

SOLUBILITY OF AMINO ACIDS IN THE EUTECTIC SOLVENT CONSTITUTED BY SODIUM ACETATE TRIHYDRATE AND UREA AND ITS AQUEOUS FORMULATION

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SUPPLEMENTARY MATERIALS

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Table S1. Solubilities (mole fraction) of different amino acids in the eutectic solvent and in its mixture with water, 50:50 (wt:wt), at different temperatures and 0.1 MPa.

| T (K) | Glycine | β -Alanine | L-Proline | <i>Eutectic</i> | | | |
|-------------------------------------|---------|------------------|-----------|---------------------------|--------------|------------|-----------|
| | | | | trans-4-Hydroxy-L-proline | L-Lysine-HCl | L-Arginine | L-Cystine |
| 308.15 | 0.1411 | 0.2223 | 0.1590 | 0.1182 | 0.0850 | 0.0910 | 0.0007 |
| 318.15 | 0.1557 | 0.2497 | 0.1980 | 0.1266 | 0.0942 | 0.1053 | 0.0018 |
| 328.15 | 0.1682 | 0.2887 | 0.2395 | 0.1422 | 0.1064 | 0.1212 | 0.0043 |
| 338.15 | 0.1812 | 0.3312 | 0.3037 | 0.1600 | 0.1181 | 0.1452 | 0.0098 |
| <i>Eutectic:water 50:50 (wt:wt)</i> | | | | | | | |
| T (K) | Glycine | β -Alanine | L-Proline | trans-4-Hydroxy-L-proline | L-Lysine-HCl | L-Arginine | L-Cystine |
| 298.15 | 0.0581 | 0.1371 | 0.2813 | 0.0515 | 0.1050 | 0.0214 | 0.0005 |
| 308.15 | 0.0743 | 0.1508 | 0.2952 | 0.0578 | 0.1205 | 0.0317 | 0.0013 |
| 318.15 | 0.0935 | 0.1714 | 0.3181 | 0.0707 | 0.1376 | 0.0501 | 0.0039 |
| 328.15 | 0.1112 | 0.1966 | 0.3401 | 0.0801 | 0.1574 | 0.0793 | 0.0073 |

Table S2. Sources and purities of amino acids used in this work.

| Amino acid | Source | Purity (wt%) |
|----------------------------|---------------|--------------|
| Glycine | Sigma-Aldrich | >99.0 |
| β -Alanine | Sigma-Aldrich | >99.0 |
| L-Proline | Panreac | >99.0 |
| trans-4-Hydroxy-L-proline | Sigma-Aldrich | >99.0 |
| L-Lysine monohydrochloride | Sigma-Aldrich | >99.5 |
| L-Arginine | Sigma-Aldrich | >98.0 |
| L-Cystine | Sigma-Aldrich | >98.0 |

Table S3. Experimental data used for calibration curves of glycine.

| <i>Eutectic</i> | | <i>Eutectic:water 50:50 (wt:wt)</i> | |
|------------------------------|--------------------------------------|-------------------------------------|---|
| mass fraction of glycine (w) | refractive index (308.15 K, 0.1 MPa) | mass fraction of glycine (w) | density (g·cm ⁻³) (298.15 K, 0.1 MPa) |
| 0.0000 | 1.44599 | 0.0000 | 1.150100 |
| 0.0202 | 1.44814 | 0.0249 | 1.157460 |
| 0.0399 | 1.44988 | 0.0508 | 1.165090 |
| 0.0601 | 1.45175 | 0.0751 | 1.172140 |
| 0.0798 | 1.45351 | 0.1000 | 1.179150 |
| 0.0996 | 1.45544 | 0.1249 | 1.186430 |

u(T)=0.01 K. u(P)=5 kPa. u(w)=0.0002. u(n_0)=0.0001 u(ρ)=0.0001

$$\text{Refractive index} = 0.0936 \cdot x + 1.4461 \quad (\text{S.1})$$

$$R^2 = 0.9988$$

$$\text{Density} = 0.2903 \cdot x + 1.1503 \quad (\text{S.2})$$

$$R^2 = 0.9998$$

Table S4. Experimental data used for calibration curves of β-alanine.

| <i>Eutectic</i> | | <i>Eutectic:water 50:50 (wt:wt)</i> | |
|--------------------------------|---|-------------------------------------|--|
| mass fraction of β-alanine (w) | refractive index (308.15 K, 0.1 MPa) | mass fraction of β-alanine (w) | density (g·cm ⁻³) (298.15 K, 0.1 MPa) |
| 0.0000 | 1.44600 | 0.0000 | 1.150104 |
| 0.0302 | 1.44875 | 0.0500 | 1.160782 |
| 0.0600 | 1.45145 | 0.1001 | 1.170575 |
| 0.0916 | 1.45409 | 0.1500 | 1.180568 |
| 0.1202 | 1.45637 | 0.2002 | 1.190214 |
| 0.1498 | 1.45906 | 0.2500 | 1.199625 |

u(T)=0.01 K. u(P)=5 kPa. u(w)=0.0002. u(n_D)=0.0001 u(ρ)=0.0003

$$\text{Refractive index} = 0.0864 \cdot x + 1.4461 \quad (\text{S.3})$$

$$R^2 = 0.9991$$

$$\text{Density} = 0.1976 \cdot x + 1.1506 \quad (\text{S.4})$$

$$R^2 = 0.9996$$

Table S5. Experimental data used for calibration curves of L-proline.

| <i>Eutectic</i> | | <i>Eutectic:water 50:50 (wt:wt)</i> | |
|--------------------------------|---|-------------------------------------|--|
| mass fraction of L-proline (w) | refractive index (308.15 K, 0.1 MPa) | mass fraction of L-proline (w) | density (g·cm ⁻³) (298.15 K, 0.1 MPa) |
| 0.0301 | 1.44841 | 0.0000 | 1.150104 |
| 0.0604 | 1.45110 | 0.1010 | 1.165964 |
| 0.0902 | 1.45360 | 0.1996 | 1.181118 |
| 0.1200 | 1.45632 | 0.3005 | 1.196699 |
| 0.1508 | 1.45891 | 0.4015 | 1.211770 |
| 0.1791 | 1.46152 | 0.4976 | 1.226005 |

u(T)=0.01 K. u(P)=5 kPa. u(w)=0.0002. u(n_D)=0.00006 u(ρ)=0.0003

$$\text{Refractive index} = 0.0877 \cdot x + 1.4458 \quad (\text{S.5})$$

$$R^2 = 0.9962$$

$$\text{Density} = 0.1526 \cdot x + 1.1505 \quad (\text{S.6})$$

$$R^2 = 0.9999$$

Table S6. Experimental data used for calibration curves of trans-4-Hydroxy-L-proline.

| Eutectic | | Eutectic:water 50:50 (wt:wt) | |
|---|---|---|--|
| mass fraction of trans-4-Hydroxy-L-proline (w) | refractive index (308.15 K, 0.1 MPa) | mass fraction of trans-4-Hydroxy-L-proline (w) | density (g·cm ⁻³) (298.15 K, 0.1 MPa) |
| 0.0000 | 1.44579 | 0.0000 | 1.150251 |
| 0.0265 | 1.44854 | 0.0501 | 1.162772 |
| 0.0500 | 1.45077 | 0.0999 | 1.175436 |
| 0.0768 | 1.45342 | 0.1492 | 1.187954 |
| 0.1012 | 1.45571 | 0.1994 | 1.199934 |
| 0.1254 | 1.45800 | 0.2501 | 1.212897 |

u(T)=0.01 K. u(P)=5 kPa. u(w)=0.0002. u(n_D)=0.00007 u(ρ)=0.0002

$$\text{Refractive index} = 0.0971 \cdot x + 1.4459 \quad (\text{S.7})$$

$$R^2 = 0.9998$$

$$\text{Density} = 0.2502 \cdot x + 1.1503 \quad (\text{S.8})$$

$$R^2 = 0.9999$$

Table S7. Experimental data used for calibration curves of L-lysine·HCl.

| Eutectic | | Eutectic:water 50:50 (wt:wt) | |
|-------------------------------|---|-------------------------------------|--|
| mass fraction of L-lysine (w) | refractive index (308.15 K, 0.1 MPa) | mass fraction of L-lysine (w) | density (g·cm ⁻³) (298.15 K, 0.1 MPa) |
| 0.0000 | 1.44579 | 0.0000 | 1.150251 |
| 0.0203 | 1.44817 | 0.0512 | 1.158801 |
| 0.0402 | 1.45034 | 0.1000 | 1.166958 |
| 0.0600 | 1.45262 | 0.1495 | 1.175155 |
| 0.0801 | 1.45488 | 0.1999 | 1.183417 |
| 0.1002 | 1.45713 | 0.2495 | 1.191512 |

u(T)=0.01 K. u(P)=5 kPa. u(w)=0.0002. u(n_D)=0.0001 u(ρ)=0.0001

$$\text{Refractive index} = 0.1132 \cdot x + 1.4459 \quad (\text{S.9})$$

$$R^2 = 0.9999$$

$$\text{Density} = 0.1660 \cdot x + 1.1503 \quad (\text{S.10})$$

$$R^2 = 1.0000$$

Table S8. Experimental data used for calibration curves of L-arginine.

| <i>Eutectic</i> | | <i>Eutectic:water 50:50 (wt:wt)</i> | |
|---------------------------------|---|-------------------------------------|--|
| mass fraction of L-arginine (w) | refractive index (308.15 K, 0.1 MPa) | mass fraction of L-arginine (w) | density (g·cm ⁻³) (298.15 K, 0.1 MPa) |
| 0.0000 | 1.44576 | 0.0000 | 1.150978 |
| 0.0203 | 1.44837 | 0.0252 | 1.154937 |
| 0.0400 | 1.45068 | 0.0505 | 1.159018 |
| 0.0600 | 1.45300 | 0.0757 | 1.162995 |
| 0.0801 | 1.45519 | 0.1003 | 1.167040 |
| 0.1001 | 1.45766 | 0.1251 | 1.170880 |

u(T)=0.01 K. u(P)=5 kPa. u(w)=0.0002. u(n_D)=0.0001 u(ρ)=0.00006

$$\text{Refractive index} = 0.1176 \cdot x + 1.4459 \quad (\text{S.11})$$

$$R^2 = 0.9997$$

$$\text{Density} = 0.1599 \cdot x + 1.1509 \quad (\text{S.12})$$

$$R^2 = 0.9999$$

Table S9. Experimental data used for calibration curves of L-cystine.

| <i>Eutectic</i> | | <i>Eutectic:water 50:50 (wt:wt)</i> | |
|--------------------------------|---|-------------------------------------|--|
| mass fraction of L-cystine (w) | refractive index (338.15 K, 0.1 MPa) | mass fraction of L-cystine (w) | density (g·cm ⁻³) (328.15 K, 0.1 MPa) |
| 0.0000 | 1.43923 | 0.0000 | 1.132343 |
| 0.0039 | 1.43996 | 0.0040 | 1.133966 |
| 0.0064 | 1.44041 | 0.0080 | 1.135490 |
| 0.0086 | 1.44084 | 0.0120 | 1.137244 |
| 0.0121 | 1.44146 | 0.0160 | 1.138934 |

u(T)=0.01 K. u(P)=5 kPa. u(w)=0.0002. u(n_D)=0.00003 u(ρ)=0.00005

$$\text{Refractive index} = 0.1858 \cdot x + 1.4392 \quad (\text{S.13})$$

$$R^2 = 0.9999$$

$$\text{Density} = 0.4111 \cdot x + 1.1323 \quad (\text{S.14})$$

$$R^2 = 0.9997$$