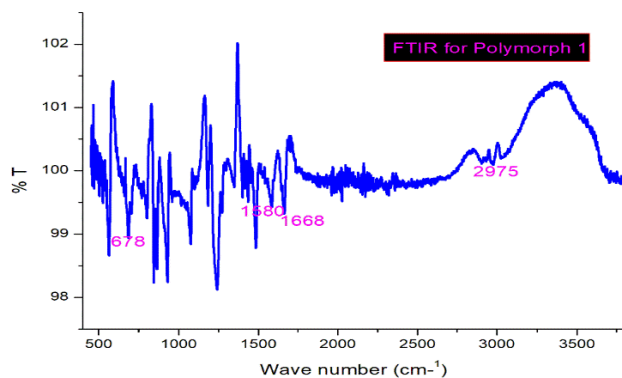


Figure S1. FT-IR spectra representation of polymorph 1.

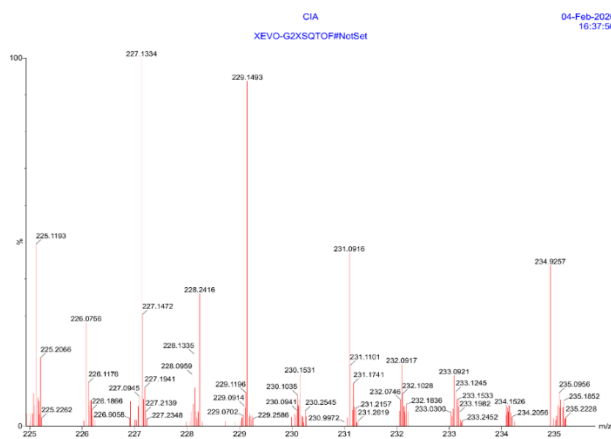


Figure S2. HRMS representation for polymorph 1.

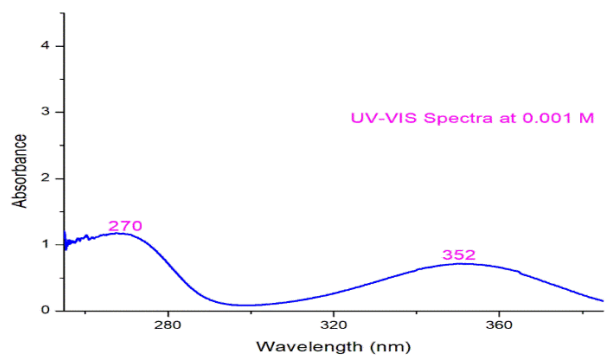


Figure S3. UV-VIS spectra representation of polymorph 1.

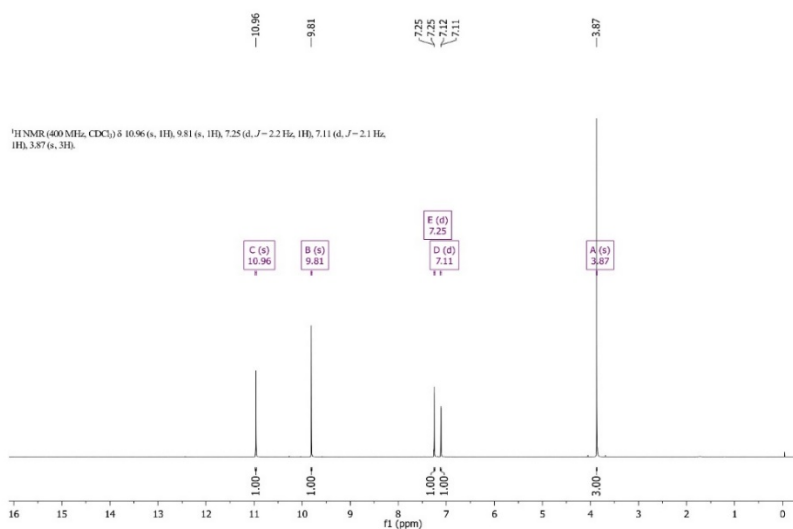


Figure S4. <sup>1</sup>H NMR representations for polymorph 1.

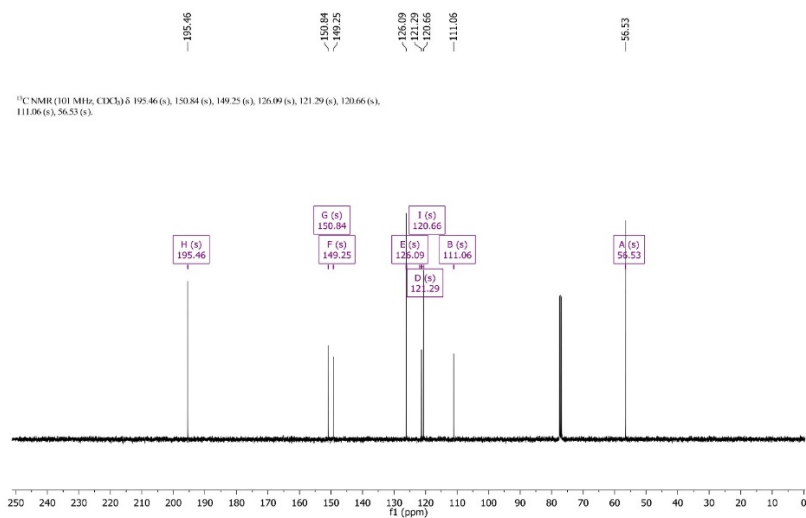
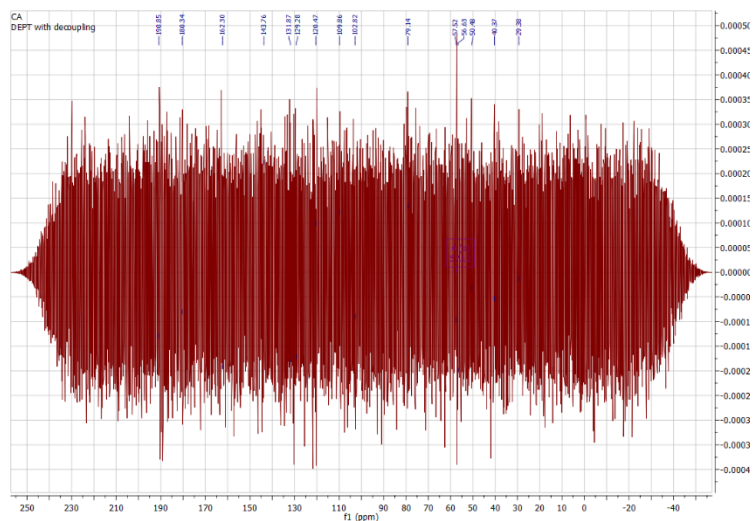


Figure S5. <sup>13</sup>C NMR representations for polymorph 1.



**Figure S6.**  $^{13}\text{C}$  DEPT Decoupling NMR representations for polymorph 1.