Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Supporting information for "Enantiotropic Inconstancy, Crystalline Solid Solutions and Co-crystal in the Salicylic acid - Anthranilic acid system"

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X(AA)	DSC endotherms	Low temperature endotherm					High temperature endotherm				
mol AA/mol SA+AA		T_{inset}	T_{onset}	T_{peak}	T_{offset}	Enthalpy	T_{inset}	T_{onset}	T_{peak}	T_{offset}	Enthalpy
		°C	°C	°C	°C	J/g	°C	°C	°C	°C	J/g
0.00	One endotherm						154.07 (0.08)	158.64 (0.006)	159.16 (0.09)	160.98 (0.23)	189.56 (4.21)
0.0109	One endotherm						153.78 (0.23)	157.81 (0.10)	158.72 (0.20)	160.15 (0.58)	181.62 (1.87)
0.0202	One endotherm						148.27 (1.45)	156.63 (0.35)	158.06 (0.18)	160.30 (0.24)	177.85 (3.84)
0.0303	One endotherm						149.82 (0.60)	156.45 (0.09)	157.69 (0.07)	159.17 (0.10)	172.36 (5.32)
0.0381	One endotherm						145.09 (1.27)	154.96 (0.14)	156.94 (0.14)	159.01 (0.11)	170.35 (4.15)
0.0523	Two separated endotherms	129.72 (0.26)	131.24 (0.10)	132.42 (0.01)	133.48 (0.08)	3.81 (0.28)	144.77 (0.47)	154.07 (0.03)	156.41 (0.08)	158.00 (0.10)	161.59 (6.06)
0.0698	Two separated endotherms	130.09 (0.31)	131.82 (0.10)	132.80 (0.05)	134.07 (0.09)	12.85 (1.16)	144.55 (0.79)	151.61 (1.29)	154.86 (0.26)	156.79 (0.33)	151.02 (8.40)
0.0953	Two separated endotherms	130.64 (0.04)	132.12 (0.02)	133.00 (0.03)	134.43 (0.16)	22.94 (1.50)	138.59 (1.45)	148.31 (0.14)	153.04 (0.16)	155.24 (0.41)	142.39 (3.35)
0.1183	Two separated endotherms	130.20 (0.92)	132.11 (0.05)	132.99 (0.07)	134.56 (0.15)	32.96 (1.75)	138.13 (0.34)	145.58 (0.30)	151.45 (0.40)	154.26 (0.68)	130.61 (5.16)
0.1375	Two separated endotherms	130.41 (0.83)	132.21 (0.04)	133.06 (0.05)	134.52 (0.17)	44.73 (3.96)	135.54 (0.16)	143.75 (0.84)	150.16 (0.25)	153.22 (0.77)	122.22 (5.87)
0.1541	Two partially overlapping endotherms	130.38 (0.94)	132.11 (0.04)	133.03 (0.06)	134.93[1] (0.35)	53.80 (3.73)		143.73 (1.34)	148.90 (0.42)	152.15 (0.88)	114.98 (7.73)
0.1843	Two partially overlapping endotherms	130.83 (0.87)	132.30 (0.02)	133.56 (0.16)	135.69[1] (0.20)	76.73 (4.68)			145.76 (1.10)	149.79 (0.65)	78.43 (2.19)
0.2449	Two partially overlapping endotherms	130.48 (0.10)	132.24 (0.02)	133.50 (0.23)	135.23[1] (0.40)	106.24 (2.6)			143.78 (0.87)	146.42 (1.02)	53.33 (5.02)
0.2853	Two partially overlapping endotherms	130.60 (0.58)	132.51 (0.47)	133.54 (0.32)		144.58 (9.83)			140.34 (3.31)	143.74 (1.06)	30.23 (15.21)
0.3584	Two endotherms mostly overlapping	130.59 (0.26)	132.78 (0.12)	133.44 (0.12)		177.18 (3.81)				138.72 (0.14)	
0.4043	One endotherm	131.31 (0.08)	133.42 (0.72)	133.91 (0.26)	135.93 (0.25)	149.86 (1.33)					
0.4404	One endotherm	129.81 (0.21)	132.89 (0.80)	134.17 (0.44)	136.07 (0.29)	176.35					
0.5000	One endotherm	130.38 (0.40)	134.24 (0.08)	134.67 (0.07)	136.41 (0.27)	180.53 (2.90)					
0.5457	Two partially	128.92 (0.32)		131.66 (0.05)		16.73 (0.23)		133.83 (0.15)	134.65 (0.01)	136.41 (0.09)	169.53 (1.76)

[1] Mid-point between endotherms is used as an approximation of the baseline offset temperature of the low-temperature endotherm. This separation also provides the calculation of the enthalpy of both the low- and high-temperature endotherms.

	overlapping endotherms										
0.6071	Two partially overlapping endotherms	130.20 (0.34)	131.13 (0.13)	132.77 (0.24)		87.81 (9.07)			134.50 (0.15)	135.67 (0.15)	53.59 (11.25)
0.6563	One endotherm	128.76 (0.40)	131.76 (0.10)	132.50 (0.27)	134.96 (0.33)	171.36 (3.57)					
0.6996	One endotherm	130.06 (0.15)	131.80 (0.26)	132.52 (0.07)	134.48 (0.25)	172.63 (7.93)					
0.7517	Two partially overlapping endotherms	128.76 (0.11)	131.97 (0.18)	132.53 (0.15)		158.55 (5.78)			139.21 (0.11)	139.76 (2.32)	50.06 (11.81)
0.8002	Two partially overlapping endotherms	128.91 (0.89)	130.51 (0.07)	132.04 (0.09)		78.33 (4.76)			137.06 (0.23)	142.28 (0.17)	103.78 (6.04)
0.8274	Two partially overlapping endotherms	128.28 (0.31)	130.38 (0.07)	131.69 (0.05)	133.34[1] (0.03)	51.29 (2.75)			137.28 (0.35)	141.91 (0.62)	96.64 (3.29)
0.8697	Two separated endotherms	129.15 (0.33)	130.62 (0.16)	131.55 (0.07)	132.59 (0.18)	5.53 (1.66)	133.31 (0.35)	138.13 (0.43)	140.69 (0.41)	143.57 (0.62)	127.16 (4.28)
0.8796	Two separated endotherms	130.16 (0.52)	131.12 (0.13)	131.58 (0.04)	132.50 (0.37)	2.34 (0.89)	133.02 (0.27)	138.15 (0.21)	140.49 (0.15)	143.52 (0.43)	125.43 (3.49)
0.8890	One endotherm						132.64 (0.14)	139.12 (0.50)	141.12 (0.37)	143.71 (0.23)	132.63 (5.73)
0.9001	One endotherm						133.18 (0.19)	139.86 (0.58)	141.75 (0.60)	143.92 (0.20)	139.44 (2.22)
0.9492	One endotherm						136.80 (0.18)	143.00 (0.42)	144.04 (0.15)	145.57 (0.14)	149.79 (1.46)
0.9663	One endotherm						139.40 (0.65)	144.39 (0.10)	145.09 (0.09)	146.47 (0.04)	154.68 (1.77)
0.9802	One endotherm						140.51 (0.62)	145.08 (0.14)	145.68 (0.07)	147.49 (0.11)	156.00 (5.35)
1.000	One endotherm						143.81 (0.90)	146.12 (0.10)	146.66 (0.05)	148.50 (0.19)	163.35 (5.18)

Solubility data at 20°C

Solid phase	Liquid	Solid	Liquid	Solid	Conc. of SA	Conc. of AA	X(SA)	A(AA)	X(solvent)
	w% AA in SA	w% AA in SA	mol% AA in SA	mol% AA in SA	mg SA/g solvent	mg AA/g solvent	mmol SA/(ml total)	mmol AA/(ml total)	mol solvent/(ml total)
SA	0%	0%	0%	0%	17.23	0.00	2.7170	0.0000	0.99728
α	4.34%	0.40%	4.31%	0.39%	18.63	0.84	2.9373	0.1341	0.99693
α	4.38%	0.25%	4.35%	0.25%	18.18	0.83	2.8661	0.1321	0.99700
α	6.97%	0.63%	6.92%	0.63%	18.70	1.40	2.9469	0.2223	0.99683
α	12.05%	1.14%	11.98%	1.13%	19.34	2.44	3.0471	0.3872	0.99657
α	20.96%	1.74%	20.84%	1.73%	19.60	5.20	3.0865	0.8241	0.99609
α+CC	24.67%	2.81%	24.54%	2.79%	21.14	6.92	3.3276	1.0975	0.99557
α+CC	24.93%	5.30%	24.80%	5.26%	21.04	6.99	3.3127	1.1083	0.99558
α+CC	24.43%	15.85%	24.29%	15.75%	19.60	6.33	3.0864	1.0047	0.99591
α+CC	24.98%	16.13%	24.85%	16.03%	19.59	6.52	3.0849	1.0346	0.99588
α+CC	25.04%	30.19%	24.90%	30.04%	20.61	6.88	3.2449	1.0916	0.99566
α+CC	25.27%	46.19%	25.13%	46.01%	20.10	6.80	3.1646	1.0777	0.99576
CC	45.43%	51.55%	45.25%	51.37%	10.67	8.88	1.6815	1.4099	0.99691
CC+βI	80.38%	51.66%	80.26%	51.48%	5.37	22.00	0.8456	3.4884	0.99567
CC+βI	80.66%	70.48%	80.55%	70.33%	5.59	23.29	0.8791	3.6924	0.99543
CC+βI	81.16%	80.43%	81.05%	80.32%	5.04	21.72	0.7938	3.4440	0.99576
CC+βI	81.14%	87.59%	81.03%	87.52%	5.16	22.18	0.8117	3.5177	0.99567
CC+βI	80.27%	97.33%	80.16%	97.32%	5.40	21.95	0.8494	3.4807	0.99567
βI	82.29%	99.42%	82.18%	99.41%	4.84	0.7622	3.5664	0.99567	0.7622
βI	89.33%	99.63%	89.26%	99.62%	2.61	0.4113	3.4682	0.99612	0.4113
βI	94.94%	99.55%	94.90%	99.55%	1.09	0.1713	3.2345	0.99659	0.1713
βI	97.81%	99.85%	97.79%	99.85%	0.45	0.0711	3.1928	0.99674	0.0711
βI	99.08%	99.90%	99.08%	99.90%	0.18	0.0291	3.1728	0.99680	0.0291
AA Form I	100%	100%	100%	100%	0.00	0.0000	3.1493	0.99685	0.0000

Solubility data at 55°C

Solid phase	Liquid	Solid	Liquid	Solid	Conc. of SA	Conc. of AA	X(SA)	A(AA)	X(solvent)
	w% AA in SA	w% AA in SA	mol% AA in SA	mol% AA in SA	mg SA/g solvent	mg AA/g solvent	mmol SA/(mol total)	mmol AA/(mol total)	mol solvent/(mol total)
SA	0.00%	0.00%	0.00%	0.00%	165.95	0.00	25.5686	0.0000	0.97443
α	0.58%	0.57%	0.57%	0.57%	165.65	0.96	25.5196	0.1491	0.97433
α	5.15%	0.95%	5.12%	0.94%	177.14	9.62	27.2046	1.4888	0.97131
α	7.53%	1.11%	7.48%	1.10%	175.56	14.29	26.9493	2.2092	0.97084
α	10.15%	1.16%	10.09%	1.15%	180.47	20.40	27.6565	3.1480	0.96920
α	14.62%	1.56%	14.53%	1.55%	198.61	34.00	30.2888	5.2220	0.96449
α+CC	23.41%	5.88%	23.28%	5.84%	227.64	69.56	34.3753	10.5801	0.95504
α+CC	22.59%	45.70%	22.47%	45.52%	222.18	64.85	33.6026	9.8783	0.95652
CC	25.05%	49.97%	24.92%	49.79%	210.42	70.34	31.8549	10.7241	0.95742
CC	23.79%	48.55%	23.66%	48.37%	224.80	70.17	33.9586	10.6763	0.95537
CC	40.08%	50.17%	39.91%	49.99%	112.30	75.12	17.2441	11.6178	0.97114
CC	51.30%	50.73%	51.12%	50.55%	82.13	86.51	12.6474	13.4172	0.97394
CC	61.71%	53.97%	61.54%	53.79%	65.53	105.61	10.0866	16.3736	0.97354
CC+βIII	76.11%	59.21%	75.98%	59.04%	54.23	172.77	8.2765	26.5557	0.96517
CC+βIII	77.45%	62.48%	77.33%	62.32%	48.96	168.17	7.4827	25.8870	0.96663
CC+βIII	77.55%	67.77%	77.43%	67.62%	52.75	181.81	8.0403	27.9133	0.96405
CC+βIII	73.63%	83.89%	73.49%	83.80%	59.67	166.66	9.1078	25.6185	0.96527
βIII	80.97%	92.72%	80.86%	92.67%	39.83	169.44	6.0946	26.1150	0.96779
βIII	83.40%	93.89%	83.30%	93.84%	33.83	170.13	5.1806	26.2424	0.96858
βIII	82.61%	94.50%	82.50%	94.46%	33.91	161.03	5.2002	24.8733	0.96993
βIII	83.25%	95.14%	83.15%	95.11%	30.92	153.67	4.7503	23.7742	0.97148
βIII	90.23%	96.99%	90.17%	96.97%	16.59	153.27	2.5546	23.7660	0.97368
βIII	94.90%	98.57%	94.87%	98.55%	8.03	149.52	1.2387	23.2292	0.97553
βIII	98.35%	98.64%	98.34%	98.63%	2.45	146.34	0.3786	22.7660	0.97686
βIII	96.81%	98.71%	96.79%	98.70%	4.74	144.06	0.7325	22.4107	0.97686
AA Form III	100%	100%	100%	100%	0.00	143.03	0.0000	22.2707	0.97773