Electronic Supplementary Information

The impact of polymorphism on the thermophysical properties of Methyl Behenate as phase-change material

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2. Materials and Methods

2.2 Differential Scanning Calorimetry (DSC)

To investigate the polymorphic behaviour of methyl behenate (MEBE) with different heating/cooling rates, the cycling regime shown in Figure A1 was employed. To summarise, samples of methyl behenate were cycled twice between 20-80°C at rates of 10, 1 and 0.1K/min. Isotherms of 5 minutes were inserted at the beginning and end of each heating/cooling cycle to allow for sample equilibration and temperature homogeneity.

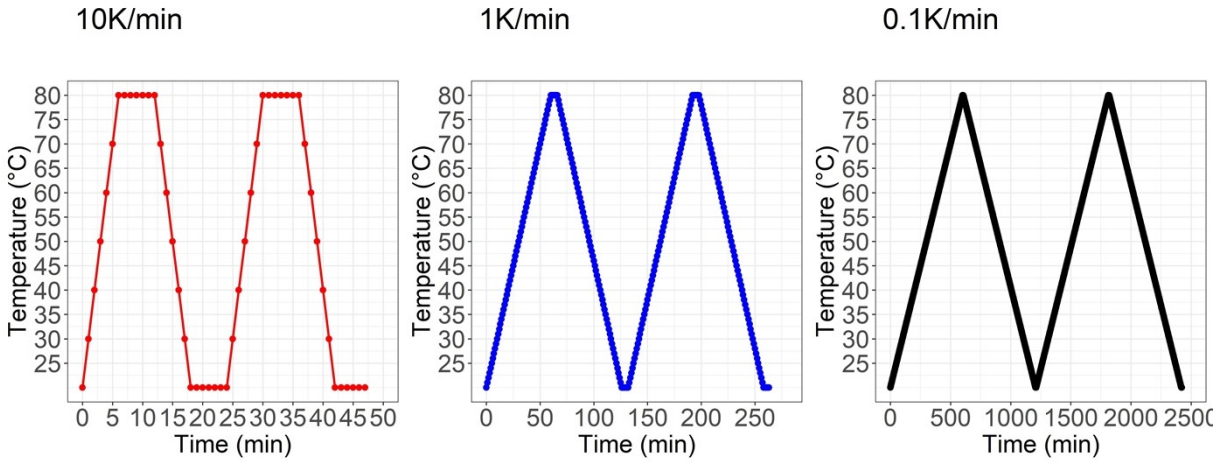

Figure A1. Heating and cooling regime used to explore thermal behaviour of MEBE.

2.3 Hot-Stage Microscopy (HSM)

A custom heating/cooling stage for a DinoLite microscope was built at HSLU to conduct in-situ hot-stage microscopy analysis. **Figure A2** shows the hot stage built according to Meerstetter Engineering's guidelines.

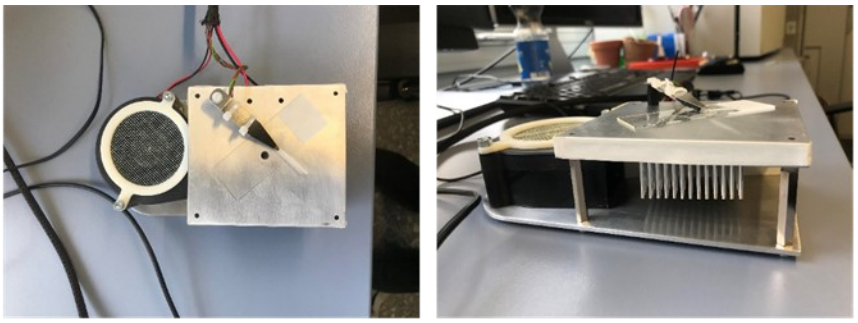

Figure A2. Custom hot-stage built at HSLU for HSM analysis

The instrument was calibrated with methyl palmitate from Merck (Gygli, CH). Details on the calibration results can be found in **Table S1**, showing a good degree of agreement between the two techniques.

Table S1. Calibration results of HSM with methyl palmitate and comparison with DSC data.

	T_{onset} [°C](DSC)		T_0 [°C](HSM)	
	Crystallisation	**Melting**	**Crystallisation**	**Melting**
10 K/min	25.7 ± 0.1	26.7 ± 0.3	25.5 ± 0.5	27.0 ± 1.0
1 K/min	26.3 ± 0.5	26.6 ± 1.2	25.5 ± 0.5	26.5 ± 0.5
0.1 K/min	26.3 ± 0.3	27.0 ± 0.1	25.0 ± 0.5	27.0 ± 1.0

2.4.2 Growth of single crystals from solution

Single crystals of Form I of Methyl Behenate were successfully grown from solution by vapour diffusion using ethyl acetate as a solvent and methanol as an antisolvent. **Figure A3** shows the setup used to grow the crystals.

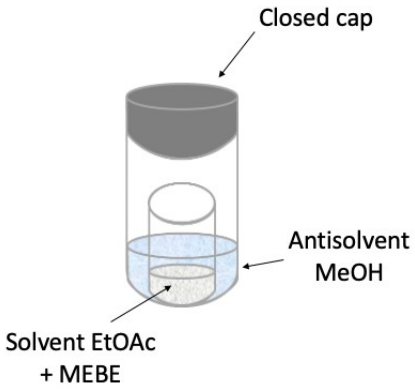

Figure A3. Solvent (Ethyl acetate, EtOAc)-antisolvent (methanol, MeOH) setup for growing single crystals of Form I.

3. Results

3.2 X-Ray diffraction Investigation

3.2.1 Form I

Table S2 shows the complete list of bond lengths of Form I of methyl behenate.

Table S2. Interatomic distances of Form I of methyl behenate from single crystal XRD

Atom 1	Atom 2	Length (Å)
C17	H17A	0.97
C17	H17B	0.97
C17	C16	1.53(1)
C17	C18	1.49(1)
C15	H15A	0.97
C15	H15B	0.97
C15	C16	1.53(1)
C15	C14	1.53(1)
C11	H11A	0.97
C11	H11B	0.97
C11	C12	1.52(1)
C11	C10	1.51(1)
C13	H13A	0.97
C13	H13B	0.969
C13	C14	1.53(1)
C13	C12	1.54(1)
C16	H16A	0.97
C16	H16B	0.97
C5	H5A	0.97
C5	H5B	0.97
C5	C6	1.53(1)
C5	C4	1.52(1)
C21	H21A	0.97
C21	H21B	0.97
C21	C22	1.51(1)
C21	C20	1.57(1)
C19	H19A	0.97
C19	H19B	0.97
C19	C18	1.55(1)
C19	C20	1.51(1)
C7	H7A	0.97
C7	H7B	0.97
C7	C6	1.50(1)
C7	C8	1.54(1)
C3	H3A	0.97
C3	H3B	0.97
C3	C4	1.53(1)
C3	C2	1.50(1)
C14	H14A	0.97
C14	H14B	0.97
C23	H23A	0.96
C23	H23B	0.96
C23	H23C	0.96
C23	C22	1.51(2)
C22	H22A	0.97

C22	H22B	0.97
C12	H12A	0.97
C12	H12B	0.97
C18	H18A	0.97
C18	H18B	0.97
C6	H6A	0.97
C6	H6B	0.97
C10	H10A	0.97
C10	H10B	0.97
C10	C9	1.53(1)
C9	H9A	0.97
C9	H9B	0.97
C9	C8	1.52(1)
C4	H4A	0.97
C4	H4B	0.97
C8	H8A	0.97
C8	H8B	0.97
C20	H20A	0.97
C20	H20B	0.97
O2	C2	1.14(1)
O1	C2	1.37(1)
O1	C1	1.47(1)
C1	H1A	0.96
C1	H1B	0.96
C1	H1C	0.96
C6A	H6AA	0.97
C6A	H6AB	0.97
C6A	C7A	1.51(2)
C6A	C5A	1.49(2)
C8A	H8AA	0.97
C8A	H8AB	0.97
C8A	C9A	1.52(2)
C8A	C7A	1.48(2)
C4A	H4AA	0.97
C4A	H4AB	0.97
C4A	C3A	1.51(2)
C4A	C5A	1.51(2)
C1A	H1AA	0.96
C1A	H1AB	0.96
C1A	H1AC	0.96
C1A	O1A	1.43(2)
O1A	C2A	1.34(2)
C16A	H16C	0.97
C16A	H16D	0.97
C16A	C17A	1.50(2)
C16A	C15A	1.48(2)
C10A	H10C	0.97
C10A	H10D	0.97
C10A	C9A	1.49(2)
C10A	C11A	1.53(2)
C2A	C3A	1.43(2)
C2A	O2A	1.22(2)

C3A	H3AA	0.97
C3A	H3AB	0.97
C12A	H12C	0.97
C12A	H12D	0.97
C12A	C11A	1.51(2)
C12A	C13A	1.50(2)
C9A	H9AA	0.97
C9A	H9AB	0.97
C7A	H7AA	0.97
C7A	H7AB	0.97
C18A	H18C	0.97
C18A	H18D	0.97
C18A	C17A	1.52(2)
C18A	C19A	1.47(2)
C5A	H5AA	0.97
C5A	H5AB	0.97
C14A	H14C	0.97
C14A	H14D	0.97
C14A	C15A	1.54(2)
C14A	C13A	1.50(2)
C11A	H11C	0.97
C11A	H11D	0.97
C22A	H22C	0.97
C22A	H22D	0.97
C22A	C21A	1.45(2)
C22A	C23A	1.51(2)
C17A	H17C	0.97
C17A	H17D	0.97
C19A	H19C	0.97
C19A	H19D	0.97
C19A	C20A	1.49(2)
C15A	H15C	0.97
C15A	H15D	0.97
C13A	H13C	0.97
C13A	H13D	0.97
C20A	H20C	0.97
C20A	H20D	0.97
C20A	C21A	1.46(2)
C21A	H21C	0.97
C21A	H21D	0.97
C23A	H23D	0.96
C23A	H23E	0.96
C23A	H23F	0.96

Table S3 shows the complete list of bond angles of Form I of methyl behenate.

Table S3. Interatomic angles of Form I of methyl behenate from single crystal XRD

Atom1	**Atom2**	**Atom3**	**Angle (°)**
H17A	C17	H17B	107.6
H17A	C17	C16	108.7
H17A	C17	C18	108.7
H17B	C17	C16	108.6

H17B	C17	C18	108.7
C16	C17	C18	114.3(6)
H15A	C15	H15B	107.7
H15A	C15	C16	108.9
H15A	C15	C14	108.9
H15B	C15	C16	108.9
H15B	C15	C14	108.9
C16	C15	C14	113.3(6)
H11A	C11	H11B	107.7
H11A	C11	C12	108.9
H11A	C11	C10	108.8
H11B	C11	C12	108.9
H11B	C11	C10	108.9
C12	C11	C10	113.5(6)
H13A	C13	H13B	107.8
H13A	C13	C14	108.9
H13A	C13	C12	108.9
H13B	C13	C14	108.9
H13B	C13	C12	109
C14	C13	C12	113.2(6)
C17	C16	C15	114.8(6)
C17	C16	H16A	108.5
C17	C16	H16B	108.5
C15	C16	H16A	108.6
C15	C16	H16B	108.6
H16A	C16	H16B	107.5
H5A	C5	H5B	107.8
H5A	C5	C6	109
H5A	C5	C4	108.9
H5B	C5	C6	109
H5B	C5	C4	108.9
C6	C5	C4	113.1(6)
H21A	C21	H21B	108.1
H21A	C21	C22	109.5
H21A	C21	C20	109.5
H21B	C21	C22	109.4
H21B	C21	C20	109.5
C22	C21	C20	110.8(8)
H19A	C19	H19B	107.8
H19A	C19	C18	109.1
H19A	C19	C20	109.1
H19B	C19	C18	109
H19B	C19	C20	109.1
C18	C19	C20	112.7(7)
H7A	C7	H7B	107.7
H7A	C7	C6	108.9
H7A	C7	C8	108.9
H7B	C7	C6	108.9
H7B	C7	C8	108.9
C6	C7	C8	113.4(6)
H3A	C3	H3B	107.8
H3A	C3	C4	109.1

H3A	C3	C2	109.1
H3B	C3	C4	109.1
H3B	C3	C2	109.1
C4	C3	C2	112.5(7)
C15	C14	C13	112.6(6)
C15	C14	H14A	109.1
C15	C14	H14B	109.1
C13	C14	H14A	109.1
C13	C14	H14B	109.1
H14A	C14	H14B	107.8
H23A	C23	H23B	109
H23A	C23	H23C	109
H23A	C23	C22	109
H23B	C23	H23C	109
H23B	C23	C22	110
H23C	C23	C22	110
C21	C22	C23	112.0(9)
C21	C22	H22A	109
C21	C22	H22B	109
C23	C22	H22A	109
C23	C22	H22B	109
H22A	C22	H22B	108
C11	C12	C13	113.5(6)
C11	C12	H12A	108.9
C11	C12	H12B	108.9
C13	C12	H12A	108.9
C13	C12	H12B	108.8
H12A	C12	H12B	107.7
C17	C18	C19	114.3(7)
C17	C18	H18A	108.7
C17	C18	H18B	108.7
C19	C18	H18A	108.6
C19	C18	H18B	108.7
H18A	C18	H18B	107.6
C5	C6	C7	113.4(6)
C5	C6	H6A	108.9
C5	C6	H6B	108.9
C7	C6	H6A	108.9
C7	C6	H6B	108.9
H6A	C6	H6B	107.7
C11	C10	H10A	108.8
C11	C10	H10B	108.7
C11	C10	C9	114.0(6)
H10A	C10	H10B	107.7
H10A	C10	C9	108.8
H10B	C10	C9	108.8
C10	C9	H9A	108.8
C10	C9	H9B	108.8
C10	C9	C8	113.6(6)
H9A	C9	H9B	107.7
H9A	C9	C8	108.9
H9B	C9	C8	108.9

C5	C4	C3	109.7(6)
C5	C4	H4A	109.7
C5	C4	H4B	109.7
C3	C4	H4A	109.7
C3	C4	H4B	109.8
H4A	C4	H4B	108.2
C7	C8	C9	112.9(6)
C7	C8	H8A	109
C7	C8	H8B	109
C9	C8	H8A	109
C9	C8	H8B	109
H8A	C8	H8B	107.8
C21	C20	C19	111.8(7)
C21	C20	H20A	109.3
C21	C20	H20B	109.3
C19	C20	H20A	109.3
C19	C20	H20B	109.2
H20A	C20	H20B	107.9
C2	O1	C1	112.7(9)
C3	C2	O2	124.2(9)
C3	C2	O1	112.5(8)
O2	C2	O1	120(1)
O1	C1	H1A	110
O1	C1	H1B	110
O1	C1	H1C	109
H1A	C1	H1B	110
H1A	C1	H1C	109
H1B	C1	H1C	109
H6AA	C6A	H6AB	107
H6AA	C6A	C7A	108
H6AA	C6A	C5A	108
H6AB	C6A	C7A	108
H6AB	C6A	C5A	108
C7A	C6A	C5A	116(1)
H8AA	C8A	H8AB	107
H8AA	C8A	C9A	108
H8AA	C8A	C7A	108
H8AB	C8A	C9A	108
H8AB	C8A	C7A	108
C9A	C8A	C7A	115(1)
H4AA	C4A	H4AB	107
H4AA	C4A	C3A	108
H4AA	C4A	C5A	108.2
H4AB	C4A	C3A	108
H4AB	C4A	C5A	108.2
C3A	C4A	C5A	116.4(9)
H1AA	C1A	H1AB	110
H1AA	C1A	H1AC	110
H1AA	C1A	O1A	110
H1AB	C1A	H1AC	109
H1AB	C1A	O1A	109
H1AC	C1A	O1A	109

C1A	O1A	C2A	120(1)
H16C	C16A	H16D	108
H16C	C16A	C17A	109
H16C	C16A	C15A	109
H16D	C16A	C17A	108
H16D	C16A	C15A	109
C17A	C16A	C15A	115(1)
H10C	C10A	H10D	108
H10C	C10A	C9A	109
H10C	C10A	C11A	109
H10D	C10A	C9A	109
H10D	C10A	C11A	109
C9A	C10A	C11A	114(1)
O1A	C2A	C3A	117(1)
O1A	C2A	O2A	112(1)
C3A	C2A	O2A	131(1)
C4A	C3A	C2A	117(1)
C4A	C3A	H3AA	108
C4A	C3A	H3AB	108
C2A	C3A	H3AA	108
C2A	C3A	H3AB	108
H3AA	C3A	H3AB	107
H12C	C12A	H12D	107
H12C	C12A	C11A	108
H12C	C12A	C13A	108
H12D	C12A	C11A	108
H12D	C12A	C13A	108
C11A	C12A	C13A	116(1)
C8A	C9A	C10A	114.2(9)
C8A	C9A	H9AA	109
C8A	C9A	H9AB	109
C10A	C9A	H9AA	109
C10A	C9A	H9AB	109
H9AA	C9A	H9AB	108
C6A	C7A	C8A	117(1)
C6A	C7A	H7AA	108
C6A	C7A	H7AB	108
C8A	C7A	H7AA	108
C8A	C7A	H7AB	108
H7AA	C7A	H7AB	107
H18C	C18A	H18D	107
H18C	C18A	C17A	108
H18C	C18A	C19A	108
H18D	C18A	C17A	108
H18D	C18A	C19A	108
C17A	C18A	C19A	117(1)
C6A	C5A	C4A	116.1(9)
C6A	C5A	H5AA	108
C6A	C5A	H5AB	108
C4A	C5A	H5AA	108.3
C4A	C5A	H5AB	108.3
H5AA	C5A	H5AB	107

H14C	C14A	H14D	108
H14C	C14A	C15A	108
H14C	C14A	C13A	108
H14D	C14A	C15A	108
H14D	C14A	C13A	108
C15A	C14A	C13A	116(1)
C10A	C11A	C12A	115(1)
C10A	C11A	H11C	108
C10A	C11A	H11D	108
C12A	C11A	H11C	108
C12A	C11A	H11D	109
H11C	C11A	H11D	108
H22C	C22A	H22D	108
H22C	C22A	C21A	109
H22C	C22A	C23A	108
H22D	C22A	C21A	109
H22D	C22A	C23A	109
C21A	C22A	C23A	115(1)
C16A	C17A	C18A	116(1)
C16A	C17A	H17C	108
C16A	C17A	H17D	108
C18A	C17A	H17C	108
C18A	C17A	H17D	108
H17C	C17A	H17D	108
C18A	C19A	H19C	107
C18A	C19A	H19D	107
C18A	C19A	C20A	121(1)
H19C	C19A	H19D	107
H19C	C19A	C20A	107
H19D	C19A	C20A	107
C16A	C15A	C14A	115(1)
C16A	C15A	H15C	109
C16A	C15A	H15D	109
C14A	C15A	H15C	109
C14A	C15A	H15D	109
H15C	C15A	H15D	108
C12A	C13A	C14A	116(1)
C12A	C13A	H13C	108
C12A	C13A	H13D	108
C14A	C13A	H13C	108
C14A	C13A	H13D	108
H13C	C13A	H13D	107
C19A	C20A	H20C	107
C19A	C20A	H20D	107
C19A	C20A	C21A	120(1)
H20C	C20A	H20D	107
H20C	C20A	C21A	107
H20D	C20A	C21A	107
C22A	C21A	C20A	111(1)
C22A	C21A	H21C	110
C22A	C21A	H21D	109
C20A	C21A	H21C	109

C20A	C21A	H21D	110
H21C	C21A	H21D	108
C22A	C23A	H23D	109
C22A	C23A	H23E	109
C22A	C23A	H23F	110
H23D	C23A	H23E	109
H23D	C23A	H23F	110
H23E	C23A	H23F	109

3.2.2 Form III

Table S4 shows the complete list of bond lengths of Form III of methyl behenate.

Table S4. Interatomic distances of Form III of methyl behenate from single crystal XRD

Atom1	Atom2	Length (Å)
C001	H00A	0.97
C001	H00B	0.97
C001	C003	1.524(2)
C001	C005	1.519(1)
C002	H00C	0.97
C002	H00D	0.97
C002	C004	1.521(2)
C002	C00A	1.521(2)
C003	H00E	0.97
C003	H00F	0.97
C003	C006	1.521(1)
C004	H00G	0.97
C004	H00H	0.97
C004	C008	1.523(1)
C005	H00I	0.97
C005	H00J	0.97
C006	H00K	0.97
C006	H00L	0.97
C006	C008	1.522(2)
C007	H00M	0.97
C007	H00N	0.97
C007	C00A	1.518(2)
C007	C00B	1.505(2)
C008	H00O	0.97
C008	H00P	0.97
O009	C00B	1.429(2)
O009	C00D	1.488(2)
C00A	H00Q	0.97
C00A	H00R	0.97
C00B	O00C	1.126(3)
C00D	H00U	0.96
C00D	H00V	0.96
C00D	H00W	0.96

Table S5 shows the complete list of bond angles of Form III of methyl behenate.

Table S5. Interatomic angles of Form III of methyl behenate from single crystal XRD

Atom1	Atom2	Atom3	Angle (°)
H00A	C001	H00B	107.7
H00A	C001	C003	108.8
H00A	C001	C005	108.8
H00B	C001	C003	108.8
H00B	C001	C005	108.8
C003	C001	C005	113.69(9)
H00C	C002	H00D	107.7
H00C	C002	C004	108.8
H00C	C002	C00A	108.8
H00D	C002	C004	108.8
H00D	C002	C00A	108.8
C004	C002	C00A	113.83(9)
C001	C003	H00E	108.8
C001	C003	H00F	108.8
C001	C003	C006	113.83(9)
H00E	C003	H00F	107.7
H00E	C003	C006	108.8
H00F	C003	C006	108.8
C002	C004	H00G	108.9
C002	C004	H00H	108.9
C002	C004	C008	113.42(9)
H00G	C004	H00H	107.7
H00G	C004	C008	108.9
H00H	C004	C008	108.9
C001	C005	H00I	108.8
C001	C005	H00J	108.8
C001	C005	C005	113.77(9)
H00I	C005	H00J	107.7
H00I	C005	C005	108.8
H00J	C005	C005	108.8
C003	C006	H00K	108.8
C003	C006	H00L	108.8
C003	C006	C008	113.62(9)
H00K	C006	H00L	107.7
H00K	C006	C008	108.8
H00L	C006	C008	108.9
H00M	C007	H00N	107.6
H00M	C007	C00A	108.7
H00M	C007	C00B	108.7
H00N	C007	C00A	108.7
H00N	C007	C00B	108.7
C00A	C007	C00B	114.1(1)
C004	C008	C006	113.95(9)
C004	C008	H00O	108.8
C004	C008	H00P	108.8
C006	C008	H00O	108.8
C006	C008	H00P	108.8
H00O	C008	H00P	107.6
C00B	O009	C00D	114.2(1)
C002	C00A	C007	112.84(9)

C002	C00A	H00Q	109
C002	C00A	H00R	109
C007	C00A	H00Q	109
C007	C00A	H00R	109
H00Q	C00A	H00R	107.8
C007	C00B	O009	112.7(1)
C007	C00B	O00C	129.5(1)
O009	C00B	O00C	115.6(1)
O009	C00D	H00U	109.5
O009	C00D	H00V	109.5
O009	C00D	H00W	109.5
H00U	C00D	H00V	109.5
H00U	C00D	H00W	109.5
H00V	C00D	H00W	109.5
H00A	C001	H00B	107.7
H00A	C001	C003	108.8
H00A	C001	C005	108.8
H00B	C001	C003	108.8
H00B	C001	C005	108.8
C003	C001	C005	113.69(9)
H00C	C002	H00D	107.7
H00C	C002	C004	108.8
H00C	C002	C00A	108.8
H00D	C002	C004	108.8
H00D	C002	C00A	108.8
C004	C002	C00A	113.83(9)
C001	C003	H00E	108.8
C001	C003	H00F	108.8
C001	C003	C006	113.83(9)
H00E	C003	H00F	107.7
H00E	C003	C006	108.8
H00F	C003	C006	108.8
C002	C004	H00G	108.9
C002	C004	H00H	108.9
C002	C004	C008	113.42(9)
H00G	C004	H00H	107.7
H00G	C004	C008	108.9
H00H	C004	C008	108.9
C005	C005	C001	113.77(9)
C005	C005	H00I	108.8
C005	C005	H00J	108.8
C001	C005	H00I	108.8
C001	C005	H00J	108.8
H00I	C005	H00J	107.7
C003	C006	H00K	108.8
C003	C006	H00L	108.8
C003	C006	C008	113.62(9)
H00K	C006	H00L	107.7
H00K	C006	C008	108.8
H00L	C006	C008	108.9
H00M	C007	H00N	107.6
H00M	C007	C00A	108.7

H00M	C007	C00B	108.7
H00N	C007	C00A	108.7
H00N	C007	C00B	108.7
C00A	C007	C00B	114.1(1)
C004	C008	C006	113.95(9)
C004	C008	H00O	108.8
C004	C008	H00P	108.8
C006	C008	H00O	108.8
C006	C008	H00P	108.8
H00O	C008	H00P	107.6
C00B	O009	C00D	114.2(1)
C002	C00A	C007	112.84(9)
C002	C00A	H00Q	109
C002	C00A	H00R	109
C007	C00A	H00Q	109
C007	C00A	H00R	109
H00Q	C00A	H00R	107.8
C007	C00B	O009	112.7(1)
C007	C00B	O00C	129.5(1)
O009	C00B	O00C	115.6(1)
O009	C00D	H00U	109.5
O009	C00D	H00V	109.5
O009	C00D	H00W	109.5
H00U	C00D	H00V	109.5
H00U	C00D	H00W	109.5
H00V	C00D	H00W	109.5

3.3 Synchrotron Powder X-Ray Diffraction studies

Powder patterns of methyl behenate were recorded *in-situ* at the I11 beamline in Diamond Light Source while performing heating/cooling cycles at 1K/min.

Figure A4 shows the patterns recorded during the first heating cycle from room temperature (circa 24°C) to 70°C at rates of 1K/min. Minor shifts to lower 2θ associated to thermal expansion were visible, but no phase transitions were observed up to the onset of melting (~ 56°C). The sample was completely molten by ~ 59°C

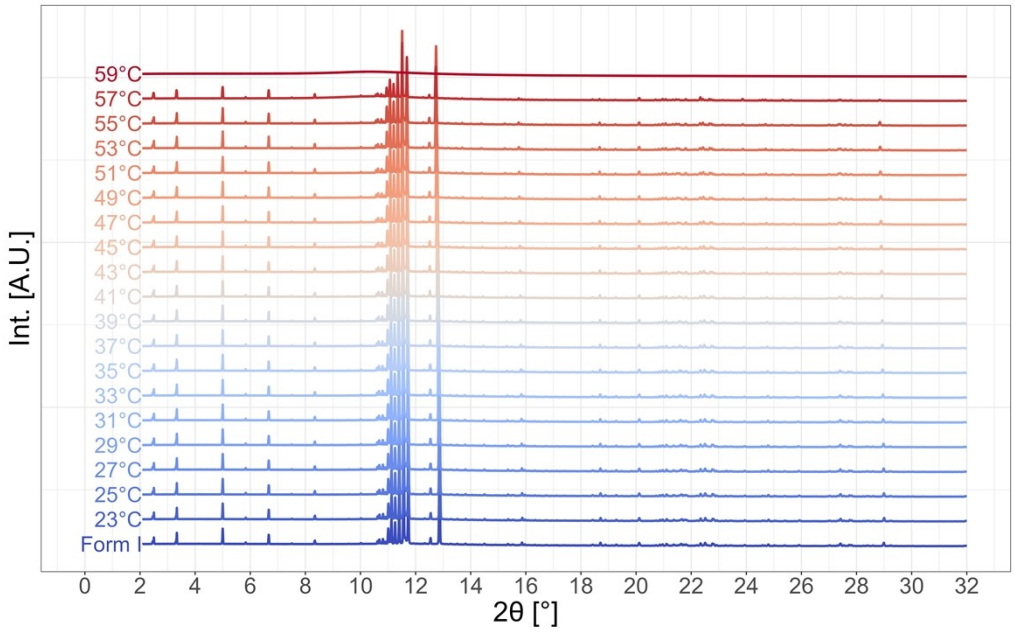

Figure A4. Powder pattern of MEBE recorded in-situ at I11 during the first heating cycle at 1K/min. The curves are colour coded based on the temperatures (blue: colder, red: hotter) and the labels indicate the temperature [°C] at which the pattern was recorded. Int. on the y-axis stands for intensity.

Figure A5 shows the patterns recorded during the first cooling cycle from 70°C to room temperature (24°C) at rates of 1K/min. The onset of crystallisation was observed at ~ 49°C analogous to the onset of crystallisation observed in the DSC experiment, and was complete by 45°C. No distinct peaks from Form II were observed, while a powder pattern consistent with that of Form III was visible at room temperature. In the plot, the powder pattern of Form I is shown to allow a comparison with the pattern of Form III, observed at room temperature.

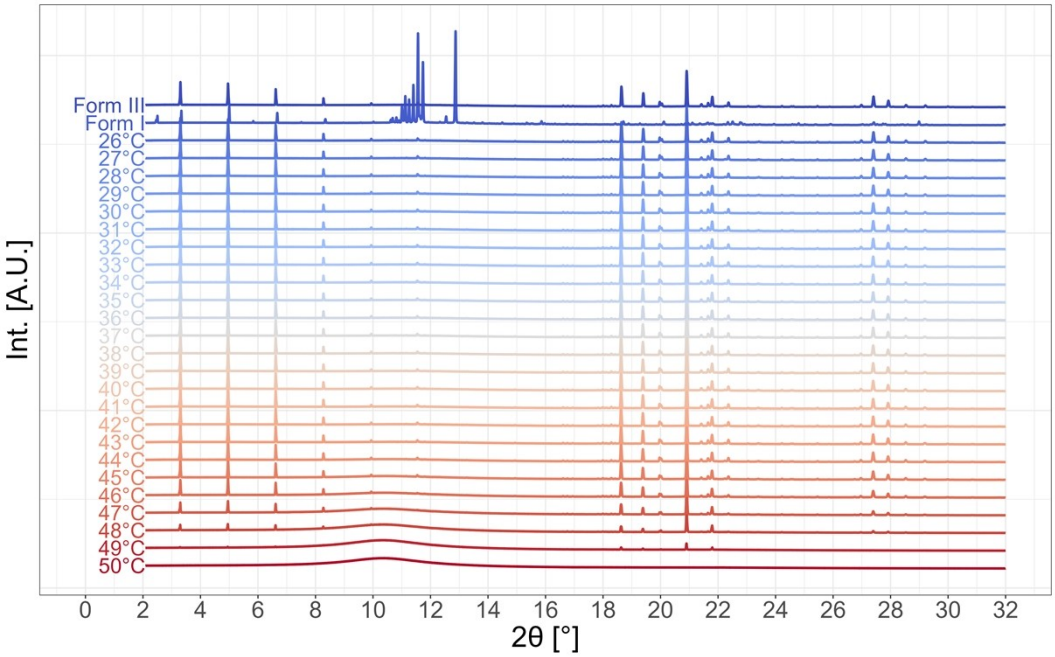

Figure A5. Powder pattern of MEBE recorded in-situ at I11 during the first cooling cycle at 1K/min. The curves are colour coded based on the temperatures (blue: colder, red: hotter) and the labels indicate the temperature [°C] at which the pattern was recorded. Int. on the y-axis stands for intensity.

Figure A6 shows the patterns recorded during the second heating cycle from room temperature (circa 24°C) to 70°C at rates of 1K/min. The onset of melting was observed at ~ 52°C analogous to the onset of melting observed in the DSC experiment, and was complete by 57°C. In the plot, the powder pattern of Form I is shown to allow a comparison with the pattern of Form III, observed at room temperature.

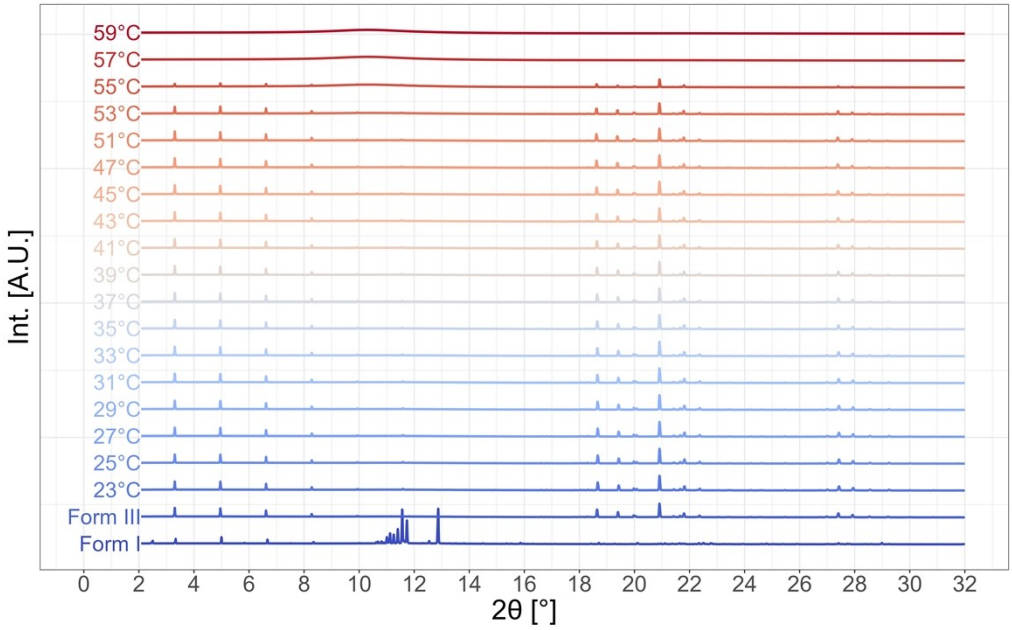

Figure A6. Powder pattern of MEBE recorded in-situ at I11 during the second heating cycle at 1K/min. The curves are colour coded based on the temperatures (blue: colder, red: hotter) and the labels indicate the temperature [°C] at which the pattern was recorded. Int. on the y-axis stands for intensity.