STRUCTURAL
CHEMISTRY

Volume 75 (2019)

Supporting information for article:

Concomitant cocrystal and salt: no interconversion in the solid state

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Table S1 The angles between the principal axes of strain ellipsoid and respective unit cell axes for a temperature difference from 293 K to 100 K for co-crystal of β-alanine with DL-tartaric acid.

	Angle of principal axis with corresponding unit cell axis (a, b or c) (°)		
Principal axis	+a	+b	+c
1	21.6(0.4)	90.0(0.0)	81.8(0.4)
2	90.0(0.0)	180.0(0.0)	90.0(0.0)
3	68.4(0.4)	90.0(0.0)	171.8(0.4)

Table S2 The angles between the principal axes of strain ellipsoid and respective unit cell axes for a temperature difference from 293 K to 100 K for molecular salt of β-alanine with DL-tartaric acid.

	Angle of principal axis with corresponding unit cell axis (a, b or c) (°)		
Principal axis	+a	+b	+c
1	118.0(9.3)	95.9(3.9)	23.7(9.6)
2	127.0(6.0)	37.7(11.7)	112.4(10.3)
3	130.3(13.4)	127.1(12.8)	97.5(1.1)

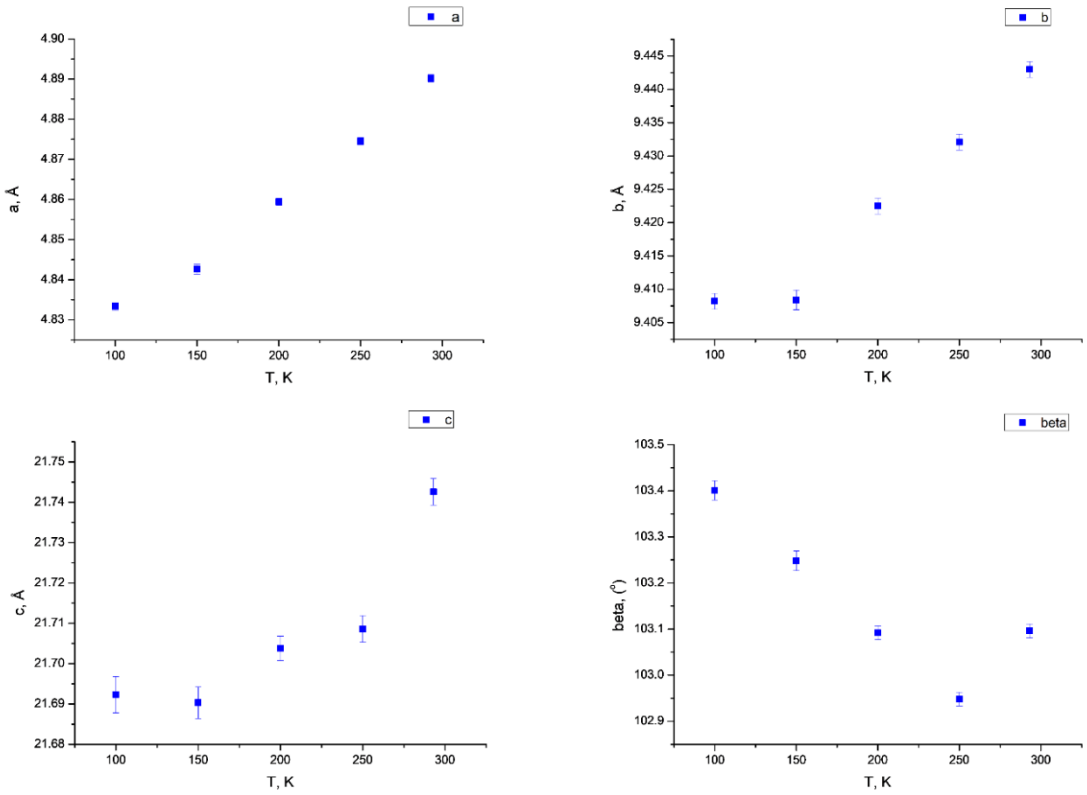

Figure S1 Unit cell parameters of co-crystal at cooling down to 100 K.

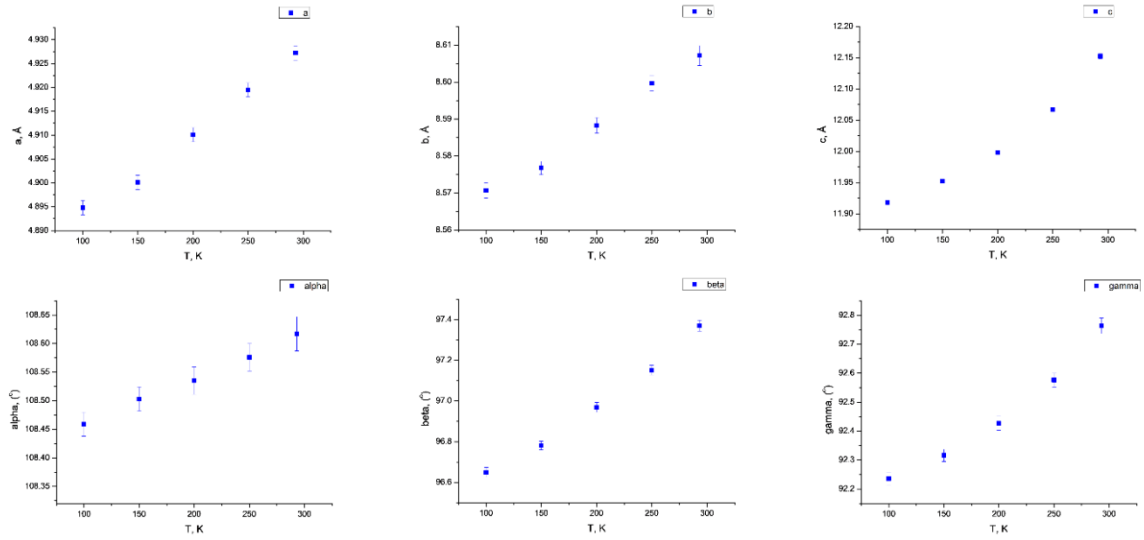

Figure S2 Unit cell parameters of molecular salt at cooling down to 100 K.

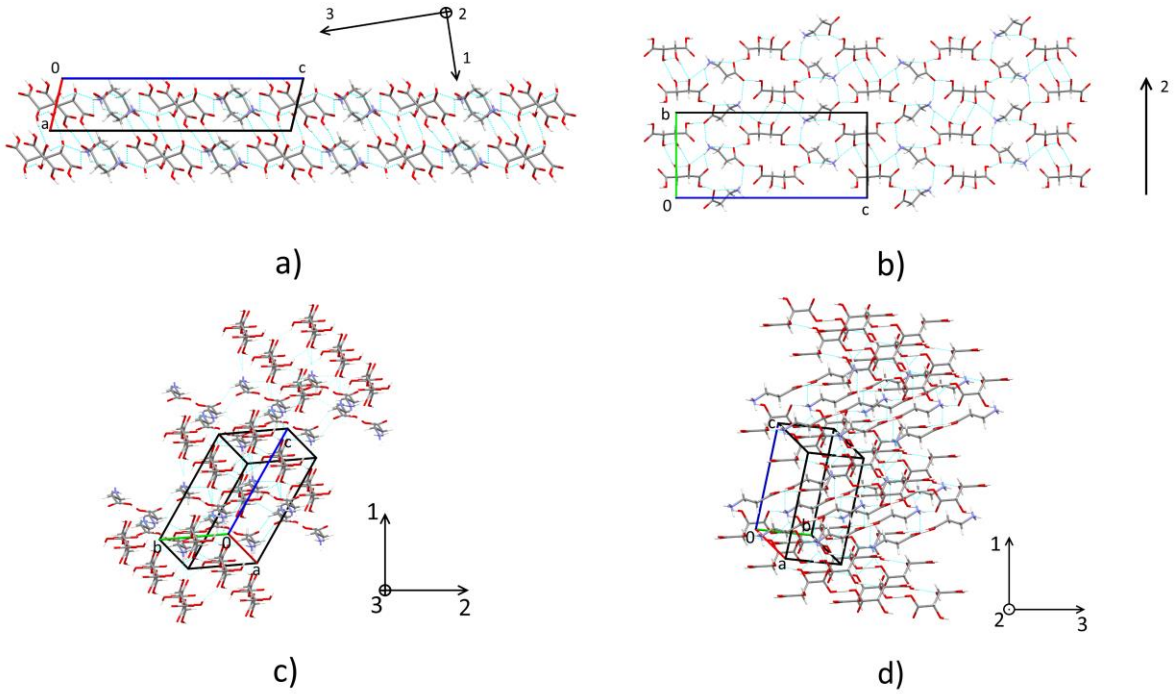

Figure S3 The approximate orientation of the principal axes of strain ellipsoids with respect to crystal structure of co-crystal (a, b) and molecular salt (c, d) of β-alanine with DL-tartaric acid. For the values of the angles formed by the principal axes of the strain ellipsoid and unit cell directions, see Tables S1 and S2.

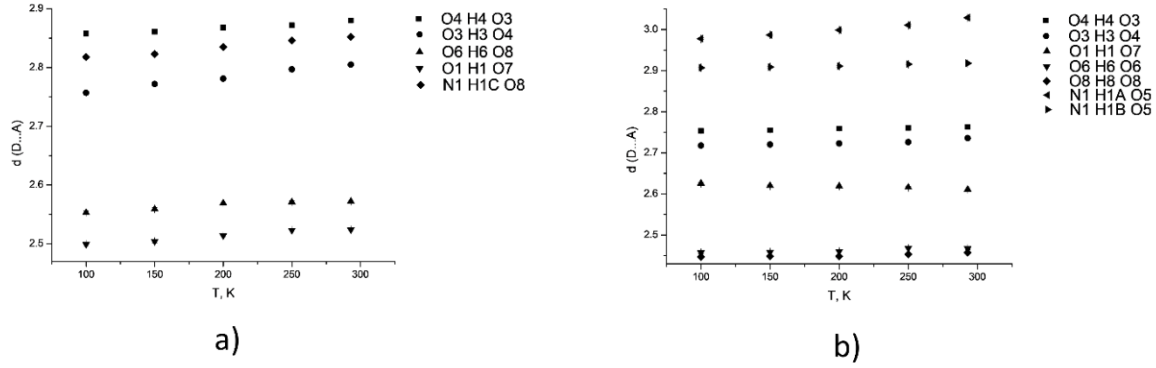

Figure S4 Donor-acceptor distances in the strongest hydrogen bonds vs temperature for co-crystal (a) and molecular salt (b).

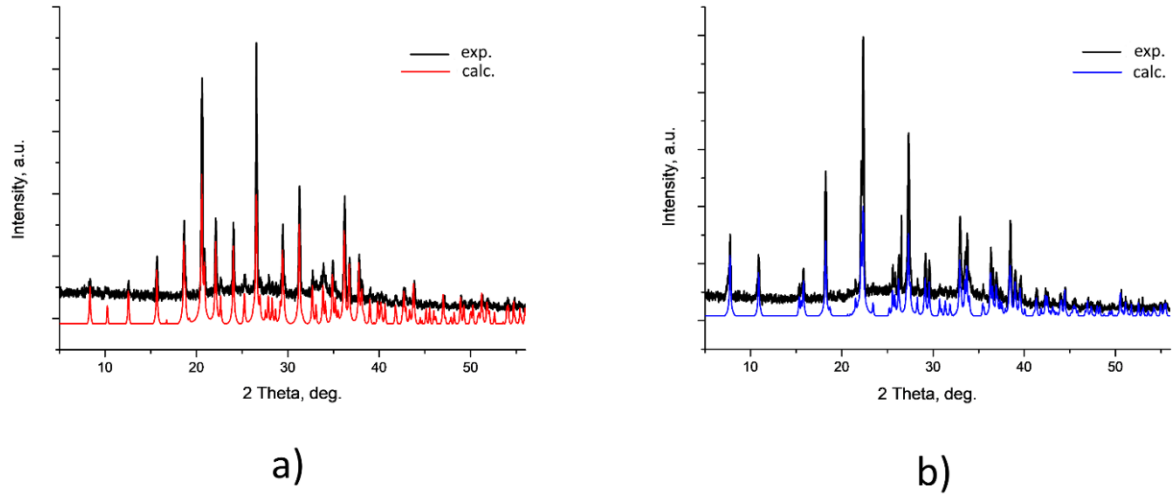

Figure S5 XRPD of co-crystal (a) and molecular salt (b) at ambient temperature. Black plots correspond to experimental data of powder diffraction, red and blue lines are calculated plots obtained from single crystal data of co-crystal and salt, respectively.