Understanding the single-crystal-to-single-crystal solid-state phase transition of DL-methionine

M.M.H. Smets,[a] S.J.T. Brugman,[a], E.R.H. van Eck,[a] P. Tinnemans,[a] H. Meekes*[a] and H.M. Cuppen[a]

[a] Radboud University, Institute for Molecules and Materials, Heyendaalseweg 135, 6525 AJ Nijmegen, The Netherlands; E-mail: h.meekes@science.ru.nl

Refinement parameters DL-methionine at 338 K and 420 K.

Table 1: Crystal data and details of the structure determination of DL-methionine at 338 K.

Crystal Data	
Formula	$C_5H_{11}NO_2S$
Formula Weight	149.21
Crystal System	monoclinic
Space group	$P2_1/c$
a (Å)	16.894(2)
b (Å)	4.7953(6)
c (Å)	9.8686(13)
β (°)	101.318(4)
V (Å^3)	783.93(17)
Z	4
D_{calc} (g/cm^3)	1.264
$\mu_{MoK\alpha}$ (mm^{-1})	0.347
F(000)	320
Crystal Size (mm)	0.06 x 0.13 x 0.35
Data Collection	
Temperature (K)	338
Radiation (Å)	MoKα 0.71073
Theta Min-Max (°)	2.5 - 23.8
Dataset	-19 < h < 19, -5 < k < 5, -11 < l < 11
Total measured reflections	21783
Independent reflections	1207
R_{int}	0.024
Observed data [I >2σ(I)]	1061
Refinement	
Reflections	1207
Parameters	111
$R[F^2 > 2\sigma(F^2)]$	0.071
wR(F^2)	0.237
S	1.05
$\Delta\rho_{max}$ (e/Å^3)	0.42
$\Delta\rho_{min}$ (e/Å^3)	-0.35

Table 2: Crystal data and details of the structure determination of DL-methionine at 420 K.

Crystal Data	
Formula	$C_5H_{11}NO_2S$
Formula Weight	149.21
Crystal System	monoclinic
Space group	$P2_1/c$
a (Å)	16.923(3)
b (Å)	4.7963(7)
c (Å)	9.8840(15)
β (°)	101.424(5)
V (Å^3)	786.4(2)
Z	4
D_{calc} (g/cm^3)	1.260
$\mu_{MoK\alpha}$ (mm^{-1})	0.346
F(000)	320
Crystal Size (mm)	0.06 x 0.13 x 0.35
Data Collection	
Temperature (K)	420
Radiation (Å)	MoKα 0.71073
Theta Min-Max (°)	2.5 - 23.8
Dataset	-19 < h < 19, -5 < k < 5, -11 < l < 11
Total measured reflections	8448
Independent reflections	1205
R_{int}	0.023
Observed data [I >2σ(I)]	1018
Refinement	
Reflections	1205
Parameters	105
$R[F^2 > 2\sigma(F^2)]$	0.072
wR(F^2)	0.238
S	1.05
$\Delta\rho_{max}$ (e/Å^3)	0.43
$\Delta\rho_{min}$ (e/Å^3)	-0.39