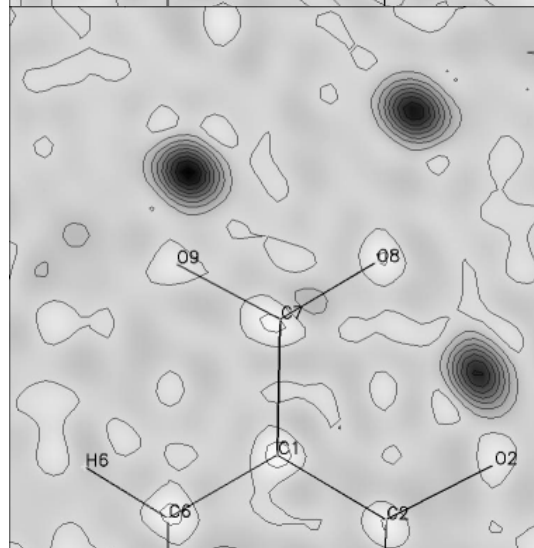
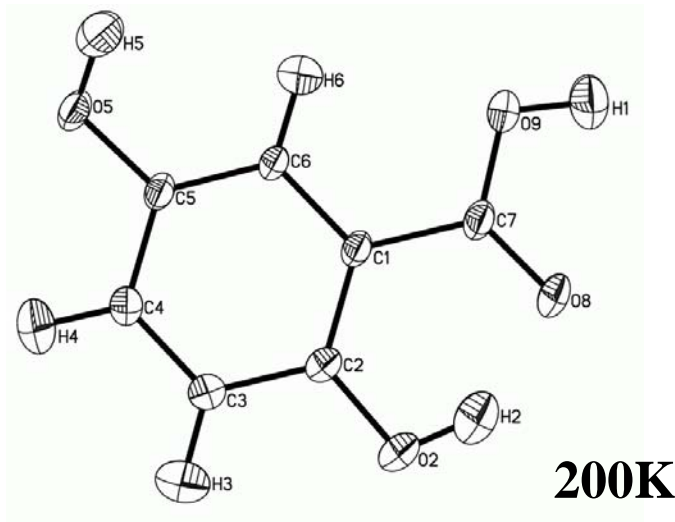
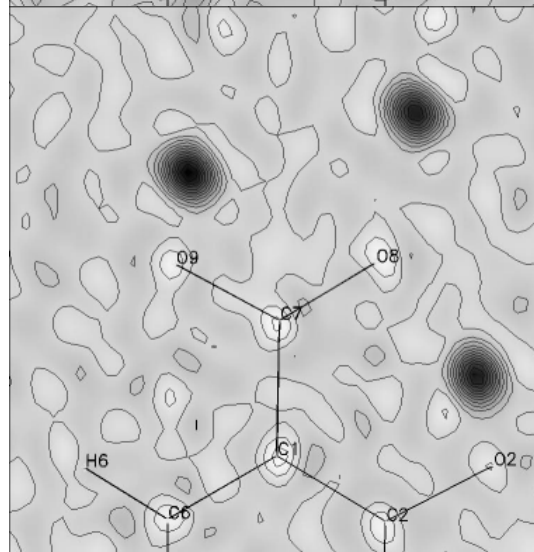
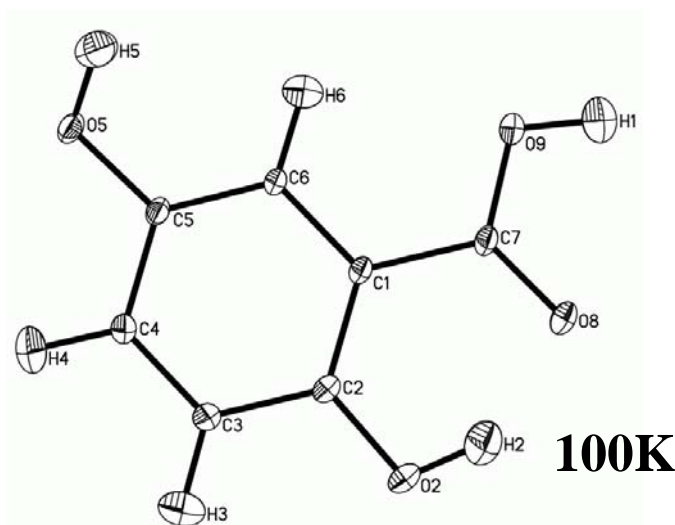
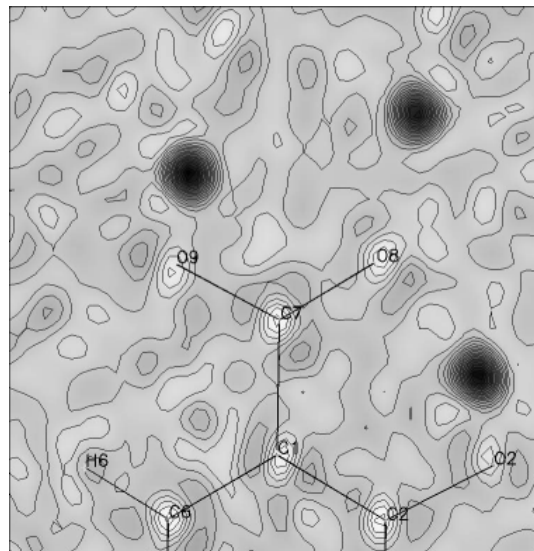
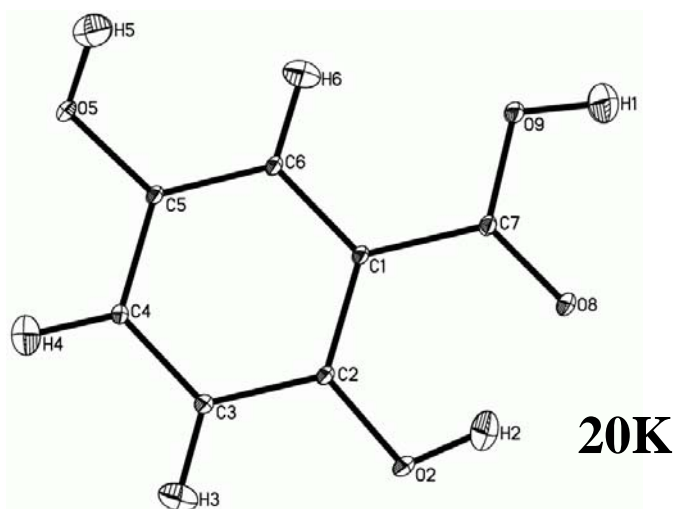


## Stability of hydrogen bonds in the cooperative hydrogen bonded system in dihydroxybenzoic acids.

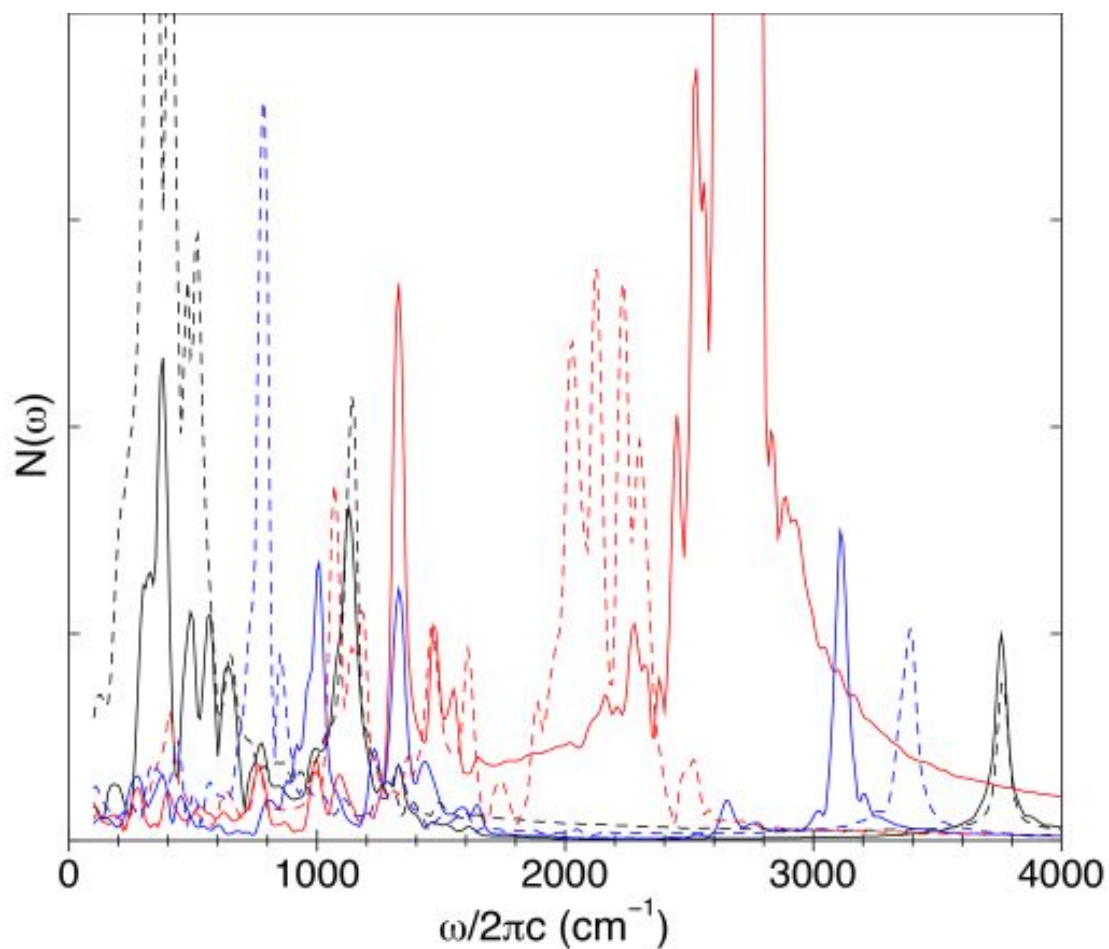
Martin S. Adam, Matthias J. Gutmann, Charlotte K. Leech, Derek S. Middlemiss, Andrew Parkin, Lynne H. Thomas and Chick C. Wilson

Supplementary figures:



**Left;** Neutron structures of 2,5-dihydroxybenzoic acid produced using ORTEP with ellipsoids plotted at 50% probability, refined from data collected on SXD at ISIS. The thermal expansion of the anisotropic displacement parameters with temperature follows the expected trend. **Right;** Difference Fourier maps of 2,5-dihydroxybenzoic acid in the plane of C7, O8 and O9 with protons H1 and H2 removed from the structural model. The resultant peaks corresponding to the hydrogen atoms show well-defined sites with no disorder present at all temperatures up to 200 K.

### Electronic Supplementary Information (Theory)



**Alternative to Figure 8.** The vibrational spectra of protons in the *para* (black), *ortho* (blue) and acid (red) OH groups in forms I (solid line) and III (dashed line) of the isolated dimer of 2,4-DHBA, derived as the Fourier transform of the atom-projected velocity autocorrelation function.