

Electronic Supplementary Information of

**Thermal Properties of Molecular Crystals through
Dispersion-corrected Quasi-harmonic Ab initio
Calculations: The Case of Urea**

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Details of Experimental Studies on the Thermal Expansion of Urea

H. Birkedal, D. Madsen, R. H. Mathiesen, K. Knudsen, H.-P. Weber, P. Pattison and D. Schwarzenbach, *Acta Crystallogr. Sec. A*, 2004, **60**, 371.

Synchrotron powder diffraction at four temperatures: 10, 80, 120 and 295 K.

S. Swaminathan, B. M. Craven and R. K. McMullan, *Acta Crystallogr. Sect. B*, 1984, **40**, 300–306

Single-crystal neutron diffraction at seven temperatures: 12, 30, 60, 90, 123, 150 and 173 K.

V. Zavodnik, A. Stash, V. Tsirelson, R. Y. de Vries and D. Feil, *Acta Crystallogr. Sec. B*, 1999, **55**, 45

Single-crystal X-ray diffraction at two temperatures: 148 and 293 K.

R. Hammond, K. Pencheva, K. J. Roberts, P. Mougín and D. Wilkinson, *J. Appl. Crystallogr.*, 2005, **38**, 1038–1039

X-ray powder diffraction at 15 temperatures between 188 and 328 K.

Larger version of Figure 1

