Table 1. Unit cell parameters of the β "-(BEDT-TTF)₄H₃O[Fe(C₂O₄)₃]·G crystals with different solvent (G) compositions below the phase transition temperature.

G composition	CB^{a}	FB^{a}	(BN) _{0.40} (FB) _{0.60} ^a	(BN) _{0.35} (CB) _{0.65}	$(BN)_{0.17}(BB)_{0.83}^{a}$
Chemical formula	$C_{52}H_{40}ClFeO_{13}S_{32}$	$C_{52}H_{40}FFeO_{13}S_{32}$	$C_{52.4}H_{40}F_{0.6}FeN_{0.4}$	$C_{52.35}H_{40}Cl_{0.65}FeN_{0.35}$	$C_{52.17}H_{40}Br_{0.83}FeN_{0.17}$
			$O_{13}S_{32}$	$O_{13}S_{32}$	$O_{13}S_{32}$
Temperature, K	100	150	120	150	120
Cell setting	triclinic	triclinic	triclinic	triclinic	triclinic
Space group, Z	$P\overline{1}, 2$	$P\overline{1}, 2$	<i>P</i> 1, 2	$P\overline{1}, 2$	$P\overline{1}, 2$
<i>a</i> (Å)	10.2041(6)	10.249(1)	10.245(2)	10.2649(3)	10.2197(5)
<i>b</i> (Å)	11.1015(6)	11.136(1)	11.109(2)	11.1956(3)	11.1518(7)
<i>c</i> (Å)	35.086(2)	35.023(4)	34.529(6)	35.1514(10)	35.247(2)
α (°)	87.709(4)	88.664(7)	87.806(8)	88.619(2)	88.339(5)
β (°)	86.580(4)	86.546(6)	86.523(8)	86.651(2)	86.435(4)
γ (°)	62.554(6)	62.455(9)	62.88(2)	62.748(3)	62.906(6)
Cell volume (Å ³)	3520.6(3)	3538(1)	3490(4)	3585.1(2)	3569.3(3)
Cell volume (Å ³) at RT^b	7269.1(6)	7264.9(7)	7248.0(7)	7284.2(7)	7287.1(7)

^aThis structure is reported as a partial determination, as the crystal data is not of sufficient quality for full determination and deposition of the crystal structure in CCDC.

^b Other crystal structure data at room temperature (RT) could be found in Table 2 of the reference [1] for a comparison with the low temperature data.

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Figure 1. (*h*0*l*) reciprocal-lattice planes calculated on the base of full experimental data which were collected for the β "-(BEDT-TTF)₄H₃O[Fe(C₂O₄)₃]·G crystals with different solvent (G) compositions below the phase transition temperature. Appearance of the additional peaks with $l \neq 2n$ (shown by arrows) in (*h*0*l*) planes is evidence of lowering symmetry (vanishing of the *c*-plane) and transition from monoclinic C2/*c* to triclinic $P\overline{1}$ structure.

a) $G = (BN)_{0.35}(CB)_{0.65}$



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(b) $\mathbf{G} = \mathbf{C}\mathbf{B}$

(c) G = FB



100 K, $l \neq 2n$

150 K, $l \neq 2n$

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d) $G = (BN)_{0.40}(FB)_{0.60}$

e) $G = (BN)_{0.17}(BB)_{0.83}$

