Thermodynamic Relationship and Phase Transition Study involving two Polymorphs of Sulfamethoxazole: Form I vs. Form II

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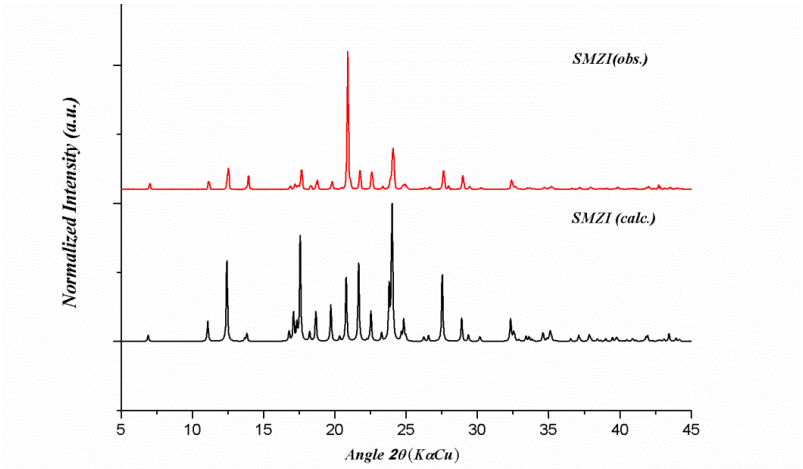
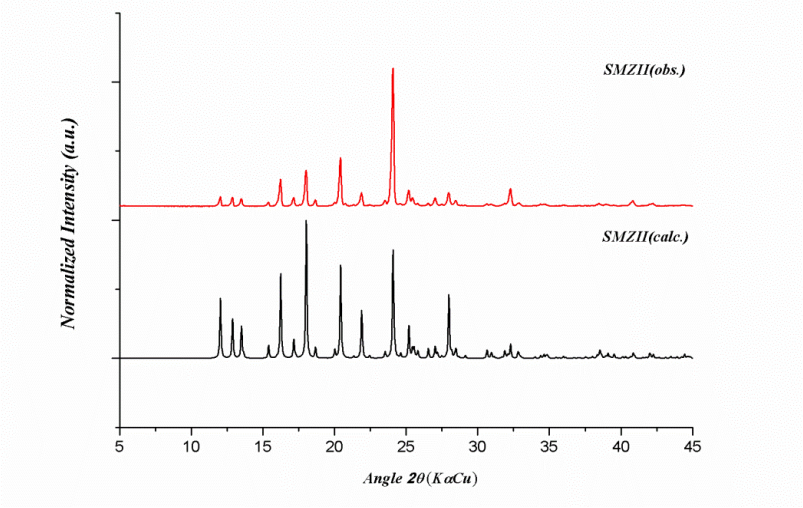
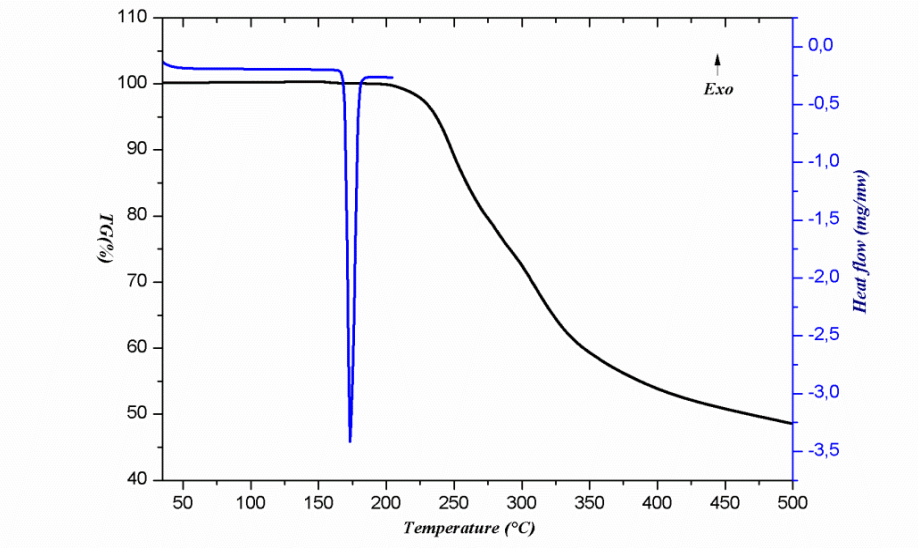


(a)



(b)

Figure S1. Direct comparison between PXRD profile calculated from single crystal data (CCDC code: SLFNMB01[12] for SMZI and SLFNMB02[12] for SMZII) and experimental for SMZI(a) and SMZII(b).



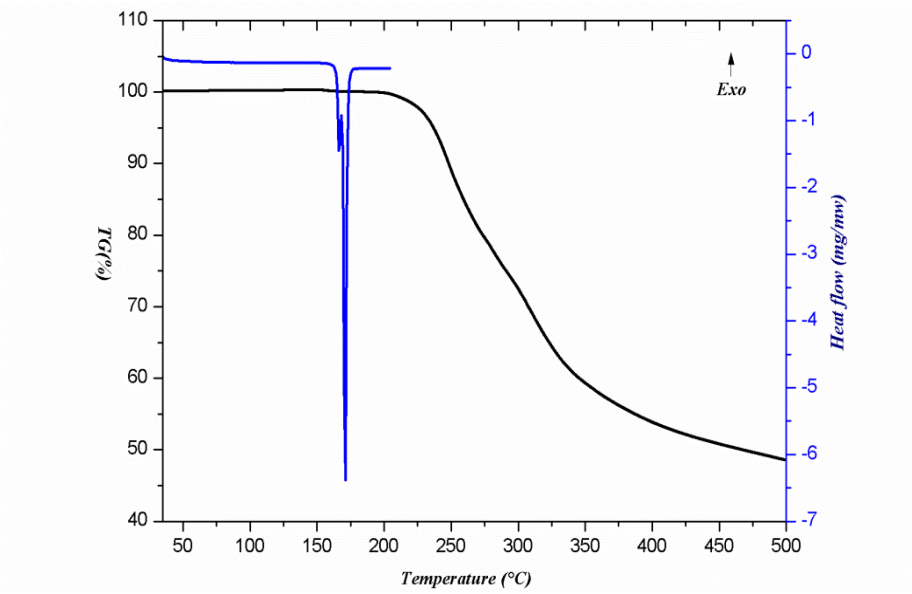


Figure S2. TG/DTA curves of solid forms (a) SMZI and (b) SMZII.

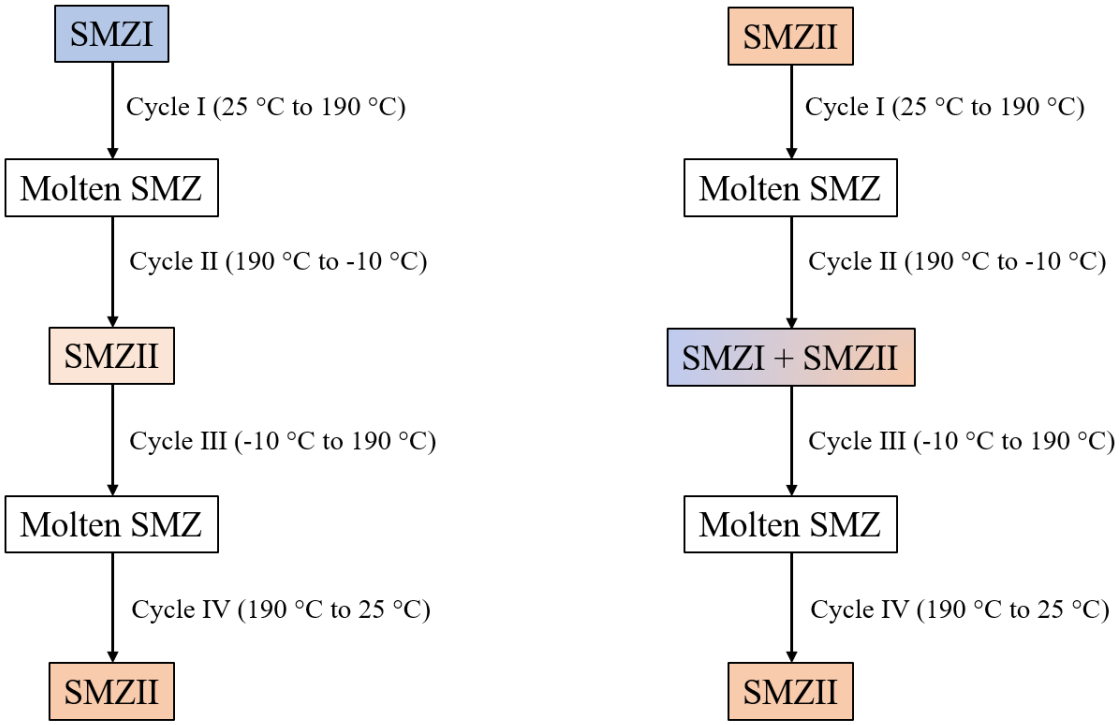


Figure S3. Scheme of heat-cool-heat protocol (B), evidencing the SMZII as final residual material.

Table S1. Hydrogen bond distances (Å) and angles (°), for SMZI. Data extracted from SLFNMB01 CIF file.

	d D···A	d D−H	<D−H···A
N1−H1···O2	3.320	0.829	140.62
N1−H2···O2	3.286	0.855	151.68
N2−H3···O1	3.240	0.855	170.48
C8−H8···N3	3.239	0.882	154.91

D = donor; A = acceptor

Table S2. Hydrogen bond distances (Å) and angles (°), for SMZII. Data extracted from SLFNMB02 CIF file.

	d D···A	d D−H	<D−H···A
N1−H1···O1	3.124	1.000	167.95
N1−H2···O2	2.997	0.902	166.87
N2−H3···N3	2.937	0.901	163.82

D = donor; A = acceptor