# Supporting information

## Solubilities of Amino Acids in the Presence of Chaotropic Anions

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## SI1 – Solubility data of AAs in pure water

**Table S1.** Summary of the literature solubility data of the amino acids in pure water, studied in this work.

| Amino acid | Solubility of AAs/ g of AA/1000 g of water | Reference | Literature average ± standard deviation |
|---|---|---|---|
| Glycine | 234.350 | [1] | 236.7 ± 3.6 |
| | 235.700 | [2] | |
| | 234.894 | [3] | |
| | 242.026 | [4] | |
| | 238.33 | This work | |
| L-leucine | 21.774 | [5] | 22.4 ± 1.1 |
| | 24.260 | [6] | |
| | 21.600 | [7] | |
| | 21.800 | [8] | |
| | 23.243 | [9] | |
| | 21.520 | [10] | |
| | 21.54 | This work | |
| L-phenylalanine | 28.000 | [8] | 28.4 ± 0.9 |
| | 29.700* | [11] | |
| | 27.800 | [3] | |
| | 27.900 | [7] | |
| | 28.35 | This work | |

*isomer not specified.

## SI2 – Solid phase studies

The identified solid phases are compiled in Erro! Fonte de referência não encontrada. for each of the studied amino acids.

**Table S2.** Cell parameters for the studied amino acids from the supplier determined by single crystal X-ray diffraction and comparison with published data in CCDC Cambridge database.

| Amino acid | Crystal form | CCDC code | Reference |
|---|---|---|---|
| Glycine (used with Na-tosylate) | Monoclinic P (α-glycine) a=5.106(4)Å; b=11.991(7)Å; c=5.452(3)Å; beta=111.53(4)º | 1416373 | Jiang *et al*. [12] |
| Glycine[a] (used with thiocyanates) | Monoclinic P (α-glycine) a=5.10 Å; b=11.99 Å; c=5.45 Å; β= 111.53º | 1416373 | Jiang *et al*. [12] |
| | Hexagonal P (γ-glycine) a=b=7.00 Å; c=5.48 Å | 1416374 | Jiang *et al.* [12] |
| L-Aspartic acid[a] | Monoclinic P a=5.112(7)Å, b=6.921(10)Å; c=7.602(10)Å, beta= 100.38(3)º | 652520 | Bendeif and Jelsch [13] |
| L-Phenylalanine[a] | Monoclinic P a=8.832(9)Å; b=6.064(8)Å; c=31.383(10)Å; beta= 97.36(5)º | 1012155 | Ihlefeldt *et al.* [14] |
| L-Leucine[a] | Monoclinic P A=9.631(4) Å; b=5.340(3) Å; 14.654(6) Å; beta=94.09(3)º | 1508364 | Binns *et al.* [15] |

[a]Data reported in a previous work [16]**.**

The crystal structure of the different amino acids in aqueous solutions of NaSCN, KSCN, and $NH_4SCN$ salts or Na-tosylate were analysed by powder X-ray diffraction and compared with the simulated powder pattern obtained from the published data deposited in CCDC Cambridge database in **Fig. S2**, **S3**, **S4**, and **S6**.

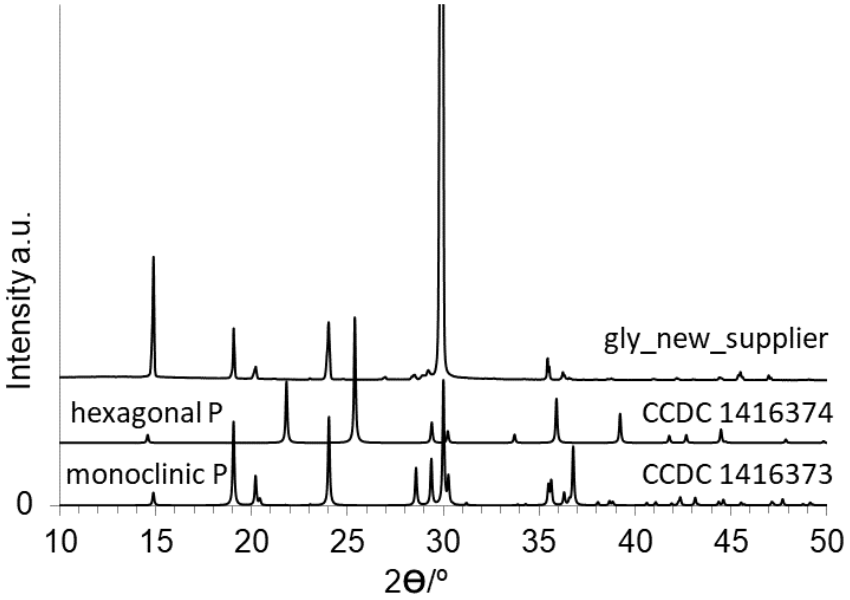


**Fig. S1.** Comparison of the experimental X–ray powder diffraction pattern of the solid phase samples of glycine (used in the solubility experiments with Na-tosylate) from supplier with the powder pattern calculated from the single-crystal X-ray diffraction data CCDC 1416373 (α form) and CCDC 1416374 (γ form).

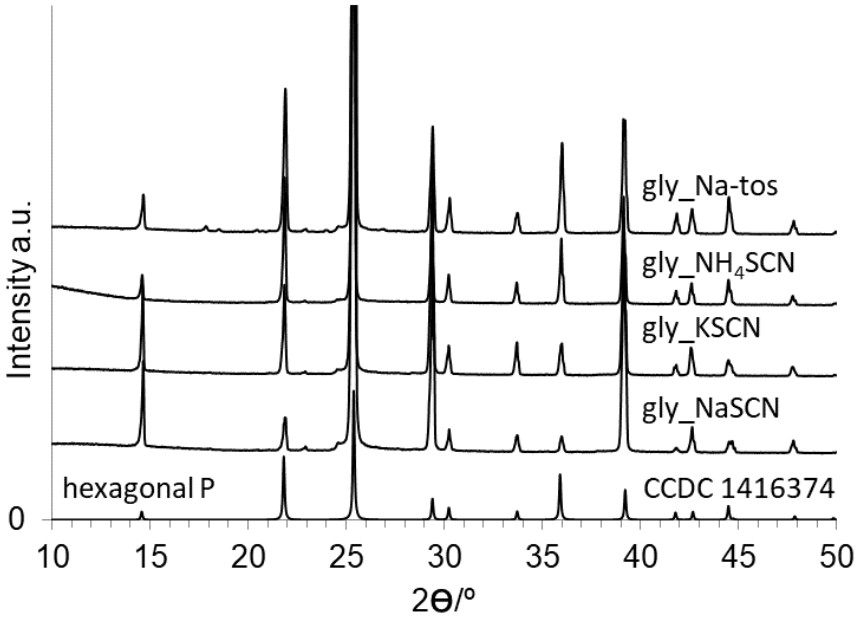


**Fig. S2.** Comparison of the experimental X–ray powder diffraction pattern of the solid phase samples of glycine (filtrated from aqueous solutions of NaSCN, KSCN, and $NH_4SCN$ salts or Na-tosylate) with the powder pattern calculated from the single-crystal X-ray diffraction data 1416374 (γ form).

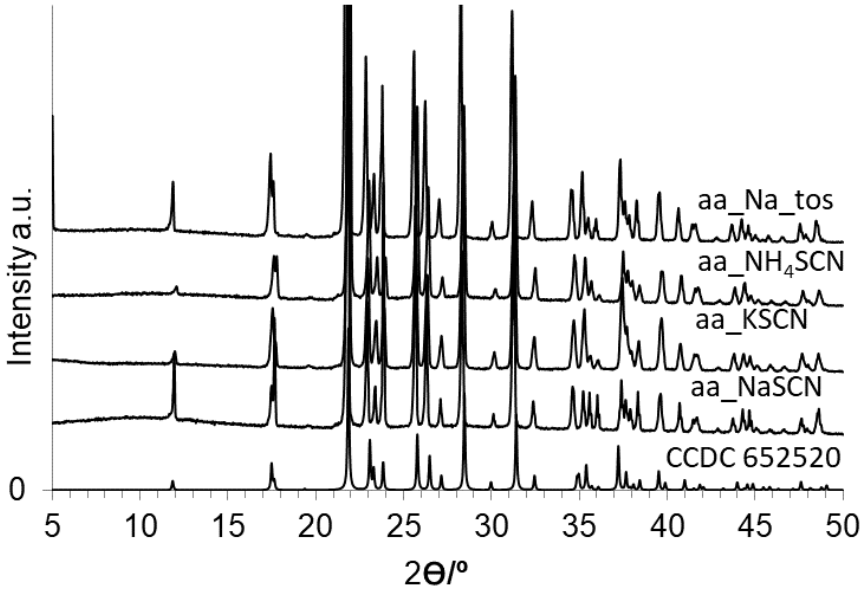


**Fig. S3.** Comparison of the experimental X–ray powder diffraction pattern of the solid phase samples of aspartic acid (filtrated from aqueous solutions of NaSCN, KSCN, and $NH_4SCN$ salts or Na-tosylate) with the powder pattern calculated from the single-crystal X-ray diffraction data CCDC 652520.

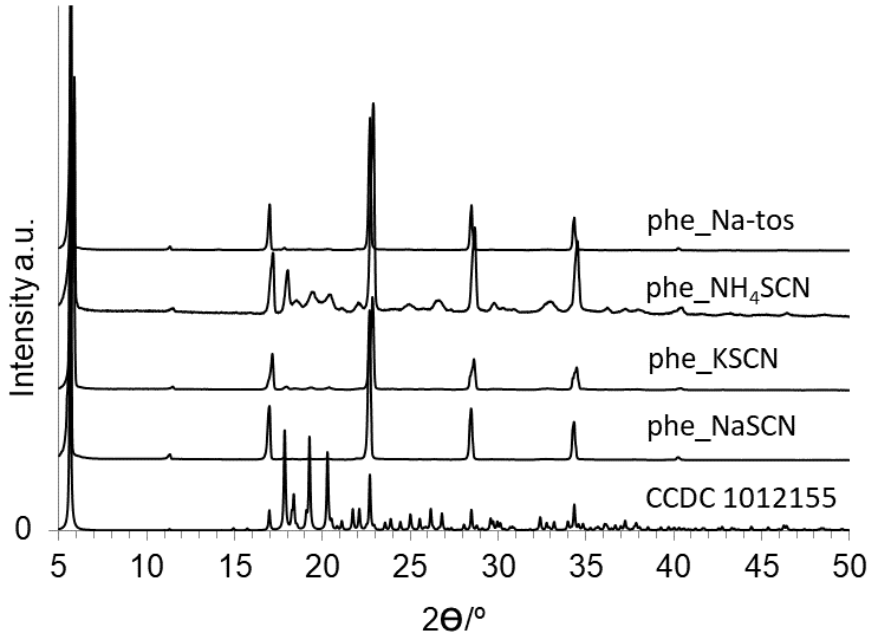


**Fig. S4.** Comparison of the experimental X–ray powder diffraction pattern of the solid phase samples of phenylalanine (filtrated from aqueous solutions of NaSCN, KSCN, and $NH_4SCN$ salts or Na-tosylate at 1.5 molal) with the powder pattern calculated from the single-crystal X-ray diffraction data CCDC 1012155.

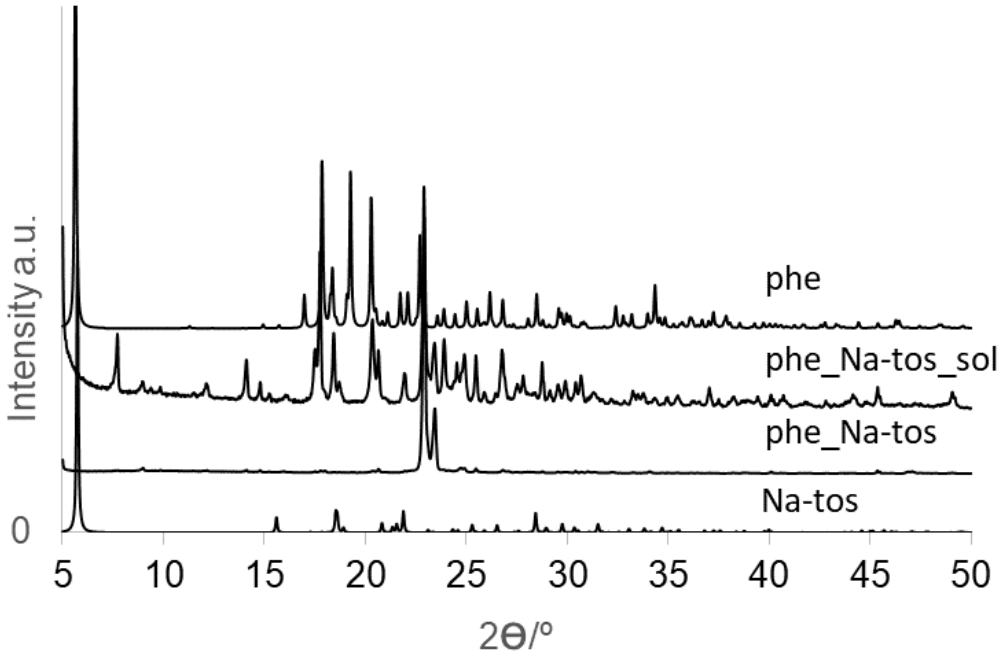


**Fig. S5.** Comparison of the experimental X–ray powder diffraction pattern of the solid phase samples of phenylalanine (filtrated from aqueous solutions of Na-tosylate at 2 molal) with the powder pattern calculated from the single-crystal X-ray diffraction data CCDC 1012155.

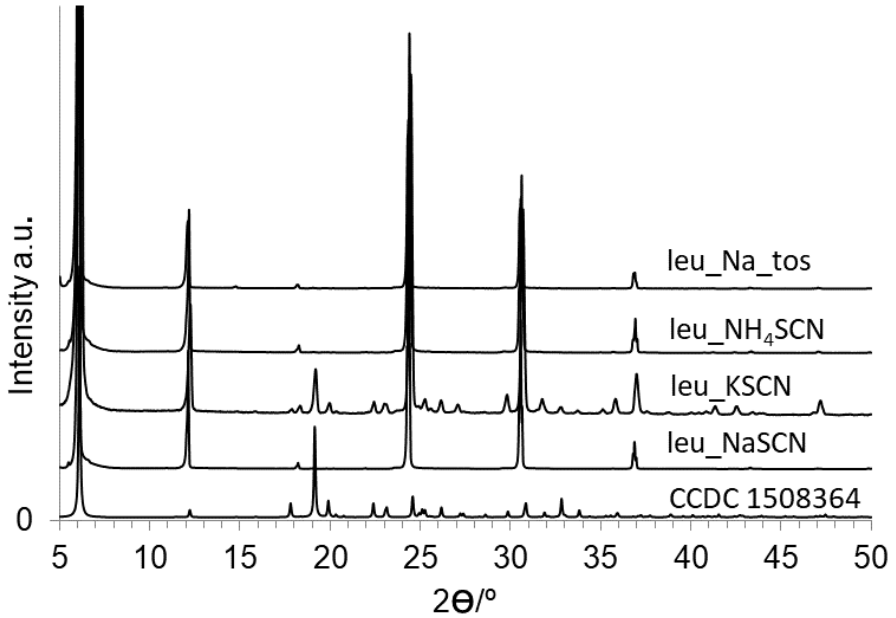


**Fig. S6.** Comparison of the experimental X–ray powder diffraction pattern of the solid phase samples of leucine (filtrated from aqueous solutions of NaSCN, KSCN, and $NH_4SCN$ salts or Na-tosylate) with the powder pattern calculated from the single-crystal X-ray diffraction data CCDC 1508364.

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