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

The role of urea in formation of the sodium acetate trihydrate (SAT)–urea eutectic liquid: a neutron diffraction and isotopic substitution study.

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Component Centre of Mass and Water Partial Radial Distribution Functions

Centre of mass radial distribution functions (COM RDFs) calculated from EPSR for pairs of components (sodium, acetate, water, and urea) are shown in Fig. S1 grouped by the central species. The first shell around sodium contains water, acetate and urea with first maxima in the RDFs (r_{max}) at 2.6, 3.2, and 3.5 Å respectively with the sodium–acetate correlation being most pronounced. There is also a notable sodium–sodium correlation peak at 3.72 Å. In addition to the strong correlation to sodium, the acetate COM shows association with both water (r_{max} = 3.6 Å), urea (r_{max} = 4.4 Å) and acetate (r_{max} = 5.0 Å) which is approximately twice the sodium–acetate correlation first peak position and corresponds to second shell associations through sodium ions. Water shows similar sharply defined water–sodium and water–water correlations with r_{max} at 2.6 and 2.8 Å respectively, and water–acetate and water–urea maxima at longer distances of 3.5 and 3.8 Å. Urea exhibits correlations with sodium, water, acetate, and other ureas with r_{max} at 3.5, 3.7, 4.5, and 4.6 Å respectively. Hence it is evident that there are significant correlations between all the components present in the SAT/urea liquid.

Partial distribution functions (pRDFs) between Hw and Ow sites in water molecules in the SAT–urea melt are shown in Fig. S2.

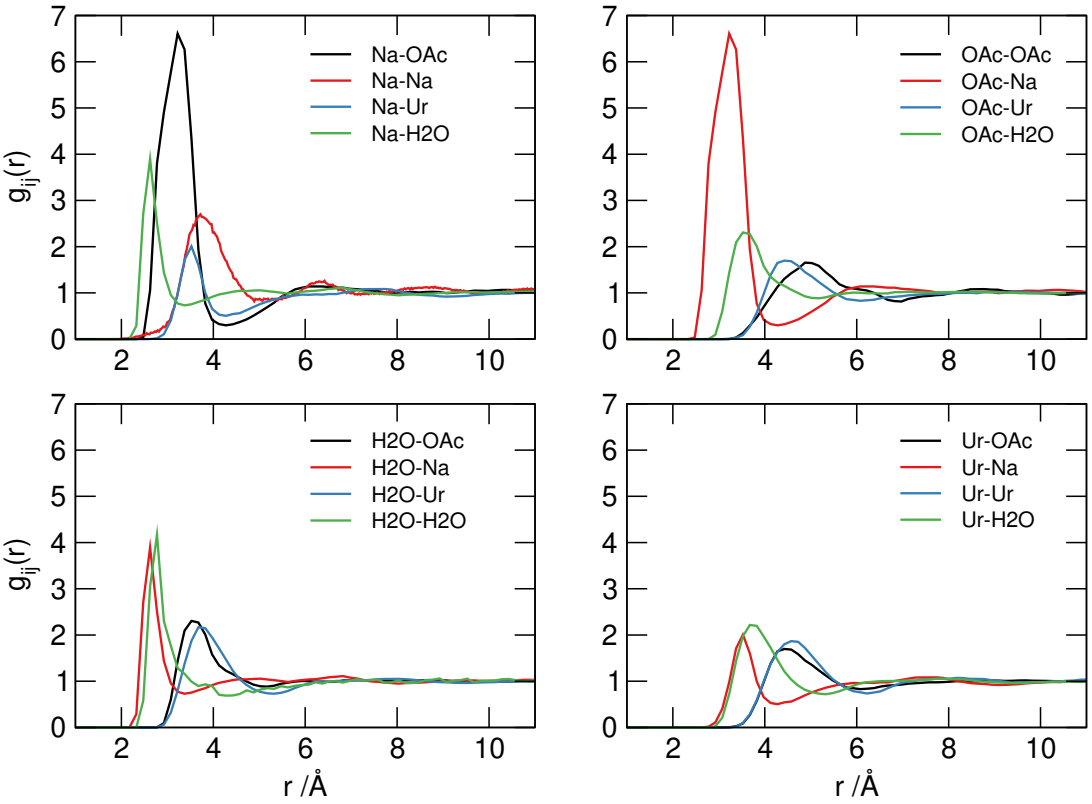

Fig. S1 Centre of mass RDFs between all components in the simulation centred around sodium (*top left*), acetate (*top right*), water (*bottom left*) and urea (*bottom right*).

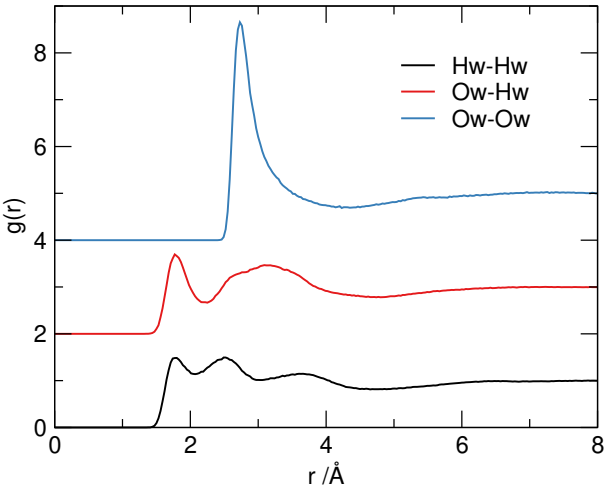

Fig. S2 Water pair correlations from the epsr model of SAT/urea. The curves are offset for clarity.

Table S1 Probability distributions of coordination numbers between Ow, OA, and OU with Na within the first coordination between 1–3.3 Å, in the EPSR model of the SAT—urea eutectic.

Coord. number	**Probability**		
	Na–OA	Na–OU	Na–Ow
0	0.0072	0.4389	0.1007
1	0.0396	0.3489	0.3992
2	0.2086	0.1439	0.2770
3	0.3201	0.0576	0.1655
4	0.2662	0.0108	0.0396
5	0.1115	0.0000	0.0180
6	0.0396	0.0000	0.0000
7	0.0072	0.0000	0.0000
8	0.0000	0.0000	0.0000

Gudrun Processing Script

```
INSTRUMENT          {
SANDALS      Instrument name
/home/jh7454/SAT+urea/Gudrun/          Gudrun input file directory:
/archive/cycle_21_1/NDXSANDALS/          Data file directory
raw          Data file type
StartupFiles/SLS/SANDALSJune2015Detector.calib          Detector calibration file name
4            User table column number for phi values
StartupFiles/SLS/groups_18.dat          Groups file name
StartupFiles/SLS/SLSdeadtime.cor          Deadtime constants file name
1 3          Spectrum number(s) for incident beam monitor
0  0         Wavelength range [Å] for monitor normalisation
2            Spectrum number(s) for transmission monitor
0.0006       Incident monitor quiet count constant
0.0006       Transmission monitor quiet count constant
0  0         Channel numbers for spike analysis
5            Spike analysis acceptance factor
0.05  4.95  0.1 Wavelength range to use [Å] and step size
100          No. of smooths on monitor
0.1  50.0  0.05 Min, Max and step in x-scale (-ve for logarithmic binning)
0  0  0  0   0 0 0 0 to end input of specified values
1.0          Groups acceptance factor
4            Merge power
1            Subtract single atom scattering?
2            By channel?
11.016       Incident flight path [m]
0            Spectrum number to output diagnostic files
StartupFiles/SLS/sears91_gudrun.dat          Neutron scattering parameters file
1            Scale selection: 1 = Q, 2 = d-space, 3 = wavelength, 4 = energy, 5 = TOF
1            Subtract wavelength-binned data?
/opt/gudrun/Gudrun          Folder where Gudrun started
/opt/gudrun/Gudrun/StartupFiles/SLS          Folder containing the startup file
0.1          Logarithmic step size
1            Hard group edges?
1            Number of iterations
0            Tweak the tweak factor(s)?
}

BEAM          {
FLATPLATE    Sample geometry
2            Number of beam profile values
1.0  1.0     Beam profile values (Maximum of 50 allowed currently)
0.05  0.2  100  Step size for absorption and m.s. calculation and no. of slices
10           Angular step for corrections [deg.]
-1.5  1.5  -1.5  1.5          Incident beam edges relative to centre of sample [cm]
-2.0  2.0  -2.1  2.1          Scattered beam edges relative to centre of sample [cm]
StartupFiles/SLS/spectrum000.dat          Filename containing incident beam spectrum par
1.0          Overall background factor
0.0          Sample dependent background factor
0.0          Shielding attenuation coefficient [per m per A]
}
```

```
NORMALISATION          {
2  1          Number of  files and period number
SLS71262.raw NORMALISATION data files
SLS71291.raw NORMALISATION data files
2  1          Number of  files and period number
SLS71263.raw NORMALISATION BACKGROUND data files
SLS71292.raw NORMALISATION BACKGROUND data files
1             Force calculation of corrections?
V  0  94.85   Normalisation atomic composition
Nb  0  5.15   Normalisation atomic composition
*  0  0       * 0 0 to specify end of composition input
SameAsBeam    Geometry
0.15  0.15    Upstream and downstream thicknesses [cm]
0  5          Angle of rotation and sample width (cm)
-0.071        Density atoms/Å^3?
300           Temperature for normalisation Placzek correction
TABLES        Total cross section source
*             Normalisation differential cross section filename
0.01          Lower limit on smoothed normalisation
1.05          Normalisation degree of smoothing
0.0           Minimum normalisation signal to background ratio
}

SAMPLE BACKGROUND          {
2  1          Number of  files and period number
SLS71263.raw SAMPLE BACKGROUND data files
SLS71292.raw SAMPLE BACKGROUND data files
}

SAMPLE S3 1mm TiZr flat plate cell          {
2  1          Number of  files and period number
SLS71264.raw SAMPLE S3 1mm TiZr flat plate cell data files
SLS71265.raw SAMPLE S3 1mm TiZr flat plate cell data files
1             Force calculation of sample corrections?
Ti  0  7.16   Composition
Zr  0  3.438  Composition
*  0  0       * 0 0 to specify end of composition input
SameAsBeam    Geometry
0.1  0.1      Upstream and downstream thicknesses [cm]
0  5          Angle of rotation and sample width (cm)
-0.0542       Density atoms/Å^3?
0             Temperature for Placzek correction:
TABLES        Total cross section source
1.0           Tweak factor
0             Top hat width (1/Å) for cleaning up Fourier Transform
0.0           Minimum radius for FT  [Å]
0.1           g(r) broadening at r = 1A [A]
0  0          0   0 to finish specifying wavelength range of resonance
0.0  1.0  0   Exponential amplitude and decay [1/A]
*  0  0       * 0 0 to specify end of exponential parameter input
1.0           Normalisation correction factor
SLS71264.msubw01          Name of file containing self scattering as a function of wavel
```

```
0           Normalise to:Nothing
20.0        Maximum radius for FT [A]
0           Output units: b/atom/sr
0.2         Power for broadening function e.g. 0.5
0.03        Step size [A]
0           Analyse this sample?
1.0  0.0    Sample environment scattering fraction and attenuation coefficient [per A]
}

GO

SAMPLE S4 1mm TiZr flat plate cell          {
2  1         Number of  files and period number
SLS71266.raw SAMPLE S4 1mm TiZr flat plate cell data files
SLS71269.raw SAMPLE S4 1mm TiZr flat plate cell data files
1           Force calculation of sample corrections?
Ti  0  7.16  Composition
Zr  0  3.438 Composition
*  0  0      * 0 0 to specify end of composition input
SameAsBeam   Geometry
0.1  0.1     Upstream and downstream thicknesses [cm]
0  5         Angle of rotation and sample width (cm)
-0.0542      Density atoms/Å^3?
0           Temperature for Placzek correction:
TABLES       Total cross section source
1.0          Tweak factor
0           Top hat width (1/Å) for cleaning up Fourier Transform
0.0          Minimum radius for FT  [Å]
0.1          g(r) broadening at r = 1A [A]
0  0         0   0 to finish specifying wavelength range of resonance
0.0  1.0  0  Exponential amplitude and decay [1/A]
*  0  0      * 0 0 to specify end of exponential parameter input
1.0          Normalisation correction factor
SLS71266.msubw01          Name of file containing self scattering as a function of wavel
0           Normalise to:Nothing
20.0         Maximum radius for FT [A]
0           Output units: b/atom/sr
0.2          Power for broadening function e.g. 0.5
0.03         Step size [A]
0           Analyse this sample?
1.0  0.0     Sample environment scattering fraction and attenuation coefficient [per A]
}

GO

SAMPLE S5 1mm TiZr flat plate cell          {
2  1          Number of  files and period number
SLS71267.raw  SAMPLE S5 1mm TiZr flat plate cell data files
SLS71270.raw  SAMPLE S5 1mm TiZr flat plate cell data files
1             Force calculation of sample corrections?
Ti  0  7.16   Composition
Zr  0  3.438  Composition
```

```
*  0  0       * 0 0 to specify end of composition input
SameAsBeam    Geometry
0.1  0.1      Upstream and downstream thicknesses [cm]
0  5          Angle of rotation and sample width (cm)
-0.0542       Density atoms/Å^3?
0             Temperature for Placzek correction:
TABLES        Total cross section source
1.0           Tweak factor
0             Top hat width (1/Å) for cleaning up Fourier Transform
0.0           Minimum radius for FT  [Å]
0.1           g(r) broadening at r = 1A [A]
0  0          0   0          to finish specifying wavelength range of resonance
0.0  1.0  0   Exponential amplitude and decay [1/A]
*  0  0       * 0 0 to specify end of exponential parameter input
1.0           Normalisation correction factor
SLS71267.msubw01          Name of file containing self scattering as a function of wavel
0             Normalise to:Nothing
20.0          Maximum radius for FT [A]
0             Output units: b/atom/sr
0.2           Power for broadening function e.g. 0.5
0.03          Step size [A]
0             Analyse this sample?
1.0  0.0      Sample environment scattering fraction and attenuation coefficient [per A]
}

GO

SAMPLE S6 1mm TiZr flat plate cell          {
2  1          Number of  files and period number
SLS71268.raw  SAMPLE S6 1mm TiZr flat plate cell data files
SLS71271.raw  SAMPLE S6 1mm TiZr flat plate cell data files
1             Force calculation of sample corrections?
Ti  0  7.16   Composition
Zr  0  3.438  Composition
*  0  0       * 0 0 to specify end of composition input
SameAsBeam    Geometry
0.1  0.1      Upstream and downstream thicknesses [cm]
0  5          Angle of rotation and sample width (cm)
-0.0542       Density atoms/Å^3?
0             Temperature for Placzek correction:
TABLES        Total cross section source
1.0           Tweak factor
0             Top hat width (1/Å) for cleaning up Fourier Transform
0.0           Minimum radius for FT  [Å]
0.1           g(r) broadening at r = 1A [A]
0  0          0   0          to finish specifying wavelength range of resonance
0.0  1.0  0   Exponential amplitude and decay [1/A]
*  0  0       * 0 0 to specify end of exponential parameter input
1.0           Normalisation correction factor
SLS71268.msubw01          Name of file containing self scattering as a function of wavel
0             Normalise to:Nothing
20.0          Maximum radius for FT [A]
```

```
0             Output units: b/atom/sr
0.2           Power for broadening function e.g. 0.5
0.03          Step size [A]
0             Analyse this sample?
1.0  0.0      Sample environment scattering fraction and attenuation coefficient [per A]
}

GO

SAMPLE S7 1mm TiZr flat plate cell          {
2  1          Number of  files and period number
SLS71272.raw   SAMPLE S7 1mm TiZr flat plate cell data files
SLS71273.raw   SAMPLE S7 1mm TiZr flat plate cell data files
1             Force calculation of sample corrections?
Ti  0  7.16    Composition
Zr  0  3.438   Composition
*  0  0        * 0 0 to specify end of composition input
SameAsBeam     Geometry
0.1  0.1       Upstream and downstream thicknesses [cm]
0  5           Angle of rotation and sample width (cm)
-0.0542        Density atoms/Å^3?
0             Temperature for Placzek correction:
TABLES         Total cross section source
1.0           Tweak factor
0             Top hat width (1/Å) for cleaning up Fourier Transform
0.0           Minimum radius for FT  [Å]
0.1           g(r) broadening at r = 1A [A]
0  0          0   0          to finish specifying wavelength range of resonance
0.0  1.0  0    Exponential amplitude and decay [1/A]
*  0  0        * 0 0 to specify end of exponential parameter input
1.0           Normalisation correction factor
SLS71272.msubw01          Name of file containing self scattering as a function of wavel
0             Normalise to:Nothing
20.0          Maximum radius for FT [A]
0             Output units: b/atom/sr
0.2           Power for broadening function e.g. 0.5
0.03          Step size [A]
0             Analyse this sample?
1.0  0.0       Sample environment scattering fraction and attenuation coefficient [per A
}

GO

SAMPLE S8 1mm TiZr flat plate cell          {
2  1          Number of  files and period number
SLS71287.raw   SAMPLE S8 1mm TiZr flat plate cell data files
SLS71289.raw   SAMPLE S8 1mm TiZr flat plate cell data files
1             Force calculation of sample corrections?
Ti  0  7.16    Composition
Zr  0  3.438   Composition
*  0  0        * 0 0 to specify end of composition input
SameAsBeam     Geometry
```

```
0.1  0.1       Upstream and downstream thicknesses [cm]
0  5           Angle of rotation and sample width (cm)
-0.0542        Density atoms/Å^3?
0              Temperature for Placzek correction:
TABLES         Total cross section source
1.0            Tweak factor
0              Top hat width (1/Å) for cleaning up Fourier Transform
0.0            Minimum radius for FT  [Å]
0.1            g(r) broadening at r = 1A [A]
0  0           0   0          to finish specifying wavelength range of resonance
0.0  1.0  0    Exponential amplitude and decay [1/A]
*  0  0        * 0 0 to specify end of exponential parameter input
1.0            Normalisation correction factor
SLS71287.msubw01          Name of file containing self scattering as a function of wavel
0              Normalise to:Nothing
20.0           Maximum radius for FT [A]
0              Output units: b/atom/sr
0.2            Power for broadening function e.g. 0.5
0.03           Step size [A]
0              Analyse this sample?
1.0  0.0       Sample environment scattering fraction and attenuation coefficient [per A
}

GO

SAMPLE T9 1mm TiZr flat plate cell          {
2  1           Number of  files and period number
SLS71288.raw   SAMPLE T9 1mm TiZr flat plate cell data files
SLS71290.raw   SAMPLE T9 1mm TiZr flat plate cell data files
1              Force calculation of sample corrections?
Ti  0  7.16    Sample atomic composition
Zr  0  3.438   Sample atomic composition
*  0  0        * 0 0 to specify end of composition input
SameAsBeam     Geometry
0.1  0.1       Upstream and downstream thicknesses [cm]
0  5           Angle of rotation and sample width (cm)
-0.0542        Density atoms/Å^3?
0              Temperature for sample Placzek correction
TABLES          Total cross section source
1.0            Sample tweak factor
0              Top hat width (1/Å) for cleaning up Fourier Transform
0.0            Minimum radius for FT  [Å]
0.1            g(r) broadening at r = 1A [A]
0  0           0   0          to finish specifying wavelength range of resonance
0.0  1.0  0    Exponential amplitude and decay [1/A]
*  0  0        * 0 0 to specify end of exponential parameter input
1.0            Normalisation correction factor
SLS71288.msubw01          Name of file containing self scattering as a function of wavel
0              Normalise to:Nothing
20.0           Maximum radius for FT [A]
0              Output units: b/atom/sr
0.2            Power for broadening function e.g. 0.5
```

```
0.03           Step size [A]
0              Analyse this sample?
1.0  0.0       Sample environment scattering fraction and attenuation coefficient [per A
}

GO

SAMPLE Sample 3 SAT-urea D-H-H can S3 50C          {
3  1           Number of  files and period number
SLS71279.raw    SAMPLE Sample 3 SAT-urea D-H-H can S3 50C data files
SLS71283.raw    SAMPLE Sample 3 SAT-urea D-H-H can S3 50C data files
SLS71293.raw    SAMPLE Sample 3 SAT-urea D-H-H can S3 50C data files
1               Force calculation of sample corrections?
Na  0  0.4      Sample atomic composition
C  0  0.8       Sample atomic composition
H  0  0.0       Sample atomic composition
H  2  1.2       Sample atomic composition
O  0  0.8       Sample atomic composition
N  0  1.2       Sample atomic composition
O  0  0.6       Sample atomic composition
C  0  0.6       Sample atomic composition
H  0  1.2       Sample atomic composition
H  2  1.2       Sample atomic composition
O  0  1.2       Sample atomic composition
H  0  2.4       Sample atomic composition
H  2  0.0       Sample atomic composition
*  0  0         * 0 0 to specify end of composition input
SameAsBeam      Geometry
0.05  0.05      Upstream and downstream thicknesses [cm]
0  5            Angle of rotation and sample width (cm)
-0.0998         Density atoms/Å^3?
0               Temperature for sample Placzek correction
TABLES          Total cross section source
1.0             Sample tweak factor
-10             Top hat width (1/Å) for cleaning up Fourier Transform
.5              Minimum radius for FT  [Å]
0.1             g(r) broadening at r = 1A [A]
0  0            0   0          to finish specifying wavelength range of resonance
0.0  1.0  0     Exponential amplitude and decay [1/A]
*  0  0         * 0 0 to specify end of exponential parameter input
1.0             Normalisation correction factor
SLS71279.msubw01          Name of file containing self scattering as a function of wavel
0               Normalise to:Nothing
20.0            Maximum radius for FT [A]
0               Output units: b/atom/sr
0.2             Power for broadening function e.g. 0.5
0.03            Step size [A]
0               Analyse this sample?
1.0  0.0        Sample environment scattering fraction and attenuation coefficient [per
}

CONTAINER S3 1mm TiZr flat plate cell          {
```

```
2  1            Number of  files and period number
SLS71264.raw    CONTAINER S3 1mm TiZr flat plate cell data files
SLS71265.raw    CONTAINER S3 1mm TiZr flat plate cell data files
Ti  0  7.16     Composition
Zr  0  3.438    Composition
*  0  0         * 0 0 to specify end of composition input
SameAsBeam      Geometry
0.1  0.1        Upstream and downstream thicknesses [cm]
0  5            Angle of rotation and sample width (cm)
-0.0542         Density atoms/Å^3?
TABLES          Total cross section source
1.0             Tweak factor
1.0  0.0        Sample environment scattering fraction and attenuation coefficient [per
}

GO

SAMPLE Sample 4 SAT-urea H/D-H/D-H/D can S4 50C          {
3  1            Number of  files and period number
SLS71280.raw    SAMPLE Sample 4 SAT-urea H/D-H/D-H/D can S4 50C data files
SLS71284.raw    SAMPLE Sample 4 SAT-urea H/D-H/D-H/D can S4 50C data files
SLS71294.raw    SAMPLE Sample 4 SAT-urea H/D-H/D-H/D can S4 50C data files
1               Force calculation of sample corrections?
Na  0  0.4      Sample atomic composition
C  0  0.8       Sample atomic composition
H  0  0.6       Sample atomic composition
H  2  0.6       Sample atomic composition
O  0  0.8       Sample atomic composition
N  0  1.2       Sample atomic composition
O  0  0.6       Sample atomic composition
C  0  0.6       Sample atomic composition
H  0  1.2       Sample atomic composition
H  2  1.2       Sample atomic composition
O  0  1.2       Sample atomic composition
H  0  1.2       Sample atomic composition
H  2  1.2       Sample atomic composition
*  0  0         * 0 0 to specify end of composition input
SameAsBeam      Geometry
0.05  0.05      Upstream and downstream thicknesses [cm]
0  5            Angle of rotation and sample width (cm)
-0.0995         Density atoms/Å^3?
0               Temperature for sample Placzek correction
TABLES          Total cross section source
1.0             Sample tweak factor
-10             Top hat width (1/Å) for cleaning up Fourier Transform
.5              Minimum radius for FT  [Å]
0.1             g(r) broadening at r = 1A [A]
0  0            0   0          to finish specifying wavelength range of resonance
0.0  1.0  0     Exponential amplitude and decay [1/A]
*  0  0         * 0 0 to specify end of exponential parameter input
1.0             Normalisation correction factor
SLS71280.msubw01          Name of file containing self scattering as a function of wavel
```

```
0               Normalise to:Nothing
20.0            Maximum radius for FT [A]
0               Output units: b/atom/sr
0.2             Power for broadening function e.g. 0.5
0.03            Step size [A]
0               Analyse this sample?
1.0  0.0        Sample environment scattering fraction and attenuation coefficient [per
}

CONTAINER S4 1mm TiZr flat plate cell          {
2  1            Number of  files and period number
SLS71266.raw    CONTAINER S4 1mm TiZr flat plate cell data files
SLS71269.raw    CONTAINER S4 1mm TiZr flat plate cell data files
Ti  0  7.16     Composition
Zr  0  3.438    Composition
*  0  0         * 0 0 to specify end of composition input
SameAsBeam      Geometry
0.1  0.1        Upstream and downstream thicknesses [cm]
0  5            Angle of rotation and sample width (cm)
-0.0542         Density atoms/Å^3?
TABLES          Total cross section source
1.0             Tweak factor
1.0  0.0        Sample environment scattering fraction and attenuation coefficient [per
}

GO

SAMPLE Sample 5 SAT-urea H-H-H can S5 50C          {
3  1            Number of  files and period number
SLS71281.raw    SAMPLE Sample 5 SAT-urea H-H-H can S5 50C data files
SLS71285.raw    SAMPLE Sample 5 SAT-urea H-H-H can S5 50C data files
SLS71295.raw    SAMPLE Sample 5 SAT-urea H-H-H can S5 50C data files
1               Force calculation of sample corrections?
Na  0  0.4      Sample atomic composition
C  0  0.8       Sample atomic composition
H  0  1.2       Sample atomic composition
H  2  0.0       Sample atomic composition
O  0  0.8       Sample atomic composition
N  0  1.2       Sample atomic composition
O  0  0.6       Sample atomic composition
C  0  0.6       Sample atomic composition
H  0  2.4       Sample atomic composition
H  2  0.0       Sample atomic composition
O  0  1.2       Sample atomic composition
H  0  2.4       Sample atomic composition
H  2  0.0       Sample atomic composition
*  0  0         * 0 0 to specify end of composition input
SameAsBeam      Geometry
0.05  0.05      Upstream and downstream thicknesses [cm]
0  5            Angle of rotation and sample width (cm)
-0.1            Density atoms/Å^3?
0               Temperature for sample Placzek correction
```

```
TABLES          Total cross section source
1.0             Sample tweak factor
-10             Top hat width (1/Å) for cleaning up Fourier Transform
.5              Minimum radius for FT  [Å]
0.1             g(r) broadening at r = 1A [A]
0  0            0   0          to finish specifying wavelength range of resonance
0.0  1.0  0     Exponential amplitude and decay [1/A]
*  0  0         * 0 0 to specify end of exponential parameter input
1.0             Normalisation correction factor
SLS71281.msubw01          Name of file containing self scattering as a function of wavel
0               Normalise to:Nothing
20.0            Maximum radius for FT [A]
0               Output units: b/atom/sr
0.2             Power for broadening function e.g. 0.5
0.03            Step size [A]
1               Analyse this sample?
1.0  0.0        Sample environment scattering fraction and attenuation coefficient [per
}

CONTAINER S5 1mm TiZr flat plate cell          {
2  1            Number of  files and period number
SLS71267.raw    CONTAINER S5 1mm TiZr flat plate cell data files
SLS71270.raw    CONTAINER S5 1mm TiZr flat plate cell data files
Ti  0  7.16     Composition
Zr  0  3.438    Composition
*  0  0         * 0 0 to specify end of composition input
SameAsBeam      Geometry
0.1  0.1        Upstream and downstream thicknesses [cm]
0  5            Angle of rotation and sample width (cm)
-0.0542         Density atoms/Å^3?
TABLES          Total cross section source
1.0             Tweak factor
1.0  0.0        Sample environment scattering fraction and attenuation coefficient [per
}

GO

SAMPLE Sample 7 SAT-urea H-D-D can S7 50C          {
2  1            Number of  files and period number
SLS71282.raw    SAMPLE Sample 7 SAT-urea H-D-D can S7 50C data files
SLS71286.raw    SAMPLE Sample 7 SAT-urea H-D-D can S7 50C data files
1               Force calculation of sample corrections?
Na  0  0.4      Sample atomic composition
C  0  0.8       Sample atomic composition
H  0  1.2       Sample atomic composition
H  2  0.0       Sample atomic composition
O  0  0.8       Sample atomic composition
N  0  1.2       Sample atomic composition
O  0  0.6       Sample atomic composition
C  0  0.6       Sample atomic composition
H  0  0.0       Sample atomic composition
H  2  2.4       Sample atomic composition
```

```
O  0  1.2       Sample atomic composition
H  0  0.0       Sample atomic composition
H  2  2.4       Sample atomic composition
*  0  0         * 0 0 to specify end of composition input
SameAsBeam      Geometry
0.05  0.05      Upstream and downstream thicknesses [cm]
0  5            Angle of rotation and sample width (cm)
-.1             Density atoms/Å^3?
0               Temperature for sample Placzek correction
TABLES          Total cross section source
1.0             Sample tweak factor
-10             Top hat width (1/Å) for cleaning up Fourier Transform
.5              Minimum radius for FT  [Å]
0.1             g(r) broadening at r = 1A [A]
0  0            0   0          to finish specifying wavelength range of resonance
0.0  1.0  0     Exponential amplitude and decay [1/A]
*  0  0         * 0 0 to specify end of exponential parameter input
1.0             Normalisation correction factor
SLS71282.msubw01          Name of file containing self scattering as a function of wavel
0               Normalise to:Nothing
20.0            Maximum radius for FT [A]
0               Output units: b/atom/sr
0.2             Power for broadening function e.g. 0.5
0.03            Step size [A]
0               Analyse this sample?
1.0  0.0        Sample environment scattering fraction and attenuation coefficient [per
}

GO

SAMPLE S7 1mm TiZr flat plate cell          {
2  1           Number of  files and period number
SLS71272.raw   SAMPLE S7 1mm TiZr flat plate cell data files
SLS71273.raw   SAMPLE S7 1mm TiZr flat plate cell data files
1              Force calculation of sample corrections?
Ti  0  7.16    Composition
Zr  0  3.438   Composition
*  0  0        * 0 0 to specify end of composition input
SameAsBeam     Geometry
0.1  0.1       Upstream and downstream thicknesses [cm]
0  5           Angle of rotation and sample width (cm)
-0.0542        Density atoms/Å^3?
0              Temperature for Placzek correction:
TABLES         Total cross section source
1.0            Tweak factor
0              Top hat width (1/Å) for cleaning up Fourier Transform
0.0            Minimum radius for FT  [Å]
0.1            g(r) broadening at r = 1A [A]
0  0           0   0          to finish specifying wavelength range of resonance
0.0  1.0  0    Exponential amplitude and decay [1/A]
*  0  0        * 0 0 to specify end of exponential parameter input
1.0            Normalisation correction factor
```

```
SLS71272.msubw01          Name of file containing self scattering as a function of wavel
0              Normalise to:Nothing
20.0           Maximum radius for FT [A]
0              Output units: b/atom/sr
0.2            Power for broadening function e.g. 0.5
0.03           Step size [A]
0              Analyse this sample?
1.0  0.0       Sample environment scattering fraction and attenuation coefficient [per A
}

GO

END
1 2 3 4 5 6 7 8 9 10
Date and time last written:  20231031 14:26:26
N
```

EPSR26 Processing Script

```
00test.EPSR                       Title of this file
feedback    .8                    Confidence factor - should be < 1. [0.8]
potfac      1.000000   1.000000   >0.0 to enable potential refinement, 0.0 to inhibit
rspcrmin    1.00                  Minimum distance for calculating the R-space coefficien
rspcfrac    0.5                   Fraction of R-space coefficient in control level [0.2]
num_threds  0                     No. of parallel threads to be used, (0 to let program c
porodpwr    0 0                   Q-value and power for Porod scattering [0 0]
nmolcell    10                    Average number of molecules in a cell [10]
control-p   none 0 0              Control pressure [a, b and/or c axes control plus value
ref_intra   0.000    0.000        Weighting on EP and Coulomb terms for intra-molecular s
sizefactor  1.00000    0.90000  0.00000E+00              Multiplying factor for box dim
nq          600                   Number of Q values. [600]
qstep       0.05                  Size of Q step [1/A]. [0.05]
qinscalefc  1.0 0.0               Scale factor on input Q values and broadening power for
ireset      0                     1: complete reset; 2: sets the Empirical Potential to z
iinit       0                     Sets accumulators to zero. Recalculates r and Q. [1]
ntimes      5                     Number of MC cycles between potential refinements. [5]
niter       1                     Number of potential refinements before exitting. [1]
nsumt       672                   Number of iterations already accumulated. [-1 with rese
intra       100                   Number of iterations between molecule shakes. [100]
rotfreq     5                     Number of iterations between internal rotation moves. [
inter       5                     Number of iterations in running averages. [5]
rho         9.94999632E-02        Atomic number density - will be derived from .ato file
cellst      0.03                  Size of r step [A]. [0.03]
rmaxgr      0.000000E+00          Range of g(r) and F.T. (0.0 will use half the cell box)
ngrsamples  0                     Requested no. of origin molecules to sample g(r). (0 wi
fwhm        0.0                   Resolution width - Q independent term. [0.0]
fwhmq       0.02                  Resolution width - Q dependent term. [0.02 for SLS]
nsmoop      1                     1 means background subtraction is ON, 0 means OFF
fnameato    SAT-urea.ato          Name of .ato file
fnamepcof   SAT-urea.pcof         Name of potential coefficients file.
revlorch    0.0 0.0               Broadening factor in Q space. [0.0 0.0]
```

```
qwidthqmax  0.01 0              Broadening and maximum Q for Bragg peak calculation
mplicities  1 1 1               No. of unit cells along a, b and c for Bragg peak calcu
hklqmin     0.0 0.0 0.0         Minimum value of qhkl to be used, minimum radius for Br
diffuse     0                   No. of unit cells along a, b and c for diffuse scatteri
nlatrefine  0                   No. of lattice refinement steps [0]
latrefine   0 0 0 0 0 0         Refinement steps for each of a, b, c, alpha, beta, gamm
rejrate     0.75                Rejection rate [0.75]
qmin        0.10000    0.10000  Qmin for Fourier transforms and for potential fits. [0.
ndata       7                   Number of data files to be fit by EPSR

data   1

datafile    SLS71316.mint01      Name of data file to be fit
wtsfile     sample-1.NWTStot.wts Name of weights file for this data set
nrtype      5                    Data type - see User Manual for more details
rshmin      0.7                  Minimum radius [A] - used for background subtraction
szeros      0.0                  Zero limit - 0 means use first data point for Q=0
tweak       1.0                  Scaling factor for this data set. [1.0]
efilereq    1                    Requested energy amplitude for this data set [1.0]
porodadd    0.0                  Additional amplitude of Porod scattering for this datas

data   2

datafile    SLS71317.mint01      Name of data file to be fit
wtsfile     sample-2.NWTStot.wts Name of weights file for this data set
nrtype      5                    Data type - see User Manual for more details
rshmin      0.7                  Minimum radius [A] - used for background subtraction
szeros      0.0                  Zero limit - 0 means use first data point for Q=0
tweak       1.0                  Scaling factor for this data set. [1.0]
efilereq    1                    Requested energy amplitude for this data set [1.0]
porodadd    0.0                  Additional amplitude of Porod scattering for this datas

data   3

datafile    SLS71279.mint01      Name of data file to be fit
wtsfile     sample-3.NWTStot.wts Name of weights file for this data set
nrtype      5                    Data type - see User Manual for more details
rshmin      0.7                  Minimum radius [A] - used for background subtraction
szeros      0.0                  Zero limit - 0 means use first data point for Q=0
tweak       1.0                  Scaling factor for this data set. [1.0]
efilereq    1                    Requested energy amplitude for this data set [1.0]
porodadd    0.0                  Additional amplitude of Porod scattering for this datas

data   4

datafile    SLS71280.mint01      Name of data file to be fit
wtsfile     sample-4.NWTStot.wts Name of weights file for this data set
nrtype      5                    Data type - see User Manual for more details
rshmin      0.7                  Minimum radius [A] - used for background subtraction
szeros      0.0                  Zero limit - 0 means use first data point for Q=0
tweak       1.0                  Scaling factor for this data set. [1.0]
efilereq    1                    Requested energy amplitude for this data set [1.0]
```

```
porodadd    0.0                 Additional amplitude of Porod scattering for this datas

data   5

datafile    SLS71281.mint01     Name of data file to be fit
wtsfile     sample-5.NWTStot.wts Name of weights file for this data set
nrtype      5                   Data type - see User Manual for more details
rshmin      0.7                 Minimum radius [A] - used for background subtraction
szeros      0.0                 Zero limit - 0 means use first data point for Q=0
tweak       1.0                 Scaling factor for this data set. [1.0]
efilereq    1                   Requested energy amplitude for this data set [1.0]
porodadd    0.0                 Additional amplitude of Porod scattering for this datas

data   6

datafile    SLS71318.mint01     Name of data file to be fit
wtsfile     sample-6.NWTStot.wts Name of weights file for this data set
nrtype      5                   Data type - see User Manual for more details
rshmin      0.7                 Minimum radius [A] - used for background subtraction
szeros      0.0                 Zero limit - 0 means use first data point for Q=0
tweak       1.0                 Scaling factor for this data set. [1.0]
efilereq    1                   Requested energy amplitude for this data set [1.0]
porodadd    0.0                 Additional amplitude of Porod scattering for this datas

data   7

datafile    SLS71282.mint01     Name of data file to be fit
wtsfile     sample-7.NWTStot.wts Name of weights file for this data set
nrtype      5                   Data type - see User Manual for more details
rshmin      0.7                 Minimum radius [A] - used for background subtraction
szeros      0.0                 Zero limit - 0 means use first data point for Q=0
tweak       1.0                 Scaling factor for this data set. [1.0]
efilereq    1                   Requested energy amplitude for this data set [1.0]
porodadd    0.0                 Additional amplitude of Porod scattering for this datas
q
```