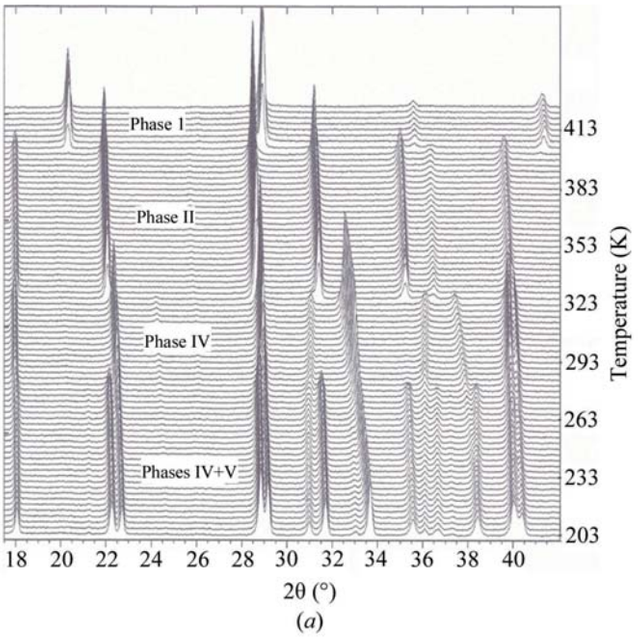

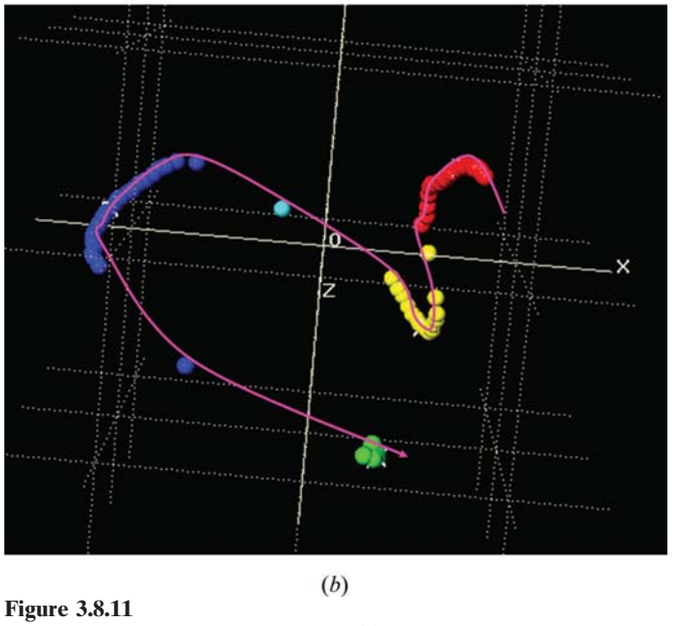

Figure 3.8.11
Ammonium nitrate phase transitions. (*a*) The raw powder data measured between 203 and 425 K. Reproduced with permission from Herrmann & Engel (1997). Copyright (1997) John Wiley and Sons. (*b*) The MMDS plot. The purple line follows the temperature change from 203 to 425 K.

$$\chi^2 = \left|\mathbf{xp} - \mathbf{S}\right|^2. \tag{3.8.29}$$

is required. Since $N \ll m$, the system is heavily overdetermined, and least-squares or singular value decomposition can be used to solve (3.8.29) for the fractional percentages arising from the scattering power of the component mixtures, $s_1, s_2, \ldots, s_N$. The values of s can be used to calculate a weight fraction for that particular phase provided that the atomic absorption coefficients are known, and this in turn requires the unit-cell dimensions and cell contents, but not the atomic coordinates (Smith *et al.*, 1988; Cressey & Schofield, 1996). The general formula for the weight fraction of component n in a mixture comprising N components is (Leroux *et al.*, 1953)

$$c_n = p_n \frac{\mu^*}{\mu_n^*}, \tag{3.8.30}$$

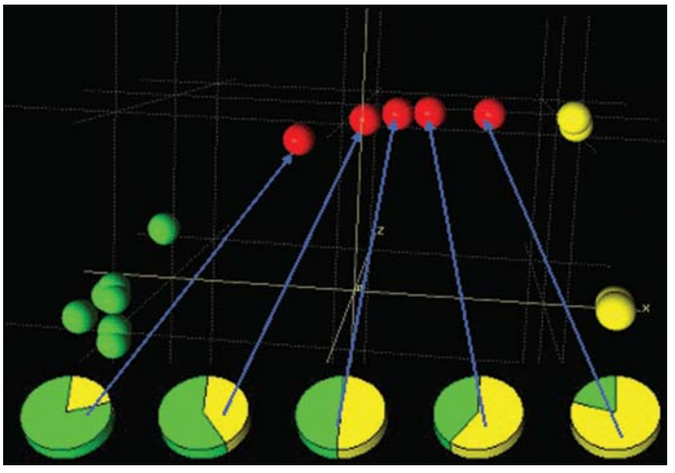

Figure 3.8.12
Identifying mixtures using lanthanum strontium copper oxide and caesium thiocyanate diffraction data taken from the ICDD Clay Minerals database. The green spheres represent pure phases of lanthanum strontium copper oxide and the yellow pure caesium thiocyanate. The red spheres represent mixtures of the two in the relative proportions of lanthanum strontium copper oxide/caesium thiocyanate 80/20, 60/40, 50/50, 40/60 and 20/80 in an arc commencing on the left-hand side of the diagram. The pie charts give the results of an independent quantitative calculation in which lanthanum strontium copper oxide and caesium thiocyanate have been included as pure phases in a reference database.

where

$$\mu^* = \sum_{j=1}^{N} c_j \mu_j^* \tag{3.8.31}$$

and

$$\mu_j^* = \mu_j / \rho_j, \tag{3.8.32}$$

where μ_j is the atomic X-ray absorption coefficient and ρ_j is the density of component j. For polymorphs, the absorption coefficients are sufficiently close and the method sufficiently approximate that the effects of absorption can be ignored.

3.8.7.1. *Example: inorganic mixtures*

As an example, a set of 19 patterns from set 78 of the ICDD database for inorganic compounds (ICDD, 2018) was imported into *DIFFRAC.EVA*. To this was added some simulated mixture data generated by adding the patterns for lanthanum strontium copper oxide and caesium thiocyanate in the proportions 80/20, 60/40, 50/50, 40/60 and 20/80. Two calculations were performed: an analysis without the pure-phase database and a second where the pure phases of lanthanum strontium copper oxide and caesium thiocyanate were present.

The results are shown in Fig. 3.8.12. In the MMDS plot the green spheres represent pure lanthanum strontium copper oxide while the yellow are pure caesium thiocyanate. The red spheres represent mixtures of the two. The latter form an arc between the green and yellow clusters. The distance of the spheres representing mixtures from the lanthanum strontium copper oxide and caesium thiocyanate spheres gives a semi-quantitative representation of the mixture contents. Running the analysis in quantitative mode gives the pie charts also shown in Fig. 3.8.12; they reproduce exactly the relative proportions of the three components.