The structure of 2-(1-hydroxy-2-methyl-propyl)-2,5-dihydro-furan-2-carboxylic acid diisopropylamide [1] has been solved at two temperatures, 150K and 250K. The high temperature structure has $Z' = 1$, but at low temperature $Z' = 2$, with the two non-crystallographically equivalent molecules related by a pseudotranslation of $\frac{1}{2}$ along the c-axis. Between these two temperatures, the crystal undergoes a reversible second order phase change, which is clearly seen in diffraction patterns produced within that temperature range.

The cell volume and cell parameters were studied as a function of temperature, first cooling the crystal, then heating it back up. The crystal exhibits a second order phase transition over the temperature range 166-206K. This phase change is seen most clearly by examining a series of diffraction patterns over a range of temperatures.

The average values of $|E|^2-1$ differ between high and low temperature structures. $\langle |E|^2-1 \rangle$ measures the absolute deviation of $E$ from its average value of unity. The more variation there is in $E$, the larger the value of $\langle |E|^2-1 \rangle$. For centric distributions, $\langle |E|^2-1 \rangle$ is ideally 0.97. At 250K $\langle |E|^2-1 \rangle = 0.871$ and at 150K $\langle |E|^2-1 \rangle = 0.955$. This indicates a larger spread in the low temperature data. This is unsurprising as $E$ attaches greater weight to high angle data and at higher resolution the differences between the two asymmetric molecules become more important.

Wilson plots

Wilson plots are generally used in order to find an average value of the scale and temperature factors. However they can also provide a quantitative comparison of the intensities of strong and weak reflections, here by plotting odd and even l reflections separately.

Acknowledgments

Many thanks to Dr. T. Donohoe, Dr. D. House and Dr. D. Carbery of the Dyson Perrins Laboratory at the University of Oxford for providing the crystals for this study.

References