The Generation and Characterisation of Standardised Forms of Trehalose Dihydrate and their Associated Solid-State Behaviour

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Variable Temperature Attenuated Total Reflection Fourier Transform Infrared spectroscopy (Variable temperature ATR-FTIR).

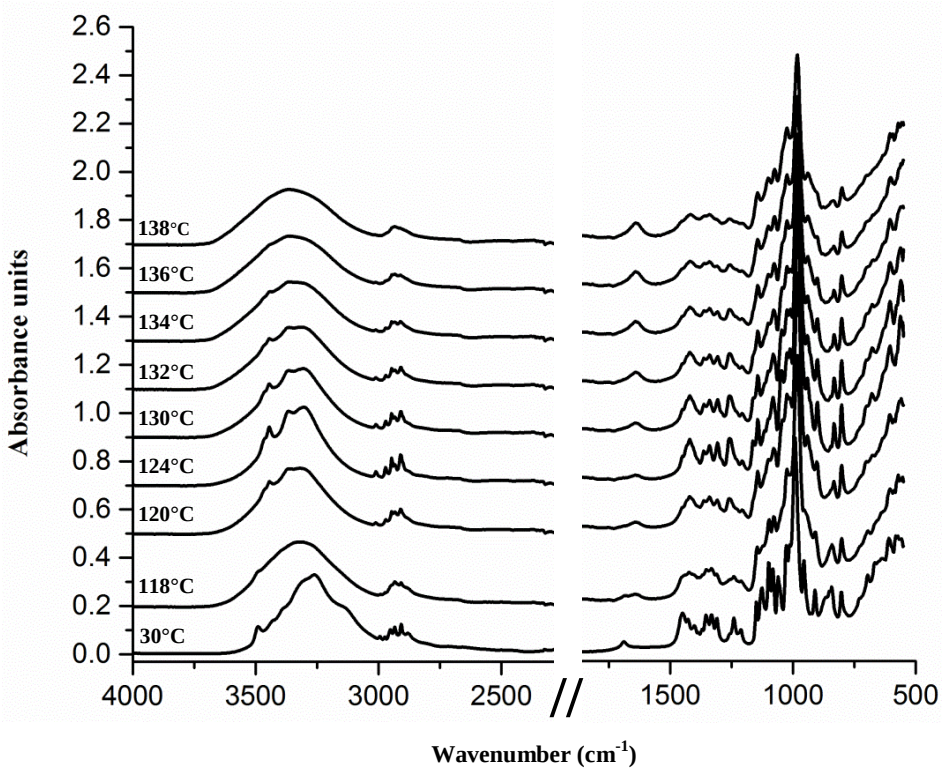

Figure SI1. Variable temperature ATR-FTIR spectra of T_{h2} measured using a constant heating rate of 2°C/min in the 500 – 1750 cm^{-1} and 1000 – 4000cm^{-1} region at 30, 118, 120, 124 and 130-138°C.

Table SI1. ATR-FTIR band assignment for T_{h2} at 124°C samples

Absorption band (cm^{-1})	
T_{h2} spectra at 124°C	**Assignment**[13, 31-37]
3446 **3366**	O-H stretch vibration of two crystal water molecules with Hydrogen bonding
3303	O-H stretching of trehalose
3010[b] 2970 2947 2933 2909	Asymmetrical and symmetrical stretching of the C-H ring
1652	Bending peak of crystal water
981 941	Two vibrational modes (asymmetrical and symmetrical) of the α,α-1↔1-glycosidic bond
929 (shoulder peak) **901**[b]	Coupled bending vibrations of C1-H, CH_2 and C-O-H
832[a] -	Bending vibration of equatorial C-H bonds in α anomers