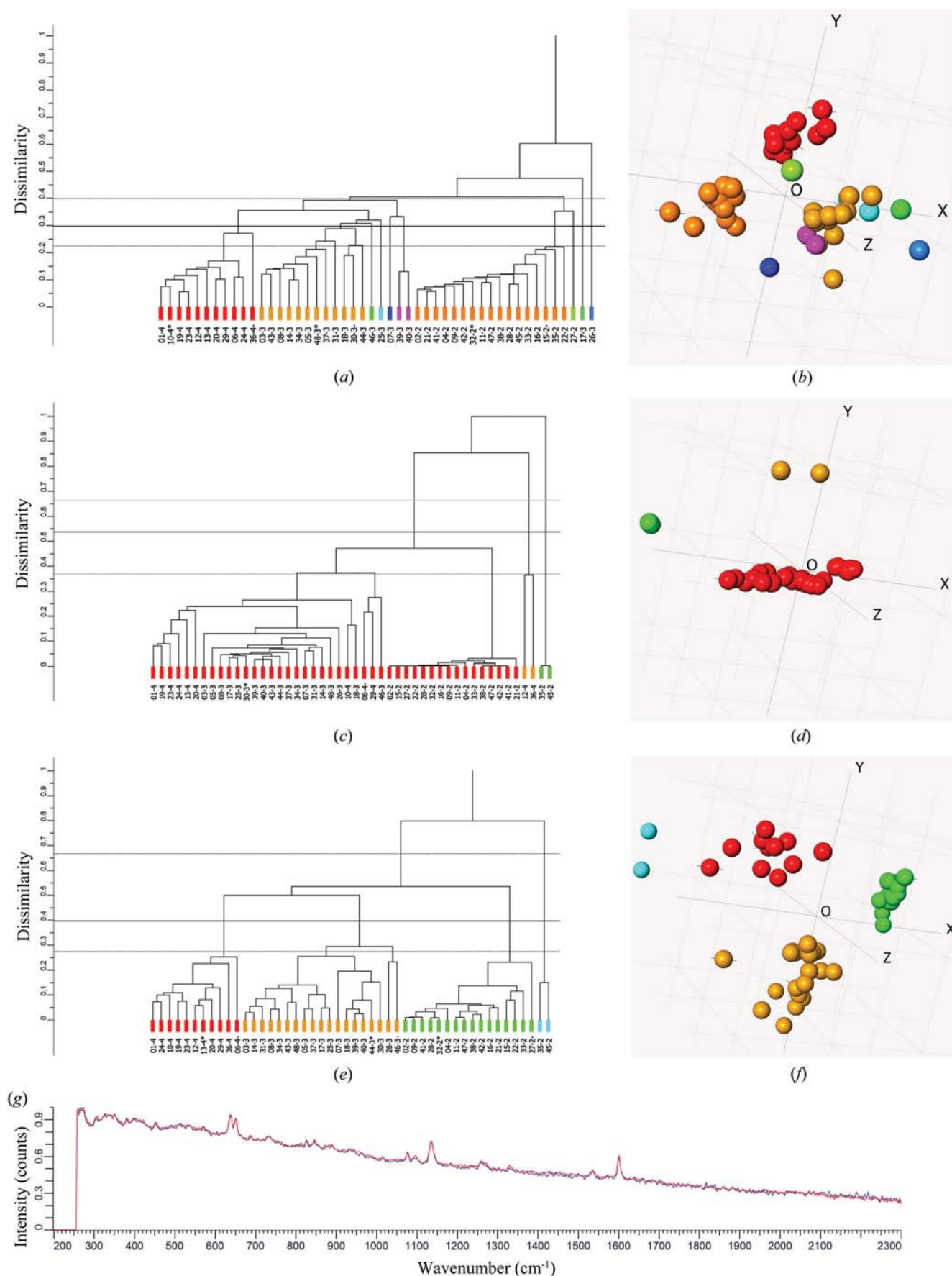


## 3.8. DATA CLUSTERING AND VISUALIZATION

**Figure 3.8.16**

Clustering 48 PXR spectra with background corrections applied for three polymorphs of sulfathiazole. (a) The dendrogram. Each sample is identified by a four-digit code. The first two digits are the well number, and the last digit defines whether the sample is form 2, 3 or 4 of sulfathiazole. (b) The MMDS plot: the red cluster is well defined but the rest of the spheres are diffuse and intermingled. (c) The dendrogram derived from clustering 48 Raman spectra of sulfathiazole with background corrections applied. (d) The corresponding MMDS plot. The clusters are poorly defined. (e) The results of the INDSCAL method. The dendrogram is shown with the default cut level. The clustering is correct; all the samples are placed in the correct group except for patterns 35-2 and 45-2. (f) The MMDS plot validates the dendrogram. (g) The Raman patterns for 35-2 and 45-2 superimposed. They are primarily background noise.