# Chapter 7 – Appendices

## Appendix 3.1 Example soft bond distance and bond angle restraints

TOPAS soft bond distance and bond angle restraint example for the MS-*C*2 phase. These text files are inputted to prevent atoms moving to unrealistic positions and angles to retain sensible structures. For all other molecules used in this project text files similar to this were created with the same level of restraint applied.

```
'=====Bond Distance Restrain=====
'C-C chain
Distance_Restrain(C3 C17, 1.54, 0, 0, 1)
Distance_Restrain(C17 C13, 1.54, 0, 0, 1)
Distance_Restrain(C13 C14, 1.54, 0, 0, 1)
Distance_Restrain(C14 C7, 1.54, 0, 0, 1)
Distance_Restrain(C7 C15, 1.54, 0, 0, 1)
Distance_Restrain(C15 C10, 1.54, 0, 0, 1)
Distance_Restrain(C10 C6, 1.54, 0, 0, 1)
Distance_Restrain(C6 C8, 1.54, 0, 0, 1)
Distance_Restrain(C8 C2, 1.54, 0, 0, 1)
Distance_Restrain(C2 C19, 1.54, 0, 0, 1)
Distance_Restrain(C19 C18, 1.54, 0, 0, 1)
Distance_Restrain(C18 C9, 1.54, 0, 0, 1)
Distance_Restrain(C9 C12, 1.54, 0, 0, 1)
Distance_Restrain(C12 C16, 1.54, 0, 0, 1)
Distance_Restrain(C16 C5, 1.54, 0, 0, 1)
Distance_Restrain(C5 C4, 1.54, 0, 0, 1)
Distance_Restrain(C4 C11, 1.54, 0, 0, 1)

Distance_Restrain(C11 O20, 1.50, 0, 0, 1)
Distance_Restrain(C11 O21, 1.50, 0, 0, 1)
Distance_Restrain(C1 O21, 2.00, 0, 0, 1)

'=====Bond Angle Restrain===
'C-C-C angles -chain
Angle_Restrain(C3 C17 C13, 109.5, 0, 0, 0.001)
Angle_Restrain(C17 C13 C14, 109.5, 0, 0, 0.001)
Angle_Restrain(C13 C14 C7, 109.5, 0, 0, 0.001)
Angle_Restrain(C14 C7 C15, 109.5, 0, 0, 0.001)
Angle_Restrain(C7 C15 C10, 109.5, 0, 0, 0.001)
Angle_Restrain(C15 C10 C6, 109.5, 0, 0, 0.001)
```

```
Angle_Restrain(C10 C6 C8, 109.5, 0, 0, 0.001)
Angle_Restrain(C6 C8 C2, 109.5, 0, 0, 0.001)
Angle_Restrain(C8 C2 C19, 109.5, 0, 0, 0.001)
Angle_Restrain(C2 C19 C18, 109.5, 0, 0, 0.001)
Angle_Restrain(C19 C18 C9, 109.5, 0, 0, 0.001)
Angle_Restrain(C18 C9 C12, 109.5, 0, 0, 0.001)
Angle_Restrain(C9 C12 C16, 109.5, 0, 0, 0.001)
Angle_Restrain(C12 C16 C5, 109.5, 0, 0, 0.001)
Angle_Restrain(C16 C5 C4, 109.5, 0, 0, 0.001)
Angle_Restrain(C5 C4 C11, 109.5, 0, 0, 0.001)

'120 degree geometry
Angle_Restrain(C4 C11 O20, 125, 0, 0, 0.001)
Angle_Restrain(O21 C11 O20, 120, 0, 0, 0.001)
Angle_Restrain(O21 C11 C4, 111, 0, 0, 0.001)
```

## Appendix 3.1.1 Atomic positions of MS-*Pnab* refinement with methyl stearate as bought lab data

**Table 7.1 Atomic positions of MS-*Pnab* refinement with methyl stearate as bought lab data.**

| Atom Number | *x* | *y* | *z* |
|---|---|---|---|
| **C1** | 0.722(5) | 0.278(4) | 0.0373(3) |
| **C2** | 0.735(4) | 0.264(3) | 0.1371(2) |
| **C3** | 0.801(4) | 0.234(4) | 0.1565(3) |
| **C4** | 0.579(4) | 0.191(4) | 0.1654(3) |
| **C5** | 0.595(5) | 0.278(4) | 0.1776(2) |
| **C6** | 0.444(4) | 0.166(4) | 0.1888(2) |
| **C7** | 0.337(4) | 0.327(4) | 0.2036(3) |
| **C8** | 0.076(4) | 0.282(5) | 0.2124(3) |
| **C9** | 0.160(4) | 0.267(5) | 0.2266(3) |
| **C10** | 0.022(4) | 0.170(5) | 0.2329(3) |
| **C11** | 0.486(3) | 0.234(4) | 0.0089(3) |
| **C12** | 0.720(5) | 0.171(4) | 0.0463(3) |
| **C13** | 0.585(4) | 0.288(5) | 0.0592(3) |
| **C14** | 0.476(5) | 0.190(4) | 0.0666(3) |
| **C15** | 0.410(4) | 0.306(4) | 0.0828(3) |
| **C16** | 0.258(4) | 0.188(3) | 0.0905(3) |
| **C17** | 0.199(4) | 0.283(4) | 0.1077(3) |
| **C18** | 0.043(4) | 0.196(5) | 0.1143(2) |
| **C19** | 0.116(3) | 0.236(4) | 0.1325(2) |
| **O1** | 0.905(3) | 0.230(3) | 0.0219(2) |
| **O2** | 0.277(2) | 0.304(2) | 0.0365(2) |

### 3.1.2 Atomic positions of MS-*Pnab* refinement with methyl stearate as bought synchrotron data

**Table 7.2 Atomic positions of MS-*Pnab* refinement with methyl stearate as bought synchrotron data.**

| Atom Number | *x* | *y* | *z* |
|---|---|---|---|
| **C1** | 0.537(4) | 0.189(3) | 0.0431(2) |
| **C2** | 0.727(3) | 0.264(4) | 0.1420(2) |
| **C3** | 0.820(3) | 0.257(4) | 0.1633(2) |
| **C4** | 0.520(4) | 0.163(3) | 0.1759(2) |
| **C5** | 0.453(4) | 0.303(4) | 0.1886(2) |
| **C6** | 0.232(3) | 0.258(4) | 0.1955(2) |
| **C7** | 0.324(5) | 0.286(4) | 0.2110(3) |
| **C8** | 0.235(5) | 0.197(4) | 0.2179(3) |
| **C9** | 0.219(5) | 0.284(5) | 0.2282(3) |
| **C10** | 0.138(5) | 0.202(4) | 0.2366(3) |
| **C11** | 0.420(3) | 0.224(3) | 0.0086(2) |
| **C12** | 0.605(4) | 0.208(4) | 0.0584(3) |
| **C13** | 0.441(4) | 0.297(3) | 0.0650(3) |
| **C14** | 0.461(5) | 0.191(3) | 0.0785(2) |
| **C15** | 0.457(4) | 0.308(3) | 0.0907(2) |
| **C16** | 0.195(4) | 0.183(3) | 0.1038(2) |
| **C17** | 0.140(4) | 0.310(3) | 0.1149(2) |
| **C18** | 0.007(4) | 0.232(4) | 0.1332(2) |
| **C19** | 0.212(3) | 0.271(4) | 0.1470(2) |
| **O1** | 0.897(2) | 0.252(2) | 0.0230(1) |
| **O2** | 0.116(2) | 0.291(2) | 0.0353(1) |

### 3.1.3 Atomic positions of MS-*C*2 refinement with the methyl stearate from the melt lab data

**Table 7.3 Atomic positions of MS-*C*2 refinement with methyl stearate from the melt lab data.**

| Atom Number | *x* | *y* | *z* |
|---|---|---|---|
| **C1** | 0.473(1) | 0.210(3) | 2.318(9) |
| **C2** | 0.235(1) | 0.194(3) | 1.25(1) |
| **C3** | 0.033(1) | 0.246(4) | 0.18(1) |
| **C4** | 0.406(1) | 0.323(3) | 1.87(1) |
| **C5** | 0.378(1) | 0.217(3) | 1.87(1) |
| **C6** | 0.188(1) | 0.200(3) | 1.05(1) |
| **C7** | 0.126(1) | 0.244(3) | 0.61(1) |
| **C8** | 0.218(1) | 0.275(3) | 1.04(1) |
| **C9** | 0.312(1) | 0.286(3) | 1.46(1) |
| **C10** | 0.171(1) | 0.282(4) | 0.84(1) |
| **C11** | 0.427(1) | 0.229(3) | 2.04(1) |
| **C12** | 0.330(1) | 0.199(3) | 1.66(1) |
| **C13** | 0.080(1) | 0.249(3) | 0.40(1) |
| **C14** | 0.094(1) | 0.235(3) | 0.64(1) |
| **C15** | 0.141(1) | 0.211(3) | 0.85(1) |
| **C16** | 0.360(1) | 0.272(3) | 1.64(1) |
| **C17** | 0.048(1) | 0.237(3) | 0.42(1) |
| **C18** | 0.284(1) | 0.185(3) | 1.44(1) |
| **C19** | 0.264(1) | 0.291(3) | 1.27(1) |
| **O20** | 0.4192(7) | 0.136(3) | 2.27(1) |
| **O21** | 0.4559(7) | 0.304(3) | 2.012(7) |

### 3.1.4 Atomic positions of MS-*Cc* refinement with methyl stearate quench cooled melt phase at 4.2 K

**Table 7.4 Atomic positions of MS-*Cc* refinement with methyl stearate quench cooled melt phase at 4.2 K.**

| Atom Number | *x* | *y* | *z* |
|---|---|---|---|
| **C1** | 0.470(2) | 0.287(7) | 1.836(3) |
| **C2** | 0.236(2) | 0.304(7) | 1.304(3) |
| **C3** | 0.032(2) | 0.223(7) | 0.633(3) |
| **C4** | 0.412(2) | 0.207(7) | 1.540(3) |
| **C5** | 0.380(2) | 0.259(7) | 1.658(4) |
| **C6** | 0.189(1) | 0.309(8) | 1.176(3) |
| **C7** | 0.124(3) | 0.203(7) | 0.901(3) |
| **C8** | 0.217(3) | 0.198(8) | 1.156(2) |
| **C9** | 0.313(3) | 0.200(7) | 1.379(3) |
| **C10** | 0.169(2) | 0.189(8) | 1.058(2) |
| **C11** | 0.431(3) | 0.270(6) | 1.717(3) |
| **C12** | 0.330(2) | 0.270(7) | 1.570(3) |
| **C13** | 0.077(2) | 0.193(6) | 0.785(3) |
| **C14** | 0.094(3) | 0.294(7) | 0.947(3) |
| **C15** | 0.142(2) | 0.304(7) | 1.063(3) |
| **C16** | 0.363(3) | 0.251(7) | 1.449(2) |
| **C17** | 0.047(4) | 0.273(7) | 0.846(2) |
| **C18** | 0.283(3) | 0.288(7) | 1.443(2) |
| **C19** | 0.265(2) | 0.195(8) | 1.275(3) |
| **O20** | 0.421(3) | 0.314(8) | 1.989(2) |
| **O21** | 0.461(3) | 0.215(7) | 1.612(3) |

### 3.1.5 Atomic positions of MS-*Cc* refinement with methyl stearate quench cooled melt phase at 193 K

**Table 7.5 Atomic positions of MS-*Cc* refinement with methyl stearate quench cooled melt phase at 193K.**

| Atom Number | *x* | *y* | *z* |
|---|---|---|---|
| **C1** | 0.474(2) | 0.298(6) | 1.810(3) |
| **C2** | 0.236(3) | 0.302(6) | 1.304(2) |
| **C3** | 0.033(3) | 0.233(6) | 0.626(3) |
| **C4** | 0.412(3) | 0.211(6) | 1.540(4) |
| **C5** | 0.380(2) | 0.254(6) | 1.664(3) |
| **C6** | 0.189(3) | 0.310(6) | 1.167(4) |
| **C7** | 0.124(3) | 0.208(6) | 0.892(3) |
| **C8** | 0.217(2) | 0.200(6) | 1.151(3) |
| **C9** | 0.313(3) | 0.207(7) | 1.375(4) |
| **C10** | 0.168(3) | 0.189(6) | 1.057(3) |
| **C11** | 0.431(3) | 0.270(5) | 1.718(2) |
| **C12** | 0.330(3) | 0.258(6) | 1.578(3) |
| **C13** | 0.077(2) | 0.195(6) | 0.775(4) |
| **C14** | 0.095(3) | 0.295(6) | 0.937(4) |
| **C15** | 0.141(2) | 0.301(6) | 1.064(4) |
| **C16** | 0.362(3) | 0.260(6) | 1.457(2) |
| **C17** | 0.047(2) | 0.2611(6) | 0.846(3) |
| **C18** | 0.282(3) | 0.283(6) | 1.450(4) |
| **C19** | 0.264(4) | 0.192(6) | 1.281(3) |
| **O20** | 0.422(4) | 0.320(6) | 1.985(3) |
| **O21** | 0.461(2) | 0.206(6) | 1.620(2) |

### 3.1.6 Atomic positions of ES-*Aa* refinement with ethyl stearate as bought lab data

**Table 7.6 Atomic positions of ES-*Aa* refinement with ethyl stearate as bought lab data.**

| Atom Number | *x* | *y* | *z* |
|---|---|---|---|
| **C1** | 0.113(3) | 0.24(2) | 0.080(2) |
| **C10** | -0.124(3) | 0.21(2) | 0.290(3) |
| **C100** | 0.139(2) | 0.24(1) | 0.036(3) |
| **C11** | -0.048(2) | 0.30(1) | 0..314(2) |
| **C12** | -0.118(3) | 0.20(2) | 0.334(3) |
| **C13** | -0.040(4) | 0.29(2) | 0.359(4) |
| **C14** | -0.173(2) | 0.19(2) | 0.374(4) |
| **C15** | -0.113(3) | 0.30(2) | 0.398(2) |
| **C16** | -0.225(4) | 0.20(1) | 0.412(3) |
| **C17** | -0.162(2) | 0.29(1) | 0.437(2) |
| **C18** | -0.351(2) | 0.23(1) | 0.446(3) |
| **C2** | -0.046(2) | 0.21(1) | 0.095(3) |
| **C200** | -0.054(3) | 0.24(1) | 0.009(3) |
| **C3** | 0.086(2) | 0.27(1) | 0.127(3) |
| **C4** | -0.063(3) | 0.21(2) | 0.145(2) |
| **C5** | 0.049(3) | 0.29(1) | 0.177(3) |
| **C6** | -0.074(2) | 0.20(2) | 0.195(4) |
| **C7** | 0.042(2) | 0.28(2) | 0.225(3) |
| **C8** | -0.095(3) | 0.21(2) | 0.244(2) |
| **C9** | -0.017(3) | 0.30(2) | 0.272(4) |
| **O1** | -0.036(2) | 0.22(1) | 0.053(3) |
| **O2** | 0.278(3) | 0.337(8) | 0.085(2) |

### 3.1.7 Atomic positions of ES-*Aa* refinement with ethyl stearate as bought synchrotron data

**Table 7.7 Atomic positions of ES-*Aa* refinement with ethyl stearate as bought synchrotron data.**

| Atom Number | *x* | *y* | *z* |
|---|---|---|---|
| **C1** | 0.077(3) | 0.25(2) | 0.083(3) |
| **C10** | -0.146(3) | 0.26(1) | 0.281(3) |
| **C100** | 0.069(3) | 0.31(1) | 0.035(4) |
| **C11** | 0.007(3) | 0.25(1) | 0.312(2) |
| **C12** | -0.123(2) | 0.156(7) | 0.328(3) |
| **C13** | -0.021(2) | 0.23(1) | 0.358(4) |
| **C14** | -0.287(3) | 0.27(1) | 0.367(2) |
| **C15** | -0.156(3) | 0.34(1) | 0.400(2) |
| **C16** | -0.193(4) | 0.200(9) | 0.415(4) |
| **C17** | -0.077(3) | 0.29(1) | 0.445(2) |
| **C18** | -0.180(3) | 0.19(1) | 0.461(3) |
| **C2** | -0.031(2) | 0.19(1) | 0.101(3) |
| **C200** | -0.135(3) | 0.22(1) | 0.008(2) |
| **C3** | 0.121(3) | 0.24(1) | 0.127(4) |
| **C4** | -0.0003(1) | 0.15(1) | 0.147(3) |
| **C5** | 0.038(3) | 0.33(1) | 0.175(4) |
| **C6** | -0.097(3) | 0.255(3) | 0.193(2) |
| **C7** | 0.066(2) | 0.26(1) | 0.220(3) |
| **C8** | -0.064(2) | 0.20(1) | 0.239(3) |
| **C9** | -0.0005(4) | 0.31(1) | 0.263(3) |
| **O1** | -0.059(2) | 0.21(1) | 0.058(2) |
| **O2** | 0.256(3) | 0.300(8) | 0.088(2) |

# Appendix 3.2 Rietveld refinements of thermal expansion scans for MS-*Pnab*

## 3.2.1 Rietveld refinement of figure 3.15 300 K scan

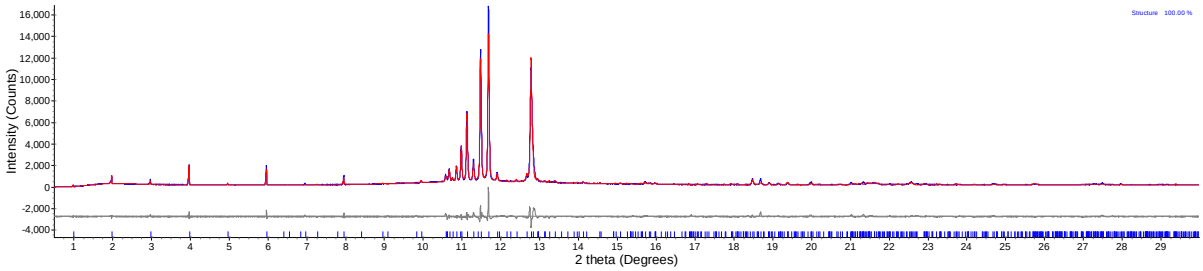


**Figure 7.1 Observed and calculated profiles for the Rietveld refinement of figure 3.15 300 K scan with the MS-*Pnab* structure. The bottom curve is the difference plot on the same intensity scale. ($R_{wp}$ = 10.30, $R_p$ = 7.36, $\chi$ = 2.76). The tick marks represent calculated peak positions.**

**Table 7.8 Refined lattice parameters for figure 3.15 300 K scan Rietveld refinement with the MS-*Pnab* structure.**

| Parameter | Value |
|---|---|
| **Phase / Space group** | MS-*Pnab* / *Pnab* |
| ***a* (Å)** | 5.6236(1) |
| ***b* (Å)** | 7.4172(2) |
| ***c* (Å)** | 95.176(5) |
| **Volume (Å$^3$)** | 3970.0(2) |

## 3.2.2 Rietveld refinement of figure 3.15 275 K scan

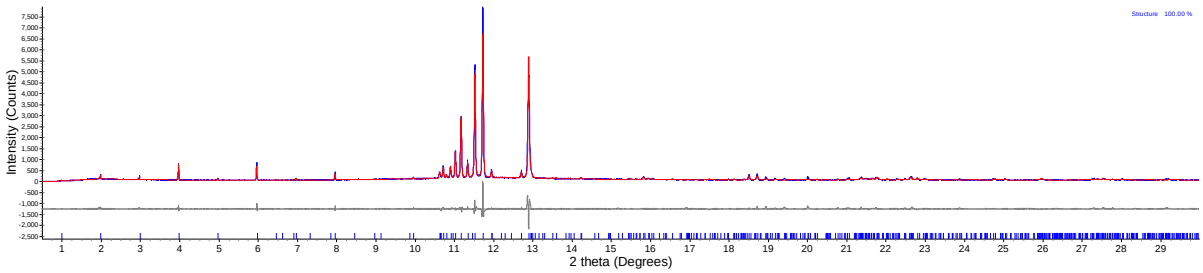


**Figure 7.2 Observed and calculated profiles for the Rietveld refinement of figure 3.15 275 K scan with the MS-*Pnab* structure. The bottom curve is the difference plot on the same intensity scale. ($R_{wp}$ = 11.59, $R_p$ = 8.50, $\chi$ = 1.78). The tick marks represent calculated peak positions.**

**Table 7.9 Refined lattice parameters for figure 3.15 275 K scan Rietveld refinement with the MS-*Pnab* structure.**

| Parameter | Value |
|---|---|
| **Phase / Space group** | MS-*Pnab* / *Pnab* |
| ***a* (Å)** | 5.6151(1) |
| ***b* (Å)** | 7.3514(1) |
| ***c* (Å)** | 95.114(4) |
| **Volume (Å$^3$)** | 3926.2(2) |

### 3.2.3 Rietveld refinement of figure 3.15 250 K scan

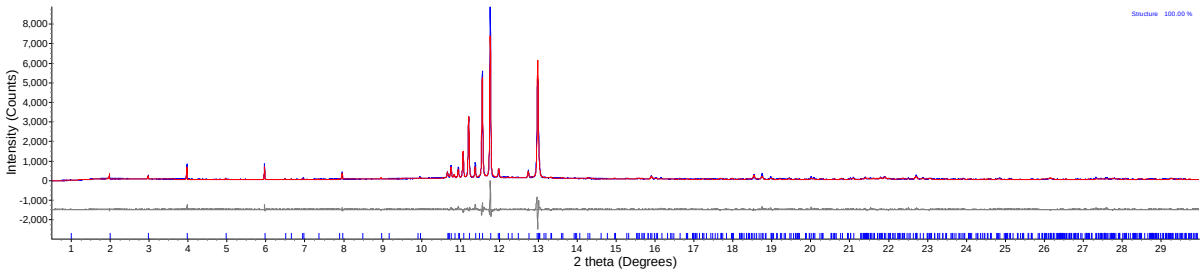


**Figure 7.3 Observed and calculated profiles for the Rietveld refinement of figure 3.15 250 K scan with the MS-*Pnab* structure. The bottom curve is the difference plot on the same intensity scale. ($R_{wp}$ = 12.46, $R_p$ = 9.28, $\chi$ = 1.91). The tick marks represent calculated peak positions.**

**Table 7.10 Refined lattice parameters for figure 3.15 250 K scan Rietveld refinement with the MS-*Pnab* structure.**

| Parameter | Value |
|---|---|
| **Phase / Space group** | MS-*Pnab* / *Pnab* |
| ***a* (Å)** | 5.6025(1) |
| ***b* (Å)** | 7.2982(1) |
| ***c* (Å)** | 95.054(4) |
| **Volume (Å$^3$)** | 3886.6(2) |

### 3.2.4 Rietveld refinement of figure 3.15 225 K scan

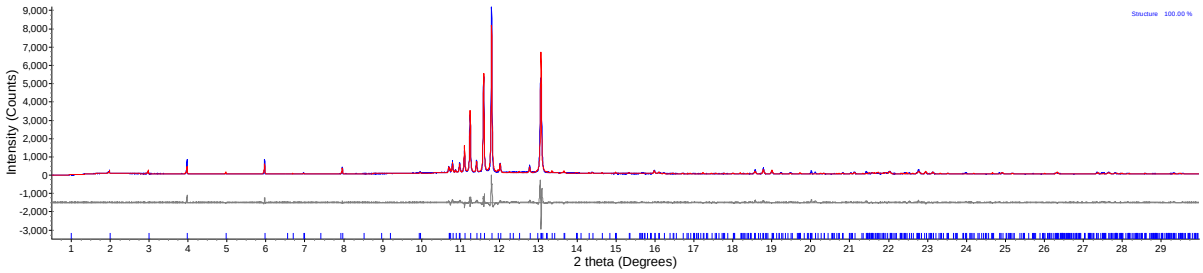


**Figure 7.4 Observed and calculated profiles for the Rietveld refinement of figure 3.15 225 K scan with the MS-*Pnab* structure. The bottom curve is the difference plot on the same intensity scale. ($R_{wp}$ = 16.23, $R_p$ = 12.12, $\chi$ = 2.50). The tick marks represent calculated peak positions.**

**Table 7.11 Refined lattice parameters for figure 3.15 225 K scan Rietveld refinement with the MS-*Pnab* structure.**

| Parameter | Value |
|---|---|
| **Phase / Space group** | MS-*Pnab* / *Pnab* |
| ***a* (Å)** | 5.5922(1) |
| ***b* (Å)** | 7.2512(2) |
| ***c* (Å)** | 95.021(4) |
| **Volume (Å$^3$)** | 3853.1(2) |

## 3.2.5 Rietveld refinement of figure 3.15 200 K scan

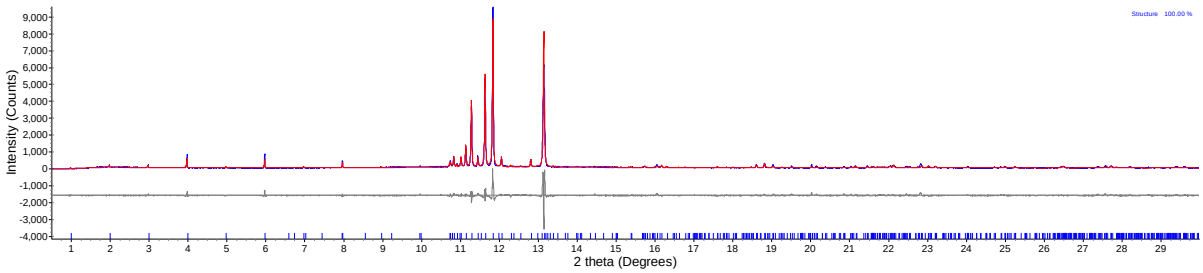


**Figure 7.5 Observed and calculated profiles for the Rietveld refinement of figure 3.15 200 K scan with the MS-*Pnab* structure. The bottom curve is the difference plot on the same intensity scale. ($R_{wp}$ = 16.41, $R_p$ = 12.08, $\chi$ = 2.55). The tick marks represent calculated peak positions.**

**Table 7.12 Refined lattice parameters for figure 3.15 200 K scan Rietveld refinement with the MS-*Pnab* structure.**

| Parameter | Value |
|---|---|
| **Phase / Space group** | MS-*Pnab* / *Pnab* |
| ***a* (Å)** | 5.5804(1) |
| ***b* (Å)** | 7.2112(2) |
| ***c* (Å)** | 94.951(5) |
| **Volume (Å$^3$)** | 3821.0(2) |

## 3.2.6 Rietveld refinement of figure 3.15 175 K scan

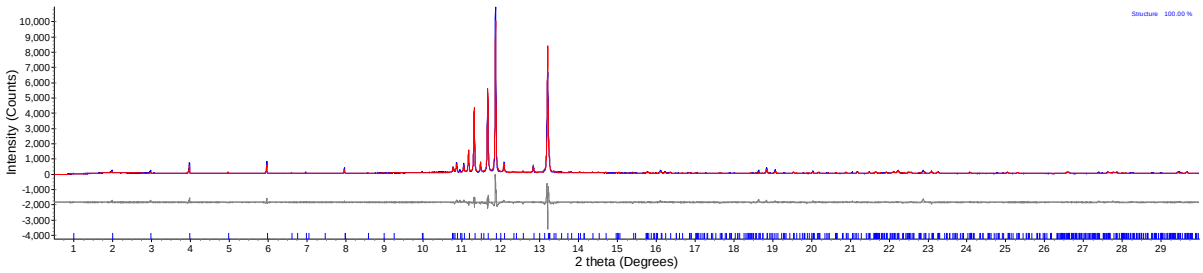


**Figure 7.6 Observed and calculated profiles for the Rietveld refinement of figure 3.15 175 K scan with the MS-*Pnab* structure. The bottom curve is the difference plot on the same intensity scale. ($R_{wp}$ = 16.95, $R_p$ = 12.50, $\chi$ = 2.65). The tick marks represent calculated peak positions.**

**Table 7.13 Refined lattice parameters for figure 3.15 175 K scan Rietveld refinement with the MS-*Pnab* structure.**

| Parameter | Value |
|---|---|
| **Phase / Space group** | MS-*Pnab* / *Pnab* |
| ***a* (Å)** | 5.5696(1) |
| ***b* (Å)** | 7.1765(1) |
| ***c* (Å)** | 94.907(4) |
| **Volume (Å$^3$)** | 3793.4(2) |

## 3.2.7 Rietveld refinement of figure 3.15 150 K scan

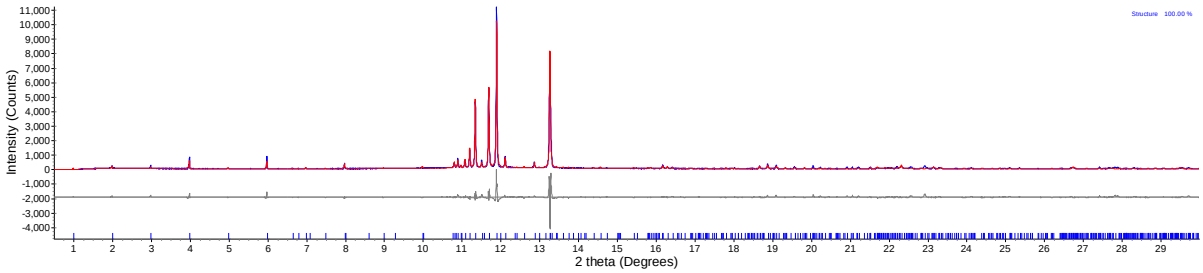


**Figure 7.7 Observed and calculated profiles for the Rietveld refinement of figure 3.15 150 K scan with the MS-*Pnab* structure. The bottom curve is the difference plot on the same intensity scale. ($R_{wp}$ = 18.27, $R_p$ = 13.32, $\chi$ = 2.88). The tick marks represent calculated peak positions.**

**Table 14.7 Refined lattice parameters for figure 3.15 150 K scan Rietveld refinement with the MS-*Pnab* structure.**

| Parameter | Value |
|---|---|
| **Phase / Space group** | MS-*Pnab* / *Pnab* |
| ***a* (Å)** | 5.5606(1) |
| ***b* (Å)** | 7.1453(2) |
| ***c* (Å)** | 94.879(5) |
| **Volume (Å$^3$)** | 3769.8(3) |

## 3.2.8 Rietveld refinement of figure 3.15 125 K scan

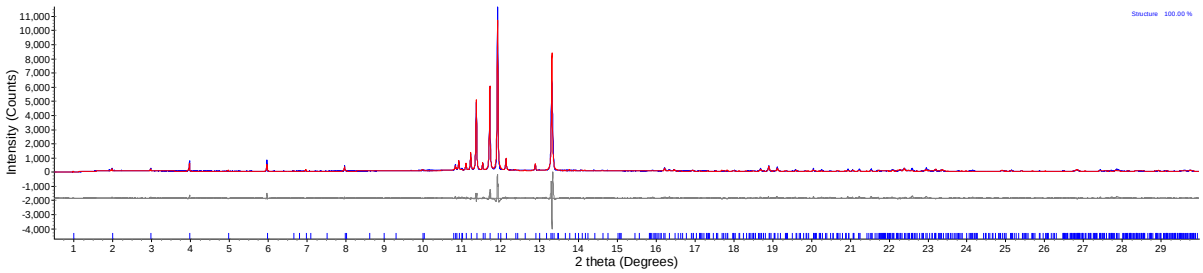


**Figure 7.8 Observed and calculated profiles for the Rietveld refinement of figure 3.15 125 K scan with the MS-*Pnab* structure. The bottom curve is the difference plot on the same intensity scale. ($R_{wp}$ = 16.82, $R_p$ = 12.38, $\chi$ = 2.67). The tick marks represent calculated peak positions.**

**Table 7.15 Refined lattice parameters for figure 3.15 125 K scan Rietveld refinement with the MS-*Pnab* structure.**

| Parameter | Value |
|---|---|
| **Phase / Space group** | MS-*Pnab* / *Pnab* |
| ***a* (Å)** | 5.5517(1) |
| ***b* (Å)** | 7.1193(1) |
| ***c* (Å)** | 94.864(4) |
| **Volume (Å$^3$)** | 3749.4(2) |

## 3.2.9 Rietveld refinement of figure 3.15 100 K scan

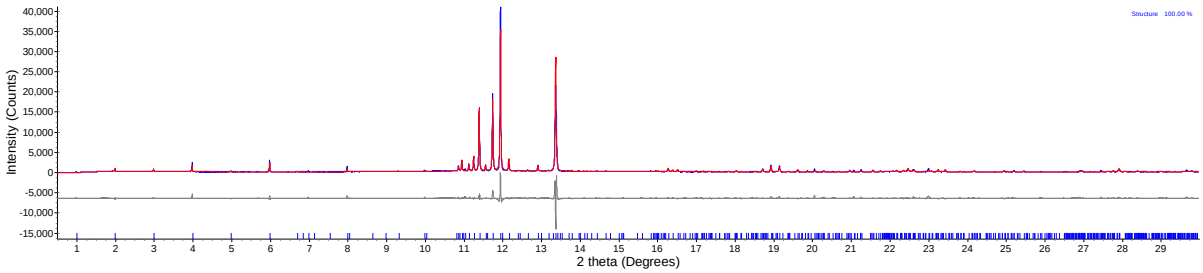


**Figure 7.9 Observed and calculated profiles for the Rietveld refinement of figure 3.15 100 K scan with the MS-*Pnab* structure. The bottom curve is the difference plot on the same intensity scale. ($R_{wp}$ = 16.12, $R_p$ = 11.34, $\chi$ = 4.47). The tick marks represent calculated peak positions.**

**Table 7.16 Refined lattice parameters for figure 3.15 100 K scan Rietveld refinement with the MS-*Pnab* structure.**

| Parameter | Value |
|---|---|
| **Phase / Space group** | MS-*Pnab* / *Pnab* |
| ***a* (Å)** | 5.5440(1) |
| ***b* (Å)** | 7.0916(1) |
| ***c* (Å)** | 94.863(4) |
| **Volume (Å$^3$)** | 3729.7(2) |

# Appendix 3.3 Rietveld refinements of thermal expansion scans for MS-*C*2

## 3.3.1 Rietveld refinement of figure 3.24 295 K scan

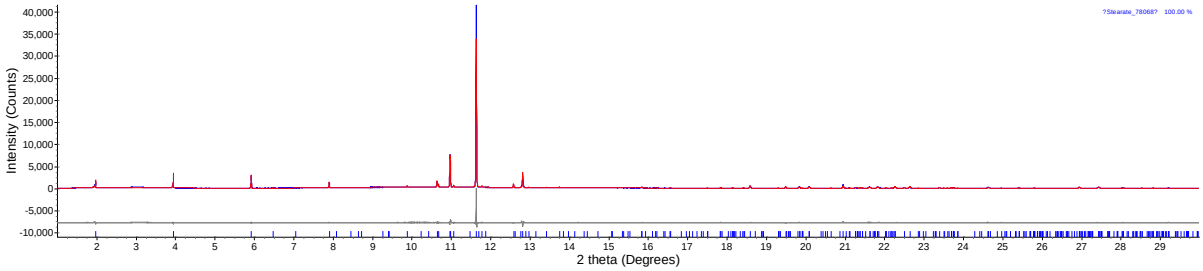


**Figure 7.10 Observed and calculated profiles for the Rietveld refinement of figure 3.24 295 K scan with the MS-*C*2 structure. The bottom curve is the difference plot on the same intensity scale. ($R_{wp}$ = 10.59, $R_p$ = 7.99, $\chi$ = 2.28). The tick marks represent calculated peak positions.**

**Table 7.17 Refined lattice parameters for figure 3.24 295 K scan Rietveld refinement with the MS-*C*2 structure.**

| Parameter | Value |
|---|---|
| **Phase / Space group** | MS-*C*2 / *C*2 |
| ***a* (Å)** | 47.95256(5) |
| ***b* (Å)** | 7.39957(3) |
| ***c* (Å)** | 5.60151(8) |
| ***β* (°)** | 91.1603(4) |
| **Volume (Å$^3$)** | 1987.17(3) |

### 3.3.2 Rietveld refinement of figure 3.24 275 K scan

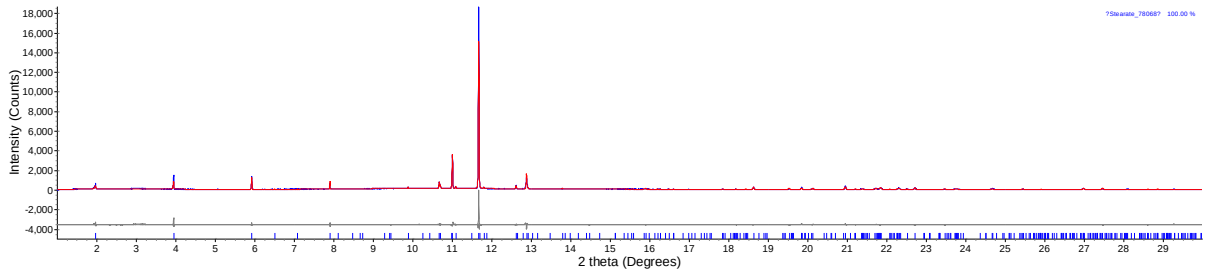


**Figure 7.11 Observed and calculated profiles for the Rietveld refinement of figure 3.24 275 K scan with the MS-*C*2 structure. The bottom curve is the difference plot on the same intensity scale. ($R_{wp}$ = 11.53, $R_p$ = 8.58, $\chi$ = 1.75). The tick marks represent calculated peak positions.**

**Table 7.18 Refined lattice parameters for figure 3.24 275 K scan Rietveld refinement with the MS-*C*2 structure.**

| Parameter | Value |
|---|---|
| **Phase / Space group** | MS-*C*2 / *C*2 |
| ***a* (Å)** | 47.9259(6) |
| ***b* (Å)** | 7.3605(1) |
| ***c* (Å)** | 5.59244(8) |
| ***β* (°)** | 91.054(1) |
| **Volume (Å$^3$)** | 1972.46(5) |

### 3.3.3 Rietveld refinement of figure 3.24 250 K scan

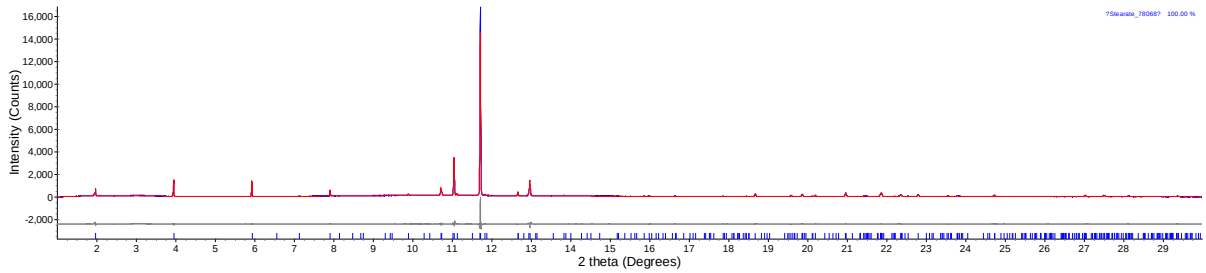


**Figure 7.12 Observed and calculated profiles for the Rietveld refinement of figure 3.24 250 K scan with the MS-*C*2 structure. The bottom curve is the difference plot on the same intensity scale. ($R_{wp}$ = 10.52, $R_p$ = 8.15, $\chi$ = 1.60). The tick marks represent calculated peak positions.**

**Table 7.19 Refined lattice parameters for figure 3.24 250 K scan Rietveld refinement with the MS-*C*2 structure.**

| Parameter | Value |
|---|---|
| **Phase / Space group** | MS-*C*2 / *C*2 |
| ***a* (Å)** | 47.8996(9) |
| ***b* (Å)** | 7.3138(1) |
| ***c* (Å)** | 5.58322(8) |
| ***β* (°)** | 90.930(1) |
| **Volume (Å$^3$)** | 1955.69(6) |

### 3.3.4 Rietveld refinement of figure 3.24 225 K scan

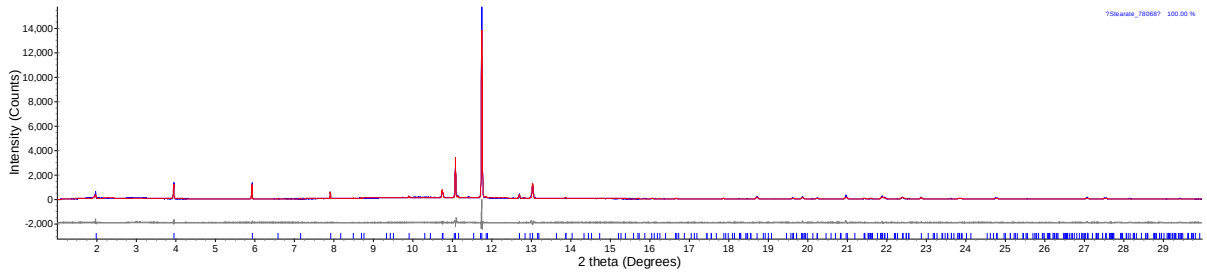


**Figure 7.13 Observed and calculated profiles for the Rietveld refinement of figure 3.24 225 K scan with the MS-*C*2 structure. The bottom curve is the difference plot on the same intensity scale. ($R_{wp}$ = 11.46, $R_p$ = 8.59, $\chi$ = 1.74). The tick marks represent calculated peak positions.**

**Table 7.20 Refined lattice parameters for figure 3.24 225 K scan Rietveld refinement with the MS-*C*2 structure.**

| Parameter | Value |
|---|---|
| **Phase / Space group** | MS-*C*2 / *C*2 |
| ***a* (Å)** | 47.8599(4) |
| ***b* (Å)** | 7.2742(1) |
| ***c* (Å)** | 5.5726(1) |
| ***β* (°)** | 90.824(3) |
| **Volume (Å$^3$)** | 1939.87(6) |

### 3.3.5 Rietveld refinement of figure 3.24 200 K scan

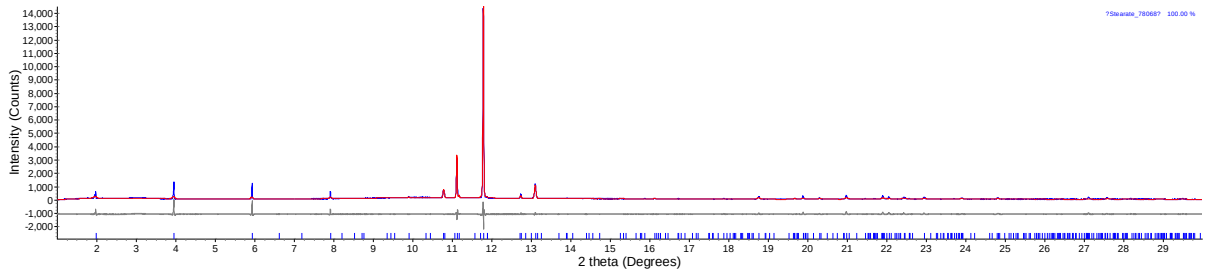


**Figure 7.14 Observed and calculated profiles for the Rietveld refinement of figure 3.24 200 K scan with the MS-*C*2 structure. The bottom curve is the difference plot on the same intensity scale. ($R_{wp}$ = 15.27, $R_p$ = 9.82, $\chi$ = 2.33). The tick marks represent calculated peak positions.**

**Table 7.21 Refined lattice parameters for figure 3.24 200 K scan Rietveld refinement with the MS-*C*2 structure.**

| Parameter | Value |
|---|---|
| **Phase / Space group** | MS-*C*2 / *C*2 |
| ***a* (Å)** | 47.839(9) |
| ***b* (Å)** | 7.2370(2) |
| ***c* (Å)** | 5.5618(5) |
| ***β* (°)** | 90.717(5) |
| **Volume (Å$^3$)** | 1925.43(4) |

## 3.3.6 Rietveld refinement of figure 3.24 175 K scan

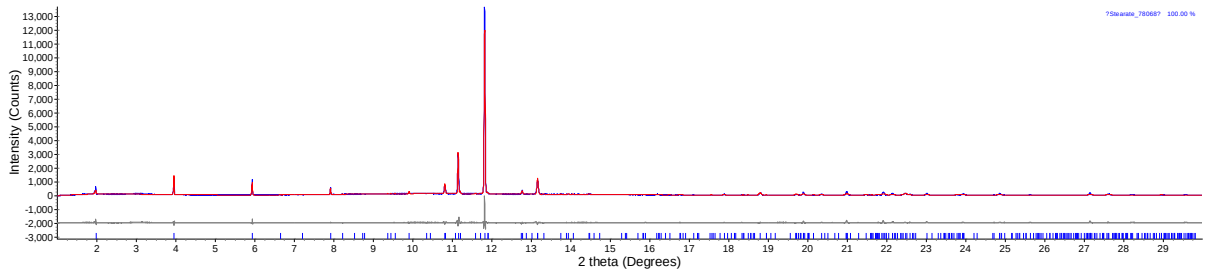


**Figure 7.15 Observed and calculated profiles for the Rietveld refinement of figure 3.24 175 K scan with the MS-*C*2 structure. The bottom curve is the difference plot on the same intensity scale. ($R_{wp}$ = 11.99, $R_p$ = 8.94, $\chi$ = 1.84). The tick marks represent calculated peak positions.**

**Table 7.22 Refined lattice parameters for figure 3.24 175 K scan Rietveld refinement with the MS-*C*2 structure.**

| Parameter | Value |
|---|---|
| **Phase / Space group** | MS-*C*2 / *C*2 |
| ***a* (Å)** | 47.817(2) |
| ***b* (Å)** | 7.2049(3) |
| ***c* (Å)** | 5.5540(2) |
| ***β* (°)** | 90.608(3) |
| **Volume (Å$^3$)** | 1913.3(2) |

## 3.3.7 Rietveld refinement of figure 3.24 150 K scan

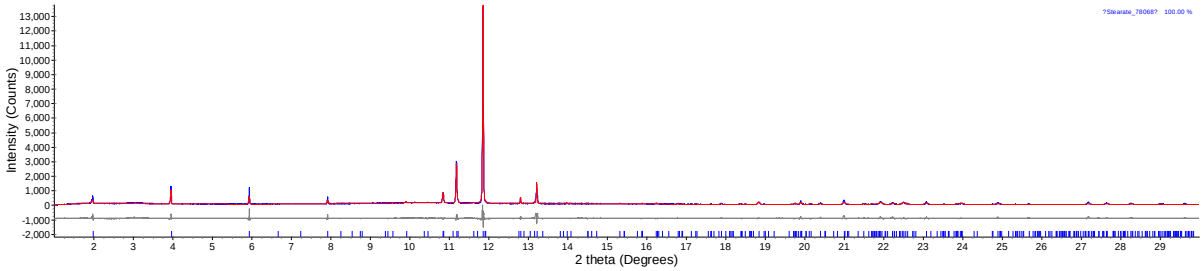


**Figure 7.16 Observed and calculated profiles for the Rietveld refinement of figure 3.24 150 K scan with the MS-*C*2 structure. The bottom curve is the difference plot on the same intensity scale. ($R_{wp}$ = 13.06, $R_p$ = 9.22, $\chi$ = 2.01). The tick marks represent calculated peak positions.**

**Table 7.23 Refined lattice parameters for figure 3.24 150 K scan Rietveld refinement with the MS-*C*2 structure.**

| Parameter | Value |
|---|---|
| **Phase / Space group** | MS-*C*2 / *C*2 |
| ***a* (Å)** | 47.795(3) |
| ***b* (Å)** | 7.1754(2) |
| ***c* (Å)** | 5.5448(2) |
| ***β* (°)** | 90.497(3) |
| **Volume (Å$^3$)** | 1901.5(2) |

### 3.3.8 Rietveld refinement of figure 3.24 125 K scan

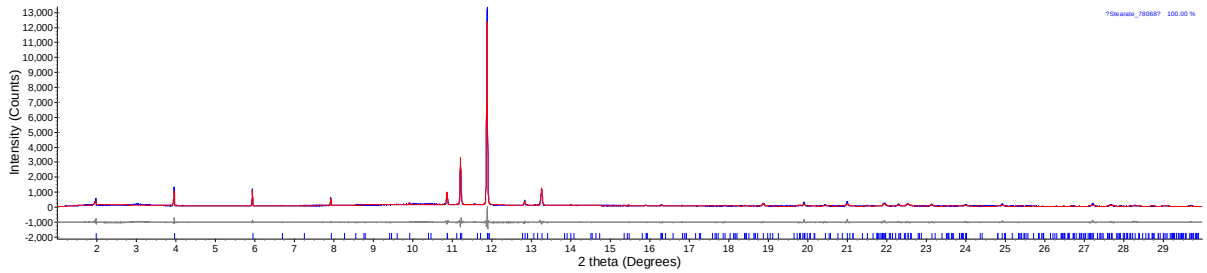


**Figure 7.17 Observed and calculated profiles for the Rietveld refinement of figure 3.24 125 K scan with the MS-*C*2 structure. The bottom curve is the difference plot on the same intensity scale. ($R_{wp}$ = 11.28, $R_p$ = 8.20, $\chi$ = 1.75). The tick marks represent calculated peak positions.**

**Table 7.24 Refined lattice parameters for figure 3.24 125 K scan Rietveld refinement with the MS-*C*2 structure.**

| Parameter | Value |
|---|---|
| **Phase / Space group** | MS-*C*2 / *C*2 |
| ***a* (Å)** | 47.7780(6) |
| ***b* (Å)** | 7.1503(1) |
| ***c* (Å)** | 5.5366(1) |
| ***β* (°)** | 90.402(3) |
| **Volume (Å$^3$)** | 1891.42(6) |

## 3.3.9 Rietveld refinement of figure 3.24 100 K scan

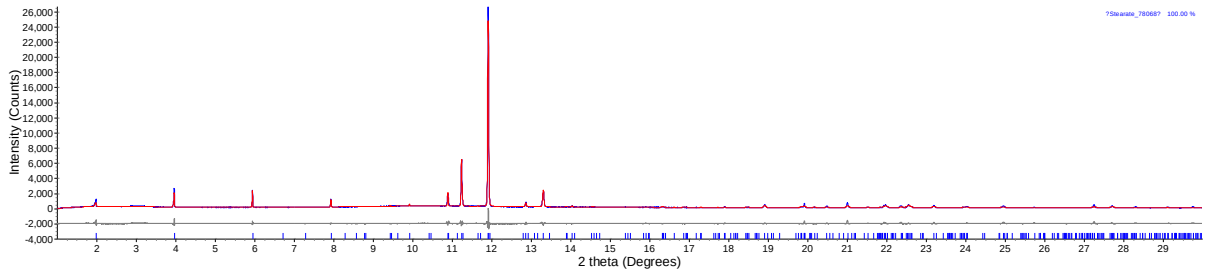


**Figure 7.18 Observed and calculated profiles for the Rietveld refinement of figure 3.24 100 K scan with the MS-*C*2 structure. The bottom curve is the difference plot on the same intensity scale. ($R_{wp}$ = 10.94, $R_p$ = 7.68, $\chi$ = 2.42). The tick marks represent calculated peak positions.**

**Table 7.25 Refined lattice parameters for figure 3.24 100 K scan Rietveld refinement with the MS-*C*2 structure.**

| Parameter | Value |
|---|---|
| **Phase / Space group** | MS-*C*2 / *C*2 |
| ***a* (Å)** | 47.759(1) |
| ***b* (Å)** | 7.12710(8) |
| ***c* (Å)** | 5.5287(3) |
| ***β* (°)** | 90.305(4) |
| **Volume (Å$^3$)** | 1881.8(1) |

# Appendix 3.4 Rietveld refinements of recrystallisations of Methyl Stearate

## 3.4.1 Rietveld refinement of figure 3.30 line C

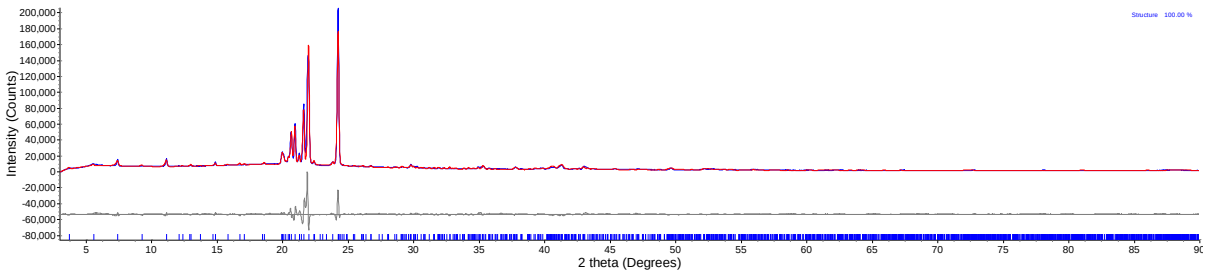


**Figure 7.19 Observed and calculated profiles for the Rietveld refinement of figure 3.30 line C with the MS-*Pnab* structure. The bottom curve is the difference plot on the same intensity scale. ($R_{wp}$ = 12.97, $R_p$ = 9.26, $\chi$ = 9.59). The tick marks represent calculated peak positions.**

**Table 7.26 Refined lattice parameters for figure 3.30 line C Rietveld refinement with the MS-*Pnab* structure.**

| Parameter | Value |
|---|---|
| **Phase / Space group** | MS-*Pnab* / *Pnab* |
| ***a* (Å)** | 5.6149(7) |
| ***b* (Å)** | 7.3375(7) |
| ***c* (Å)** | 95.27(2) |
| **Volume (Å$^3$)** | 3925.3(9) |

## 3.4.2 Rietveld refinement of figure 3.30 line D

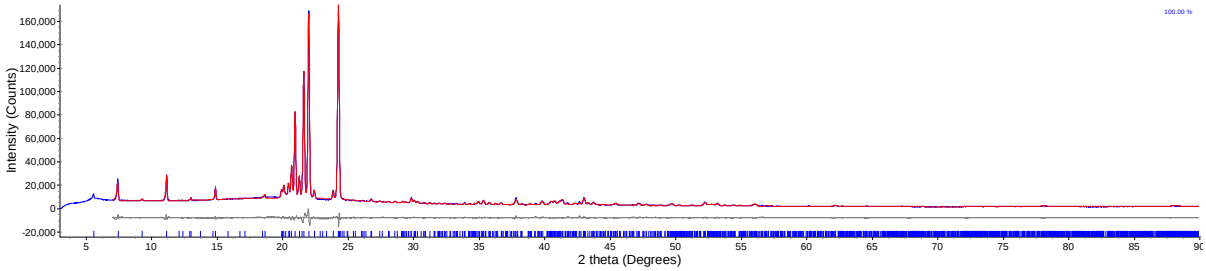


**Figure 7.20 Observed and calculated profiles for the Rietveld refinement of figure 3.30 line D with the MS-*Pnab* structure. The bottom curve is the difference plot on the same intensity scale. ($R_{wp}$ = 5.20, $R_p$ = 3.83, $\chi$ = 3.84). The tick marks represent calculated peak positions.**

**Table 7.27 Refined lattice parameters for figure 3.30 line D Rietveld refinement with the MS-*Pnab* structure.**

| Parameter | Value |
|---|---|
| **Phase / Space group** | MS-*Pnab* / *Pnab* |
| ***a* (Å)** | 5.6144(3) |
| ***b* (Å)** | 7.3338(4) |
| ***c* (Å)** | 95.150(6) |
| **Volume (Å$^3$)** | 3917.8(4) |

### 3.4.3 Rietveld refinement of figure 3.30 line E

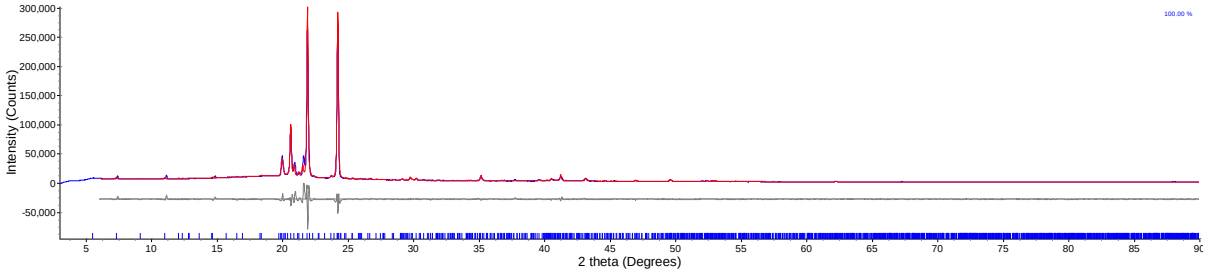


**Figure 7.21 Observed and calculated profiles for the Rietveld refinement of figure 3.30 line E with the MS-*Pnab* structure. The bottom curve is the difference plot on the same intensity scale. ($R_{wp}$ = 11.12, $R_p$ = 7.31, $\chi$ = 8.83). The tick marks represent calculated peak positions.**

**Table 7.28 Refined lattice parameters for figure 3.30 line E Rietveld refinement with the MS-*Pnab* structure.**

| Parameter | Value |
|---|---|
| **Phase / Space group** | MS-*Pnab* / *Pnab* |
| ***a* (Å)** | 5.6349(5) |
| ***b* (Å)** | 7.3569(5) |
| ***c* (Å)** | 96.66(1) |
| **Volume (Å$^3$)** | 4006.9(6) |

### 3.4.4 Rietveld refinement of figure 3.30 line F

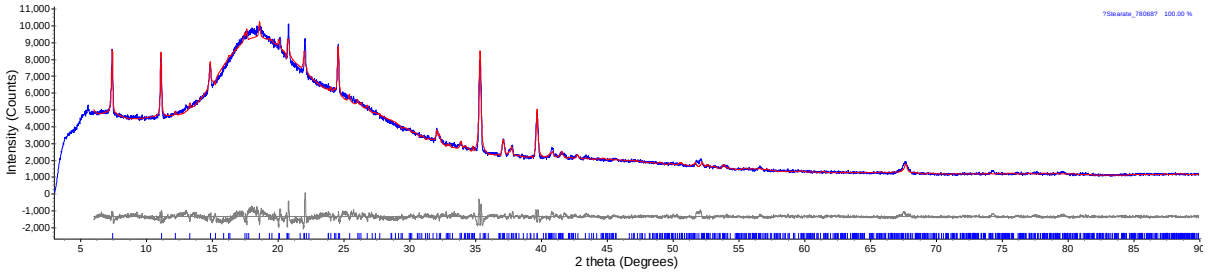


**Figure 7.22 Observed and calculated profiles for the Rietveld refinement of figure 3.30 line F with the MS-*C*2 structure. The bottom curve is the difference plot on the same intensity scale. ($R_{wp}$ = 3.44, $R_p$ = 2.57, $\chi$ = 1.92). The tick marks represent calculated peak positions.**

**Table 7.29 Refined lattice parameters for figure 3.30 line F Rietveld refinement with the MS-*C*2 structure.**

| Parameter | Value |
|---|---|
| **Phase / Space group** | MS-*C*2 / *C*2 |
| ***a* (Å)** | 47.680(5) |
| ***b* (Å)** | 7.3275(6) |
| ***c* (Å)** | 5.5791(2) |
| ***β* (°)** | 90.676(4) |
| **Volume (Å$^3$)** | 1949.5(2) |

### 3.4.5 Rietveld refinement of figure 3.30 line G

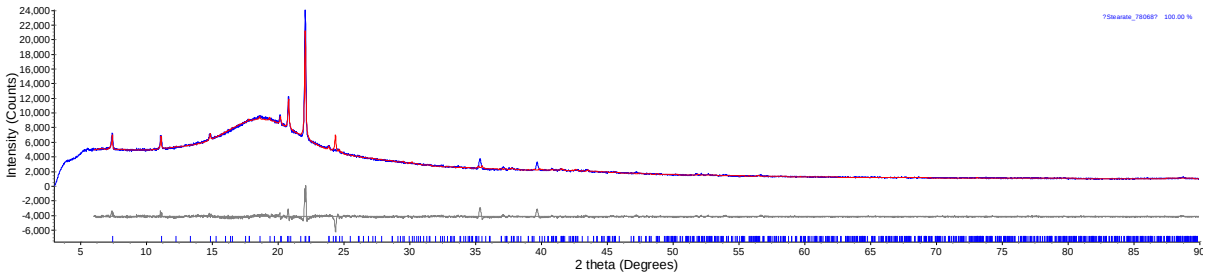


**Figure 7.23 Observed and calculated profiles for the Rietveld refinement of figure 3.30 line G with the MS-*C*2 structure. The bottom curve is the difference plot on the same intensity scale. ($R_{wp}$ = 4.20, $R_p$ = 2.50, $\chi$ = 2.28). The tick marks represent calculated peak positions.**

**Table 7.30 Refined lattice parameters for figure 3.30 line G Rietveld refinement with the MS-*C*2 structure.**

| Parameter | Value |
|---|---|
| **Phase / Space group** | MS-*C*2 / *C*2 |
| ***a* (Å)** | 47.684(8) |
| ***b* (Å)** | 7.301(1) |
| ***c* (Å)** | 5.533(1) |
| ***β* (°)** | 91.07(2) |
| **Volume (Å$^3$)** | 1925.8(6) |

## 3.4.6 Rietveld refinement of figure 3.31 line C

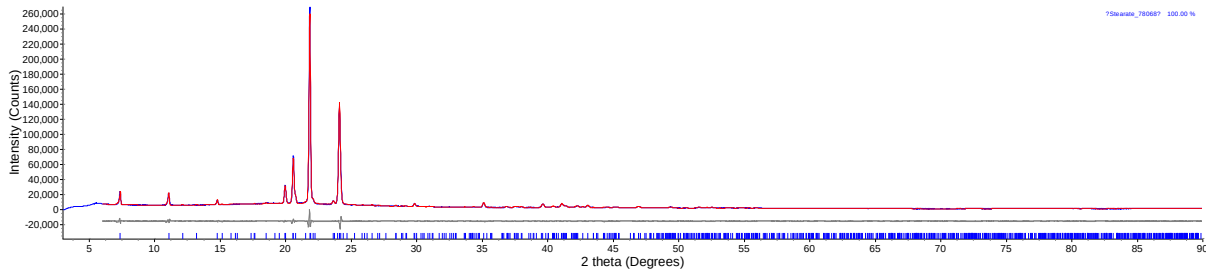


**Figure 7.24 Observed and calculated profiles for the Rietveld refinement of figure 3.31 line C with the MS-*C*2 structure. The bottom curve is the difference plot on the same intensity scale. ($R_{wp}$ = 5.09, $R_p$ = 3.78, $\chi$ = 3.59). The tick marks represent calculated peak positions.**

**Table 7.31 Refined lattice parameters for figure 3.31 line C Rietveld refinement with the MS-*C*2 structure.**

| Parameter | Value |
|---|---|
| **Phase / Space group** | MS-*C*2 / *C*2 |
| ***a* (Å)** | 47.920(4) |
| ***b* (Å)** | 7.3797(3) |
| ***c* (Å)** | 5.5998(3) |
| ***β* (°)** | 91.050(4) |
| **Volume (Å$^3$)** | 1980.0(2) |

## 3.4.7 Rietveld refinement of figure 3.31 line D

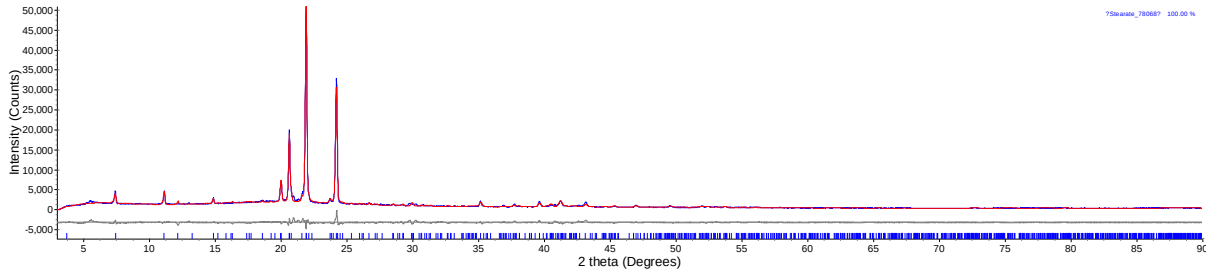


**Figure 7.25 Observed and calculated profiles for the Rietveld refinement of figure 3.31 line D with the MS-*C*2 structure. The bottom curve is the difference plot on the same intensity scale. ($R_{wp}$ = 9.04, $R_p$ = 6.57, $\chi$ = 3.06). The tick marks represent calculated peak positions.**

**Table 7.32 Refined lattice parameters for figure 3.31 line D Rietveld refinement with the MS-*C*2 structure.**

| Parameter | Value |
|---|---|
| **Phase / Space group** | MS-*C*2 / *C*2 |
| ***a* (Å)** | 47.712(7) |
| ***b* (Å)** | 7.3554(5) |
| ***c* (Å)** | 5.6048(5) |
| ***β* (°)** | 90.893(7) |
| **Volume (Å$^3$)** | 1966.7(4) |

## 3.4.8 Rietveld refinement of figure 3.31 line E

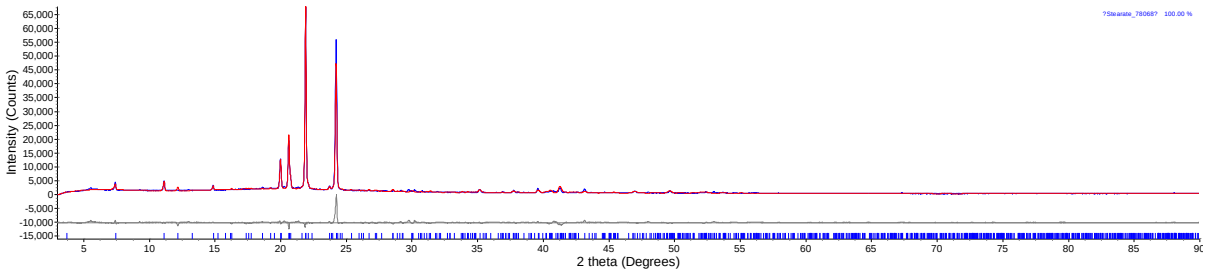


**Figure 7.26 Observed and calculated profiles for the Rietveld refinement of figure 3.31 line E with the MS-*C*2 structure. The bottom curve is the difference plot on the same intensity scale. ($R_{wp}$ = 11.77, $R_p$ = 8.31, $\chi$ = 4.07). The tick marks represent calculated peak positions.**

**Table 7.33 Refined lattice parameters for figure 3.31 line E Rietveld refinement with the MS-*C*2 structure.**

| Parameter | Value |
|---|---|
| **Phase / Space group** | MS-*C*2 / *C*2 |
| ***a* (Å)** | 47.618(7) |
| ***b* (Å)** | 7.3401(5) |
| ***c* (Å)** | 5.6059(5) |
| ***β* (°)** | 90.829(6) |
| **Volume (Å$^3$)** | 1959.2(4) |

### 3.4.9 Rietveld refinement of figure 3.31 line F

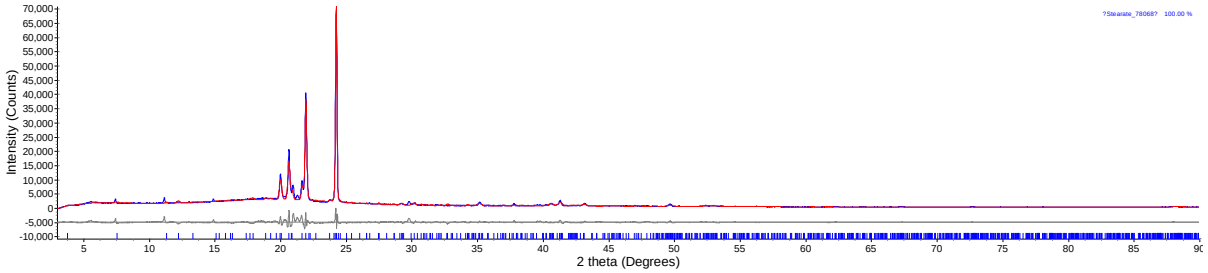


**Figure 7.27 Observed and calculated profiles for the Rietveld refinement of figure 3.31 line F with the MS-*C*2 structure. The bottom curve is the difference plot on the same intensity scale. ($R_{wp}$ = 11.23, $R_p$ = 8.20, $\chi$ = 4.30). The tick marks represent calculated peak positions.**

**Table 7.34 Refined lattice parameters for figure 3.31 line F Rietveld refinement with the MS-*C*2 structure.**

| Parameter | Value |
|---|---|
| **Phase / Space group** | MS-*C*2 / *C*2 |
| ***a* (Å)** | 47.02(1) |
| ***b* (Å)** | 7.341(2) |
| ***c* (Å)** | 5.606(1) |
| ***β* (°)** | 91.366(6) |
| **Volume (Å$^3$)** | 1934.7(8) |

## 3.4.10 Rietveld refinement of figure 3.32 line C

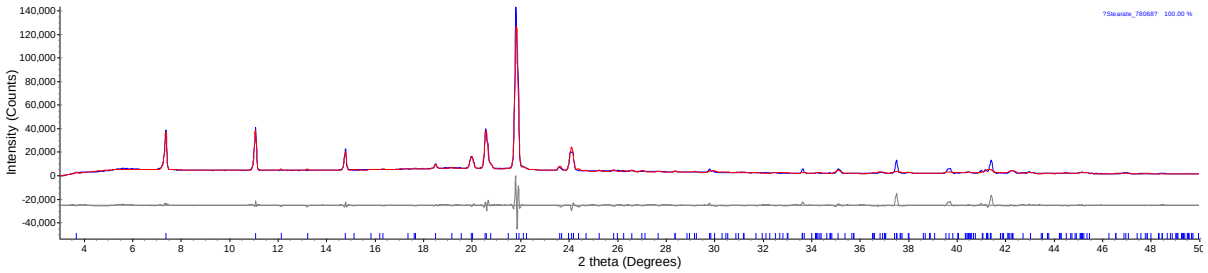


**Figure 7.28 Observed and calculated profiles for the Rietveld refinement of figure 3.32 line C with the MS-*C*2 structure. The bottom curve is the difference plot on the same intensity scale. ($R_{wp}$ = 11.83, $R_p$ = 7.54, $\chi$ = 8.27). The tick marks represent calculated peak positions.**

**Table 7.35 Refined lattice parameters for figure 3.32 line C Rietveld refinement with the MS-*C*2 structure.**

| Parameter | Value |
|---|---|
| **Space group** | MS-*C*2 / *C*2 |
| ***a* (Å)** | 47.957(7) |
| ***b* (Å)** | 7.3816(7) |
| ***c* (Å)** | 5.59664(8) |
| ***β* (°)** | 91.18(2) |
| **Volume (Å$^3$)** | 1980.7(5) |

### 3.4.11 Rietveld refinement of figure 3.32 line D

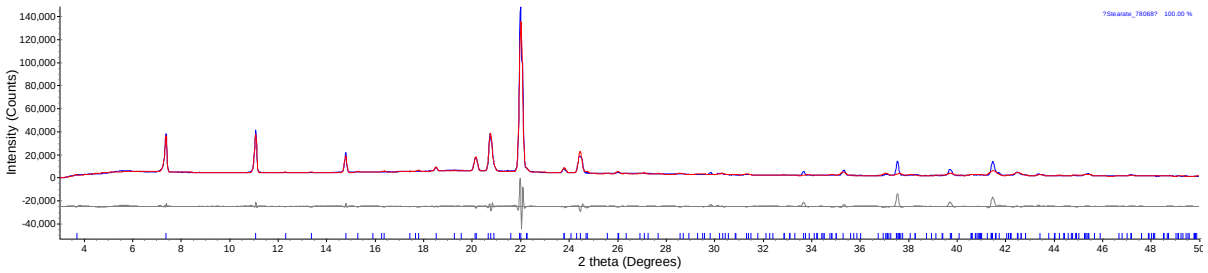


**Figure 7.29 Observed and calculated profiles for the Rietveld refinement of figure 3.32 line D with the MS-*C*2 structure. The bottom curve is the difference plot on the same intensity scale. ($R_{wp}$ = 12.59, $R_p$ = 7.80, $\chi$ = 8.81). The tick marks represent calculated peak positions.**

**Table 7.36 Refined lattice parameters for figure 3.32 line D Rietveld refinement with the MS-*C*2 structure.**

| Parameter | Value |
|---|---|
| **Phase / Space group** | MS-*C*2 / *C*2 |
| ***a* (Å)** | 47.899(8) |
| ***b* (Å)** | 7.2747(7) |
| ***c* (Å)** | 5.5714(8) |
| ***β* (°)** | 90.90(1) |
| **Volume (Å$^3$)** | 1941.1(5) |

## 3.4.12 Rietveld refinement of figure 3.32 line F

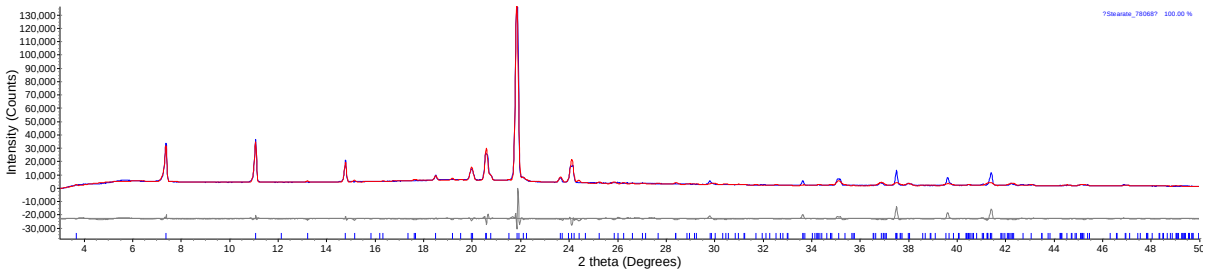


**Figure 7.30 Observed and calculated profiles for the Rietveld refinement of figure 3.32 line F with the MS-*C*2 structure. The bottom curve is the difference plot on the same intensity scale. ($R_{wp}$ = 11.37, $R_p$ = 6.92, $\chi$ = 7.80). The tick marks represent calculated peak positions.**

**Table 7.37 Refined lattice parameters for figure 3.32 line F Rietveld refinement with the MS-*C*2 structure.**

| Parameter | Value |
|---|---|
| **Phase / Space group** | MS-*C*2 / *C*2 |
| ***a* (Å)** | 47.932(6) |
| ***b* (Å)** | 7.3771(7) |
| ***c* (Å)** | 5.5958(7) |
| ***β* (°)** | 91.10(1) |
| **Volume (Å$^3$)** | 1978.3(4) |

### 3.4.13 Rietveld refinement of figure 3.32 line G

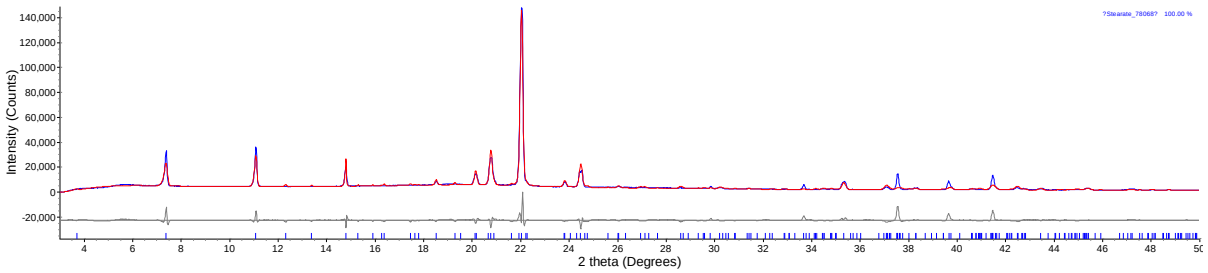


**Figure 7.31 Observed and calculated profiles for the Rietveld refinement of figure 3.32 line G with the MS-*C*2 structure. The bottom curve is the difference plot on the same intensity scale. ($R_{wp}$ = 13.31, $R_p$ = 8.28, $\chi$ = 9.18). The tick marks represent calculated peak positions.**

**Table 7.38 Refined lattice parameters for figure 3.32 line G Rietveld refinement with the MS-*C*2 structure.**

| Parameter | Value |
|---|---|
| **Phase / Space group** | MS-*C*2 / *C*2 |
| ***a* (Å)** | 47.903(6) |
| ***b* (Å)** | 7.2691(7) |
| ***c* (Å)** | 5.5733(7) |
| ***β* (°)** | 90.78(1) |
| **Volume (Å$^3$)** | 1940.5(4) |

## 3.4.14 Rietveld refinement of figure 3.32 line I

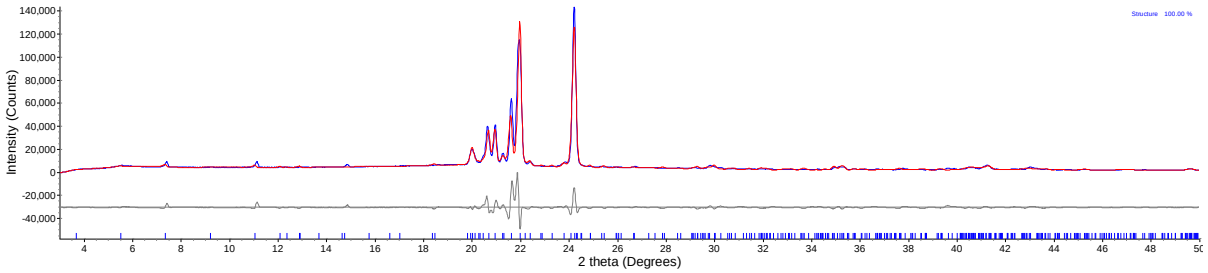


**Figure 7.32 Observed and calculated profiles for the Rietveld refinement of figure 3.32 line I with the MS-*Pnab* structure. The bottom curve is the difference plot on the same intensity scale. ($R_{wp}$ = 14.59, $R_p$ = 10.40, $\chi$ = 11.16). The tick marks represent calculated peak positions.**

**Table 7.39 Refined lattice parameters for figure 3.32 line I Rietveld refinement with the MS-*Pnab* structure.**

| Parameter | Value |
|---|---|
| **Phase / Space group** | MS-*Pnab* / *Pnab* |
| ***a* (Å)** | 5.602(1) |
| ***b* (Å)** | 7.342(1) |
| ***c* (Å)** | 96.08(3) |
| **Volume (Å$^3$)** | 3951(1) |

# Appendix 3.5 Rietveld refinements of thermal expansion scans for MS-*Cc*

## 3.5.1 Rietveld refinement of figure 3.39 260 K scan

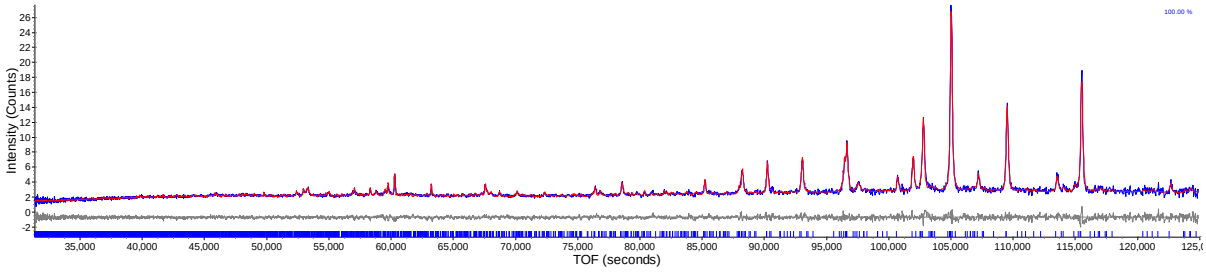


**Figure 7.33 Observed and calculated profiles for the Rietveld refinement of figure 3.39 260 K scan with the MS-*Cc* structure. The bottom curve is the difference plot on the same intensity scale. ($R_{wp}$ = 6.97, $R_p$ = 5.66, $\chi$ = 0.20). The tick marks represent calculated peak positions.**

**Table 7.40 Refined lattice parameters for figure 3.39 260 K scan Rietveld refinement with the MS-*Cc* structure.**

| Parameter | Value |
|---|---|
| **Phase / Space group** | MS-*Cc* / *Cc* |
| ***a* (Å)** | 49.0093(4) |
| ***b* (Å)** | 7.3148(2) |
| ***c* (Å)** | 5.5786(1) |
| ***β* (°)** | 77.704(1) |
| **Volume (Å$^3$)** | 1953.99(7) |

### 3.5.2 Rietveld refinement of figure 3.39 240 K scan

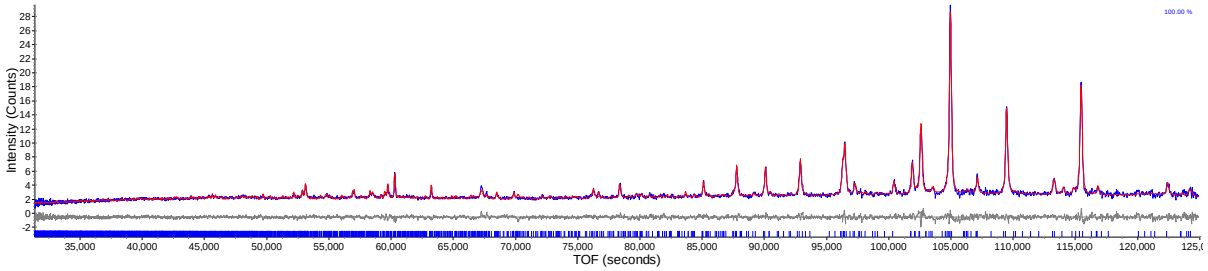


**Figure 7.34 Observed and calculated profiles for the Rietveld refinement of figure 3.39 240 K scan with the MS-*Cc* structure. The bottom curve is the difference plot on the same intensity scale. ($R_{wp}$ = 6.93, $R_p$ = 5.74, $\chi$ = 0.20). The tick marks represent calculated peak positions.**

**Table 7.41 Refined lattice parameters for figure 3.39 240 K scan Rietveld refinement with the MS-*Cc* structure.**

| Parameter | Value |
|---|---|
| **Phase / Space group** | MS-*Cc* / *Cc* |
| ***a* (Å)** | 49.0018(3) |
| ***b* (Å)** | 7.2765(1) |
| ***c* (Å)** | 5.5698(1) |
| ***β* (°)** | 77.627(1) |
| **Volume (Å$^3$)** | 1939.86(6) |

### 3.5.3 Rietveld refinement of figure 3.39 220 K scan

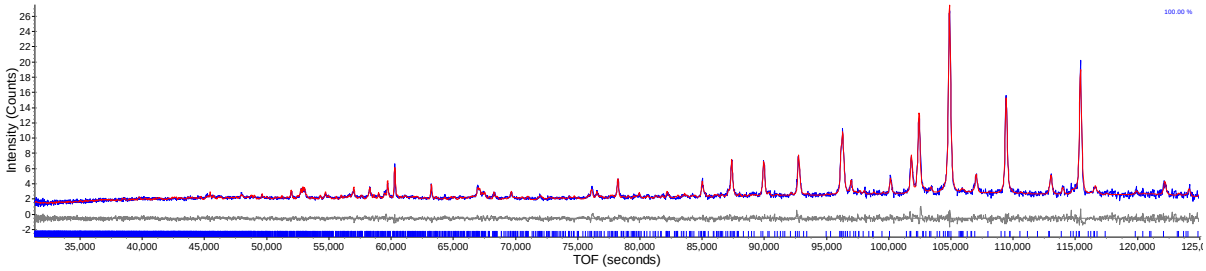


**Figure 7.35 Observed and calculated profiles for the Rietveld refinement of figure 3.39 220 K scan with the MS-*Cc* structure. The bottom curve is the difference plot on the same intensity scale. ($R_{wp}$ = 6.83, $R_p$ = 5.71, $\chi$ = 0.20). The tick marks represent calculated peak positions.**

**Table 7.42 Refined lattice parameters for figure 3.39 220 K scan Rietveld refinement with the MS-*Cc* structure.**

| Parameter | Value |
|---|---|
| **Phase / Space group** | MS-*Cc* / *Cc* |
| ***a* (Å)** | 48.9961(3) |
| ***b* (Å)** | 7.2436(1) |
| ***c* (Å)** | 5.5615(1) |
| ***β* (°)** | 77.550(1) |
| **Volume (Å$^3$)** | 1927.42(5) |

### 3.5.4 Rietveld refinement of figure 3.39 200 K scan

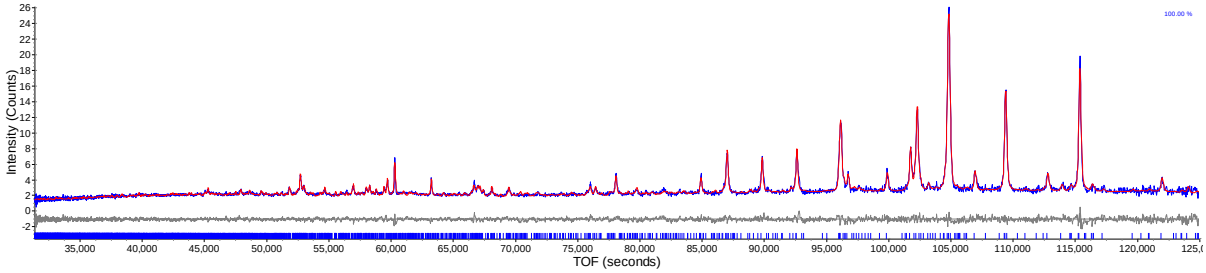


**Figure 7.36 Observed and calculated profiles for the Rietveld refinement of figure 3.39 200 K scan with the MS-*Cc* structure. The bottom curve is the difference plot on the same intensity scale. ($R_{wp}$ = 6.84, $R_p$ = 5.73, $\chi$ = 0.20). The tick marks represent calculated peak positions.**

**Table 7.43 Refined lattice parameters for figure 3.39 200 K scan Rietveld refinement with the MS-*Cc* structure.**

| Parameter | Value |
|---|---|
| **Phase / Space group** | MS-*Cc* / *Cc* |
| ***a* (Å)** | 48.9891(3) |
| ***b* (Å)** | 7.2132(1) |
| ***c* (Å)** | 5.5539(1) |
| ***β* (°)** | 77.483(1) |
| **Volume (Å$^3$)** | 1915.90(5) |

### 3.5.5 Rietveld refinement of figure 3.39 180 K scan

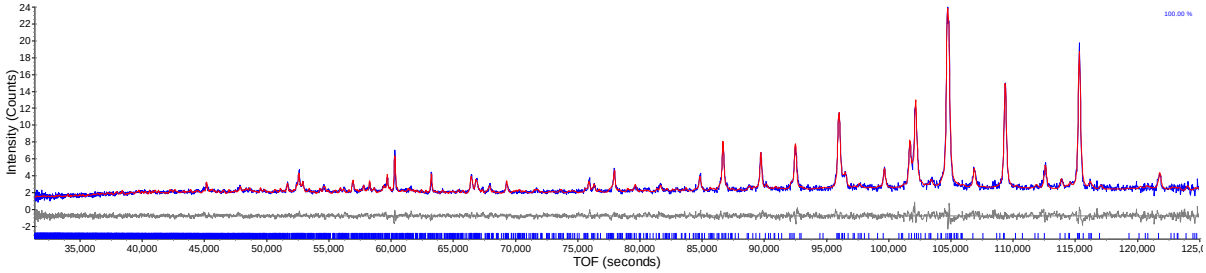


**Figure 7.37 Observed and calculated profiles for the Rietveld refinement of figure 3.39 180 K scan with the MS-*Cc* structure. The bottom curve is the difference plot on the same intensity scale. ($R_{wp}$ = 7.14, $R_p$ = 5.95, $\chi$ = 0.21). The tick marks represent calculated peak positions.**

**Table 7.44 Refined lattice parameters for figure 3.39 180 K scan Rietveld refinement with the MS-*Cc* structure.**

| Parameter | Value |
|---|---|
| **Phase / Space group** | MS-*Cc* / *Cc* |
| ***a* (Å)** | 48.9824(4) |
| ***b* (Å)** | 7.1860(1) |
| ***c* (Å)** | 5.5470(1) |
| ***β* (°)** | 77.418(1) |
| **Volume (Å$^3$)** | 1905.57(5) |

### 3.5.6 Rietveld refinement of figure 3.39 160 K scan

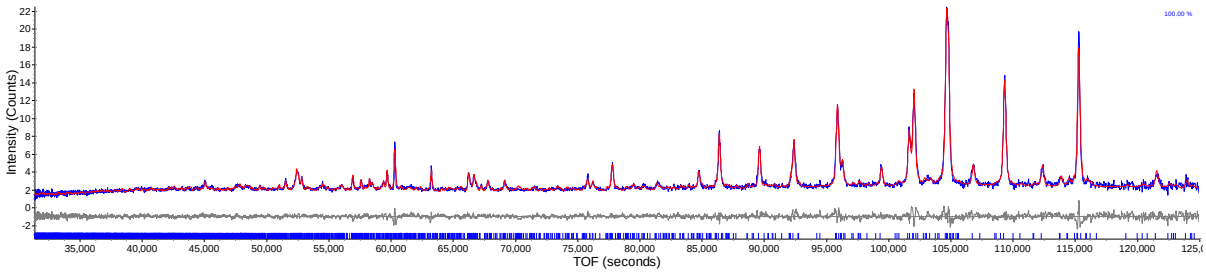


**Figure 7.38 Observed and calculated profiles for the Rietveld refinement of figure 3.39 160 K scan with the MS-*Cc* structure. The bottom curve is the difference plot on the same intensity scale. ($R_{wp}$ = 7.34, $R_p$ = 6.01, $\chi$ = 0.21). The tick marks represent calculated peak positions.**

**Table 7.45 Refined lattice parameters for figure 3.39 160 K scan Rietveld refinement with the MS-*Cc* structure.**

| Parameter | Value |
|---|---|
| **Phase / Space group** | MS-*Cc* / *Cc* |
| ***a* (Å)** | 48.9768(4) |
| ***b* (Å)** | 7.1609(1) |
| ***c* (Å)** | 5.5387(1) |
| ***β* (°)** | 77.345(2) |
| **Volume (Å$^3$)** | 1895.33(6) |

### 3.5.7 Rietveld refinement of figure 3.39 140 K scan

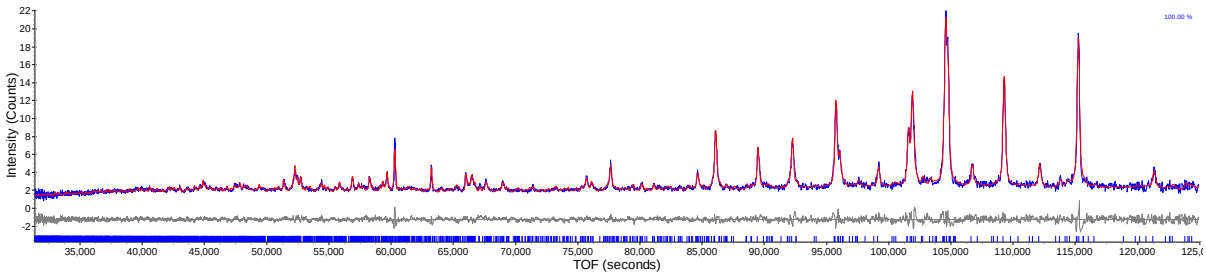


**Figure 7.39 Observed and calculated profiles for the Rietveld refinement of figure 3.39 140 K scan with the MS-*Cc* structure. The bottom curve is the difference plot on the same intensity scale. ($R_{wp}$ = 7.47, $R_p$ = 6.15, $\chi$ = 0.22). The tick marks represent calculated peak positions.**

**Table 7.46 Refined lattice parameters for figure 3.39 140 K scan Rietveld refinement with the MS-*Cc* structure.**

| Parameter | Value |
|---|---|
| **Phase / Space group** | MS-*Cc* / *Cc* |
| ***a* (Å)** | 48.9741(4) |
| ***b* (Å)** | 7.1370(1) |
| ***c* (Å)** | 5.5307(1) |
| ***β* (°)** | 77.277(1) |
| **Volume (Å$^3$)** | 1885.68(6) |

### 3.5.8 Rietveld refinement of figure 3.39 120 K scan

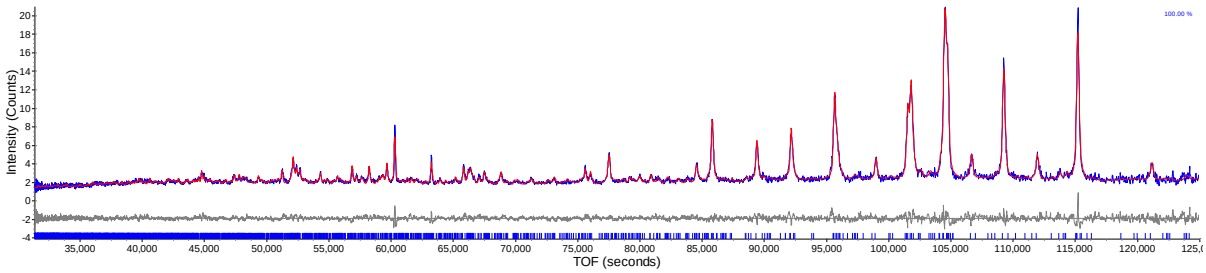


**Figure 7.40 Observed and calculated profiles for the Rietveld refinement of figure 3.39 120 K scan with the MS-*Cc* structure. The bottom curve is the difference plot on the same intensity scale. ($R_{wp}$ = 7.36, $R_p$ = 6.11, $\chi$ = 0.22). The tick marks represent calculated peak positions.**

**Table 7.47 Refined lattice parameters for figure 3.39 120 K scan Rietveld refinement with the MS-*Cc* structure.**

| Parameter | Value |
|---|---|
| **Phase / Space group** | MS-*Cc* / *Cc* |
| ***a* (Å)** | 48.9687(4) |
| ***b* (Å)** | 7.1147(1) |
| ***c* (Å)** | 5.5245(1) |
| ***β* (°)** | 77.217(2) |
| **Volume (Å$^3$)** | 1877.00(6) |

### 3.5.9 Rietveld refinement of figure 3.39 100 K scan

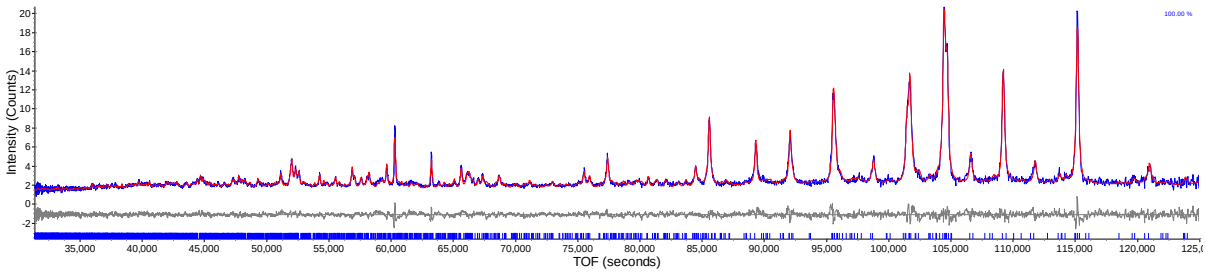


**Figure 7.41 Observed and calculated profiles for the Rietveld refinement of figure 3.39 100 K scan with the MS-*Cc* structure. The bottom curve is the difference plot on the same intensity scale. ($R_{wp}$ = 7.67, $R_p$ = 6.41, $\chi$ = 0.22). The tick marks represent calculated peak positions.**

**Table 7.48 Refined lattice parameters for figure 3.39 100 K scan Rietveld refinement with the MS-*Cc* structure.**

| Parameter | Value |
|---|---|
| **Phase / Space group** | MS-*Cc* / *Cc* |
| ***a* (Å)** | 48.9624(4) |
| ***b* (Å)** | 7.0945(1) |
| ***c* (Å)** | 5.5180(1) |
| ***β* (°)** | 77.164(2) |
| **Volume (Å$^3$)** | 1868.85(6) |

### 3.5.10 Rietveld refinement of figure 3.39 80 K scan

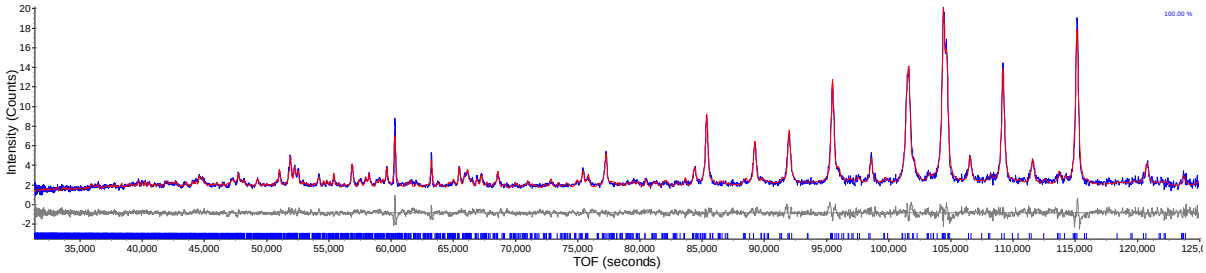


**Figure 7.42 Observed and calculated profiles for the Rietveld refinement of figure 3.39 80 K scan with the MS-*Cc* structure. The bottom curve is the difference plot on the same intensity scale. ($R_{wp}$ = 7.73, $R_p$ = 6.39, $\chi$ = 0.23). The tick marks represent calculated peak positions.**

**Table 7.49 Refined lattice parameters for figure 3.39 80 K scan Rietveld refinement with the MS-*Cc* structure.**

| Parameter | Value |
|---|---|
| **Phase / Space group** | MS-*Cc* / *Cc* |
| ***a* (Å)** | 48.9604(5) |
| ***b* (Å)** | 7.0768(1) |
| ***c* (Å)** | 5.5108(1) |
| ***β* (°)** | 77.095(2) |
| **Volume (Å$^3$)** | 1861.18(7) |

### 3.5.11 Rietveld refinement of figure 3.39 60 K scan

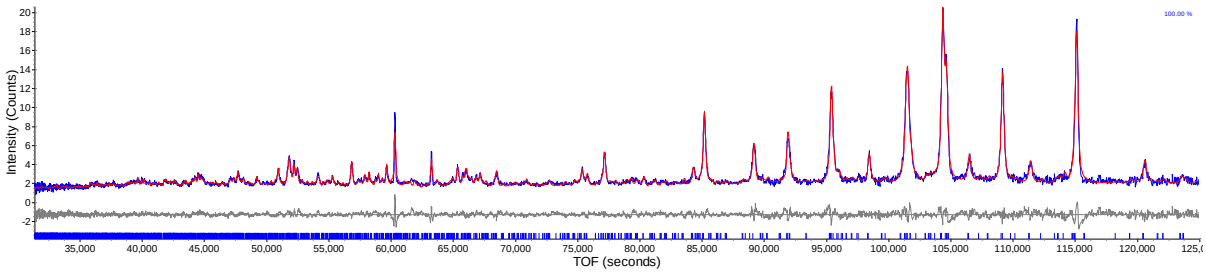


**Figure 7.43 Observed and calculated profiles for the Rietveld refinement of figure 3.39 60 K scan with the MS-*Cc* structure. The bottom curve is the difference plot on the same intensity scale. ($R_{wp}$ = 7.91, $R_p$ = 6.52, $\chi$ = 0.23). The tick marks represent calculated peak positions.**

**Table 7.50 Refined lattice parameters for figure 3.39 60 K scan Rietveld refinement with the MS-*Cc* structure.**

| Parameter | Value |
|---|---|
| **Phase / Space group** | MS-*Cc* / *Cc* |
| ***a* (Å)** | 48.9588(5) |
| ***b* (Å)** | 7.0623(1) |
| ***c* (Å)** | 5.5044(1) |
| ***β* (°)** | 77.046(2) |
| **Volume (Å$^3$)** | 1854.46(6) |

### 3.5.12 Rietveld refinement of figure 3.39 40 K scan

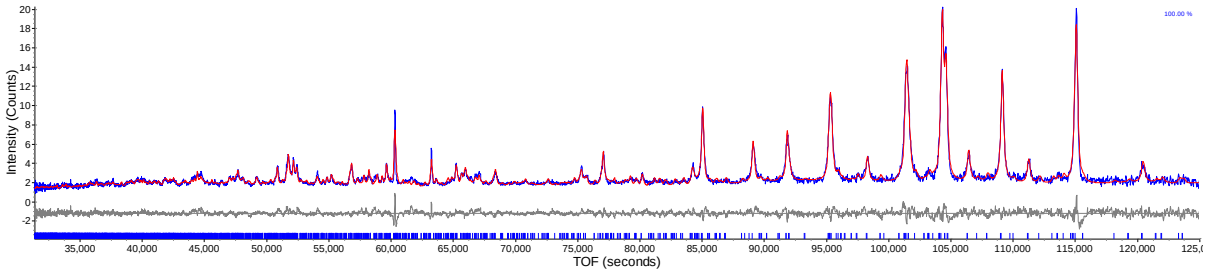


**Figure 7.44 Observed and calculated profiles for the Rietveld refinement of figure 3.39 40 K scan with the MS-*Cc* structure. The bottom curve is the difference plot on the same intensity scale. ($R_{wp}$ = 8.53, $R_p$ = 7.17, $\chi$ = 0.25). The tick marks represent calculated peak positions.**

**Table 7.51 Refined lattice parameters for figure 3.39 40 K scan Rietveld refinement with the MS-*Cc* structure.**

| Parameter | Value |
|---|---|
| **Phase / Space group** | MS-*Cc* / *Cc* |
| ***a* (Å)** | 48.9556(5) |
| ***b* (Å)** | 7.0498(2) |
| ***c* (Å)** | 5.4991(1) |
| ***β* (°)** | 76.991(2) |
| **Volume (Å$^3$)** | 1849.18(7) |

### 3.5.13 Rietveld refinement of figure 3.39 20 K scan

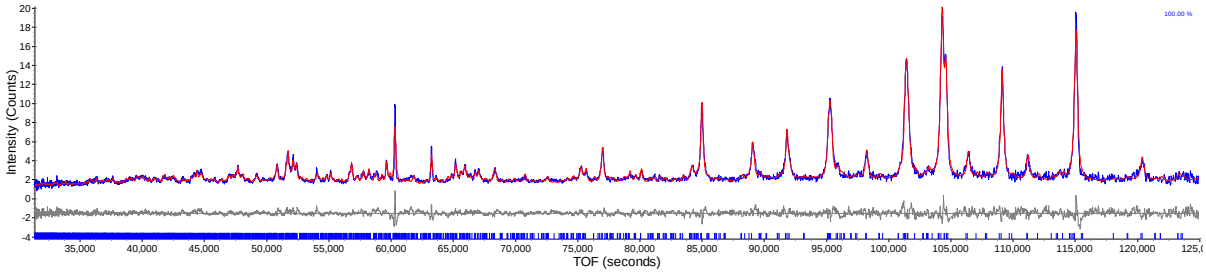


**Figure 7.45 Observed and calculated profiles for the Rietveld refinement of figure 3.39 20 K scan with the MS-*Cc* structure. The bottom curve is the difference plot on the same intensity scale. ($R_{wp}$ = 8.37, $R_p$ = 6.91, $\chi$ = 0.25). The tick marks represent calculated peak positions.**

**Table 7.52 Refined lattice parameters for figure 3.39 20 K scan Rietveld refinement with the MS-*Cc* structure.**

| Parameter | Value |
|---|---|
| **Phase / Space group** | MS-*Cc* / *Cc* |
| ***a* (Å)** | 48.9554(5) |
| ***b* (Å)** | 7.0447(2) |
| ***c* (Å)** | 5.4964(1) |
| ***β* (°)** | 76.962(2) |
| **Volume (Å$^3$)** | 1846.71(6) |

# Appendix 3.6 Rietveld refinements of recrystallisations of Ethyl Stearate

## 3.6.1 Rietveld refinement of figure 3.65 line B

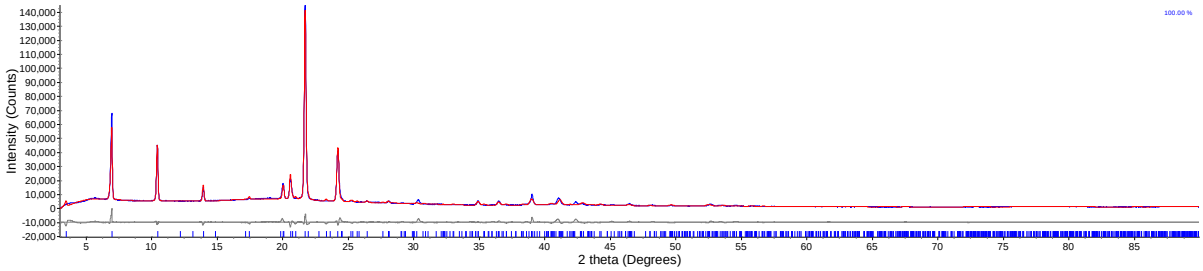


**Figure 7.46 Observed and calculated profiles for the Rietveld refinement of figure 3.65 line B with the ES-*Aa* structure. The bottom curve is the difference plot on the same intensity scale. ($R_{wp}$ = 8.46, $R_p$ = 5.39, $\chi$ = 5.22). The tick marks represent calculated peak positions.**

**Table 7.53 Refined lattice parameters for figure 3.65 line B Rietveld refinement with the ES-*Aa* structure.**

| Parameter | Value |
|---|---|
| **Phase / Space group** | ES-*Aa* / *Aa* |
| ***a* (Å)** | 5.5724(4) |
| ***b* (Å)** | 7.3445(5) |
| ***c* (Å)** | 55.080(6) |
| ***β* (°)** | 112.853(9) |
| **Volume (Å$^3$)** | 2077.3(3) |

## 3.6.2 Rietveld refinement of figure 3.65 line C

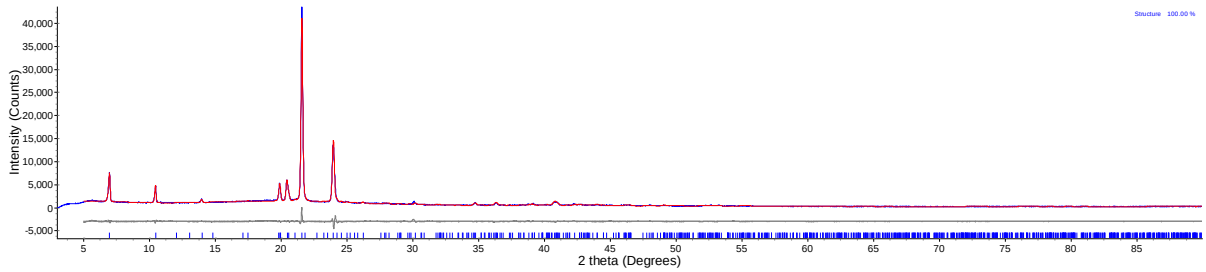


**Figure 7.47 Observed and calculated profiles for the Rietveld refinement of figure 3.65 line C with the ES-*Aa* structure. The bottom curve is the difference plot on the same intensity scale. ($R_{wp}$ = 6.92, $R_p$ = 5.20, $\chi$ = 2.00). The tick marks represent calculated peak positions.**

**Table 7.54 Refined lattice parameters for figure 3.65 line C Rietveld refinement with the ES-*Aa* structure.**

| Parameter | Value |
|---|---|
| **Phase / Space group** | Ethyl Stearate 1968 / *Aa* |
| ***a* (Å)** | 5.6091(5) |
| ***b* (Å)** | 7.4180(4) |
| ***c* (Å)** | 55.055(8) |
| ***β* (°)** | 113.080(8) |
| **Volume (Å$^3$)** | 2107.4 (4) |

### 3.6.3 Rietveld refinement of figure 3.65 line D

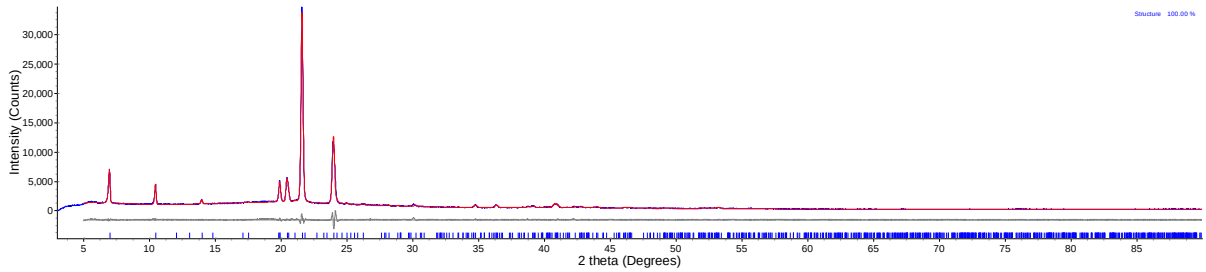


**Figure 7.48 Observed and calculated profiles for the Rietveld refinement of figure 3.65 line D with the ES-*Aa* structure. The bottom curve is the difference plot on the same intensity scale. ($R_{wp}$ = 6.01, $R_p$ = 4.40, $\chi$ = 1.72). The tick marks represent calculated peak positions.**

**Table 7.55 Refined lattice parameters for figure 3.65 line D Rietveld refinement with the ES-*Aa* structure.**

| Parameter | Value |
|---|---|
| **Phase / Space group** | ES-*Aa* / *Aa* |
| ***a* (Å)** | 5.6118(10) |
| ***b* (Å)** | 7.4136(6) |
| ***c* (Å)** | 55.07(1) |
| ***β* (°)** | 113.20(2) |
| **Volume (Å$^3$)** | 2105.9(7) |

## 3.6.4 Rietveld refinement of figure 3.66 line B

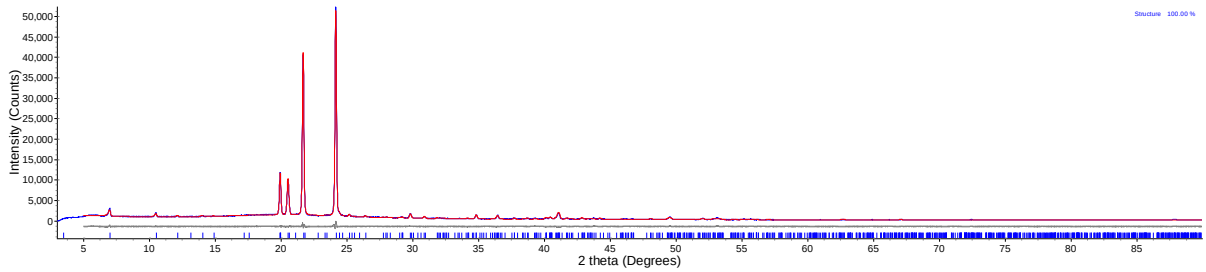


**Figure 7.49 Observed and calculated profiles for the Rietveld refinement of figure 3.66 line B with the ES-*Aa* structure. The bottom curve is the difference plot on the same intensity scale. ($R_{wp}$ = 5.78, $R_p$ = 4.11, $\chi$ = 1.72). The tick marks represent calculated peak positions.**

**Table 7.56 Refined lattice parameters for figure 3.66 line B Rietveld refinement with the ES-*Aa* structure.**

| Parameter | Value |
|---|---|
| **Phase / Space group** | ES-*Aa* / *Aa* |
| ***a* (Å)** | 5.6157(3) |
| ***b* (Å)** | 7.3572(3) |
| ***c* (Å)** | 55.048(7) |
| ***β* (°)** | 113.569(4) |
| **Volume (Å$^3$)** | 2084.6(3) |

## 3.6.5 Rietveld refinement of figure 3.66 line C

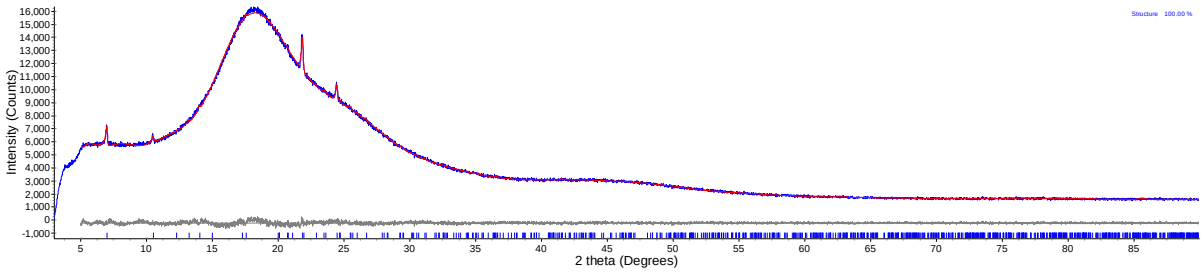


**Figure 7.50 Observed and calculated profiles for the Rietveld refinement of figure 3.66 line C with the ES-*Aa* structure. The bottom curve is the difference plot on the same intensity scale. ($R_{wp}$ = 1.74, $R_p$ = 1.35, $\chi$ = 1.56). The tick marks represent calculated peak positions.**

**Table 7.57 Refined lattice parameters for figure 3.66 line C Rietveld refinement with the ES-*Aa* structure.**

| Parameter | Value |
|---|---|
| **Phase / Space group** | ES-*Aa* / *Aa* |
| ***a* (Å)** | 5.587(2) |
| ***b* (Å)** | 7.271(2) |
| ***c* (Å)** | 55.06(3) |
| ***β* (°)** | 113.59(4) |
| **Volume (Å$^3$)** | 2050 (2) |

## 3.6.6 Rietveld refinement of figure 3.66 line D

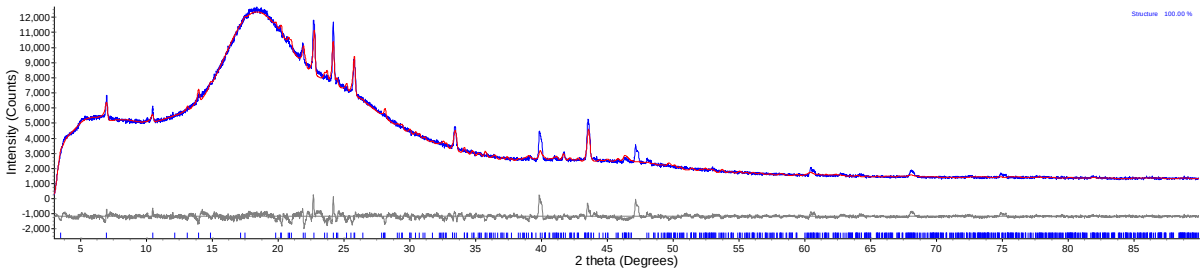


**Figure 7.51 Observed and calculated profiles for the Rietveld refinement of figure 3.66 line D with the ES-*Aa* structure. The bottom curve is the difference plot on the same intensity scale. ($R_{wp}$ = 3.86, $R_p$ = 2.54, $\chi$ = 2.34). The tick marks represent calculated peak positions.**

**Table 7.58 Refined lattice parameters for figure 3.66 line D Rietveld refinement with the ES-*Aa* structure.**

| Parameter | Value |
|---|---|
| **Phase / Space group** | ES-*Aa* / *Aa* |
| ***a* (Å)** | 5.4990(9) |
| ***b* (Å)** | 7.356(1) |
| ***c* (Å)** | 55.53(1) |
| ***β* (°)** | 113.97(1) |
| **Volume (Å$^3$)** | 2052.5(6) |

## 3.6.7 Rietveld refinement of figure 3.66 line E

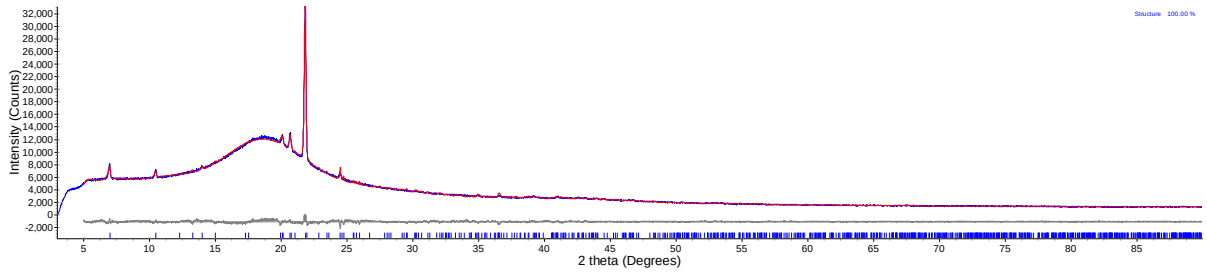


**Figure 7.52 Observed and calculated profiles for the Rietveld refinement of figure 3.66 line E with the ES-*Aa* structure. The bottom curve is the difference plot on the same intensity scale. ($R_{wp}$ = 2.62, $R_p$ = 2.06, $\chi$ = 1.57). The tick marks represent calculated peak positions.**

**Table 7.59 Refined lattice parameters for figure 3.66 line E Rietveld refinement with the ES-*Aa* structure.**

| Parameter | Value |
|---|---|
| **Phase / Space group** | ES-*Aa* / *Aa* |
| ***a* (Å)** | 5.5847(9) |
| ***b* (Å)** | 7.2621(9) |
| ***c* (Å)** | 55.11(1) |
| ***β* (°)** | 113.35(1) |
| **Volume (Å$^3$)** | 2051.8 (6) |

## 3.6.8 Rietveld refinement of figure 3.67 line B

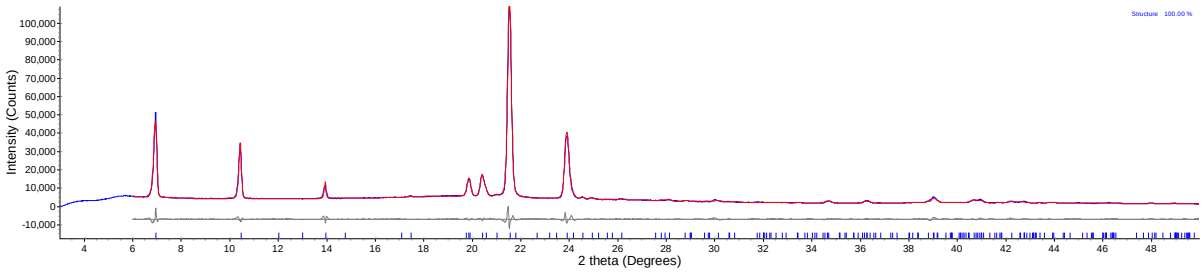


**Figure 7.53 Observed and calculated profiles for the Rietveld refinement of figure 3.67 line B with the ES-*Aa* structure. The bottom curve is the difference plot on the same intensity scale. ($R_{wp}$ = 4.68, $R_p$ = 3.26, $\chi$ = 3.24). The tick marks represent calculated peak positions.**

**Table 7.60 Refined lattice parameters for figure 3.67 line B Rietveld refinement with the ES-*Aa* structure.**

| Parameter | Value |
|---|---|
| **Phase / Space group** | ES-*Aa* / *Aa* |
| ***a* (Å)** | 5.6141(8) |
| ***b* (Å)** | 7.4339(4) |
| ***c* (Å)** | 55.101(8) |
| ***β* (°)** | 113.03(1) |
| **Volume (Å$^3$)** | 2116.3(5) |

## 3.6.9 Rietveld refinement of figure 3.67 line C

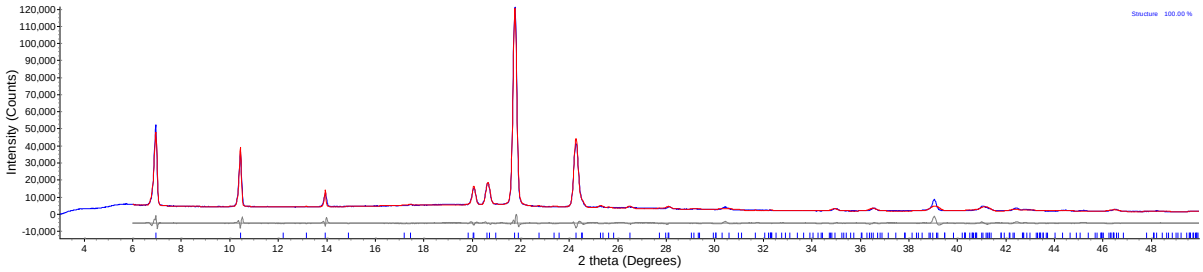


**Figure 7.54 Observed and calculated profiles for the Rietveld refinement of figure 3.67 line C with the ES-*Aa* structure. The bottom curve is the difference plot on the same intensity scale. ($R_{wp}$ = 6.74, $R_p$ = 4.36, $\chi$ = 4.67). The tick marks represent calculated peak positions.**

**Table 7.61 Refined lattice parameters for figure 3.67 line C Rietveld refinement with the ES-*Aa* structure.**

| Parameter | Value |
|---|---|
| **Phase / Space group** | ES-*Aa* / *Aa* |
| ***a* (Å)** | 5.5821(7) |
| ***b* (Å)** | 7.3276(4) |
| ***c* (Å)** | 55.259(8) |
| ***β* (°)** | 113.17(1) |
| **Volume (Å$^3$)** | 2078.0 (5) |

## 3.6.10 Rietveld refinement of figure 3.67 line E

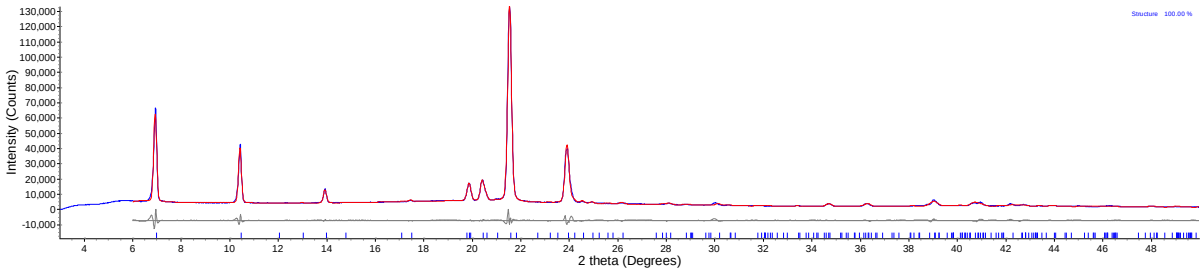


**Figure 7.55 Observed and calculated profiles for the Rietveld refinement of figure 3.67 line E with the ES-*Aa* structure. The bottom curve is the difference plot on the same intensity scale. ($R_{wp}$ = 5.51, $R_p$ = 3.77, $\chi$ = 3.97). The tick marks represent calculated peak positions.**

**Table 7.62 Refined lattice parameters for figure 3.67 line E Rietveld refinement with the ES-*Aa* structure.**

| Parameter | Value |
|---|---|
| **Phase / Space group** | ES-*Aa* / *Aa* |
| ***a* (Å)** | 5.6042(9) |
| ***b* (Å)** | 7.4231(7) |
| ***c* (Å)** | 55.03(1) |
| ***β* (°)** | 113.02(5) |
| **Volume (Å$^3$)** | 2106.9(6) |

## 3.6.11 Rietveld refinement of figure 3.67 line F

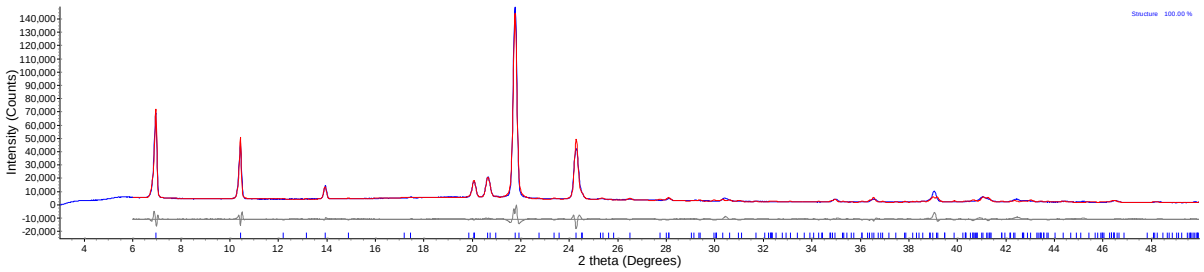


**Figure 7.56 Observed and calculated profiles for the Rietveld refinement of figure 3.67 line F with the ES-*Aa* structure. The bottom curve is the difference plot on the same intensity scale. ($R_{wp}$ = 9.14, $R_p$ = 6.23, $\chi$ = 6.62). The tick marks represent calculated peak positions.**

**Table 7.63 Refined lattice parameters for figure 3.67 line F Rietveld refinement with the ES-*Aa* structure.**

| Parameter | Value |
|---|---|
| **Phase / Space group** | ES-*Aa* / *Aa* |
| ***a* (Å)** | 5.5789(5) |
| ***b* (Å)** | 7.3241(4) |
| ***c* (Å)** | 55.240 (6) |
| ***β* (°)** | 113.160(9) |
| **Volume (Å$^3$)** | 2075.2(3) |

## 3.6.12 Rietveld refinement of figure 3.67 line H

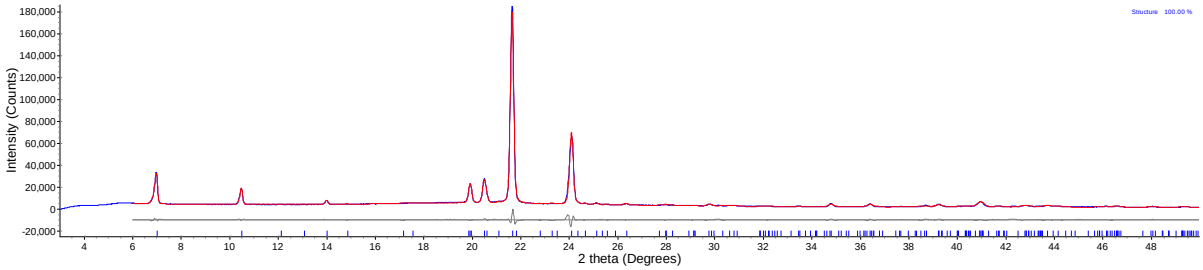


**Figure 7.57 Observed and calculated profiles for the Rietveld refinement of figure 3.67 line H with the ES-*Aa* structure. The bottom curve is the difference plot on the same intensity scale. ($R_{wp}$ = 5.20, $R_p$ = 3.60, $\chi$ = 3.76). The tick marks represent calculated peak positions.**

**Table 7.64 Refined lattice parameters for figure 3.67 line H Rietveld refinement with the ES-*Aa* structure.**

| Parameter | Value |
|---|---|
| **Phase / Space group** | ES-*Aa* / *Aa* |
| ***a* (Å)** | 5.6150(6) |
| ***b* (Å)** | 7.3783(3) |
| ***c* (Å)** | 55.038(6) |
| ***β* (°)** | 113.432(1) |
| **Volume (Å$^3$)** | 2092.1 (4) |

# Appendix 4.1 Atomic positions for methyl palmitate refinements

## 4.1.1 Atomic positions of MP-*Pnab* refinement with methyl palmitate as bought lab data

**Table 7.65 Atomic positions of MP-*Pnab* refinement with methyl palmitate as bought lab data.**

| Atom Number | *x* | *y* | *z* |
|---|---|---|---|
| **C1** | 0.801(8) | 0.243(7) | 0.0442(7) |
| **C2** | 0.635(7) | 0.256(6) | 0.1532(6) |
| **C3** | 0.807(7) | 0.316(7) | 0.1708(6) |
| **C4** | 0.748(6) | 0.215(7) | 0.1825(6) |
| **C5** | 0.584(7) | 0.333(7) | 0.1957(7) |
| **C6** | 0.577(6) | 0.231(7) | 0.2121(6) |
| **C7** | 0.422(7) | 0.252(7) | 0.2186(6) |
| **C8** | 0.198(6) | 0.167(7) | 0.2082(6) |
| **C11** | 1.087(7) | 0.244(6) | 0.0275(6) |
| **C12** | 0.704(8) | 0.176(8) | 0.0595(7) |
| **C13** | 0.513(7) | 0.289(6) | 0.0651(6) |
| **C14** | 0.476(6) | 0.176(8) | 0.0846(7) |
| **C15** | 0.307(7) | 0.297(7) | 0.0971(6) |
| **C16** | 0.309(7) | 0.213(7) | 0.1114(6) |
| **C17** | 0.081(7) | 0.294(7) | 0.1242(6) |
| **C18** | 0.016(7) | 0.198(8) | 0.1393(7) |
| **C19** | 0.127(7) | 0.304(6) | 0.1516(6) |
| **O1** | 0.981(5) | 0.187(4) | 0.0400(4) |
| **O2** | 0.677(6) | 0.314(5) | 0.0356(5) |

### 4.1.2 Atomic positions of MP-*C*2 refinement with methyl palmitate from the melt lab data

**Table 7.66 Atomic positions of MP-*C*2 refinement with methyl palmitate from the melt lab data.**

| Atom Number | *x* | *y* | *z* |
|---|---|---|---|
| **C1** | 0.472(5) | 0.161(3) | 2.28(5) |
| **C2** | 0.210(3) | 0.263(4) | 1.18(4) |
| **C4** | 0.405(4) | 0.314(3) | 1.86(8) |
| **C5** | 0.373(3) | 0.213(4) | 1.83(6) |
| **C6** | 0.158(3) | 0.193(3) | 0.91(4) |
| **C7** | 0.087(3) | 0.174(4) | 0.56(4) |
| **C8** | 0.196(4) | 0.243(3) | 0.91(5) |
| **C9** | 0.298(4) | 0.218(3) | 1.42(5) |
| **C10** | 0.141(2) | 0.290(2) | 0.70(7) |
| **C11** | 0.424(7) | 0.249(3) | 2.11(6) |
| **C12** | 0.315(4) | 0.228(4) | 1.67(4) |
| **C13** | 0.042(2) | 0.232(2) | 0.234(4) |
| **C14** | 0.053(3) | 0.248(4) | 0.51(4) |
| **C15** | 0.102(3) | 0.269(2) | 0.75(4) |
| **C16** | 0.353(3) | 0.290(3) | 1.63(3) |
| **C18** | 0.259(5) | 0.243(3) | 1.44(6) |
| **C19** | 0.241(2) | 0.168(3) | 1.21(3) |
| **O20** | 0.4119(4) | 0.242(3) | 2.35(2) |
| **O21** | 0.456(1) | 0.313(4) | 2.11(3) |

# Appendix 4.2 Rietveld refinements for thermal expansion scans of MP-*Pnab*

## 4.2.1 Rietveld refinement of figure 4.8 293 K scan

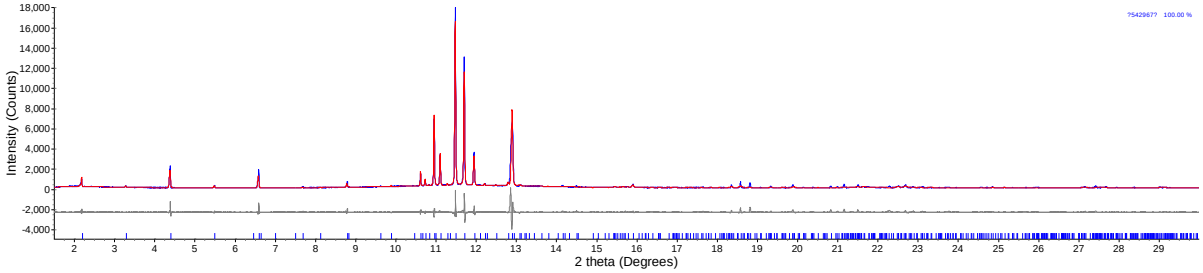


**Figure 7.58 Observed and calculated profiles for the Rietveld refinement of figure 4.8 293 K scan with the MP-*Pnab* structure. The bottom curve is the difference plot on the same intensity scale. ($R_{wp}$ = 12.97, $R_p$ = 4.25, $\chi$ = 3.05). The tick marks represent calculated peak positions.**

**Table 7.67 Refined lattice parameters for figure 4.8 293 K scan Rietveld refinement with the MP-*Pnab* structure.**

| Parameter | Value |
|---|---|
| **Phase / Space group** | MP-*Pnab* / *Pnab* |
| ***a* (Å)** | 5.6213(2) |
| ***b* (Å)** | 7.3496(2) |
| ***c* (Å)** | 86.193(5) |
| **Volume (Å$^3$)** | 3561.0 (3) |

## 4.2.2 Rietveld refinement of figure 4.8 275 K scan

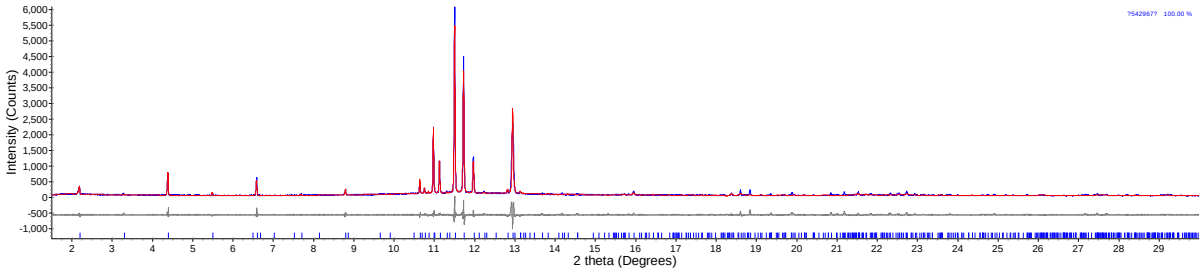


**Figure 7.59 Observed and calculated profiles for the Rietveld refinement of figure 4.8 275 K scan with the MP-*Pnab* structure. The bottom curve is the difference plot on the same intensity scale. ($R_{wp}$ = 13.00, $R_p$ = 7.38, $\chi$ = 1.76). The tick marks represent calculated peak positions.**

**Table 7.68 Refined lattice parameters for figure 4.8 275 K scan Rietveld refinement with the MP-*Pnab* structure.**

| Parameter | Value |
|---|---|
| **Phase / Space group** | MP-*Pnab* / *Pnab* |
| ***a* (Å)** | 5.6135(2) |
| ***b* (Å)** | 7.3207(2) |
| ***c* (Å)** | 86.103(5) |
| **Volume (Å$^3$)** | 3538.4(3) |

### 4.2.3 Rietveld refinement of figure 4.8 250 K scan

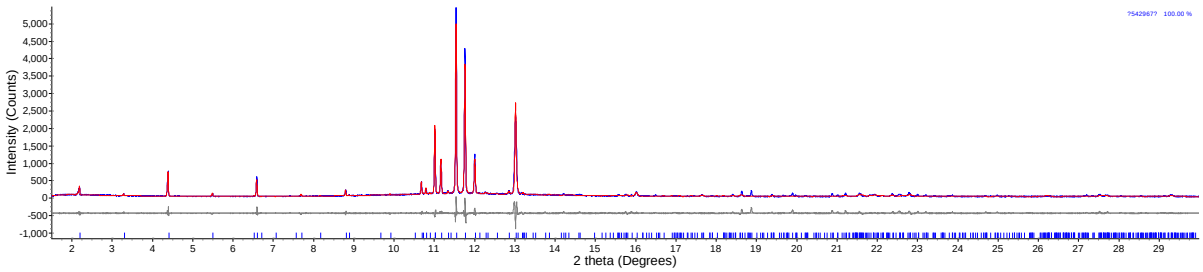


**Figure 7.60 Observed and calculated profiles for the Rietveld refinement of figure 4.8 250 K scan with the MP-*Pnab* structure. The bottom curve is the difference plot on the same intensity scale. ($R_{wp}$ = 12.81, $R_p$ = 8.93, $\chi$ = 1.73). The tick marks represent calculated peak positions.**

**Table 7.69 Refined lattice parameters for figure 4.8 250 K scan Rietveld refinement with the MP-*Pnab* structure.**

| Parameter | Value |
|---|---|
| **Phase / Space group** | MP-*Pnab* / *Pnab* |
| ***a* (Å)** | 5.6014(2) |
| ***b* (Å)** | 7.2792(2) |
| ***c* (Å)** | 86.045(5) |
| **Volume (Å$^3$)** | 3508.4(3) |

## 4.2.4 Rietveld refinement of figure 4.8 225 K scan

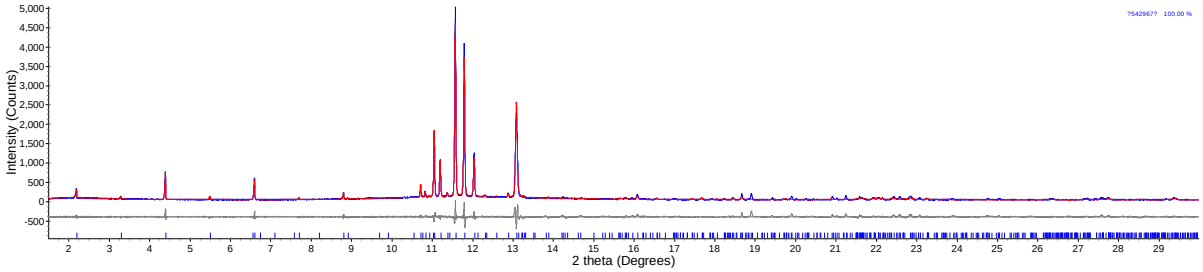


**Figure 7.61 Observed and calculated profiles for the Rietveld refinement of figure 4.8 225 K scan with the MP-*Pnab* structure. The bottom curve is the difference plot on the same intensity scale. ($R_{wp}$ = 12.96, $R_p$ = 9.14, $\chi$ = 1.77). The tick marks represent calculated peak positions.**

**Table 7.70 Refined lattice parameters for figure 4.8 225 K scan Rietveld refinement with the MP-*Pnab* structure.**

| Parameter | Value |
|---|---|
| **Phase / Space group** | MP-*Pnab* / *Pnab* |
| ***a* (Å)** | 5.5900(2) |
| ***b* (Å)** | 7.2430(2) |
| ***c* (Å)** | 85.998(5) |
| **Volume (Å$^3$)** | 3481.9(3) |

### 4.2.5 Rietveld refinement of figure 4.8 200 K scan

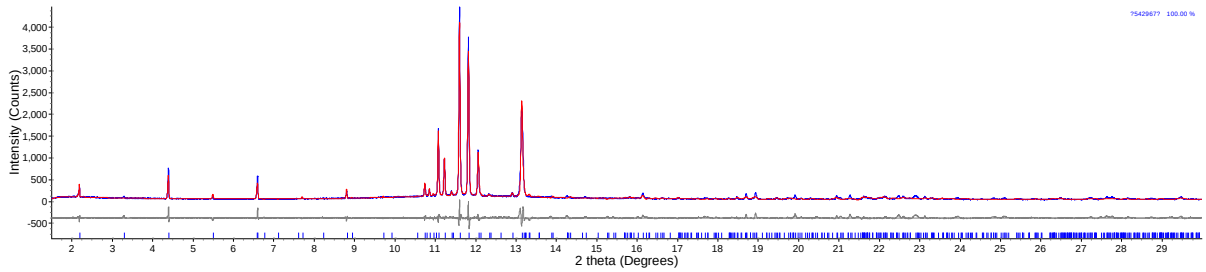


**Figure 7.62 Observed and calculated profiles for the Rietveld refinement of figure 4.8 200 K scan with the MP-*Pnab* structure. The bottom curve is the difference plot on the same intensity scale. ($R_{wp}$ = 12.70, $R_p$ = 8.90, $\chi$ = 1.74). The tick marks represent calculated peak positions.**

**Table 7.71 Refined lattice parameters for figure 4.8 200 K scan Rietveld refinement with the MP-*Pnab* structure.**

| Parameter | Value |
|---|---|
| **Phase / Space group** | MP-*Pnab* / *Pnab* |
| ***a* (Å)** | 5.5787(2) |
| ***b* (Å)** | 7.2093(2) |
| ***c* (Å)** | 85.943(5) |
| **Volume (Å$^3$)** | 3456.5(3) |

## 4.2.6 Rietveld refinement of figure 4.8 175 K scan

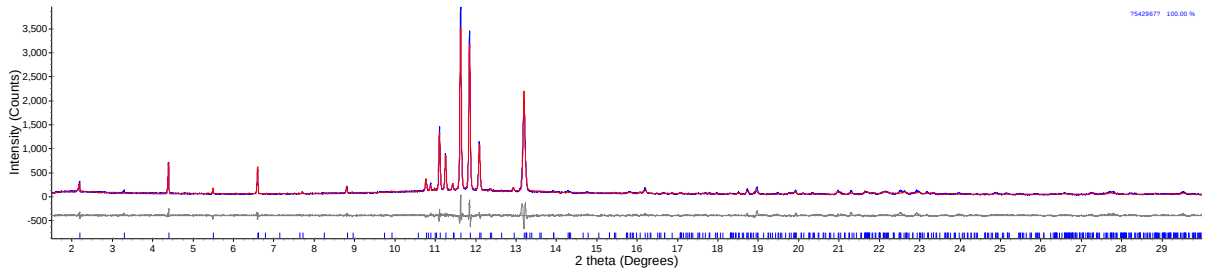


**Figure 7.63 Observed and calculated profiles for the Rietveld refinement of figure 4.8 175 K scan with the MP-*Pnab* structure. The bottom curve is the difference plot on the same intensity scale. ($R_{wp}$ = 11.45, $R_p$ = 8.28, $\chi$ = 1.57). The tick marks represent calculated peak positions.**

**Table 7.72 Refined lattice parameters for figure 4.8 175 K scan Rietveld refinement with the MP-*Pnab* structure.**

| Parameter | Value |
|---|---|
| **Phase / Space group** | MP-*Pnab* / *Pnab* |
| ***a* (Å)** | 5.5688(2) |
| ***b* (Å)** | 7.1816(2) |
| ***c* (Å)** | 85.939(6) |
| **Volume (Å$^3$)** | 3437.0 (3) |

## 4.2.7 Rietveld refinement of figure 4.8 150 K scan

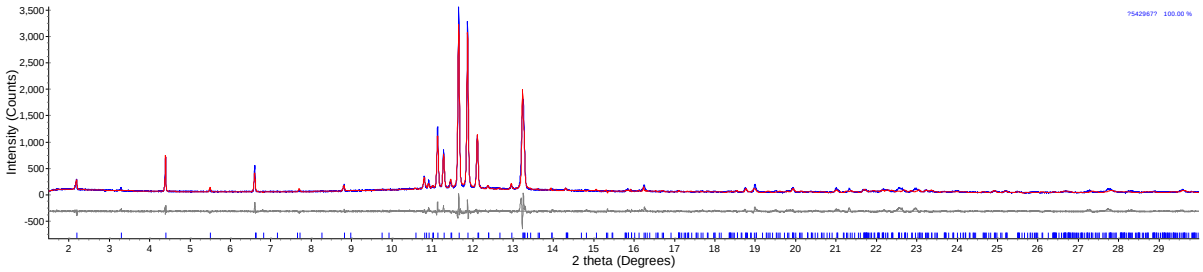


**Figure 7.64 Observed and calculated profiles for the Rietveld refinement of figure 4.8 150 K scan with the MP-*Pnab* structure. The bottom curve is the difference plot on the same intensity scale. ($R_{wp}$ = 12.02, $R_p$ = 8.56, $\chi$ = 1.65). The tick marks represent calculated peak positions.**

**Table 7.73 Refined lattice parameters for figure 4.8 150 K scan Rietveld refinement with the MP-*Pnab* structure.**

| Parameter | Value |
|---|---|
| **Phase / Space group** | MP-*Pnab* / *Pnab* |
| ***a* (Å)** | 5.5573(2) |
| ***b* (Å)** | 7.1617(2) |
| ***c* (Å)** | 85.925(5) |
| **Volume (Å$^3$)** | 3419.8(2) |

## 4.2.8 Rietveld refinement of figure 4.8 125 K scan

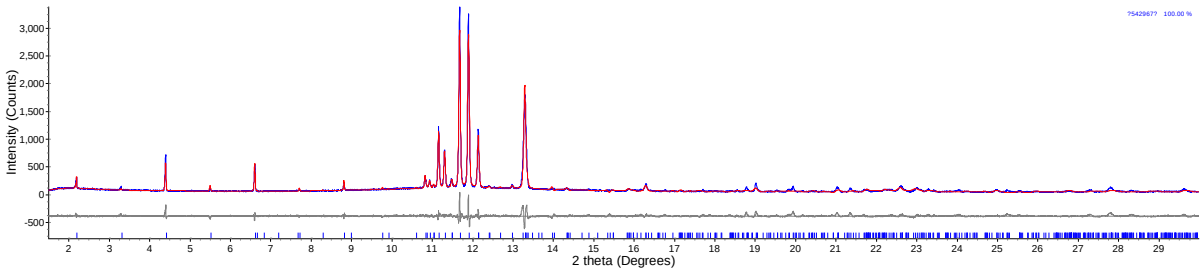


**Figure 7.65 Observed and calculated profiles for the Rietveld refinement of figure 4.8 125 K scan with the MP-*Pnab* structure. The bottom curve is the difference plot on the same intensity scale. ($R_{wp}$ = 11.76, $R_p$ = 8.43, $\chi$ = 1.63). The tick marks represent calculated peak positions.**

**Table 7.74 Refined lattice parameters for figure 4.8 125 K scan Rietveld refinement with the MP-*Pnab* structure.**

| Parameter | Value |
|---|---|
| **Phase / Space group** | MP-*Pnab* / *Pnab* |
| ***a* (Å)** | 5.5504(2) |
| ***b* (Å)** | 7.1312(2) |
| ***c* (Å)** | 85.885(5) |
| **Volume (Å$^3$)** | 3399.4(3) |

# Appendix 4.3 Rietveld refinement of recrystallisations of Methyl Palmitate

## 4.3.1 Rietveld refinement of figure 4.23 line C

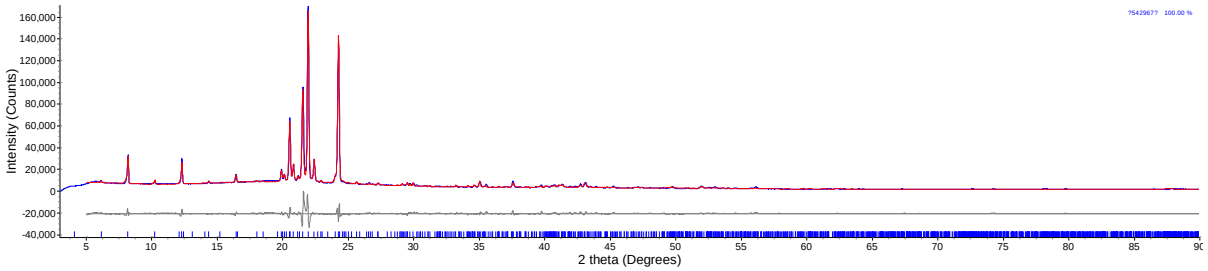


**Figure 7.66 Observed and calculated profiles for the Rietveld refinement of figure 4.23 line C with the MP-*Pnab* structure. The bottom curve is the difference plot on the same intensity scale. ($R_{wp}$ = 8.73, $R_p$ = 6.22, $\chi$ = 6.31). The tick marks represent calculated peak positions.**

**Table 7.75 Refined lattice parameters for figure 4.23 line C scan Rietveld refinement with the MP-*Pnab* structure.**

| Parameter | Value |
|---|---|
| **Phase / Space group** | MP-*Pnab* / *Pnab* |
| ***a* (Å)** | 5.6274(3) |
| ***b* (Å)** | 7.3360(4) |
| ***c* (Å)** | 86.28(1) |
| **Volume (Å$^3$)** | 3562.0(5) |

## 4.3.2 Rietveld refinement of figure 4.23 line D

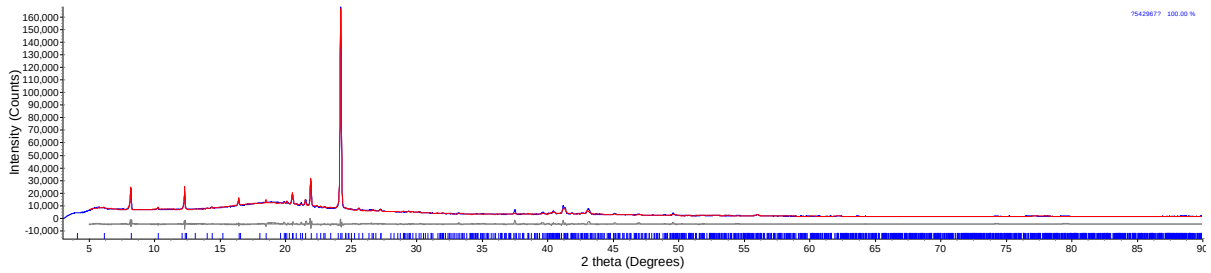


**Figure 7.67 Observed and calculated profiles for the Rietveld refinement of figure 4.23 line D with the MP-*Pnab* structure. The bottom curve is the difference plot on the same intensity scale. ($R_{wp}$ = 6.07, $R_p$ = 4.20, $\chi$ = 4.10). The tick marks represent calculated peak positions.**

**Table 7.76 Refined lattice parameters for figure 4.23 line D scan Rietveld refinement with the MP-*Pnab* structure.**

| Parameter | Value |
|---|---|
| **Phase / Space group** | MP-*Pnab* / *Pnab* |
| ***a* (Å)** | 5.6270(4) |
| ***b* (Å)** | 7.3447(4) |
| ***c* (Å)** | 86.223(9) |
| **Volume (Å$^3$)** | 3563.5(5) |

### 4.3.3 Rietveld refinement of figure 4.23 line E

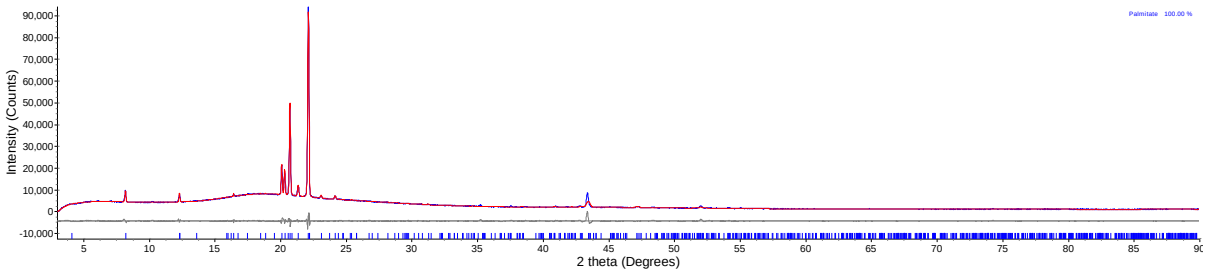


**Figure 7.68 Observed and calculated profiles for the Rietveld refinement of figure 4.23 line E with the MP-*C*2 structure. The bottom curve is the difference plot on the same intensity scale. ($R_{wp}$ = 4.92, $R_p$ = 2.83, $\chi$ = 2.75). The tick marks represent calculated peak positions.**

**Table 7.77 Refined lattice parameters for figure 4.23 line E Rietveld refinement with the MP-*C*2 structure.**

| Parameter | Value |
|---|---|
| **Phase / Space group** | MP-*C*2 / *C*2 |
| ***a* (Å)** | 43.227(8) |
| ***b* (Å)** | 7.288(3) |
| ***c* (Å)** | 5.559(2) |
| ***β* (°)** | 93.785(4) |
| **Volume (Å$^3$)** | 1747.2(9) |

### 4.3.4 Rietveld refinement of figure 4.23 line F

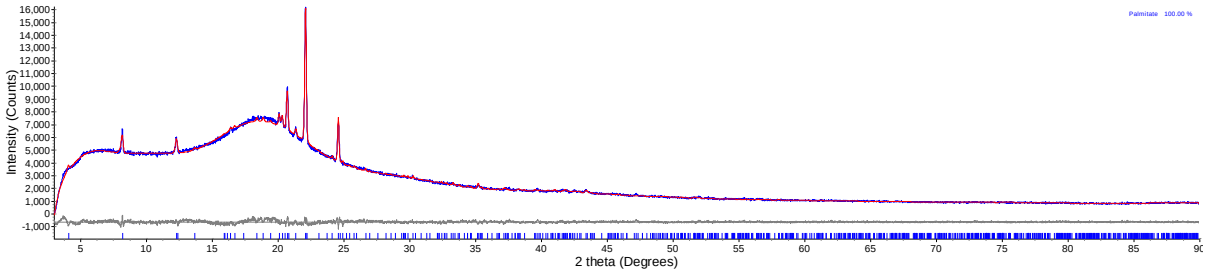


**Figure 7.69 Observed and calculated profiles for the Rietveld refinement of figure 4.23 line F with the MP-*C*2 structure. The bottom curve is the difference plot on the same intensity scale. ($R_{wp}$ = 2.93, $R_p$ = 2.17, $\chi$ = 1.46). The tick marks represent calculated peak positions.**

**Table 7.78 Refined lattice parameters for figure 4.23 line F Rietveld refinement with the MP-*C*2 structure.**

| Parameter | Value |
|---|---|
| **Phase / Space group** | MP-*C*2 / *C*2 |
| ***a* (Å)** | 43.32(1) |
| ***b* (Å)** | 7.240(1) |
| ***c* (Å)** | 5.583(1) |
| ***β* (°)** | 93.95(1) |
| **Volume (Å$^3$)** | 1746.9(6) |

## 4.3.5 Rietveld refinement of figure 4.24 line C

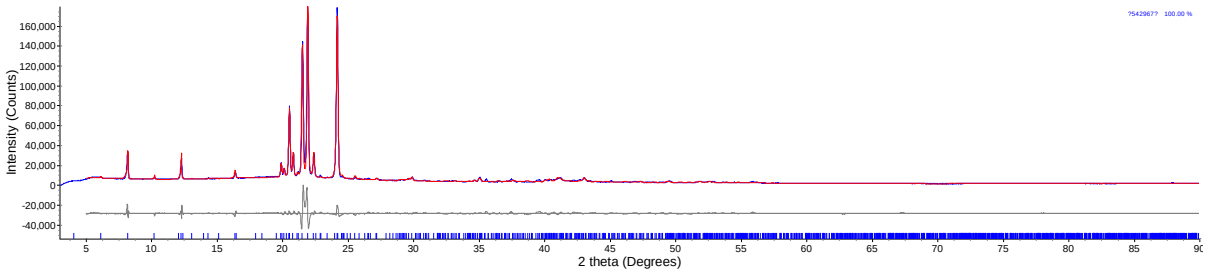


**Figure 7.70 Observed and calculated profiles for the Rietveld refinement of figure 4.24 line C with the MP-*Pnab* structure. The bottom curve is the difference plot on the same intensity scale. ($R_{wp}$ = 10.39, $R_p$ = 7.05, $\chi$ = 7.69). The tick marks represent calculated peak positions.**

**Table 7.79 Refined lattice parameters for figure 4.24 line C scan Rietveld refinement with the MP-*Pnab* structure.**

| Parameter | Value |
|---|---|
| **Phase / Space group** | MP-*Pnab* / *Pnab* |
| ***a* (Å)** | 5.6257(4) |
| ***b* (Å)** | 7.3704(7) |
| ***c* (Å)** | 86.72(1) |
| **Volume (Å$^3$)** | 3595.9(7) |

## 4.3.6 Rietveld refinement of figure 4.24 line D

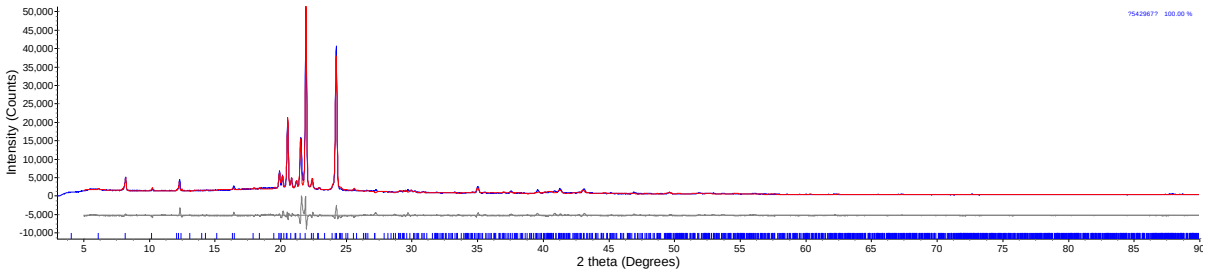


**Figure 7.71 Observed and calculated profiles for the Rietveld refinement of figure 4.24 line D with the MP-*Pnab* structure. The bottom curve is the difference plot on the same intensity scale. ($R_{wp}$ = 10.80, $R_p$ = 7.67, $\chi$ = 3.74). The tick marks represent calculated peak positions.**

**Table 7.80 Refined lattice parameters for figure 4.24 line D scan Rietveld refinement with the MP-*Pnab* structure.**

| Parameter | Value |
|---|---|
| **Phase / Space group** | MP-*Pnab* / *Pnab* |
| ***a* (Å)** | 5.6367(5) |
| ***b* (Å)** | 7.3587(6) |
| ***c* (Å)** | 86.87(1) |
| **Volume (Å$^3$)** | 3603.4(7) |

## 4.3.7 Rietveld refinement of figure 4.24 line E

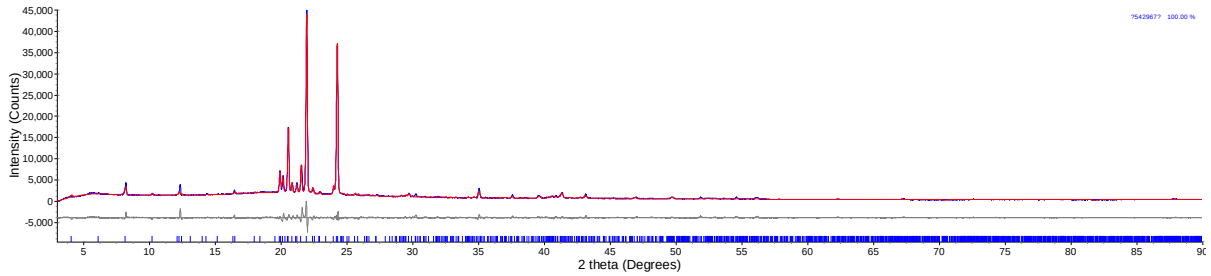


**Figure 7.72 Observed and calculated profiles for the Rietveld refinement of figure 4.24 line E with the MP-*Pnab* structure. The bottom curve is the difference plot on the same intensity scale. ($R_{wp}$ = 9.95, $R_p$ = 6.76, $\chi$ = 3.20). The tick marks represent calculated peak positions.**

**Table 7.81 Refined lattice parameters for figure 4.24 line E scan Rietveld refinement with the MP-*Pnab* structure.**

| Parameter | Value |
|---|---|
| **Phase / Space group** | MP-*Pnab* / *Pnab* |
| ***a* (Å)** | 5.6314(6) |
| ***b* (Å)** | 7.3452(6) |
| ***c* (Å)** | 86.77(1) |
| **Volume (Å$^3$)** | 3589.3(7) |

### 4.3.8 Rietveld refinement of figure 4.24 line F

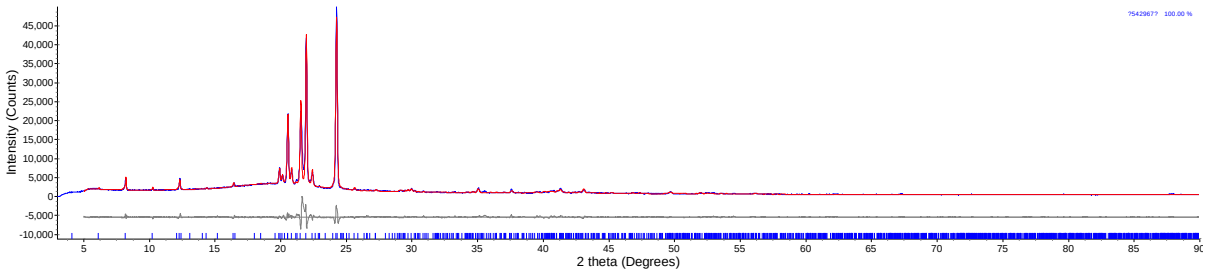


**Figure 7.73 Observed and calculated profiles for the Rietveld refinement of figure 4.24 line F with the MP-*Pnab* structure. The bottom curve is the difference plot on the same intensity scale. ($R_{wp}$ = 8.50, $R_p$ = 5.75, $\chi$ = 3.24). The tick marks represent calculated peak positions.**

**Table 7.82 Refined lattice parameters for figure 4.24 line F scan Rietveld refinement with the MP-*Pnab* structure.**

| Parameter | Value |
|---|---|
| **Phase / Space group** | MP-*Pnab* / *Pnab* |
| ***a* (Å)** | 5.6302(4) |
| ***b* (Å)** | 7.3453(5) |
| ***c* (Å)** | 86.478(1) |
| **Volume (Å$^3$)** | 3576.4(6) |

## 4.3.9 Rietveld refinement of figure 4.25 line C

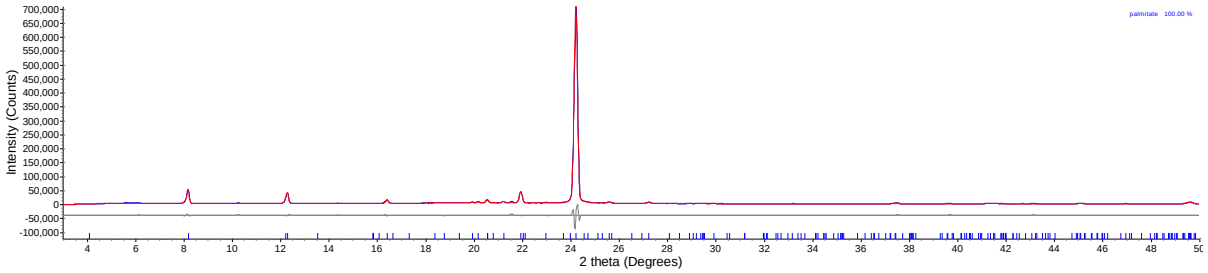


**Figure 7.74 Observed and calculated profiles for the Rietveld refinement of figure 4.25 line C with the MP-*C*2 structure. The bottom curve is the difference plot on the same intensity scale. ($R_{wp}$ = 8.32, $R_p$ = 6.09, $\chi$ = 7.38). The tick marks represent calculated peak positions.**

**Table 7.83 Refined lattice parameters for figure 4.25 line C Rietveld refinement with the MP-*C*2 structure.**

| Parameter | Value |
|---|---|
| **Phase / Space group** | MP-*C*2 / *C*2 |
| ***a* (Å)** | 43.313(6) |
| ***b* (Å)** | 7.3485(4) |
| ***c* (Å)** | 5.6045(9) |
| ***β* (°)** | 94.08(2) |
| **Volume (Å$^3$)** | 1779.3(4) |

## 4.3.10 Rietveld refinement of figure 4.25 line D

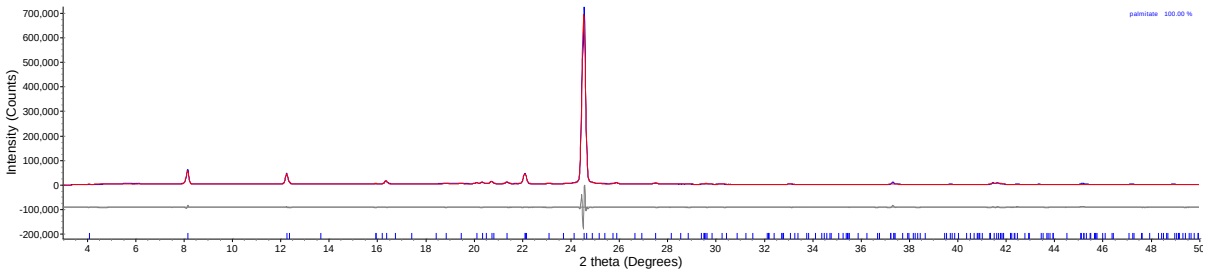


**Figure 7.75 Observed and calculated profiles for the Rietveld refinement of figure 4.25 line D with the MP-*C*2 structure. The bottom curve is the difference plot on the same intensity scale. ($R_{wp}$ = 10.53, $R_p$ = 7.63, $\chi$ = 9.28). The tick marks represent calculated peak positions.**

**Table 7.84 Refined lattice parameters for figure 4.25 line D Rietveld refinement with the MP-*C*2 structure.**

| Parameter | Value |
|---|---|
| **Phase / Space group** | MP-*C*2 / *C*2 |
| ***a* (Å)** | 43.397(7) |
| ***b* (Å)** | 7.2499(6) |
| ***c* (Å)** | 5.5689(9) |
| ***β* (°)** | 93.91(2) |
| **Volume (Å$^3$)** | 1748.0(4) |

## 4.3.11 Rietveld refinement of figure 4.25 line F

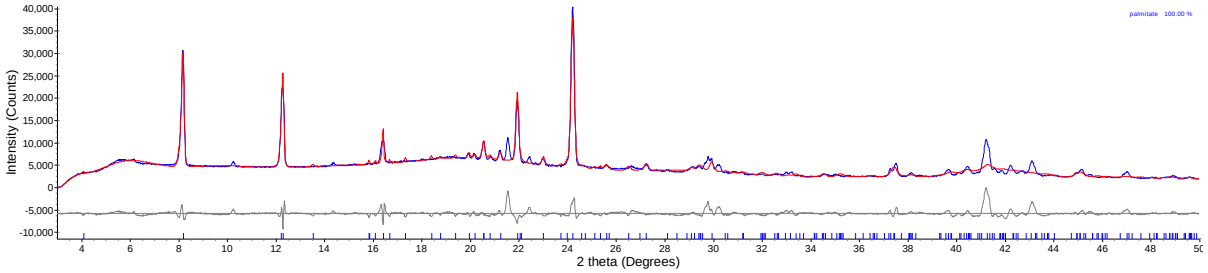


**Figure 7.76 Observed and calculated profiles for the Rietveld refinement of figure 4.25 line F with the MP-*C*2 structure. The bottom curve is the difference plot on the same intensity scale. ($R_{wp}$ = 10.36, $R_p$ = 6.61, $\chi$ = 7.09). The tick marks represent calculated peak positions.**

**Table 7.85 Refined lattice parameters for figure 4.25 line F Rietveld refinement with the MP-*C*2 structure.**

| Parameter | Value |
|---|---|
| **Phase / Space group** | MP-*C*2 / *C*2 |
| ***a* (Å)** | 43.3(1) |
| ***b* (Å)** | 7.3470(8) |
| ***c* (Å)** | 5.599(1) |
| ***β* (°)** | 94.16(2) |
| **Volume (Å$^3$)** | 1777.0(6) |

## 4.3.12 Rietveld refinement of figure 4.25 line G

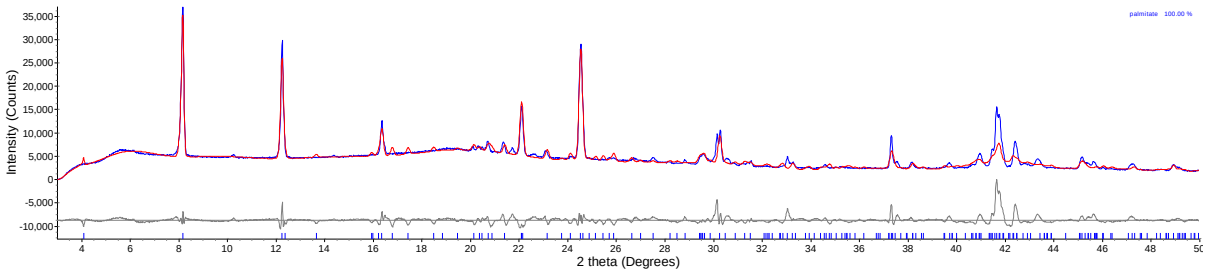


**Figure 7.77 Observed and calculated profiles for the Rietveld refinement of figure 4.25 line G with the MP-*C*2 structure. The bottom curve is the difference plot on the same intensity scale. ($R_{wp}$ = 11.90, $R_p$ = 7.84, $\chi$ = 8.09). The tick marks represent calculated peak positions.**

**Table 7.86 Refined lattice parameters for figure 4.25 line G Rietveld refinement with the MP-*C*2 structure.**

| Parameter | Value |
|---|---|
| **Phase / Space group** | MP-*C*2 / *C*2 |
| ***a* (Å)** | 43.451(6) |
| ***b* (Å)** | 7.2530(6) |
| ***c* (Å)** | 5.5573(9) |
| ***β* (°)** | 94.091(1) |
| **Volume (Å$^3$)** | 1746.9(4) |

## 4.3.13 Rietveld refinement of figure 4.25 line I

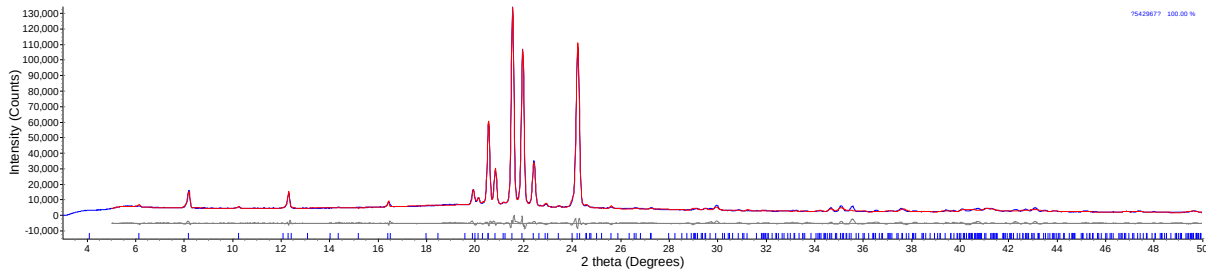


**Figure 7.78 Observed and calculated profiles for the Rietveld refinement of figure 4.25 line I with the MP-*Pnab* structure. The bottom curve is the difference plot on the same intensity scale. ($R_{wp}$ = 6.68, $R_p$ = 4.38, $\chi$ = 5.17). The tick marks represent calculated peak positions.**

**Table 7.87 Refined lattice parameters for figure 4.25 line I scan Rietveld refinement with the MP-*Pnab* structure.**

| Parameter | Value |
|---|---|
| **Phase / Space group** | MP-*Pnab* / *Pnab* |
| ***a* (Å)** | 5.6212(4) |
| ***b* (Å)** | 7.3482(6) |
| ***c* (Å)** | 86.41(1) |
| **Volume (Å$^3$)** | 3569.3(7) |

# Appendix 5.1 Atomic positions of hydrocarbon refinements

## 5.1.1 Atomic positions of octadecane 1972 refinement with octadecane as bought

**Table 7.88 Atomic positions of octadecane 1972 refinement with octadecane as bought.**

| Atom Number | *x* | *y* | *z* |
|---|---|---|---|
| **C1** | 0.06(1) | 0.271(1) | -0.4379(4) |
| **C2** | 0.15(1) | 0.079(3) | -0.3917(2) |
| **C3** | 0.055(5) | 0.230(1) | -0.3379(4) |
| **C4** | 0.091(2) | 0.038(2) | -0.290(2) |
| **C5** | 0.03(7) | 0.185(2) | -0.235(4) |
| **C6** | 0.069(6) | 0.008(2) | -0.18(1) |
| **C7** | 0.009(9) | 0.137(4) | 0.13(3) |
| **C8** | 0.066(1) | -0.047(2) | -0.079(3) |
| **C9** | -0.052(1) | 0.084(4) | -0.025(3) |
| **C9A** | 0.052(2) | -0.084(3) | 0.025(3) |
| **C8A** | -0.066(1) | 0.047(3) | 0.079(3) |
| **C7A** | -0.008(2) | -0.137(3) | 0.129(4) |
| **C6A** | -0.08(3) | 0.005(4) | 0.184(2) |
| **C5A** | -0.034(3) | -0.187(5) | 0.234(3) |
| **C4A** | -0.091(3) | -0.038(1) | 0.290(1) |
| **C3A** | -0.055(3) | -0.230(2) | 0.338(3) |
| **C2A** | -0.154(1) | -0.079(3) | 0.392(2) |
| **C1A** | -0.063(2) | -0.271(2) | 0.438(1) |

### 5.1.2 Atomic positions of eicosane 1992 refinement with eicosane as bought

**Table 7.89 Atomic positions of eicosane 1992 refinement with eicosane as bought.**

| Atom Number | *x* | *y* | *z* |
|---|---|---|---|
| **C1** | 0.252(8) | 0.310(6) | -0.462(1) |
| **C2** | 0.254(9) | 0.016(7) | -0.407(1) |
| **C3** | 0.20(1) | 0.148(7) | -0.356(2) |
| **C4** | -0.01(1) | 0.071(8) | -0.319(1) |
| **C5** | -0.079(9) | 0.245(8) | -0.253(2) |
| **C6** | 0.085(1) | 0 | -0.214(2) |
| **C7** | 0.14(1) | 0.122(9) | -0.182(1) |
| **C8** | 0.186(9) | -0.082(8) | -0.133(1) |
| **C9** | 0.06(1) | 0.134(9) | -0.072(2) |
| **C10** | 0.14(1) | -0.048(9) | -0.030(2) |
| **C10A** | 0.03(1) | 0.118(8) | 0.021(2) |
| **C9A** | 0.12(1) | -0.075(9) | 0.063(2) |
| **C8A** | 0.04(1) | 0.062(8) | 0.105(1) |
| **C7A** | 0.07(1) | -0.175(9) | 0.159(1) |
| **C6A** | -0.085(1) | 0 | 0.214(2) |
| **C5A** | -0.12(1) | -0.199(9) | 0.262(2) |
| **C4A** | -0.185(9) | -0.065(8) | 0.304(1) |
| **C3A** | -0.05(1) | -0.294(8) | 0.349(2) |
| **C2A** | -0.036(9) | -0.121(8) | 0.396(1) |
| **C1A** | 0.120(8) | -0.376(7) | 0.445(1) |

# Appendix 5.2 Rietveld refinements of recrystallisations of Octadecane

## 5.2.1 Rietveld refinement of figure 5.16 line B

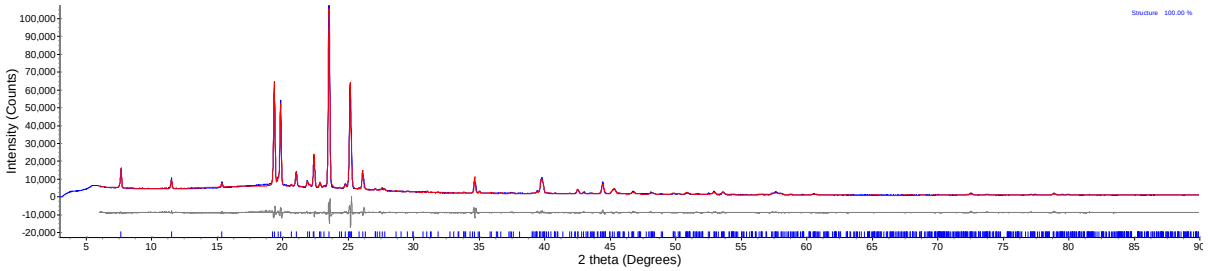


**Figure 7.79 Observed and calculated profiles for the Rietveld refinement of figure 5.16 line B with the octadecane structure. The bottom curve is the difference plot on the same intensity scale. ($R_{wp}$ = 7.31, $R_p$ = 5.16, $\chi$ = 4.18). The tick marks represent calculated peak positions.**

**Table 7.90 Refined lattice parameters for figure 5.16 line B Rietveld refinement with the octadecane structure.**

| Parameter | Value |
|---|---|
| **Phase / Space group** | Octadecane / *P*-1 |
| ***a* (Å)** | 4.2389(2) |
| ***b* (Å)** | 4.7833(2) |
| ***c* (Å)** | 24.875(1) |
| ***α* (°)** | 85.153(4) |
| ***β* (°)** | 67.943(5) |
| ***γ* (°)** | 73.401(2) |
| **Volume (Å$^3$)** | 477.82(4) |

## 5.2.2 Rietveld refinement of figure 5.16 line C

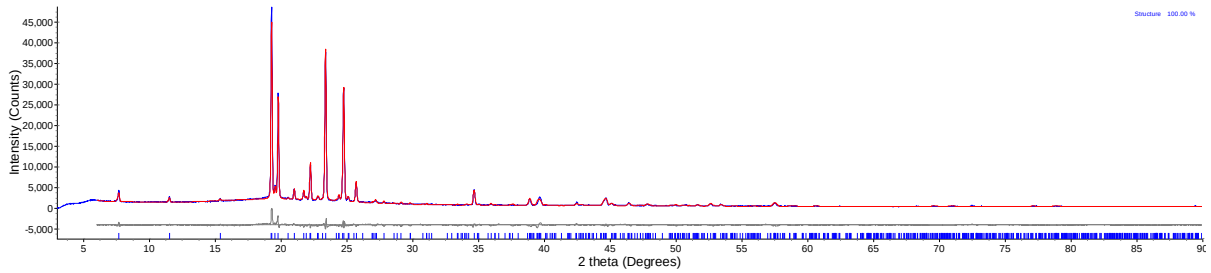


**Figure 7.80 Observed and calculated profiles for the Rietveld refinement of figure 5.16 line C with the octadecane structure. The bottom curve is the difference plot on the same intensity scale. ($R_{wp}$ = 7.92, $R_p$ = 5.81, $\chi$ = 2.72). The tick marks represent calculated peak positions.**

**Table 7.91 Refined lattice parameters for figure 5.16 line C Rietveld refinement with the octadecane structure.**

| Parameter | Value |
|---|---|
| **Phase / Space group** | Octadecane / *P*-1 |
| ***a* (Å)** | 4.2884(2) |
| ***b* (Å)** | 4.82350(9) |
| ***c* (Å)** | 24.880(2) |
| ***α* (°)** | 85.140(4) |
| ***β* (°)** | 67.904(6) |
| ***γ* (°)** | 72.605(2) |
| **Volume (Å$^3$)** | 454.82(4) |

## 5.2.3 Rietveld refinement of figure 5.16 line D

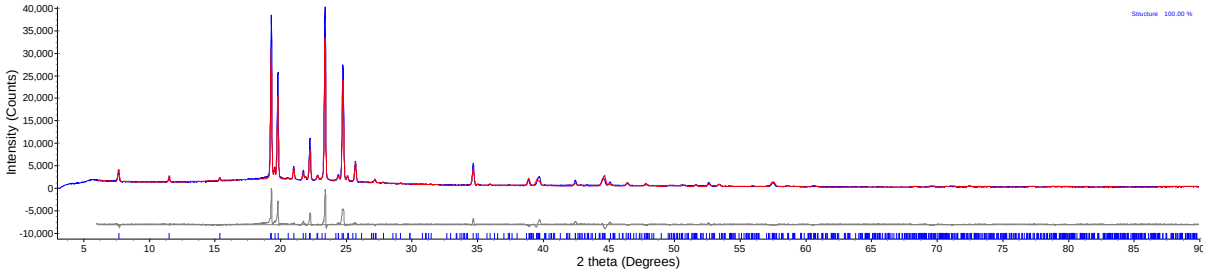


**Figure 7.81 Observed and calculated profiles for the Rietveld refinement of figure 5.16 line D with the octadecane structure. The bottom curve is the difference plot on the same intensity scale. ($R_{wp}$ = 11.23, $R_p$ = 8.14, $\chi$ = 3.82). The tick marks represent calculated peak positions.**

**Table 7.92 Refined lattice parameters for figure 5.16 line D Rietveld refinement with the octadecane structure.**

| Parameter | Value |
|---|---|
| **Phase / Space group** | Octadecane / *P*-1 |
| ***a* (Å)** | 4.2867(3) |
| ***b* (Å)** | 4.8206(3) |
| ***c* (Å)** | 24.875(3) |
| ***α* (°)** | 85.124(7) |
| ***β* (°)** | 67.86(1) |
| ***γ* (°)** | 72.600(3) |
| **Volume (Å$^3$)** | 454.11(7) |

## 5.2.4 Rietveld refinement of figure 5.16 line E

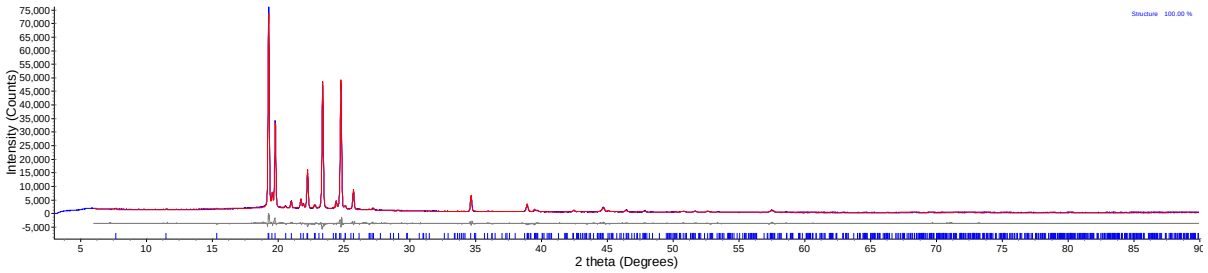


**Figure 7.82 Observed and calculated profiles for the Rietveld refinement of figure 5.16 line E with the octadecane structure. The bottom curve is the difference plot on the same intensity scale. ($R_{wp}$ = 6.92, $R_p$ = 5.02, $\chi$ = 2.48). The tick marks represent calculated peak positions.**

**Table 7.93 Refined lattice parameters for figure 5.16 line E Rietveld refinement with the octadecane structure.**

| Parameter | Value |
|---|---|
| **Phase / Space group** | Octadecane / *P*-1 |
| ***a* (Å)** | 4.2871(2) |
| ***b* (Å)** | 4.8227(2) |
| ***c* (Å)** | 24.908(2) |
| ***α* (°)** | 85.091(4) |
| ***β* (°)** | 67.900(5) |
| ***γ* (°)** | 72.626(1) |
| **Volume (Å$^3$)** | 455.17(5) |

## 5.2.5 Rietveld refinement of figure 5.16 line F

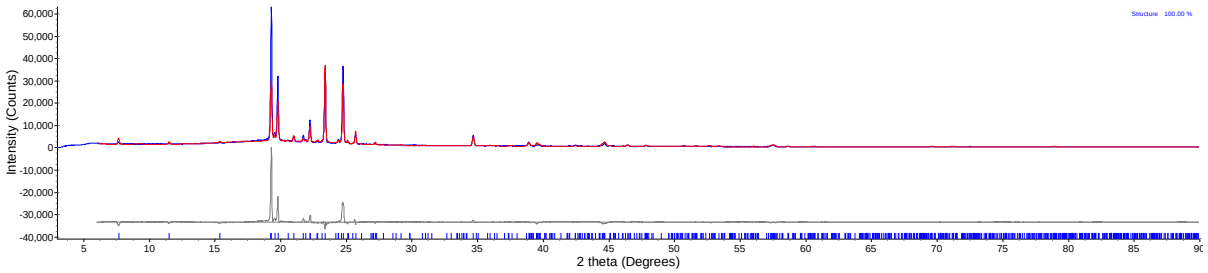


**Figure 7.83 Observed and calculated profiles for the Rietveld refinement of figure 5.16 line F with the octadecane structure. The bottom curve is the difference plot on the same intensity scale. ($R_{wp}$ = 18.68, $R_p$ = 12.94, $\chi$ = 6.91). The tick marks represent calculated peak positions.**

**Table 7.94 Refined lattice parameters for figure 5.16 line F Rietveld refinement with the octadecane structure.**

| Parameter | Value |
|---|---|
| **Phase / Space group** | Octadecane / *P*-1 |
| ***a* (Å)** | 4.2873(5) |
| ***b* (Å)** | 4.8183(6) |
| ***c* (Å)** | 24.892(5) |
| ***α* (°)** | 85.06(1) |
| ***β* (°)** | 67.77(2) |
| ***γ* (°)** | 72.600(6) |
| **Volume (Å$^3$)** | 454.0(1) |

# Appendix 5.3 Rietveld refinements of recrystallisations of Eicosane

## 5.3.1 Rietveld refinement of figure 5.19 line B

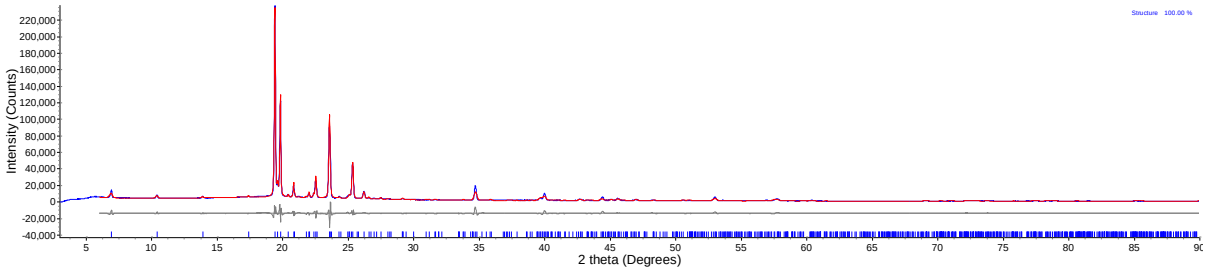


**Figure 7.84 Observed and calculated profiles for the Rietveld refinement of figure 5.19 line B with the eicosane structure. The bottom curve is the difference plot on the same intensity scale. ($R_{wp}$ = 9.93, $R_p$ = 6.97, $\chi$ = 6.06). The tick marks represent calculated peak positions.**

**Table 7.95 Refined lattice parameters for figure 5.19 line B Rietveld refinement with the eicosane structure.**

| Parameter | Value |
|---|---|
| **Phase / Space group** | Eicosane / *P*-1 |
| ***a* (Å)** | 4.2153(3) |
| ***b* (Å)** | 4.7614(4) |
| ***c* (Å)** | 27.406(3) |
| ***α* (°)** | 85.597(5) |
| ***β* (°)** | 68.345(9) |
| ***γ* (°)** | 73.678(3) |
| **Volume (Å$^3$)** | 490.40(8) |

## 5.3.2 Rietveld refinement of figure 5.19 line C

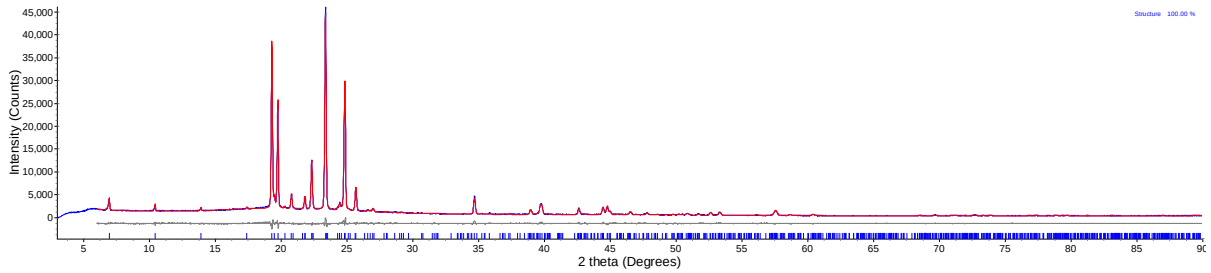


**Figure 7.85 Observed and calculated profiles for the Rietveld refinement of figure 5.19 line C with the eicosane structure. The bottom curve is the difference plot on the same intensity scale. ($R_{wp}$ = 4.76, $R_p$ = 3.66, $\chi$ = 1.63). The tick marks represent calculated peak positions.**

**Table 7.96 Refined lattice parameters for figure 5.19 line C Rietveld refinement with the eicosane structure.**

| Parameter | Value |
|---|---|
| **Phase / Space group** | Eicosane / *P*-1 |
| ***a* (Å)** | 4.2798(1) |
| ***b* (Å)** | 4.8180(1) |
| ***c* (Å)** | 27.4244(7) |
| ***α* (°)** | 85.584(2) |
| ***β* (°)** | 68.308(3) |
| ***γ* (°)** | 72.667(1) |
| **Volume (Å$^3$)** | 501.23(2) |

### 5.3.3 Rietveld refinement of figure 5.19 line D

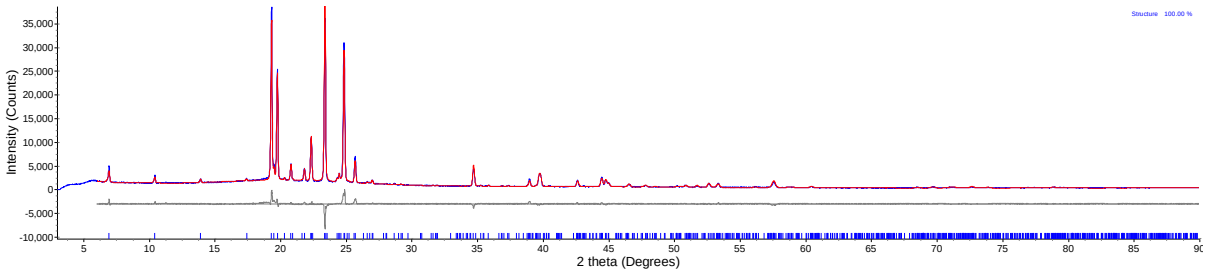


**Figure 7.86 Observed and calculated profiles for the Rietveld refinement of figure 5.19 line D with the eicosane structure. The bottom curve is the difference plot on the same intensity scale. ($R_{wp}$ = 6.77, $R_p$ = 5.20, $\chi$ = 2.32). The tick marks represent calculated peak positions.**

**Table 7.97 Refined lattice parameters for figure 5.19 line D Rietveld refinement with the eicosane structure.**

| Parameter | Value |
|---|---|
| **Phase / Space group** | Eicosane / *P*-1 |
| ***a* (Å)** | 4.2798(1) |
| ***b* (Å)** | 4.8178(2) |
| ***c* (Å)** | 27.4252(8) |
| ***α* (°)** | 85.587(3) |
| ***β* (°)** | 68.303(4) |
| ***γ* (°)** | 72.661(1) |
| **Volume (Å$^3$)** | 501.21(3) |

## 5.3.4 Rietveld refinement of figure 5.19 line E

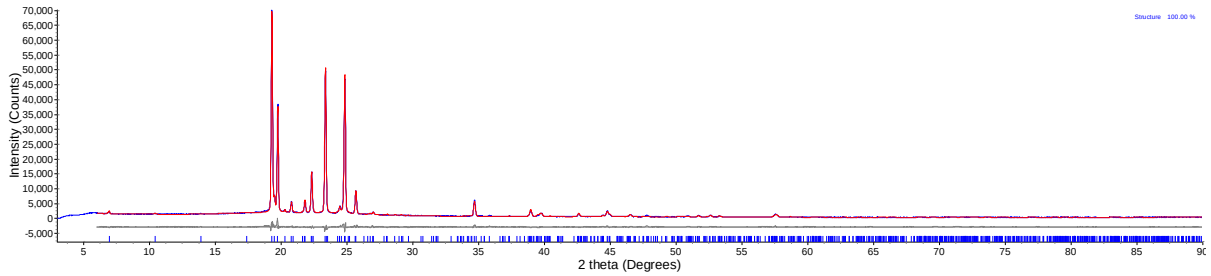


**Figure 7.87 Observed and calculated profiles for the Rietveld refinement of figure 5.19 line E with the eicosane structure. The bottom curve is the difference plot on the same intensity scale. ($R_{wp}$ = 6.06, $R_p$ = 4.46, $\chi$ = 2.20). The tick marks represent calculated peak positions.**

**Table 7.98 Refined lattice parameters for figure 5.19 line E Rietveld refinement with the eicosane structure.**

| Parameter | Value |
|---|---|
| **Phase / Space group** | Eicosane / *P*-1 |
| ***a* (Å)** | 4.2809(2) |
| ***b* (Å)** | 4.8185(2) |
| **c (Å)** | 27.441(1) |
| ***α* (°)** | 85.552(3) |
| ***β* (°)** | 68.297(4) |
| ***γ* (°)** | 72.660(1) |
| **Volume (Å$^3$)** | 501.67(4) |

## 5.3.5 Rietveld refinement of figure 5.19 line F

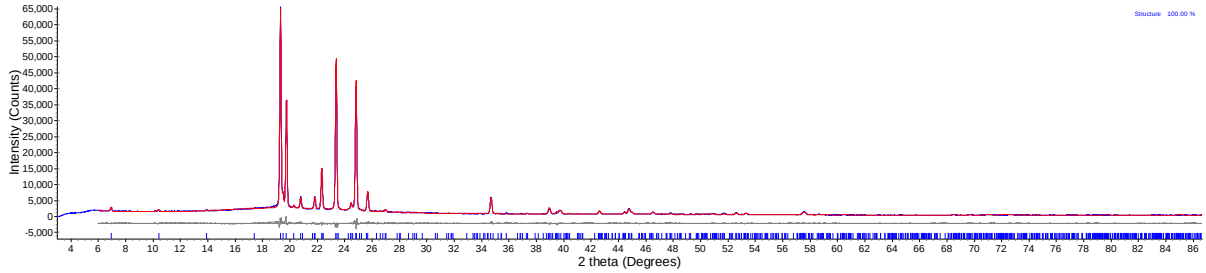


**Figure 7.88 Observed and calculated profiles for the Rietveld refinement of figure 5.19 line F with the eicosane structure. The bottom curve is the difference plot on the same intensity scale. ($R_{wp}$ = 5.53, $R_p$ = 4.21, $\chi$ = 2.10). The tick marks represent calculated peak positions.**

**Table 7.99 Refined lattice parameters for figure 5.19 line F Rietveld refinement with the eicosane structure.**

| Parameter | Value |
|---|---|
| **Phase / Space group** | Eicosane / *P*-1 |
| ***a* (Å)** | 4.2806(2) |
| ***b* (Å)** | 4.8186(2) |
| ***c* (Å)** | 27.436(1) |
| ***α* (°)** | 85.569(3) |
| ***β* (°)** | 68.304(5) |
| ***γ* (°)** | 72.661(1) |
| **Volume (Å$^3$)** | 501.57(4) |

# Appendix 5.4 Rietveld refinements of recrystallisations of Docosane

## 5.4.1 Rietveld refinement of figure 5.26 line B

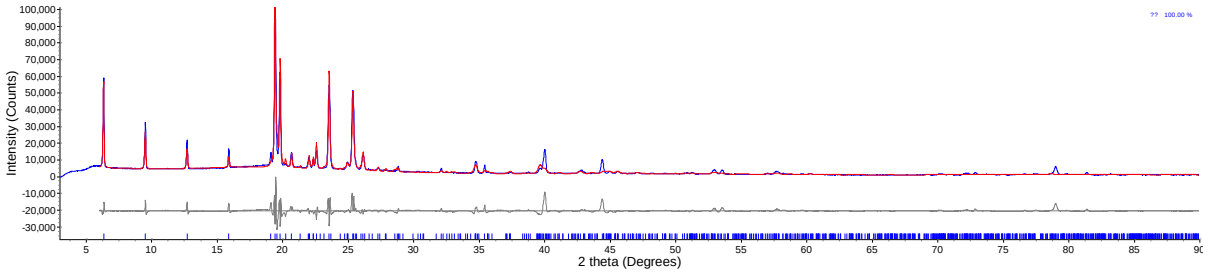


**Figure 7.89 Observed and calculated profiles for the Rietveld refinement of figure 5.26 line B with the docosane structure. The bottom curve is the difference plot on the same intensity scale. ($R_{wp}$ = 16.63, $R_p$ = 11.17, $\chi$ = 9.99). The tick marks represent calculated peak positions.**

**Table 7.100 Refined lattice parameters for figure 5.26 line B Rietveld refinement with the docosane structure.**

| Parameter | Value |
|---|---|
| **Phase / Space group** | Docosane / *P*-1 |
| ***a* (Å)** | 4.2210(4) |
| ***b* (Å)** | 4.7630(4) |
| ***c* (Å)** | 29.967(6) |
| ***α* (°)** | 86.03(2) |
| ***β* (°)** | 68.49(2) |
| ***γ* (°)** | 73.696 (6) |
| **Volume (Å$^3$)** | 537.6(1) |

## 5.4.2 Rietveld refinement of figure 5.26 line C

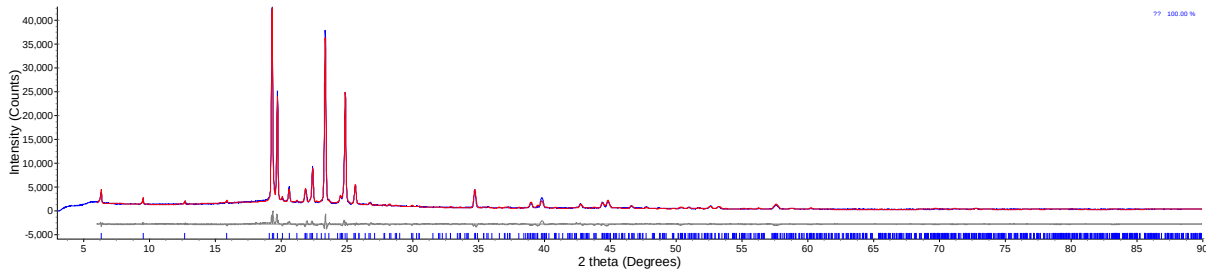


**Figure 7.90 Observed and calculated profiles for the Rietveld refinement of figure 5.26 line C with the docosane structure. The bottom curve is the difference plot on the same intensity scale. ($R_{wp}$ = 8.06, $R_p$ = 6.00, $\chi$ = 2.70). The tick marks represent calculated peak positions.**

**Table 7.101 Refined lattice parameters for figure 5.26 line C Rietveld refinement with the docosane structure.**

| Parameter | Value |
|---|---|
| **Phase / Space group** | Docosane / *P*-1 |
| ***a* (Å)** | 4.2733(2) |
| ***b* (Å)** | 4.8147(2) |
| ***c* (Å)** | 29.957(2) |
| ***α* (°)** | 85.973(5) |
| ***β* (°)** | 68.733(6) |
| ***γ* (°)** | 72.674(2) |
| **Volume (Å$^3$)** | 547.82(5) |

## 5.4.3 Rietveld refinement of figure 5.26 line D

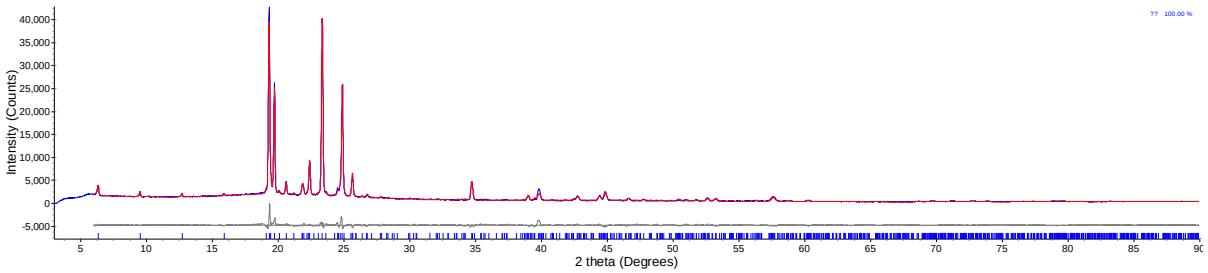


**Figure 7.91 Observed and calculated profiles for the Rietveld refinement of figure 5.26 line D with the docosane structure. The bottom curve is the difference plot on the same intensity scale. ($R_{wp}$ = 8.01, $R_p$ = 5.75, $\chi$ = 2.73). The tick marks represent calculated peak positions.**

**Table 7.102 Refined lattice parameters for figure 5.26 line D Rietveld refinement with the docosane structure.**

| Parameter | Value |
|---|---|
| **Phase / Space group** | Docosane / *P*-1 |
| ***a* (Å)** | 4.2726(2) |
| ***b* (Å)** | 4.8131(2) |
| ***c* (Å)** | 29.967(2) |
| ***α* (°)** | 85.976(4) |
| ***β* (°)** | 68.708(6) |
| ***γ* (°)** | 72.690(2) |
| **Volume (Å$^3$)** | 547.69(5) |

## 5.4.4 Rietveld refinement of figure 5.26 line E

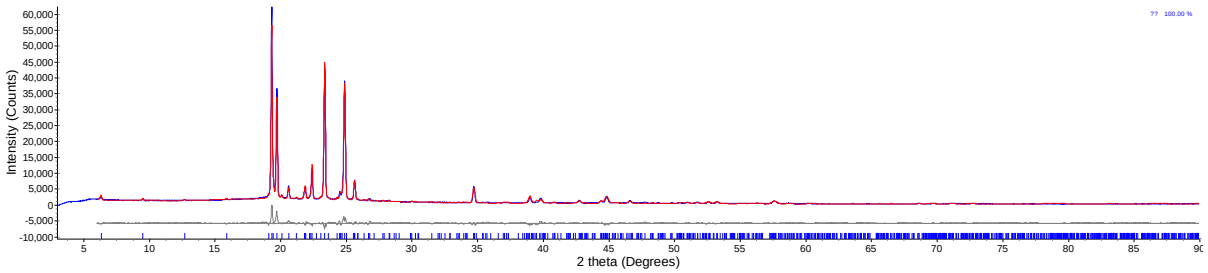


**Figure 7.92 Observed and calculated profiles for the Rietveld refinement of figure 5.26 line E with the docosane structure. The bottom curve is the difference plot on the same intensity scale. ($R_{wp}$ = 9.82, $R_p$ = 7.26, $\chi$ = 3.51). The tick marks represent calculated peak positions.**

**Table 7.103 Refined lattice parameters for figure 5.26 line E Rietveld refinement with the docosane structure.**

| Parameter | Value |
|---|---|
| **Phase / Space group** | Docosane / *P*-1 |
| ***a* (Å)** | 4.2736(2) |
| ***b* (Å)** | 4.8141(3) |
| ***c* (Å)** | 29.970(3) |
| ***α* (°)** | 85.965(6) |
| ***β* (°)** | 68.699(7) |
| ***γ* (°)** | 72.682(2) |
| **Volume (Å$^3$)** | 547.93(7) |

## 5.4.5 Rietveld refinement of figure 5.26 line F

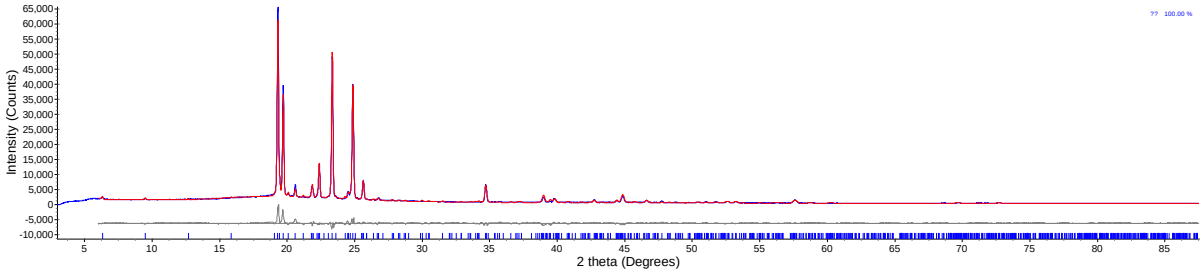


**Figure 7.93 Observed and calculated profiles for the Rietveld refinement of figure 5.26 line F with the docosane structure. The bottom curve is the difference plot on the same intensity scale. ($R_{wp}$ = 9.58, $R_p$ = 7.05, $\chi$ = 3.66). The tick marks represent calculated peak positions.**

**Table 7.104 Refined lattice parameters for figure 5.26 line F Rietveld refinement with the docosane structure.**

| Parameter | Value |
|---|---|
| **Space group** | Docosane / *P*-1 |
| ***a* (Å)** | 4.2724(2) |
| ***b* (Å)** | 4.8129(3) |
| ***c* (Å)** | 29.972(2) |
| ***α* (°)** | 85.975(5) |
| ***β* (°)** | 68.692(7) |
| ***γ* (°)** | 72.711(2) |
| **Volume (Å$^3$)** | 547.74(7) |

# Appendix 5.5 Rietveld refinements of cocrystallisation experiments with Methyl Stearate and Dodecane

## 5.5.1 Rietveld refinement of figure 5.27 line D

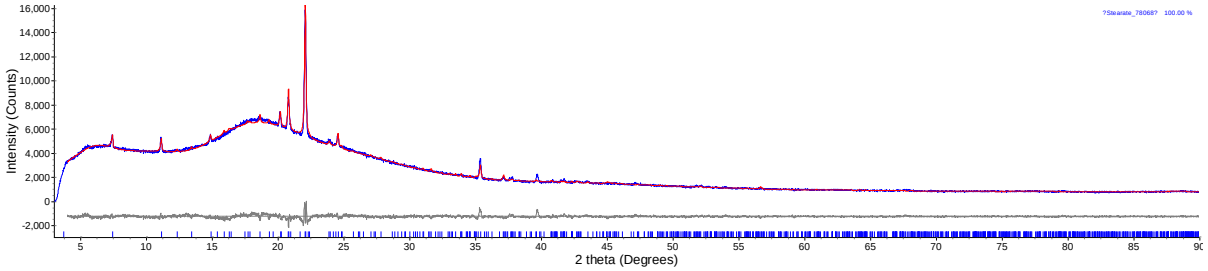


**Figure 7.94 Observed and calculated profiles for the Rietveld refinement of figure 5.27 line D with the MS-*C*2 structure. The bottom curve is the difference plot on the same intensity scale. ($R_{wp}$ = 3.28, $R_p$ = 2.42, $\chi$ = 1.59). The tick marks represent calculated peak positions.**

**Table 7.105 Refined lattice parameters for figure 5.27 line D Rietveld refinement with the MS-*C*2 structure.**

| Parameter | Value |
|---|---|
| **Phase / Space group** | MS-*C*2 / *C*2 |
| ***a* (Å)** | 47.593(7) |
| ***b* (Å)** | 7.2429(7) |
| ***c* (Å)** | 5.5651(8) |
| ***β* (°)** | 90.95(1) |
| **Volume (Å$^3$)** | 1918.1(4) |

## 5.5.2 Rietveld refinement of figure 5.27 line E

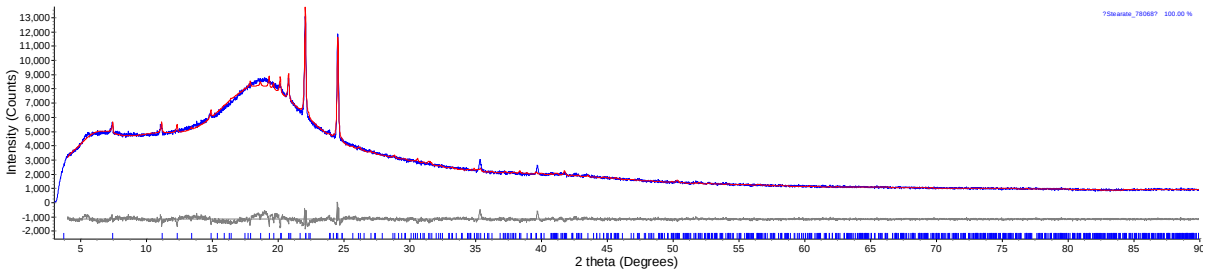


**Figure 7.95 Observed and calculated profiles for the Rietveld refinement of figure 5.27 line E with the MS-*C*2 structure. The bottom curve is the difference plot on the same intensity scale. ($R_{wp}$ = 3.21, $R_p$ = 2.47, $\chi$ = 1.66). The tick marks represent calculated peak positions.**

**Table 7.106 Refined lattice parameters for figure 5.27 line E Rietveld refinement with the MS-*C*2 structure.**

| Parameter | Value |
|---|---|
| **Phase / Space group** | MS-*C*2 / *C*2 |
| ***a* (Å)** | 47.502(8) |
| ***b* (Å)** | 7.2473(3) |
| ***c* (Å)** | 5.5609(8) |
| ***β* (°)** | 91.05(1) |
| **Volume (Å$^3$)** | 1914.0(4) |

## 5.5.3 Rietveld refinement of figure 5.27 line F

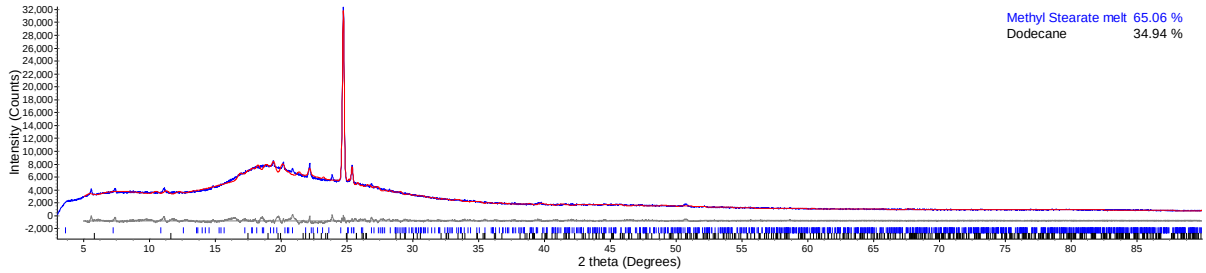


**Figure 7.96 Observed and calculated profiles for the mixed phase Rietveld refinement of figure 5.27 line F with the MS-*C*2 and dodecane structures. The bottom curve is the difference plot on the same intensity scale. ($R_{wp}$ = 3.79, $R_p$ = 2.97, $\chi$ = 1.89). The tick marks represent calculated peak positions.**

**Table 7.107 Refined lattice parameters for figure 5.27 line F mixed phase Rietveld refinement with the MS-*C*2 and dodecane structures.**

| Parameter | Value |
|---|---|
| **Phase / Space group** | MS-*C*2 / *C*2 |
| ***a* (Å)** | 48.83(2) |
| ***b* (Å)** | 7.102(3) |
| ***c* (Å)** | 6.482(4) |
| ***β* (°)** | 91.78 (2) |
| **Volume (Å$^3$)** | 2246(2) |
| **Phase / Space group** | Dodecane / *P*-1 |
| ***a* (Å)** | 4.268(2) |
| ***b* (Å)** | 4.840(2) |
| ***c* (Å)** | 15.408(8) |
| ***α* (°)** | 91.51(2) |
| ***β* (°)** | 80.51(4) |
| ***γ* (°)** | 105.1(2) |
| **Volume (Å$^3$)** | 303.0(3) |
| **Phase fractions (%)** | MS-*C*2 65.06 : 34.94 Dodecane |

## 5.5.4 Rietveld refinement of figure 5.27 line G

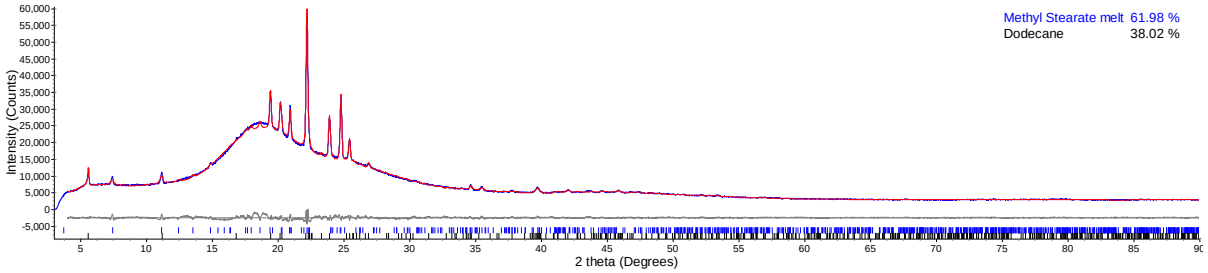


**Figure 7.97 Observed and calculated profiles for the mixed phase Rietveld refinement of figure 5.27 line G with the MS-*C*2 and dodecane structures. The bottom curve is the difference plot on the same intensity scale. ($R_{wp}$ = 2.52, $R_p$ = 2.01, $\chi$ = 2.15). The tick marks represent calculated peak positions.**

**Table 7.108 Refined lattice parameters for figure 5.27 line G mixed phase Rietveld refinement with the MS-*C*2 and dodecane structures.**

| Parameter | Value |
|---|---|
| **Phase / Space group** | MS-*C*2 / *C*2 |
| ***a* (Å)** | 47.62(1) |
| ***b* (Å)** | 7.1844(7) |
| ***c* (Å)** | 5.562(1) |
| ***β* (°)** | 90.52(2) |
| **Volume (Å$^3$)** | 1902.7(7) |
| **Phase / Space group** | Dodecane / *P*-1 |
| ***a* (Å)** | 4.1966(6) |
| ***b* (Å)** | 4.7497(6) |
| ***c* (Å)** | 16.027(5) |
| ***α* (°)** | 93.28(2) |
| ***β* (°)** | 80.10(2) |
| ***γ* (°)** | 105.842(8) |
| **Volume (Å$^3$)** | 302.7(1) |
| **Phase fractions (%)** | MS-*C*2 61.98 : 38.02 Dodecane |

## 5.5.5 Rietveld refinement of figure 5.28 line D

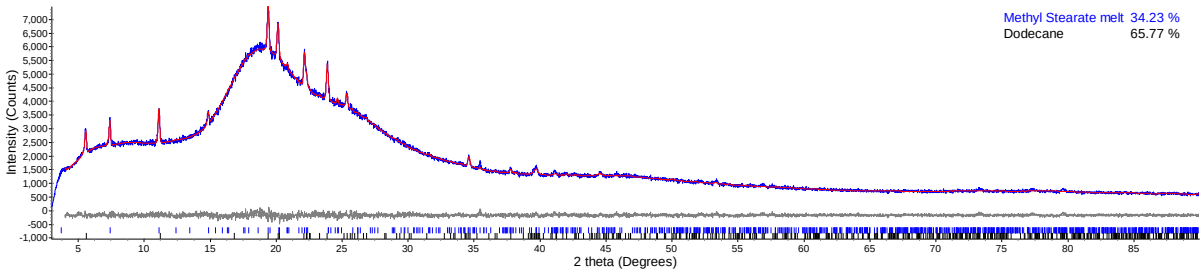


**Figure 7.98 Observed and calculated profiles for the mixed phase Rietveld refinement of figure 5.28 line D with the MS-*C*2 and dodecane structures. The bottom curve is the difference plot on the same intensity scale. ($R_{wp}$ = 2.69, $R_p$ = 1.99, $\chi$ = 1.15). The tick marks represent calculated peak positions.**

**Table 7.109 Refined lattice parameters for figure 5.27 line D mixed phase Rietveld refinement with the MS-*C*2 and dodecane structures.**

| Parameter | Value |
|---|---|
| **Phase / Space group** | MS-*C*2 / *C*2 |
| ***a* (Å)** | 47.64(2) |
| ***b* (Å)** | 7.215(2) |
| ***c* (Å)** | 5.565(2) |
| ***β* (°)** | 90.53(3) |
| **Volume (Å$^3$)** | 1912(1) |
| **Phase / Space group** | Dodecane / *P*-1 |
| ***a* (Å)** | 4.200(1) |
| ***b* (Å)** | 4.7553(9) |
| ***c* (Å)** | 16.024(7) |
| ***α* (°)** | 93.348(4) |
| ***β* (°)** | 80.16(4) |
| ***γ* (°)** | 105.96(2) |
| **Volume (Å$^3$)** | 303.1(2) |
| **Phase fractions (%)** | MS-*C*2 34.23 : 65.77 Dodecane |

# Appendix 5.6 Rietveld refinements of cocrystallisation experiments with Methyl Stearate and Tetradecane

## 5.6.1 Rietveld refinement of figure 5.29 line D

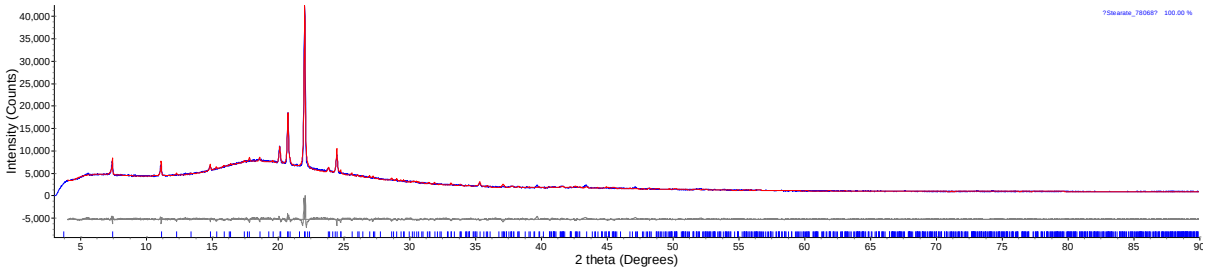


**Figure 7.99 Observed and calculated profiles for the Rietveld refinement of figure 5.29 line D with the MS-*C*2 structure. The bottom curve is the difference plot on the same intensity scale. ($R_{wp}$ = 4.37, $R_p$ = 3.03, $\chi$ = 2.28). The tick marks represent calculated peak positions.**

**Table 7.110 Refined lattice parameters for figure 5.29 line D Rietveld refinement with the MS-*C*2 structure.**

| Parameter | Value |
|---|---|
| **Phase / Space group** | MS-*C*2 / *C*2 |
| ***a* (Å)** | 47.672(4) |
| ***b* (Å)** | 7.2703(3) |
| ***c* (Å)** | 5.5707(4) |
| ***β* (°)** | 90.971(8) |
| **Volume (Å$^3$)** | 1930.5(2) |

## 5.6.2 Rietveld refinement of figure 5.29 line E

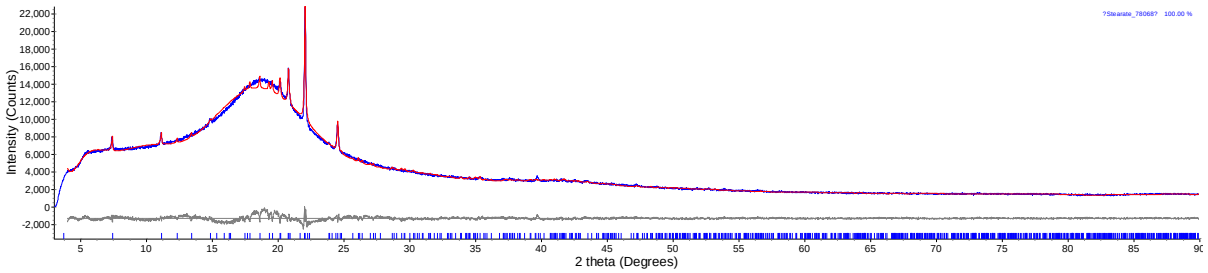


**Figure 7.100 Observed and calculated profiles for the Rietveld refinement of figure 5.29 line E with the MS-*C*2 structure. The bottom curve is the difference plot on the same intensity scale. ($R_{wp}$ = 3.11, $R_p$ = 2.54, $\chi$ = 1.97). The tick marks represent calculated peak positions.**

**Table 7.111 Refined lattice parameters for figure 5.29 line E Rietveld refinement with the MS-*C*2 structure.**

| Parameter | Value |
|---|---|
| **Phase / Space group** | MS-*C*2 / *C*2 |
| ***a* (Å)** | 47.631(7) |
| ***b* (Å)** | 7.2492(5) |
| ***c* (Å)** | 5.5742(8) |
| ***β* (°)** | 90.79(1) |
| **Volume (Å$^3$)** | 1924.5(4) |

## 5.6.3 Rietveld refinement of figure 5.29 line F

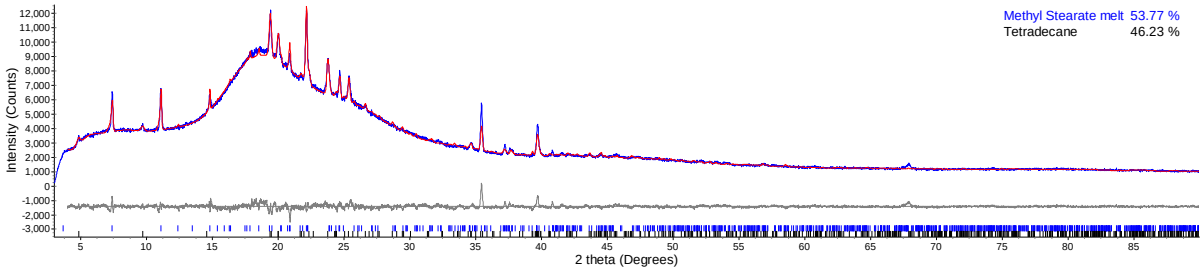


**Figure 7.101 Observed and calculated profiles for the mixed phase Rietveld refinement of figure 5.29 line F with the MS-*C*2 and tetradecane structures. The bottom curve is the difference plot on the same intensity scale. ($R_{wp}$ = 3.40, $R_p$ = 2.40, $\chi$ = 1.84). The tick marks represent calculated peak positions.**

**Table 7.112 Refined lattice parameters for figure 5.29 line F mixed phase Rietveld refinement with the MS-*C*2 and tetradecane structures.**

| Parameter | Value |
|---|---|
| **Phase / Space group** | MS-*C*2 / *C*2 |
| ***a* (Å)** | 47.89(1) |
| ***b* (Å)** | 7.218(1) |
| ***c* (Å)** | 5.569(1) |
| ***β* (°)** | 90.50(2) |
| **Volume (Å$^3$)** | 1924.9(6) |
| **Phase / Space group** | Tetradecane / *P*-1 |
| ***a* (Å)** | 4.2090(7) |
| ***b* (Å)** | 4.7602(7) |
| ***c* (Å)** | 18.552(3) |
| ***α* (°)** | 92.83(1) |
| ***β* (°)** | 78.99(2) |
| ***γ* (°)** | 106.03(1) |
| **Volume (Å$^3$)** | 350.68(9) |
| **Phase fractions (%)** | MS-*C*2 53.77 : 46.23 Tetradecane |

## 5.6.4 Rietveld refinement of figure 5.29 line G

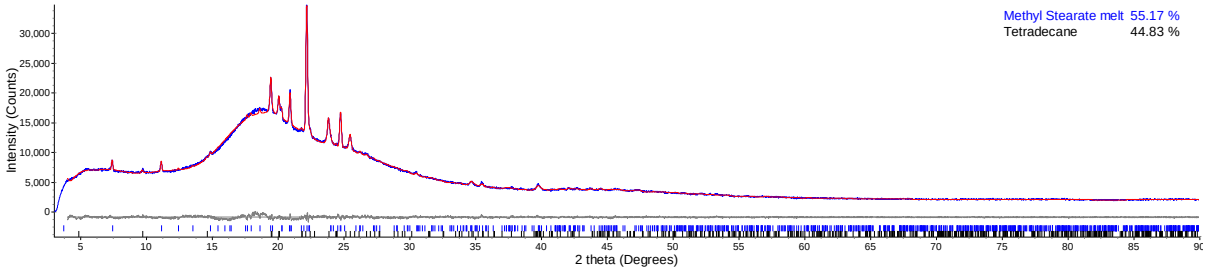


**Figure 7.102 Observed and calculated profiles for the mixed phase Rietveld refinement of figure 5.29 line G with the MS-*C*2 and tetradecane structures. The bottom curve is the difference plot on the same intensity scale. ($R_{wp}$ = 2.03, $R_p$ = 1.62, $\chi$ = 1.49). The tick marks represent calculated peak positions.**

**Table 7.113 Refined lattice parameters for figure 5.29 line G mixed phase Rietveld refinement with the MS-*C*2 and tetradecane structures.**

| Parameter | Value |
|---|---|
| **Phase / Space group** | MS-*C*2 / *C*2 |
| ***a* (Å)** | 47.60(2) |
| ***b* (Å)** | 7.185(2) |
| ***c* (Å)** | 5.555(2) |
| ***β* (°)** | 90.51(2) |
| **Volume (Å$^3$)** | 1900(1) |
| **Phase / Space group** | Tetradecane / *P*-1 |
| ***a* (Å)** | 4.188(2) |
| ***b* (Å)** | 4.739(1) |
| ***c* (Å)** | 18.53(1) |
| ***α* (°)** | 92.93(4) |
| ***β* (°)** | 79.03(7) |
| ***γ* (°)** | 105.96(2) |
| **Volume (Å$^3$)** | 347.1(3) |
| **Phase fractions (%)** | MS-*C*2 55.17 : 44.83 Tetradecane |

## 5.6.5 Rietveld refinement of figure 5.30 line D

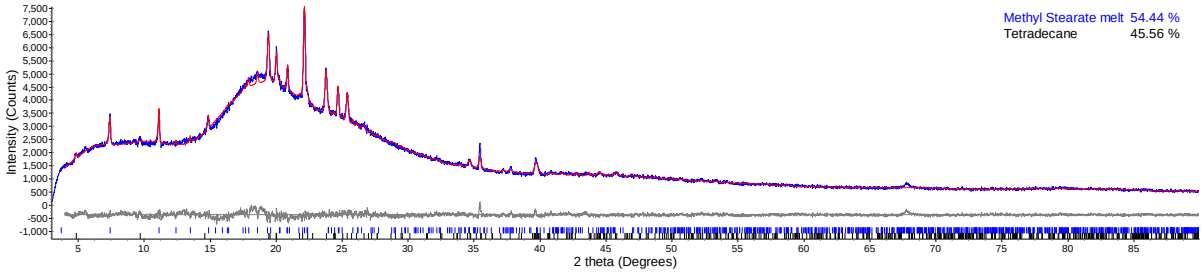


**Figure 7.103 Observed and calculated profiles for the mixed phase Rietveld refinement of figure 5.30 line D with the MS-*C*2 and tetradecane structures. The bottom curve is the difference plot on the same intensity scale. ($R_{wp}$ = 3.48, $R_p$ = 2.65, $\chi$ = 1.40). The tick marks represent calculated peak positions.**

**Table 7.114 Refined lattice parameters for figure 5.30 line D mixed phase Rietveld refinement with the MS-*C*2 and tetradecane structures.**

| Parameter | Value |
|---|---|
| **Phase / Space group** | MS-*C*2 / *C*2 |
| ***a* (Å)** | 47.65(1) |
| ***b* (Å)** | 7.202(1) |
| ***c* (Å)** | 5.558(1) |
| ***β* (°)** | 90.72(3) |
| **Volume (Å$^3$)** | 1907.2(8) |
| **Phase / Space group** | Tetradecane / *P*-1 |
| ***a* (Å)** | 4.199(1) |
| ***b* (Å)** | 4.7529(8) |
| ***c* (Å)** | 18.520(5) |
| ***α* (°)** | 93.0(4) |
| ***β* (°)** | 79.05(4) |
| ***γ* (°)** | 106.09(2) |
| **Volume (Å$^3$)** | 348.7(2) |
| **Phase fractions** | MS-*C*2 54.44 : 45.56 Tetradecane |

# Appendix 5.7 Rietveld refinements of cocrystallisation experiments with Methyl Stearate and Octadecane

## 5.7.1 Rietveld refinement of figure 5.31 line E

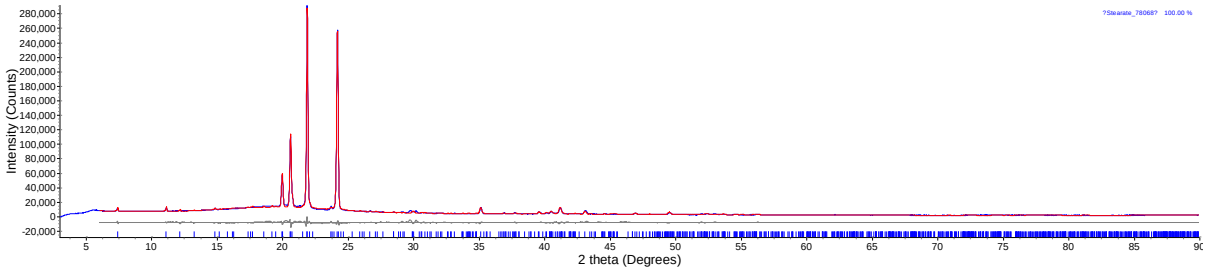


**Figure 7.104 Observed and calculated profiles for the Rietveld refinement of figure 5.31 line E with the MS-*C*2 structure. The bottom curve is the difference plot on the same intensity scale. ($R_{wp}$ = 6.47, $R_p$ = 4.54, $\chi$ = 5.12). The tick marks represent calculated peak positions.**

**Table 7.115 Refined lattice parameters for figure 5.31 line E Rietveld refinement with the MS-*C*2 structure.**

| Parameter | Value |
|---|---|
| **Phase / Space group** | MS-*C*2 / *C*2 |
| ***a* (Å)** | 47.788 (3) |
| ***b* (Å)** | 7.3636(3) |
| ***c* (Å)** | 5.6140(4) |
| ***β* (°)** | 90.886(5) |
| **Volume (Å$^3$)** | 1975.3(2) |

## 5.7.2 Rietveld refinement of figure 5.31 line F

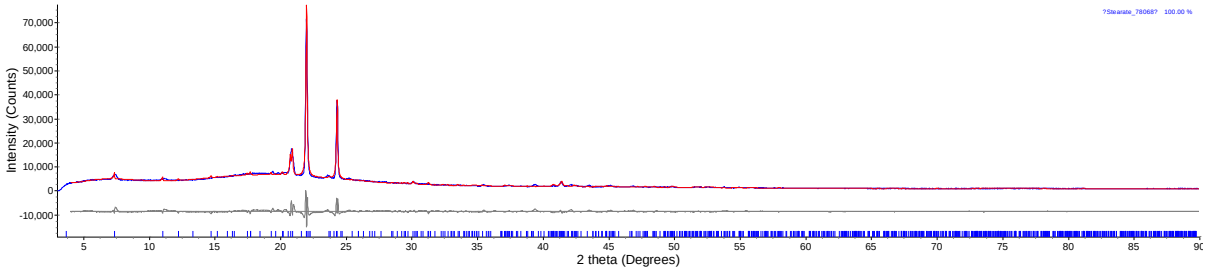


**Figure 7.105 Observed and calculated profiles for the Rietveld refinement of figure 5.31 line F with the MS-*C*2 structure. The bottom curve is the difference plot on the same intensity scale. ($R_{wp}$ = 7.86, $R_p$ = 5.81, $\chi$ = 4.19). The tick marks represent calculated peak positions.**

**Table 7.116 Refined lattice parameters for figure 5.31 line F Rietveld refinement with the MS-*C*2 structure.**

| Parameter | Value |
|---|---|
| **Phase / Space group** | MS-*C*2 / *C*2 |
| ***a* (Å)** | 48.132(6) |
| ***b* (Å)** | 7.3163(2) |
| ***c* (Å)** | 5.5499(4) |
| ***β* (°)** | 91.036(7) |
| **Volume (Å$^3$)** | 1954.1(3) |

## 5.7.3 Rietveld refinement of figure 5.31 line G

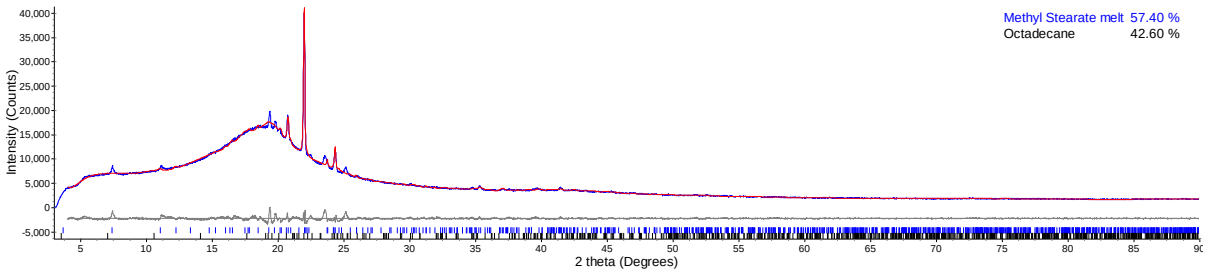


**Figure 7.106 Observed and calculated profiles for the mixed phase Rietveld refinement of figure 5.31 line G with the MS-*C*2 and octadecane structures. The bottom curve is the difference plot on the same intensity scale. ($R_{wp}$ = 3.16, $R_p$ = 2.30, $\chi$ = 2.20). The tick marks represent calculated peak positions.**

**Table 7.117 Refined lattice parameters for figure 5.31 line G mixed phase Rietveld refinement with the MS-*C*2 and octadecane structures.**

| Parameter | Value |
|---|---|
| **Phase / Space group** | MS-*C*2 / *C*2 |
| ***a* (Å)** | 48.01(2) |
| ***b* (Å)** | 7.3071(6) |
| ***c* (Å)** | 5.5353(8) |
| ***β* (°)** | 91.43) |
| **Volume (Å$^3$)** | 1941.3(7) |
| **Phase / Space group** | Octadecane / *P*-1 |
| ***a* (Å)** | 4.38(2) |
| ***b* (Å)** | 4.85(1) |
| ***c* (Å)** | 26.94(8) |
| ***α* (°)** | 86.62(3) |
| ***β* (°)** | 69.01(5) |
| ***γ* (°)** | 73.96(2) |
| **Volume (Å$^3$)** | 513.2(3) |
| **Phase fractions** | MS-*C*2 57.40 : 42.60 Octadecane |

## 5.7.4 Rietveld refinement of figure 5.33 line E

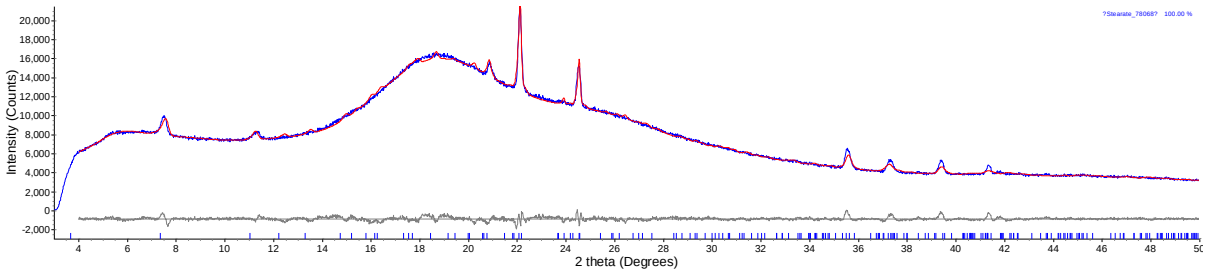


**Figure 7.107 Observed and calculated profiles for the Rietveld refinement of figure 5.33 line E with the MS-*C*2 structure. The bottom curve is the difference plot on the same intensity scale. ($R_{wp}$ = 2.19, $R_p$ = 1.57, $\chi$ = 1.96). The tick marks represent calculated peak positions.**

**Table 7.118 Refined lattice parameters for figure 5.33 line E Rietveld refinement with the MS-*C*2 structure.**

| Parameter | Value |
|---|---|
| **Phase / Space group** | MS-*C*2 / *C*2 |
| ***a* (Å)** | 48.09(2) |
| ***b* (Å)** | 7.323(1) |
| ***c* (Å)** | 5.613(1) |
| ***β* (°)** | 90.89(2) |
| **Volume (Å$^3$)** | 1976.2(9) |

## 5.7.5 Rietveld refinement of figure 5.33 line F

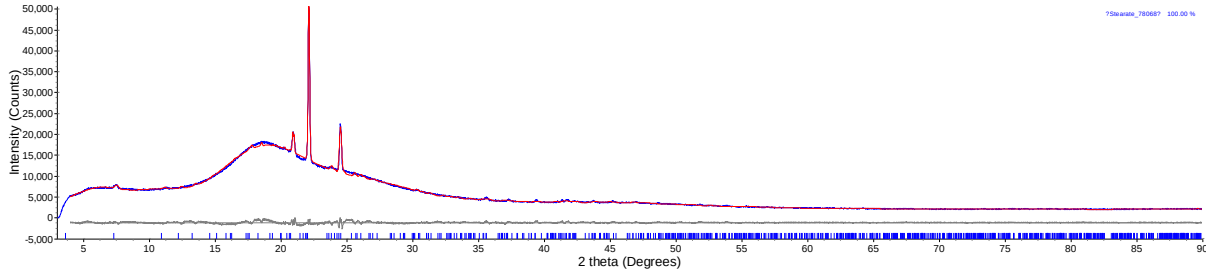


**Figure 7.108 Observed and calculated profiles for the Rietveld refinement of figure 5.33 line F with the MS-*C*2 structure. The bottom curve is the difference plot on the same intensity scale. ($R_{wp}$ = 2.67, $R_p$ = 2.11, $\chi$ = 1.96). The tick marks represent calculated peak positions.**

**Table 7.119 Refined lattice parameters for figure 5.33 line F Rietveld refinement with the MS-*C*2 structure.**

| Parameter | Value |
|---|---|
| **Phase / Space group** | MS-*C*2 / *C*2 |
| ***a* (Å)** | 48.60(2) |
| ***b* (Å)** | 7.337(3) |
| ***c* (Å)** | 5.609(2) |
| ***β* (°)** | 90.72(1) |
| **Volume (Å$^3$)** | 1200(2) |

## 5.7.6 Rietveld refinement of figure 5.34 line D

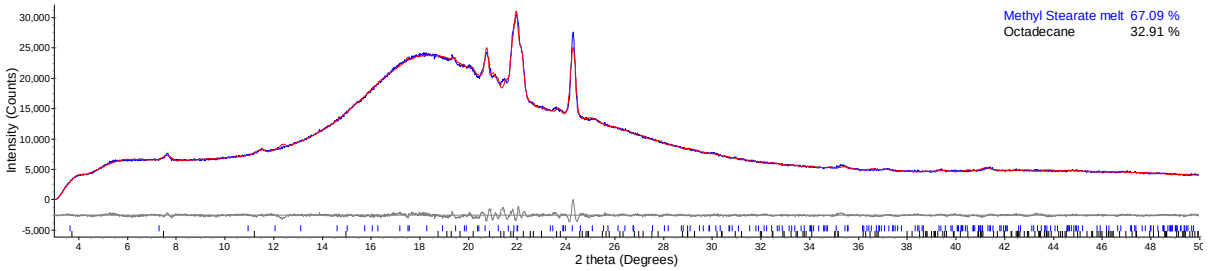


**Figure 7.109 Observed and calculated profiles for the mixed phase Rietveld refinement of figure 5.34 line D with the MS-*C*2 and octadecane structures. The bottom curve is the difference plot on the same intensity scale. ($R_{wp}$ = 1.93, $R_p$ = 1.41, $\chi$ = 1.92). The tick marks represent calculated peak positions.**

**Table 7.120 Refined lattice parameters for figure 5.34 line D mixed phase Rietveld refinement with the MS-*C*2 and octadecane structures.**

| Parameter | Value |
|---|---|
| **Phase / Space group** | MS-*C*2 / *C*2 |
| ***a* (Å)** | 48.49(5) |
| ***b* (Å)** | 7.421(4) |
| ***c* (Å)** | 5.629(5) |
| ***β* (°)** | 91.71(4) |
| **Volume (Å$^3$)** | 2024(3) |
| **Phase / Space group** | Octadecane / *P*-1 |
| ***a* (Å)** | 4.327(4) |
| ***b* (Å)** | 4.824(5) |
| ***c* (Å)** | 25.567(3) |
| ***α* (°)** | 86.7(1) |
| ***β* (°)** | 67.90(7) |
| ***γ* (°)** | 74.5() |
| **Volume (Å$^3$)** | 476(1) |
| **Phase fractions** | MS-*C*2 67.09 : 32.91 Octadecane |

# Appendix 5.8 Rietveld refinements of cocrystallisation experiments with Methyl Stearate and Eicosane

## 5.8.1 Rietveld refinement of figure 5.35 line D

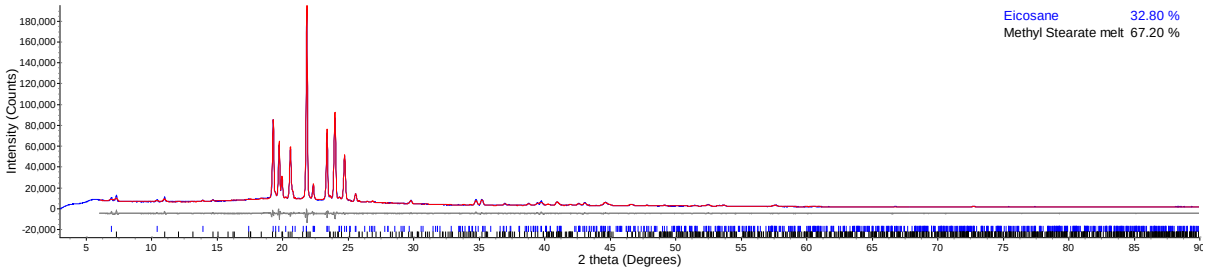


**Figure 7.110 Observed and calculated profiles for the mixed phase Rietveld refinement of figure 5.35 line D with the MS-*C*2 and eicosane structures. The bottom curve is the difference plot on the same intensity scale. ($R_{wp}$ = 4.30, $R_p$ = 3.12, $\chi$ = 3.19). The tick marks represent calculated peak positions.**

**Table 7.121 Refined lattice parameters for figure 5.35 line D mixed phase Rietveld refinement with the MS-*C*2 and eicosane structures.**

| Parameter | Value |
|---|---|
| **Phase / Space group** | MS-*C*2 / *C*2 |
| ***a* (Å)** | 48.232(3) |
| ***b* (Å)** | 7.4145(5) |
| ***c* (Å)** | 5.5904(6) |
| ***β* (°)** | 90.719(5) |
| **Volume (Å$^3$)** | 1999.1(3) |
| **Phase / Space group** | Eicosane / *P*-1 |
| ***a* (Å)** | 4.2856(2) |
| ***b* (Å)** | 4.8334(4) |
| ***c* (Å)** | 27.394(4) |
| ***α* (°)** | 85.654(8) |
| ***β* (°)** | 68.28(2) |
| ***γ* (°)** | 72.39(3) |
| **Volume (Å$^3$)** | 502.0(1) |
| **Phase fractions** | MS-*C*2 32.80 : 67.20 Eicosane |

## 5.8.2 Rietveld refinement of figure 5.35 line E

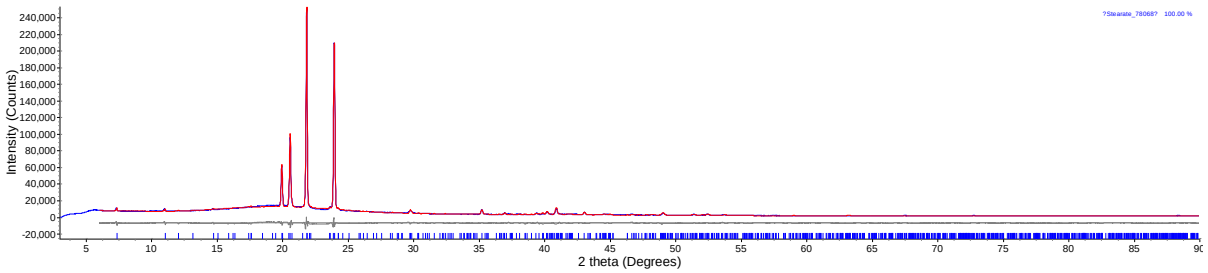


**Figure 7.111 Observed and calculated profiles for the Rietveld refinement of figure 5.35 line E with the MS-*C*2 structure. The bottom curve is the difference plot on the same intensity scale. ($R_{wp}$ = 6.03, $R_p$ = 4.52, $\chi$ = 4.54). The tick marks represent calculated peak positions.**

**Table 7.122 Refined lattice parameters for figure 5.35 line E Rietveld refinement with the MS-*C*2 structure.**

| Parameter | Value |
|---|---|
| **Phase / Space group** | MS-*C*2 / *C*2 |
| ***a* (Å)** | 48.091(5) |
| ***b* (Å)** | 7.4260(3) |
| ***c* (Å)** | 5.5873(4) |
| ***β* (°)** | 90.833(5) |
| **Volume (Å$^3$)** | 1995.1(3) |

## 5.8.3 Rietveld refinement of figure 5.35 line F

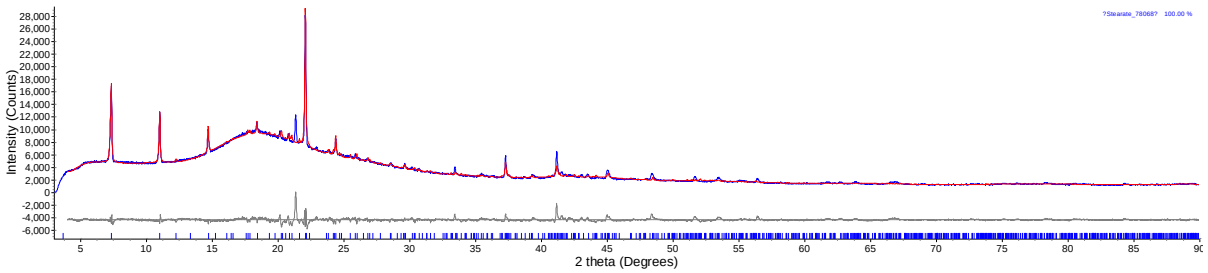


**Figure 7.112 Observed and calculated profiles for the Rietveld refinement of figure 5.35 line F with the MS-*C*2 structure. The bottom curve is the difference plot on the same intensity scale. ($R_{wp}$ = 5.51, $R_p$ = 3.57, $\chi$ = 3.15). The tick marks represent calculated peak positions.**

**Table 7.123 Refined lattice parameters for figure 5.35 line F Rietveld refinement with the MS-*C*2 structure.**

| Parameter | Value |
|---|---|
| **Phase / Space group** | MS-*C*2 / *C*2 |
| ***a* (Å)** | 48.172(3) |
| ***b* (Å)** | 7.2950(6) |
| ***c* (Å)** | 5.5031(5) |
| ***β* (°)** | 91.274(8) |
| **Volume (Å$^3$)** | 1933.4(3) |

## 5.8.4 Rietveld refinement of figure 5.35 line G

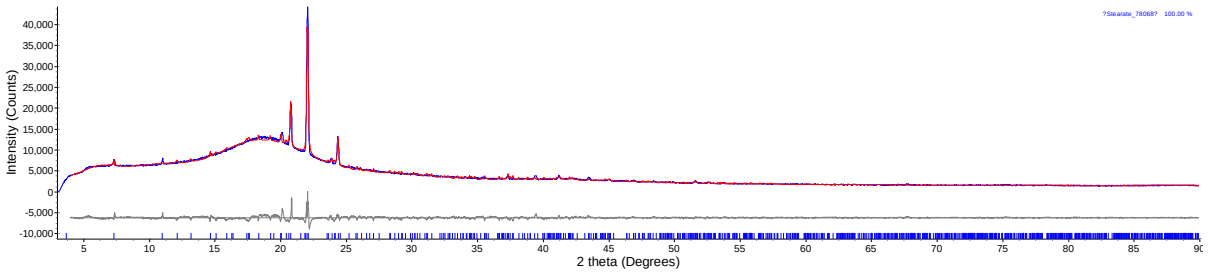


**Figure 7.113 Observed and calculated profiles for the Rietveld refinement of figure 5.35 line G with the MS-*C*2 structure. The bottom curve is the difference plot on the same intensity scale. ($R_{wp}$ = 4.90, $R_p$ = 3.56, $\chi$ = 3.09). The tick marks represent calculated peak positions.**

**Table 7.124 Refined lattice parameters for figure 5.35 line G Rietveld refinement with the MS-*C*2 structure.**

| Parameter | Value |
|---|---|
| **Phase / Space group** | MS-*C*2 / *C*2 |
| ***a* (Å)** | 48.401(2) |
| ***b* (Å)** | 7.3823(5) |
| ***c* (Å)** | 5.5690(3) |
| ***β* (°)** | 90.868(5) |
| **Volume (Å$^3$)** | 1989.6(2) |

## 5.8.5 Rietveld refinement of figure 5.36 line D

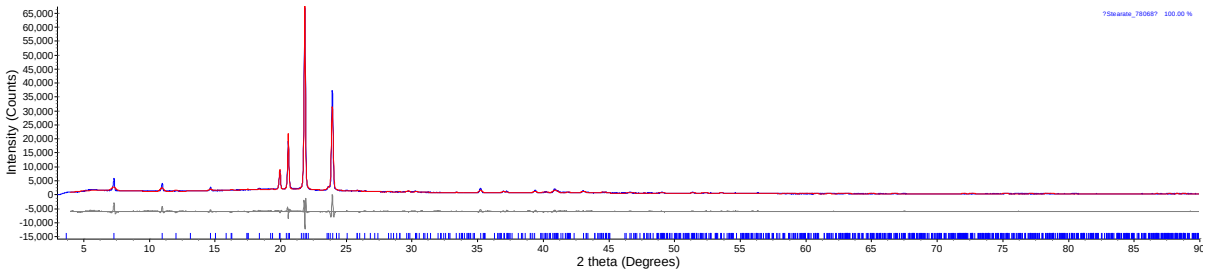


**Figure 7.114 Observed and calculated profiles for the Rietveld refinement of figure 5.36 line D with the MS-*C*2 structure. The bottom curve is the difference plot on the same intensity scale. ($R_{wp}$ = 10.04, $R_p$ = 7.34, $\chi$ = 3.30). The tick marks represent calculated peak positions.**

**Table 7.125 Refined lattice parameters for figure 5.36 line D Rietveld refinement with the MS-*C*2 structure.**

| Parameter | Value |
|---|---|
| **Phase / Space group** | MS-*C*2 / *C*2 |
| ***a* (Å)** | 48.274(8) |
| ***b* (Å)** | 7.4283(7) |
| ***c* (Å)** | 5.5944(7) |
| ***β* (°)** | 90.477(6) |
| **Volume (Å$^3$)** | 2006.0(5) |

## 5.8.6 Rietveld refinement of figure 5.36 line E

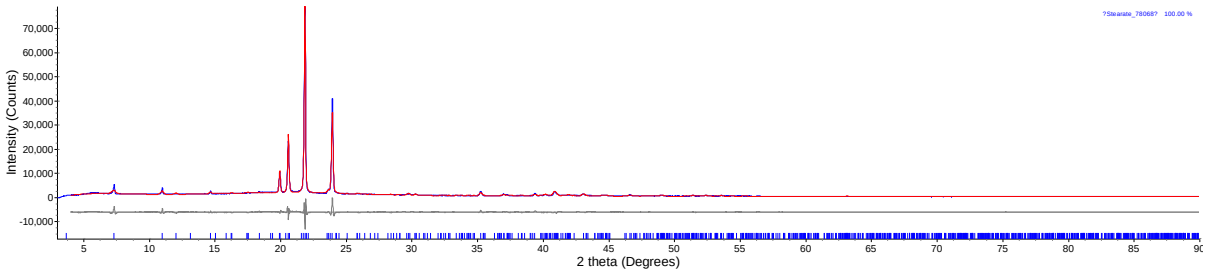


**Figure 7.115 Observed and calculated profiles for the Rietveld refinement of figure 5.36 line E with the MS-*C*2 structure. The bottom curve is the difference plot on the same intensity scale. ($R_{wp}$ = 9.63, $R_p$ = 7.45, $\chi$ = 3.38). The tick marks represent calculated peak positions.**

**Table 7.126 Refined lattice parameters for figure 5.36 line E Rietveld refinement with the MS-*C*2 structure.**

| Parameter | Value |
|---|---|
| **Phase / Space group** | MS-*C*2 / *C*2 |
| ***a* (Å)** | 48.279(6) |
| ***b* (Å)** | 7.4300(5) |
| ***c* (Å)** | 5.5936(5) |
| ***β* (°)** | 90.481(6) |
| **Volume (Å$^3$)** | 2006.4(3) |

## 5.8.7 Rietveld refinement of figure 5.36 line F

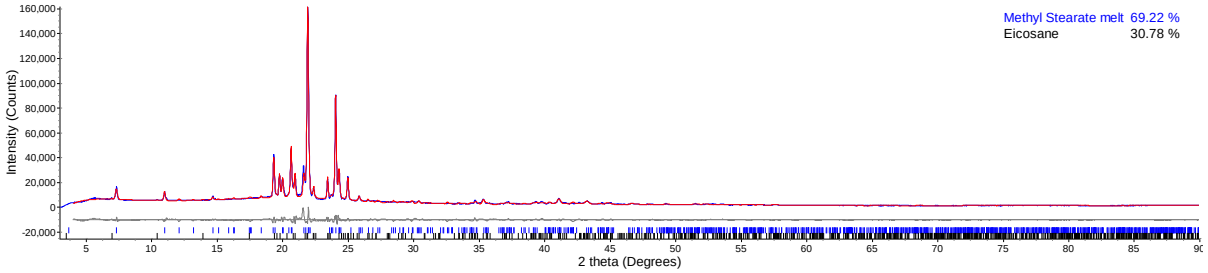


**Figure 7.116 Observed and calculated profiles for the mixed phase Rietveld refinement of figure 5.36 line F with the MS-*C*2 and eicosane structures. The bottom curve is the difference plot on the same intensity scale. ($R_{wp}$ = 8.03, $R_p$ = 5.88, $\chi$ = 5.37). The tick marks represent calculated peak positions.**

**Table 7.127 Refined lattice parameters for figure 5.36 line F mixed phase Rietveld refinement with the MS-*C*2 and eicosane structures.**

| Parameter | Value |
|---|---|
| **Phase / Space group** | MS-*C*2 / *C*2 |
| ***a* (Å)** | 48.231(8) |
| ***b* (Å)** | 7.390(1) |
| ***c* (Å)** | 5.5787(9) |
| ***β* (°)** | 90.356(8) |
| **Volume (Å$^3$)** | 1988.4(5) |
| **Phase / Space group** | Eicosane / *P*-1 |
| ***a* (Å)** | 4.2553(7) |
| ***b* (Å)** | 4.7979(8) |
| ***c* (Å)** | 29.349(5) |
| ***α* (°)** | 85.59(1) |
| ***β* (°)** | 68.39(2) |
| ***γ* (°)** | 72.98(9) |
| **Volume (Å$^3$)** | 496.1(2) |
| **Phase fractions** | MS-*C*2 69.22 : 30.78 Eicosane |

## 5.8.8 Rietveld refinement of figure 5.37 line D

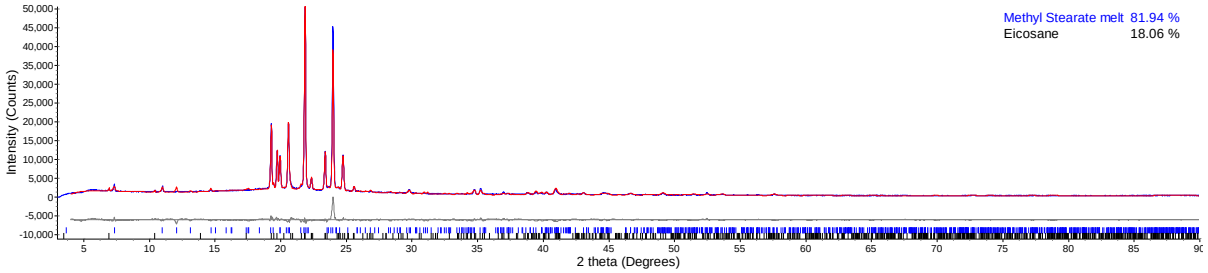


**Figure 7.117 Observed and calculated profiles for the mixed phase Rietveld refinement of figure 5.37 line D with the MS-*C*2 and eicosane structures. The bottom curve is the difference plot on the same intensity scale. ($R_{wp}$ = 9.63, $R_p$ = 6.85, $\chi$ = 3.39). The tick marks represent calculated peak positions.**

**Table 7.128 Refined lattice parameters for figure 5.37 line D mixed phase Rietveld refinement with the MS-*C*2 and eicosane structures.**

| Parameter | Value |
|---|---|
| **Phase / Space group** | MS-*C*2 / C2 |
| **a (Å)** | 48.250(6) |
| **b (Å)** | 7.4174(5) |
| **c (Å)** | 5.5921(5) |
| **β (°)** | 90.616(7) |
| **Volume (Å$^3$)** | 2001.3(4) |
| **Phase / Space group** | Eicosane / P-1 |
| **a (Å)** | 4.2821(6) |
| **b (Å)** | 4.8303(4) |
| **c (Å)** | 27.426(7) |
| **α (°)** | 85.59(2) |
| **β (°)** | 68.35(2) |
| **γ (°)** | 72.407(6) |
| **Volume (Å$^3$)** | 502.2(2) |
| **Phase fractions** | MS-*C*2 81.94 : 18.06 Eicosane |

## 5.8.9 Rietveld refinement of figure 5.37 line E

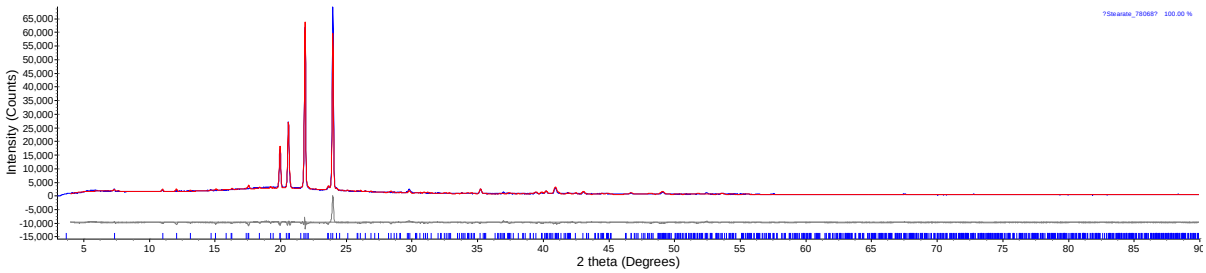


**Figure 7.118 Observed and calculated profiles for the Rietveld refinement of figure 5.37 line E with the MS-*C*2 structure. The bottom curve is the difference plot on the same intensity scale. ($R_{wp}$ = 10.41, $R_p$ = 7.79, $\chi$ = 3.84). The tick marks represent calculated peak positions.**

**Table 7.129 Refined lattice parameters for figure 5.37 line E Rietveld refinement with the MS-*C*2 structure.**

| Parameter | Value |
|---|---|
| **Phase / Space group** | MS-*C*2 / C2 |
| **a (Å)** | 48.195(6) |
| **b (Å)** | 7.4216(5) |
| **c (Å)** | 5.5938(5) |
| **β (°)** | 90.628(5) |
| **Volume (Å$^3$)** | 2000.7(3) |

## 5.8.10 Rietveld refinement of figure 5.37 line F

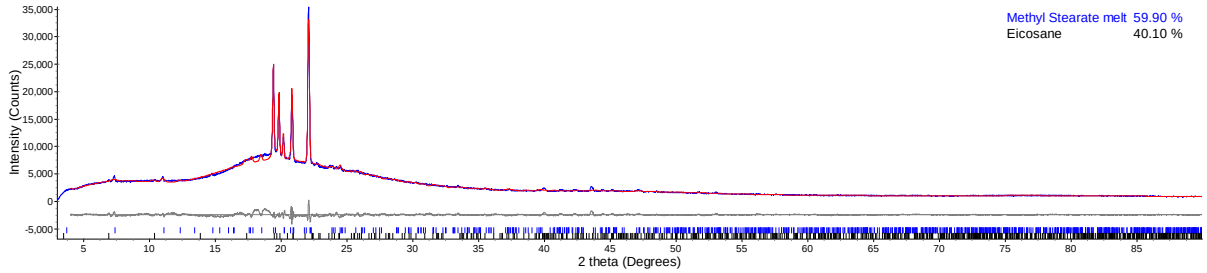


**Figure 7.119 Observed and calculated profiles for the mixed phase Rietveld refinement of figure 5.37 line F with the MS-*C*2 and eicosane structures. The bottom curve is the difference plot on the same intensity scale. ($R_{wp}$ = 4.39, $R_p$ = 3.35, $\chi$ = 2.31). The tick marks represent calculated peak positions.**

**Table 7.130 Refined lattice parameters for figure 5.37 line F mixed phase Rietveld refinement with the MS-*C*2 and eicosane structures.**

| Parameter | Value |
|---|---|
| **Phase / Space group** | MS-*C*2 / *C*2 |
| ***a* (Å)** | 47.81(3) |
| ***b* (Å)** | 7.244(4) |
| ***c* (Å)** | 5.543(3) |
| ***β* (°)** | 90.382(8) |
| **Volume (Å$^3$)** | 1920(2) |
| **Phase / Space group** | Eicosane / *P*-1 |
| ***a* (Å)** | 4.132(8) |
| ***b* (Å)** | 4.721(6) |
| ***c* (Å)** | 27.56 (3) |
| ***α* (°)** | 85.93(9) |
| ***β* (°)** | 67.8(1) |
| ***γ* (°)** | 74.7(3) |
| **Volume (Å$^3$)** | 480 (1) |
| **Phase fractions** | MS-*C*2 59.90 : 40.10 Eicosane |

## 5.8.11 Rietveld refinement of figure 5.37 line G

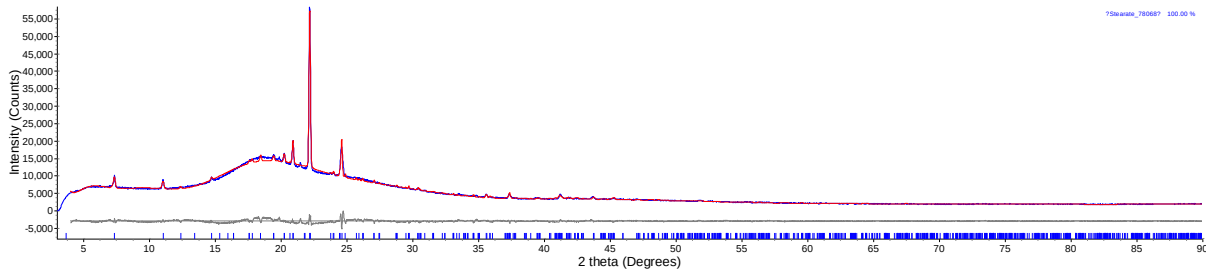


**Figure 7.120 Observed and calculated profiles for the Rietveld refinement of figure 5.37 line G with the MS-*C*2 structure. The bottom curve is the difference plot on the same intensity scale. ($R_{wp}$ = 3.62, $R_p$ = 2.88, $\chi$ = 2.53). The tick marks represent calculated peak positions.**

**Table 7.131 Refined lattice parameters for figure 5.37 line G Rietveld refinement with the MS-*C*2 structure.**

| Parameter | Value |
|---|---|
| **Phase / Space group** | MS-*C*2 / *C*2 |
| ***a* (Å)** | 48.074(8) |
| ***b* (Å)** | 7.2320(8) |
| ***c* (Å)** | 5.5528(7) |
| ***β* (°)** | 90.10(1) |
| **Volume (Å$^3$)** | 1930.6(5) |

## 5.8.12 Rietveld refinement of figure 5.38 line D

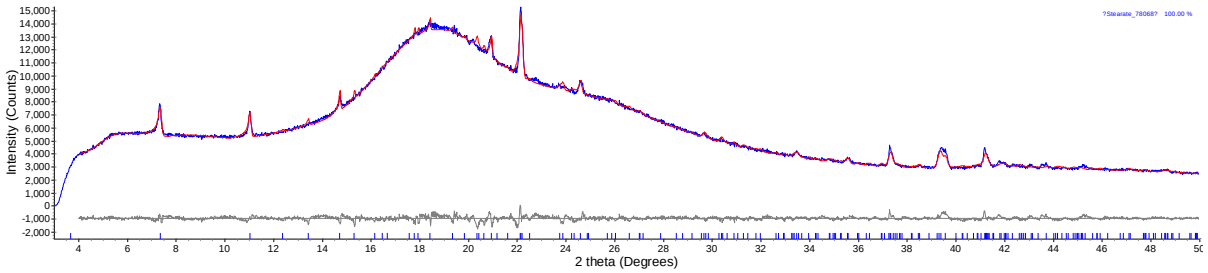


**Figure 7.121 Observed and calculated profiles for the Rietveld refinement of figure 5.38 line D with the MS-*C*2 structure. The bottom curve is the difference plot on the same intensity scale. ($R_{wp}$ = 2.25, $R_p$ = 1.66, $\chi$ = 1.77). The tick marks represent calculated peak positions.**

**Table 7.132 Refined lattice parameters for figure 5.38 line D Rietveld refinement with the MS-*C*2 structure.**

| Parameter | Value |
|---|---|
| **Phase / Space group** | MS-*C*2 / *C*2 |
| ***a* (Å)** | 48.175(7) |
| ***b* (Å)** | 7.2350(8) |
| ***c* (Å)** | 5.4889(8) |
| ***β* (°)** | 91.56(1) |
| **Volume (Å$^3$)** | 1912.4(4) |

# Appendix 5.9 Rietveld refinements of cocrystallisation experiments with Methyl Stearate and Docosane

## 5.9.1 Rietveld refinement of figure 5.39 line D

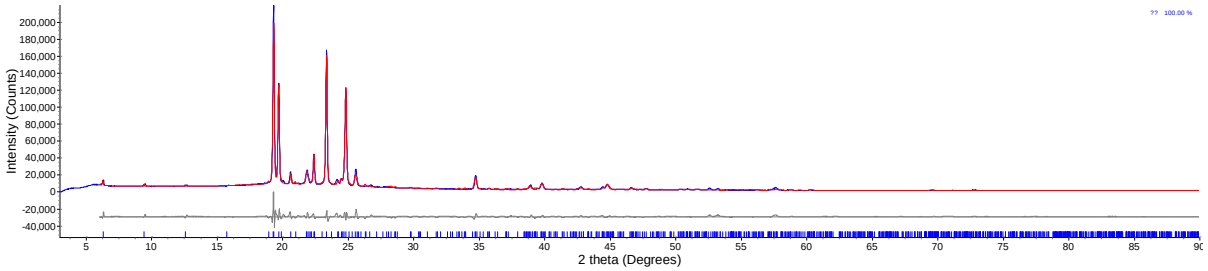


**Figure 7.122 Observed and calculated profiles for the Rietveld refinement of figure 5.39 line D with the docosane structure. The bottom curve is the difference plot on the same intensity scale. ($R_{wp}$ = 10.35, $R_p$ = 7.51, $\chi$ = 7.70). The tick marks represent calculated peak positions.**

**Table 7.133 Refined lattice parameters for figure 5.39 line D Rietveld refinement with the docosane structure.**

| Parameter | Value |
|---|---|
| **Phase / Space group** | Docosane / *P*-1 |
| ***a* (Å)** | 4.2698(2) |
| ***b* (Å)** | 4.8274(1) |
| ***c* (Å)** | 30.177(3) |
| ***α* (°)** | 86.947(7) |
| ***β* (°)** | 68.95(1) |
| ***γ* (°)** | 72.852(3) |
| **Volume (Å$^3$)** | 553.71(7) |

## 5.9.2 Rietveld refinement of figure 5.39 line E

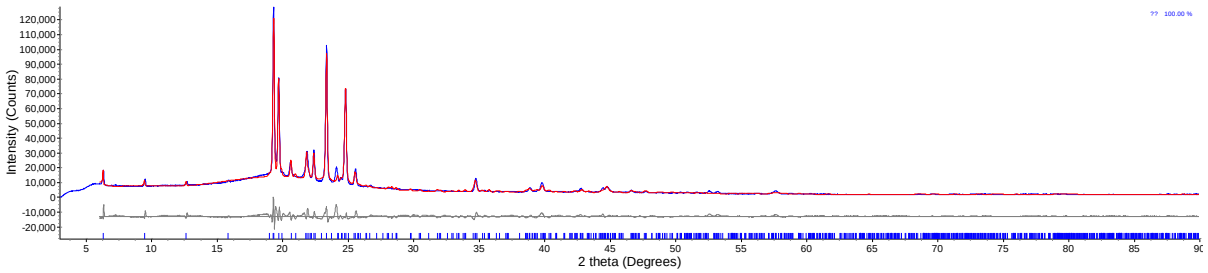


**Figure 7.123 Observed and calculated profiles for the Rietveld refinement of figure 5.39 line E with the docosane structure. The bottom curve is the difference plot on the same intensity scale. ($R_{wp}$ = 8.96, $R_p$ = 6.62, $\chi$ = 6.82). The tick marks represent calculated peak positions.**

**Table 7.134 Refined lattice parameters for figure 5.39 line E Rietveld refinement with the docosane structure.**

| Parameter | Value |
|---|---|
| **Phase / Space group** | Docosane / *P*-1 |
| ***a* (Å)** | 4.2756(8) |
| ***b* (Å)** | 4.5295(3) |
| ***c* (Å)** | 30.091(7) |
| ***α* (°)** | 86.86(1) |
| ***β* (°)** | 68.74(1) |
| ***γ* (°)** | 72.806(4) |
| **Volume (Å$^3$)** | 552.2(2) |

## 5.9.3 Rietveld refinement of figure 5.39 line F

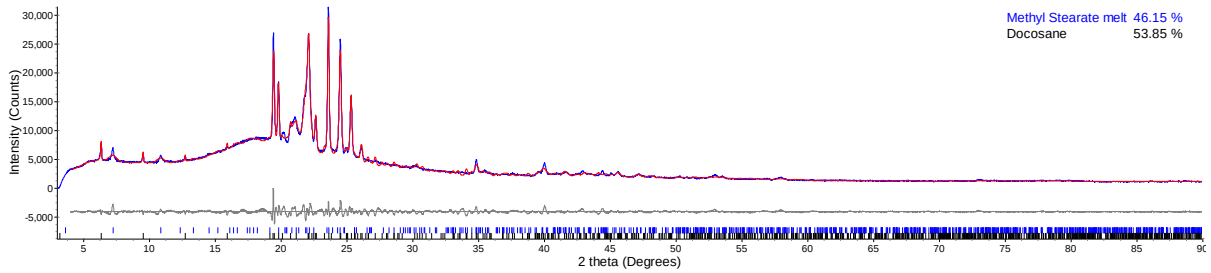


**Figure 7.124 Observed and calculated profiles for the mixed phase Rietveld refinement of figure 5.39 line F with the MS-*C*2 and docosane structures. The bottom curve is the difference plot on the same intensity scale. ($R_{wp}$ = 5.23, $R_p$ = 3.90, $\chi$ = 3.05). The tick marks represent calculated peak positions.**

**Table 7.135 Refined lattice parameters for figure 5.39 line F mixed phase Rietveld refinement with the MS-*C*2 and docosane structures.**

| Parameter | Value |
|---|---|
| **Phase / Space group** | MS-*C*2 / *C*2 |
| ***a* (Å)** | 48.80(2) |
| ***b* (Å)** | 7.263(2) |
| ***c* (Å)** | 5.503(1) |
| ***β* (°)** | 92.14(2) |
| **Volume (Å$^3$)** | 1949(1) |
| **Phase / Space group** | Docosane / *P*-1 |
| ***a* (Å)** | 4.2013(2) |
| ***b* (Å)** | 4.7773(3) |
| ***c* (Å)** | 29.819(3) |
| ***α* (°)** | 86.994(6) |
| ***β* (°)** | 69.095(8) |
| ***γ* (°)** | 73.722(4) |
| **Volume (Å$^3$)** | 535.93(8) |
| **Phase fractions** | MS-*C*2 46.15 : 53.85 Docosane |

## 5.9.4 Rietveld refinement of figure 5.39 line G

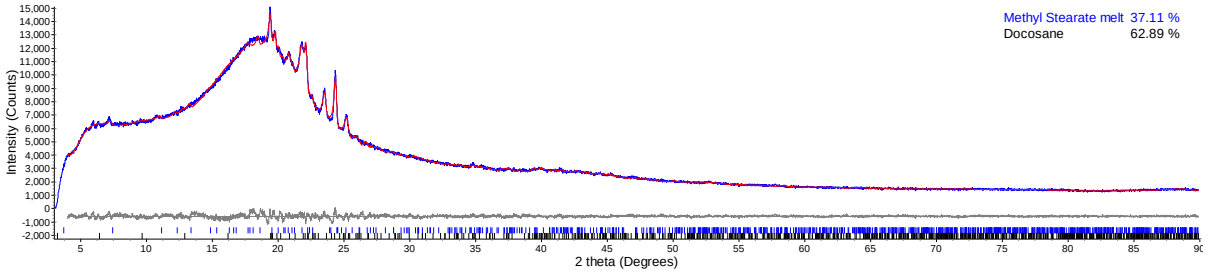


**Figure 7.125 Observed and calculated profiles for the mixed phase Rietveld refinement of figure 5.39 line G with the MS-*C*2 and docosane structures. The bottom curve is the difference plot on the same intensity scale. ($R_{wp}$ = 2.21, $R_p$ = 1.73, $\chi$ = 1.37). The tick marks represent calculated peak positions.**

**Table 7.136 Refined lattice parameters for figure 5.39 line G mixed phase Rietveld refinement with the MS-*C*2 and docosane structures.**

| Parameter | Value |
|---|---|
| **Phase / Space group** | MS-*C*2 / *C*2 |
| ***a* (Å)** | 47.67(2) |
| ***b* (Å)** | 7.260(2) |
| ***c* (Å)** | 5.444(2) |
| ***β* (°)** | 91.43(2) |
| **Volume (Å$^3$)** | 1883(1) |
| **Phase / Space group** | Docosane / *P*-1 |
| ***a* (Å)** | 4.229(2) |
| ***b* (Å)** | 4.756(2) |
| ***c* (Å)** | 29.64(2) |
| ***α* (°)** | 86.78 (3) |
| ***β* (°)** | 67.70(3) |
| ***γ* (°)** | 73.68(2) |
| **Volume (Å$^3$)** | 528.4(4) |
| **Phase fractions** | MS-*C*2 37.11 : 62.89 Docosane |

## 5.9.5 Rietveld refinement of figure 5.41 line D

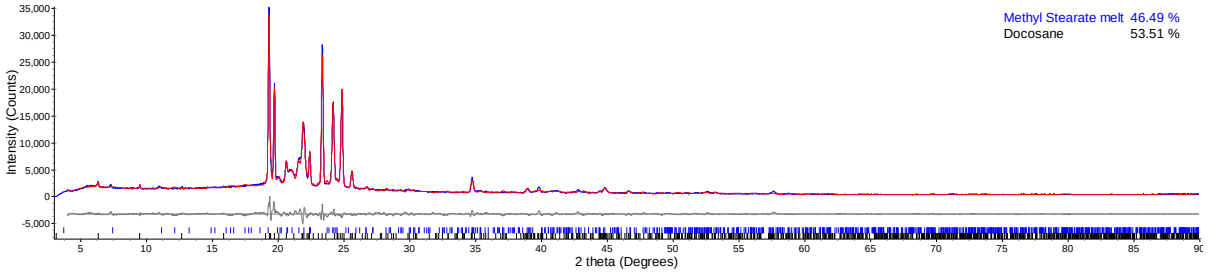


**Figure 7.126 Observed and calculated profiles for the mixed phase Rietveld refinement of figure 5.41 line D with the MS-*C*2 and docosane structures. The bottom curve is the difference plot on the same intensity scale. ($R_{wp}$ = 8.49, $R_p$ = 6.51, $\chi$ = 3.08). The tick marks represent calculated peak positions.**

**Table 7.137 Refined lattice parameters for figure 5.41 line D mixed phase Rietveld refinement with the MS-*C*2 and docosane structures.**

| Parameter | Value |
|---|---|
| **Phase / Space group** | MS-*C*2 / *C*2 |
| ***a* (Å)** | 47.60(2) |
| ***b* (Å)** | 7.3603(7) |
| ***c* (Å)** | 5.516(1) |
| ***β* (°)** | 92.12 (2) |
| **Volume (Å$^3$)** | 1931.1(9) |
| **Phase / Space group** | Docosane / *P*-1 |
| ***a* (Å)** | 4.2750(4) |
| ***b* (Å)** | 4.8173(5) |
| ***c* (Å)** | 30.006(5) |
| ***α* (°)** | 86.012(9) |
| ***β* (°)** | 68.67(1) |
| ***γ* (°)** | 72.603(4) |
| **Volume (Å$^3$)** | 548.7(1) |
| **Phase fractions** | MS-*C*2 46.49 : 53.51 Docosane |

## 5.9.6 Rietveld refinement of figure 5.41 line E

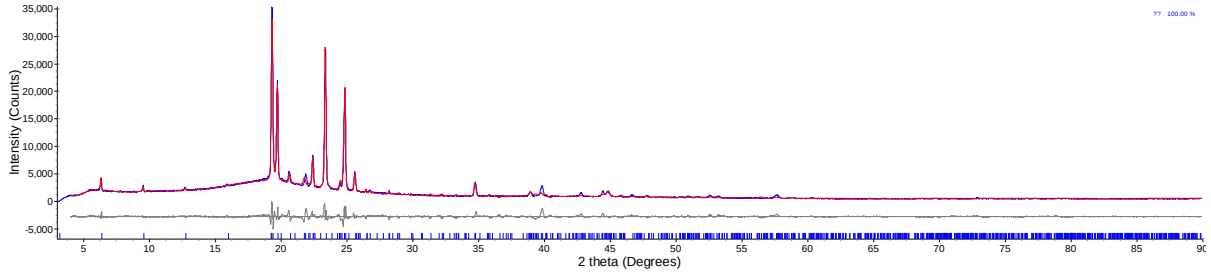


**Figure 7.127 Observed and calculated profiles for the Rietveld refinement of figure 5.41 line E with the docosane structure. The bottom curve is the difference plot on the same intensity scale. ($R_{wp}$ = 9.27, $R_p$ = 6.41, $\chi$ = 3.48). The tick marks represent calculated peak positions.**

**Table 7.138 Refined lattice parameters for figure 5.41 line E Rietveld refinement with the docosane structure.**

| Parameter | Value |
|---|---|
| **Phase / Space group** | Docosane / *P*-1 |
| ***a* (Å)** | 4.2687(4) |
| ***b* (Å)** | 4.8138(5) |
| ***c* (Å)** | 29.804(3) |
| ***α* (°)** | 86.883(8) |
| ***β* (°)** | 68.50(1) |
| ***γ* (°)** | 72.946(4) |
| **Volume (Å$^3$)** | 543.8(1) |

## 5.9.7 Rietveld refinement of figure 5.41 line F

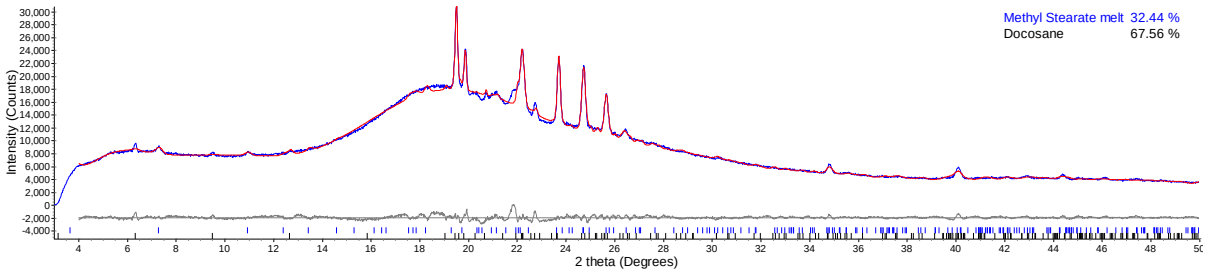


**Figure 7.128 Observed and calculated profiles for the mixed phase Rietveld refinement of figure 5.41 line F with the MS-*C*2 and docosane structures. The bottom curve is the difference plot on the same intensity scale. ($R_{wp}$ = 2.52, $R_p$ = 1.95, $\chi$ = 2.39). The tick marks represent calculated peak positions.**

**Table 7.139 Refined lattice parameters for figure 5.41 line F mixed phase Rietveld refinement with the MS-*C*2 and docosane structures.**

| Parameter | Value |
|---|---|
| **Phase / Space group** | MS-*C*2 / *C*2 |
| ***a* (Å)** | 48.61(3) |
| ***b* (Å)** | 7.209(3) |
| ***c* (Å)** | 5.498(3) |
| ***β* (°)** | 91.36(5) |
| **Volume (Å$^3$)** | 1927(2) |
| **Phase / Space group** | Docosane / *P*-1 |
| ***a* (Å)** | 4.175(1) |
| ***b* (Å)** | 4.747(2) |
| ***c* (Å)** | 29.94(1) |
| ***α* (°)** | 86.05(2) |
| ***β* (°)** | 69.2(2) |
| ***γ* (°)** | 74.08(1) |
| **Volume (Å$^3$)** | 533.1(3) |
| **Phase fractions** | MS-*C*2 32.44 : 67.56 Docosane |

## 5.9.8 Rietveld refinement of figure 5.41 line G

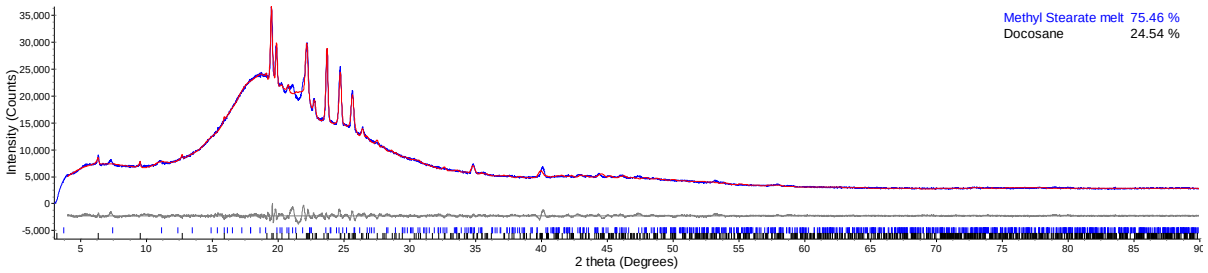


**Figure 7.129 Observed and calculated profiles for the mixed phase Rietveld refinement of figure 5.41 line G with the MS-*C*2 and docosane structures. The bottom curve is the difference plot on the same intensity scale. ($R_{wp}$ = 2.63, $R_p$ = 1.94, $\chi$ = 2.18). The tick marks represent calculated peak positions.**

**Table 7.140 Refined lattice parameters for figure 5.41 line G mixed phase Rietveld refinement with the MS-*C*2 and docosane structures.**

| Parameter | Value |
|---|---|
| **Phase / Space group** | MS-*C*2 / *C*2 |
| ***a* (Å)** | 47.63(7) |
| ***b* (Å)** | 7.22(1) |
| ***c* (Å)** | 5.57(1) |
| ***β* (°)** | 92.7(2) |
| **Volume (Å$^3$)** | 1916(6) |
| **Phase / Space group** | Docosane / *P*-1 |
| ***a* (Å)** | 4.1576(7) |
| ***b* (Å)** | 4.7269(8) |
| ***c* (Å)** | 29.753(7) |
| ***α* (°)** | 86.69(1) |
| ***β* (°)** | 69.27(1) |
| ***γ* (°)** | 74.26(1) |
| **Volume (Å$^3$)** | 525.9(2) |
| **Phase fractions** | MS-*C*2 75.46 : 24.54 Docosane |

## 5.9.9 Rietveld refinement of figure 5.42 line D

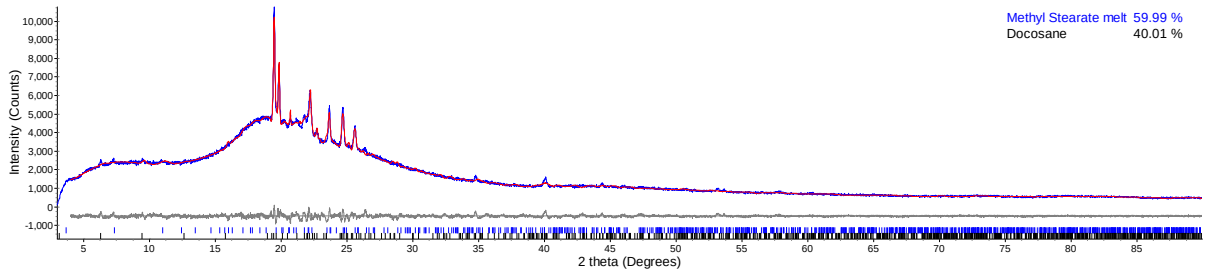


**Figure 7.130 Observed and calculated profiles for the mixed phase Rietveld refinement of figure 5.42 line D with the MS-*C*2 and docosane structures. The bottom curve is the difference plot on the same intensity scale. ($R_{wp}$ = 3.69, $R_p$ = 2.82, $\chi$ = 1.47). The tick marks represent calculated peak positions.**

**Table 7.141 Refined lattice parameters for figure 5.42 line D mixed phase Rietveld refinement with the MS-*C*2 and docosane structures.**

| Parameter | Value |
|---|---|
| **Phase / Space group** | MS-*C*2 / *C*2 |
| ***a* (Å)** | 48.27(6) |
| ***b* (Å)** | 7.205(7) |
| ***c* (Å)** | 5.634(5) |
| ***β* (°)** | 92.42(7) |
| **Volume (Å$^3$)** | 1957(4) |
| **Phase / Space group** | Docosane / *P*-1 |
| ***a* (Å)** | 4.242(2) |
| ***b* (Å)** | 4.826(2) |
| ***c* (Å)** | 30.07(1) |
| ***α* (°)** | 85.60(2) |
| ***β* (°)** | 69.10(1) |
| ***γ* (°)** | 72.61(2) |
| **Volume (Å$^3$)** | 548.6(4) |
| **Phase fractions** | MS-*C*2 59.99 : 40.01 Docosane |

# Appendix 5.10 Rietveld refinements of cocrystallisation experiments with Methyl Palmitate and Dodecane

## 5.10.1 Rietveld refinement of figure 5.43 line D

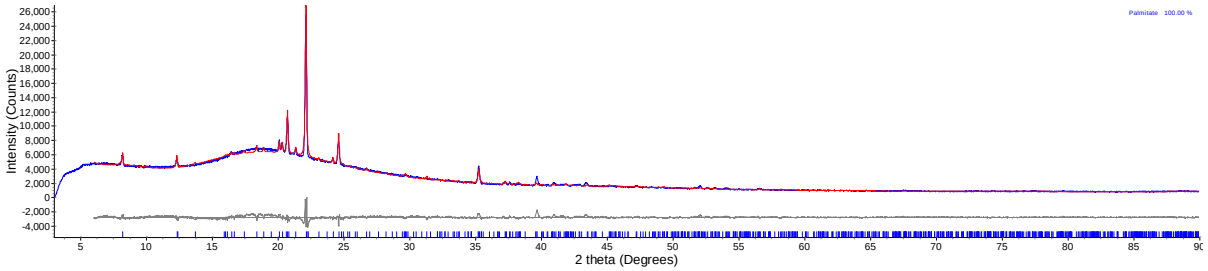


**Figure 7.131 Observed and calculated profiles for the Rietveld refinement of figure 5.43 line D with the MP-*C*2 structure. The bottom curve is the difference plot on the same intensity scale. ($R_{wp}$ = 4.54, $R_p$ = 3.34, $\chi$ = 2.24). The tick marks represent calculated peak positions.**

**Table 7.142 Refined lattice parameters for figure 5.43 line D Rietveld refinement with the MP-*C*2 structure.**

| Parameter | Value |
|---|---|
| **Phase / Space group** | MP-*C*2 / *C*2 |
| ***a* (Å)** | 43.154(5) |
| ***b* (Å)** | 7.2302(4) |
| ***c* (Å)** | 5.5830(5) |
| ***β* (°)** | 93.800(8) |
| **Volume (Å$^3$)** | 1738.1(3) |

## 5.10.2 Rietveld refinement of figure 5.43 line E

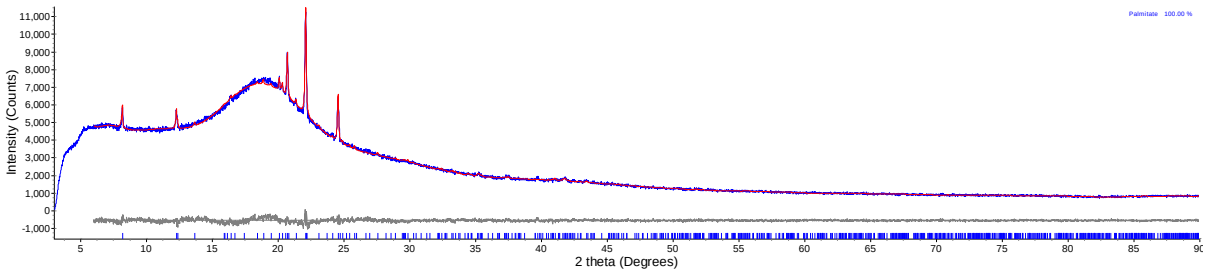


**Figure 7.132 Observed and calculated profiles for the Rietveld refinement of figure 5.43 line E with the MP-*C*2 structure. The bottom curve is the difference plot on the same intensity scale. ($R_{wp}$ = 2.59, $R_p$ = 2.02, $\chi$ = 1.26). The tick marks represent calculated peak positions.**

**Table 7.143 Refined lattice parameters for figure 5.43 line E Rietveld refinement with the MP-*C*2 structure.**

| Parameter | Value |
|---|---|
| **Phase / Space group** | MP-*C*2 / *C*2 |
| ***a* (Å)** | 43.280(6) |
| ***b* (Å)** | 7.2426(4) |
| ***c* (Å)** | 5.5755(7) |
| ***β* (°)** | 93.94(1) |
| **Volume (Å$^3$)** | 1743.5(3) |

## 5.10.3 Rietveld refinement of figure 5.43 line F

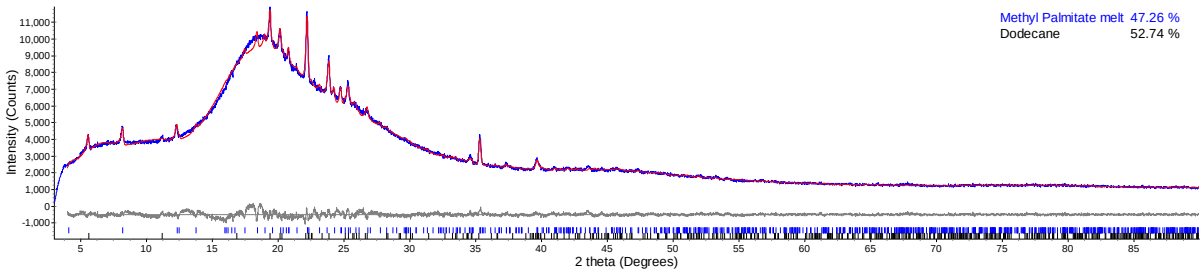


**Figure 7.133 Observed and calculated profiles for the mixed phase Rietveld refinement of figure 5.43 line F with the MP-*C*2 and dodecane structures. The bottom curve is the difference plot on the same intensity scale. ($R_{wp}$ = 2.84, $R_p$ = 2.28, $\chi$ = 1.56). The tick marks represent calculated peak positions.**

**Table 7.144 Refined lattice parameters for figure 5.43 line F mixed phase Rietveld refinement with the MP-*C*2 and dodecane structures.**

| Parameter | Value |
|---|---|
| **Phase / Space group** | MP-*C*2 / *C*2 |
| ***a* (Å)** | 43.132(9) |
| ***b* (Å)** | 7.183(1) |
| ***c* (Å)** | 5.568(1) |
| ***β* (°)** | 93.66(1) |
| **Volume (Å$^3$)** | 1721.6(6) |
| **Phase / Space group** | Dodecane / *P*-1 |
| ***a* (Å)** | 4.202(1) |
| ***b* (Å)** | 4.759(1) |
| ***c* (Å)** | 16.010(7) |
| ***α* (°)** | 93.32(5) |
| ***β* (°)** | 80.23(4) |
| ***γ* (°)** | 106.12 (3) |
| **Volume (Å$^3$)** | 303.1(2) |
| **Phase fractions** | MP-*C*2 47.26 : 52.74 Dodecane |

## 5.10.4 Rietveld refinement of figure 5.43 line G

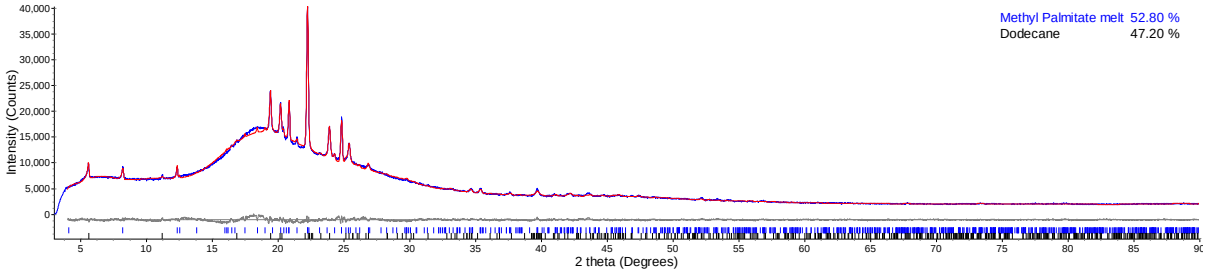


**Figure 7.134 Observed and calculated profiles for the mixed phase Rietveld refinement of figure 5.43 line G with the MP-*C*2 and dodecane structures. The bottom curve is the difference plot on the same intensity scale. ($R_{wp}$ = 2.55, $R_p$ = 2.04, $\chi$ = 1.84). The tick marks represent calculated peak positions.**

**Table 7.145 Refined lattice parameters for figure 5.43 line G mixed phase Rietveld refinement with the MP-*C*2 and dodecane structures.**

| Parameter | Value |
|---|---|
| **Phase / Space group** | MP-*C*2 / *C*2 |
| ***a* (Å)** | 43.137(8) |
| ***b* (Å)** | 7.1701(7) |
| ***c* (Å)** | 5.5701(7) |
| ***β* (°)** | 93.63(1) |
| **Volume (Å$^3$)** | 1719.4(4) |
| **Phase / Space group** | Dodecane / *P*-1 |
| ***a* (Å)** | 4.203(1) |
| ***b* (Å)** | 4.7503(7) |
| ***c* (Å)** | 16.024(6) |
| ***α* (°)** | 93.43 (4) |
| ***β* (°)** | 79.87 (4) |
| ***γ* (°)** | 105.95(1) |
| **Volume (Å$^3$)** | 302.8(2) |
| **Phase fractions** | MP-*C*2 52.80 : 47.20 Dodecane |

## 5.10.5 Rietveld refinement of figure 5.44 line D

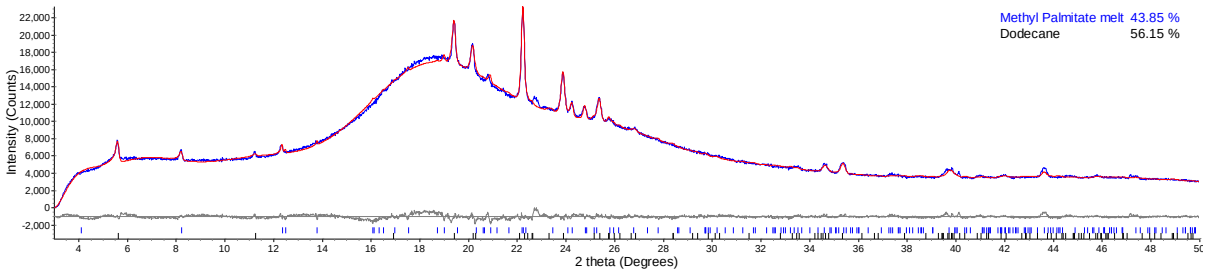


**Figure 7.135 Observed and calculated profiles for the mixed phase Rietveld refinement of figure 5.44 line D with the MP-*C*2 and dodecane structures. The bottom curve is the difference plot on the same intensity scale. ($R_{wp}$ = 2.57, $R_p$ = 1.95, $\chi$ = 2.21). The tick marks represent calculated peak positions.**

**Table 7.146 Refined lattice parameters for figure 5.44 line D mixed phase Rietveld refinement with the MP-*C*2 and dodecane structures.**

| Parameter | Value |
|---|---|
| **Phase / Space group** | MP-*C*2 / *C*2 |
| ***a* (Å)** | 43.09(2) |
| ***b* (Å)** | 7.177(2) |
| ***c* (Å)** | 5.507(1) |
| ***β* (°)** | 94.60(2) |
| **Volume (Å$^3$)** | 1697.9(8) |
| **Phase / Space group** | Dodecane / *P*-1 |
| ***a* (Å)** | 4.200(1) |
| ***b* (Å)** | 4.748(1) |
| ***c* (Å)** | 15.948(9) |
| ***α* (°)** | 93.20(4) |
| ***β* (°)** | 80.09 (6) |
| ***γ* (°)** | 105.91(2) |
| **Volume (Å$^3$)** | 301.3(2) |
| **Phase fractions** | MP-*C*2 43.85 : 56.15 Dodecane |

# Appendix 5.11 Rietveld refinements of cocrystallisation experiments with Methyl Palmitate and Tetradecane

## 5.11.1 Rietveld refinement of figure 5.45 line D

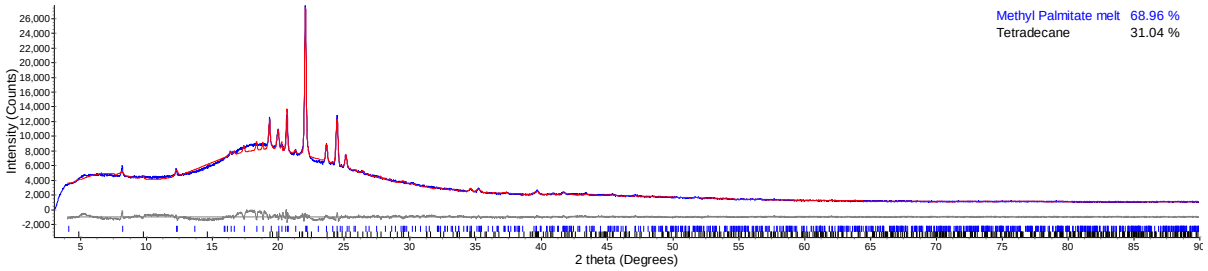


**Figure 7.136 Observed and calculated profiles for the mixed phase Rietveld refinement of figure 5.45 line D with the MP-*C*2 and tetradecane structures. The bottom curve is the difference plot on the same intensity scale. ($R_{wp}$ = 3.92, $R_p$ = 3.10, $\chi$ = 2.14). The tick marks represent calculated peak positions.**

**Table 7.147 Refined lattice parameters for figure 5.45 line D mixed phase Rietveld refinement with the MP-*C*2 and tetradecane structures.**

| Parameter | Value |
|---|---|
| **Phase / Space group** | MP-*C*2 / *C*2 |
| ***a* (Å)** | 43.28(1) |
| ***b* (Å)** | 7.2630(5) |
| ***c* (Å)** | 5.5826(7) |
| ***β* (°)** | 93.78(1) |
| **Volume (Å$^3$)** | 1751.0(5) |
| **Phase / Space group** | Tetradecane / *P*-1 |
| ***a* (Å)** | 4.238(2) |
| ***b* (Å)** | 4.7739(6) |
| ***c* (Å)** | 18.50(4) |
| ***α* (°)** | 92.61(4) |
| ***β* (°)** | 78.7(6) |
| ***γ* (°)** | 106.35(2) |
| **Volume (Å$^3$)** | 352.1(2) |
| **Phase fractions** | MP-*C*2 68.96 : 31.04 Tetradecane |

## 5.11.2 Rietveld refinement of figure 5.45 line E

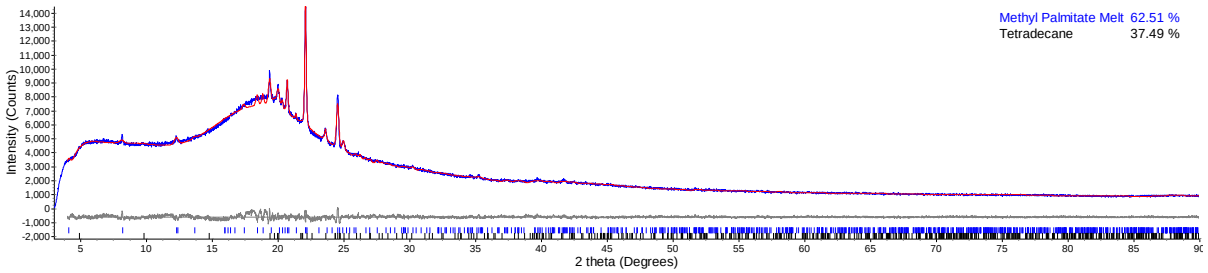


**Figure 7.137 Observed and calculated profiles for the mixed phase Rietveld refinement of figure 5.45 line E with the MP-*C*2 and tetradecane structures. The bottom curve is the difference plot on the same intensity scale. ($R_{wp}$ = 2.73, $R_p$ = 2.16, $\chi$ = 1.40). The tick marks represent calculated peak positions.**

**Table 7.148 Refined lattice parameters for figure 5.45 line E mixed phase Rietveld refinement with the MP-*C*2 and tetradecane structures.**

| Parameter | Value |
|---|---|
| **Phase / Space group** | MP-*C*2 / *C*2 |
| ***a* (Å)** | 43.35(1) |
| ***b* (Å)** | 7.2492(8) |
| ***c* (Å)** | 5.572(1) |
| ***β* (°)** | 93.99(2) |
| **Volume (Å$^3$)** | 1746.8(7) |
| **Phase / Space group** | Tetradecane / *P*-1 |
| ***a* (Å)** | 4.256(2) |
| ***b* (Å)** | 4.782(1) |
| ***c* (Å)** | 18.32(1) |
| ***α* (°)** | 92.75(7) |
| ***β* (°)** | 79.08(7) |
| ***γ* (°)** | 106.87(3) |
| **Volume (Å$^3$)** | 350.4(3) |
| **Phase fractions** | MP-*C*2 62.51 : 37.49 Tetradecane |

## 5.11.3 Rietveld refinement of figure 5.45 line F

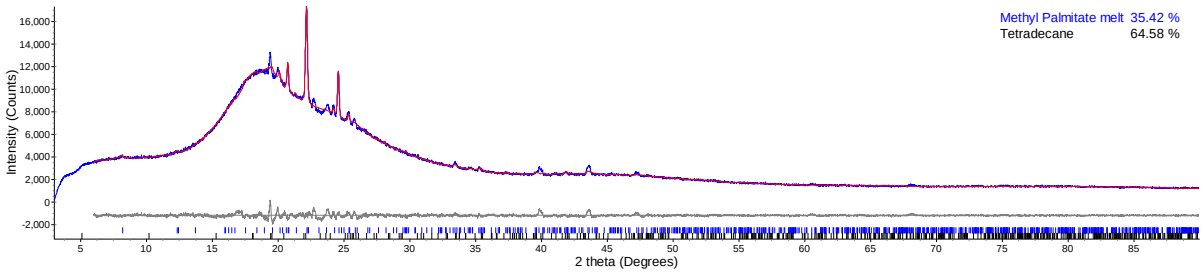


**Figure 7.138 Observed and calculated profiles for the mixed phase Rietveld refinement of figure 5.45 line F with the MP-*C*2 and tetradecane structures. The bottom curve is the difference plot on the same intensity scale. ($R_{wp}$ = 2.72, $R_p$ = 1.96, $\chi$ = 1.58). The tick marks represent calculated peak positions.**

**Table 7.149 Refined lattice parameters for figure 5.45 line F mixed phase Rietveld refinement with the MP-*C*2 and tetradecane structures.**

| Parameter | Value |
|---|---|
| **Phase / Space group** | MP-*C*2 / *C*2 |
| ***a* (Å)** | 43.13(2) |
| ***b* (Å)** | 7.222(3) |
| ***c* (Å)** | 5.567(3) |
| ***β* (°)** | 93.46(2) |
| **Volume (Å$^3$)** | 1731(1) |
| **Phase / Space group** | Tetradecane / *P*-1 |
| ***a* (Å)** | 3.94(2) |
| ***b* (Å)** | 5.10(1) |
| ***c* (Å)** | 17.98(8) |
| ***α* (°)** | 85.7(3) |
| ***β* (°)** | 77.2(6) |
| ***γ* (°)** | 103.5(6) |
| **Volume (Å$^3$)** | 340(3) |
| **Phase fractions** | MP-*C*2 35.42 : 64.58 Tetradecane |

## 5.11.4 Rietveld refinement of figure 5.45 line G

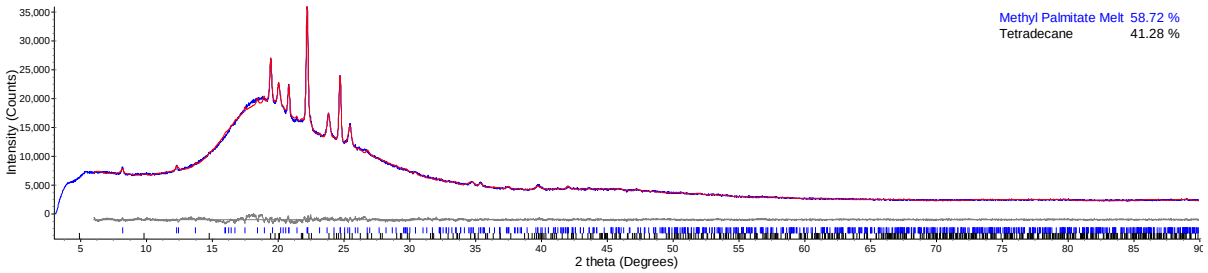


**Figure 7.139 Observed and calculated profiles for the mixed phase Rietveld refinement of figure 5.45 line G with the MP-*C*2 and tetradecane structures. The bottom curve is the difference plot on the same intensity scale. ($R_{wp}$ = 2.02, $R_p$ = 1.61, $\chi$ = 1.56). The tick marks represent calculated peak positions.**

**Table 7.150 Refined lattice parameters for figure 5.45 line G mixed phase Rietveld refinement with the MP-*C*2 and tetradecane structures.**

| Parameter | Value |
|---|---|
| **Phase / Space group** | MP-*C*2 / *C*2 |
| ***a* (Å)** | 43.24(1) |
| ***b* (Å)** | 7.204(1) |
| ***c* (Å)** | 5.561(1) |
| ***β* (°)** | 93.67(1) |
| **Volume (Å$^3$)** | 1728.9(7) |
| **Phase / Space group** | Tetradecane / *P*-1 |
| ***a* (Å)** | 4.222(3) |
| ***b* (Å)** | 4.744(1) |
| ***c* (Å)** | 18.38(2) |
| ***α* (°)** | 93.53(5) |
| ***β* (°)** | 78.0(1) |
| ***γ* (°)** | 105.90(2) |
| **Volume (Å$^3$)** | 346.3(5) |
| **Phase fractions** | MP-*C*2 58.72 : 41.28 Tetradecane |

## 5.11.5 Rietveld refinement of figure 5.46 line D

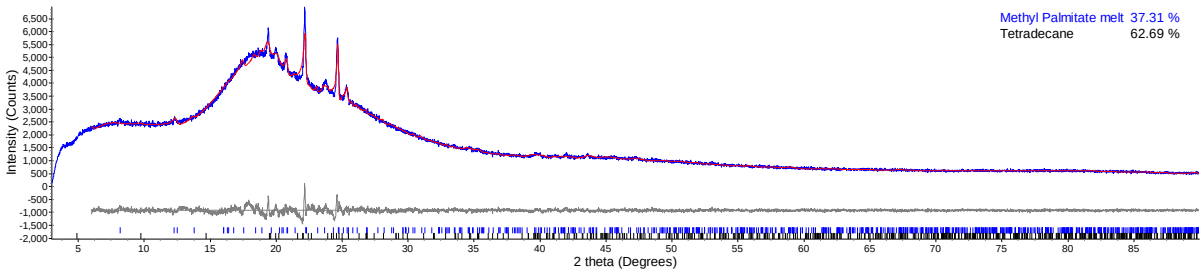


**Figure 7.140 Observed and calculated profiles for the mixed phase Rietveld refinement of figure 5.46 line D with the MP-*C*2 and tetradecane structures. The bottom curve is the difference plot on the same intensity scale. ($R_{wp}$ = 3.39, $R_p$ = 2.62, $\chi$ = 1.36). The tick marks represent calculated peak positions.**

**Table 7.151 Refined lattice parameters for figure 5.46 line D mixed phase Rietveld refinement with the MP-*C*2 and tetradecane structures.**

| Parameter | Value |
|---|---|
| **Phase / Space group** | MP-*C*2 / *C*2 |
| ***a* (Å)** | 43.29(3) |
| ***b* (Å)** | 7.18(4) |
| ***c* (Å)** | 5.543(4) |
| ***β* (°)** | 93.426(2) |
| **Volume (Å$^3$)** | 1721(2) |
| **Phase / Space group** | Tetradecane / *P*-1 |
| ***a* (Å)** | 4.210(5) |
| ***b* (Å)** | 4.747(5) |
| ***c* (Å)** | 18.52(4) |
| ***α* (°)** | 94.71(9) |
| ***β* (°)** | 77.8(1) |
| ***γ* (°)** | 106.39(8) |
| **Volume (Å$^3$)** | 347.0(9) |
| **Phase fractions** | MP-*C*2 37.31 : 62.69 Tetradecane |

# Appendix 5.12Rietveld refinements of cocrystallisation experiments with Methyl Palmitate and Octadecane

## 5.12.1 Rietveld refinement of figure 5.47 line D

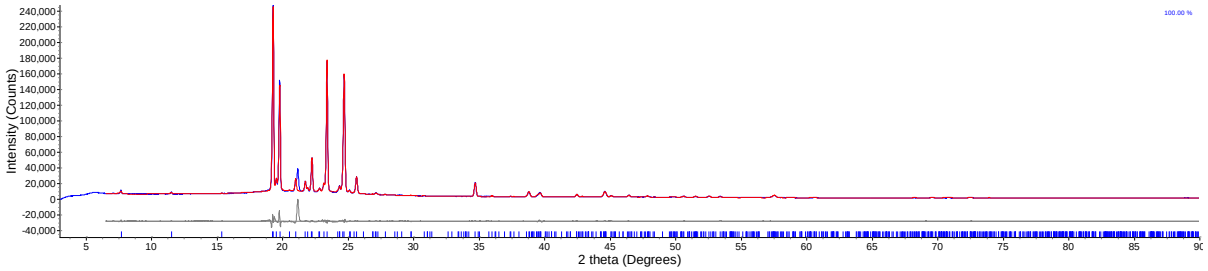


**Figure 7.141 Observed and calculated profiles for the Rietveld refinement of figure 5.47 line D with the octadecane structure. The bottom curve is the difference plot on the same intensity scale. ($R_{wp}$ = 8.27, $R_p$ = 3.99, $\chi$ = 6.29). The tick marks represent calculated peak positions.**

**Table 7.152 Refined lattice parameters for figure 5.47 line D Rietveld refinement with the octadecane structure.**

| Parameter | Value |
|---|---|
| **Phase / Space group** | Octadecane / *P*-1 |
| ***a* (Å)** | 4.2905(2) |
| ***b* (Å)** | 4.8309(2) |
| ***c* (Å)** | 24.885(3) |
| ***α* (°)** | 85.145(5) |
| ***β* (°)** | 67.886(7) |
| ***γ* (°)** | 72.438(2) |
| **Volume (Å$^3$)** | 455.32(6) |

## 5.12.2 Rietveld refinement of figure 5.47 line E

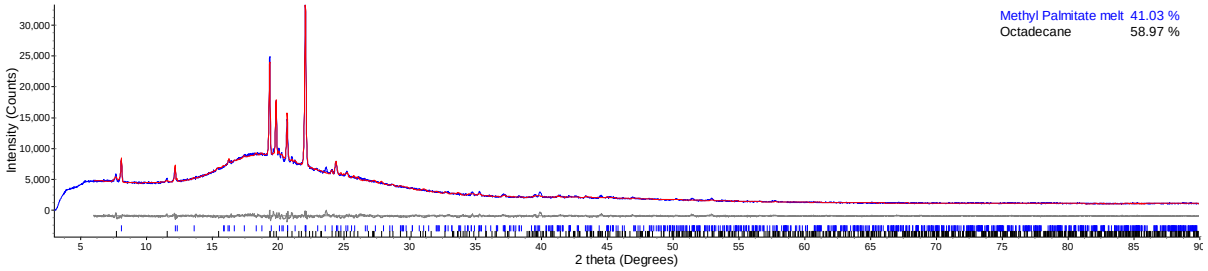


**Figure 7.142 Observed and calculated profiles for the mixed phase Rietveld refinement of figure 5.47 line E with the MP-*C*2 and octadecane structures. The bottom curve is the difference plot on the same intensity scale. ($R_{wp}$ = 3.22, $R_p$ = 2.40, $\chi$ = 1.77). The tick marks represent calculated peak positions.**

**Table 7.153 Refined lattice parameters for figure 5.47 line E mixed phase Rietveld refinement with the MP-*C*2 and octadecane structures.**

| Parameter | Value |
|---|---|
| **Phase / Space group** | MP-*C*2 / *C*2 |
| ***a* (Å)** | 43.630(4) |
| ***b* (Å)** | 7.279(1) |
| ***c* (Å)** | 5.574(1) |
| ***β* (°)** | 93.59(2) |
| **Volume (Å$^3$)** | 1766.7(5) |
| **Phase / Space group** | Octadecane / *P*-1 |
| ***a* (Å)** | 4.3155(5) |
| ***b* (Å)** | 4.7952(4) |
| ***c* (Å)** | 24.812(8) |
| ***α* (°)** | 84.72(1) |
| ***β* (°)** | 67.44(2) |
| ***γ* (°)** | 72.78(2) |
| **Volume (Å$^3$)** | 454.8(2) |
| **Phase fractions** | MP-*C*2 41.03 : 58.97 Octadecane |

## 5.12.3 Rietveld refinement of figure 5.47 line F

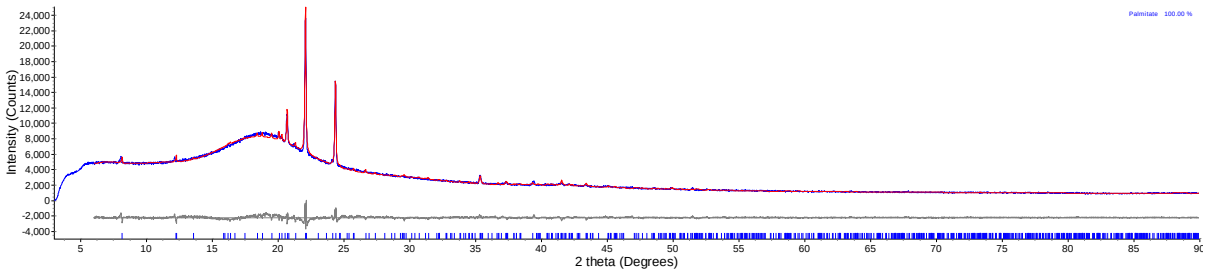


**Figure 7.143 Observed and calculated profiles for the Rietveld refinement of figure 5.47 line F with the MP-*C*2 structure. The bottom curve is the difference plot on the same intensity scale. ($R_{wp}$ = 3.54, $R_p$ = 2.69, $\chi$ = 1.84). The tick marks represent calculated peak positions.**

**Table 7.154 Refined lattice parameters for figure 5.47 line F Rietveld refinement with the MP-*C*2 structure.**

| Parameter | Value |
|---|---|
| **Phase / Space group** | MP-*C*2 / *C*2 |
| ***a* (Å)** | 43.376(7) |
| ***b* (Å)** | 7.2998(2) |
| ***c* (Å)** | 5.5613(5) |
| ***β* (°)** | 93.76(1) |
| **Volume (Å$^3$)** | 1757.1(3) |

## 5.12.4 Rietveld refinement of figure 5.48 line D

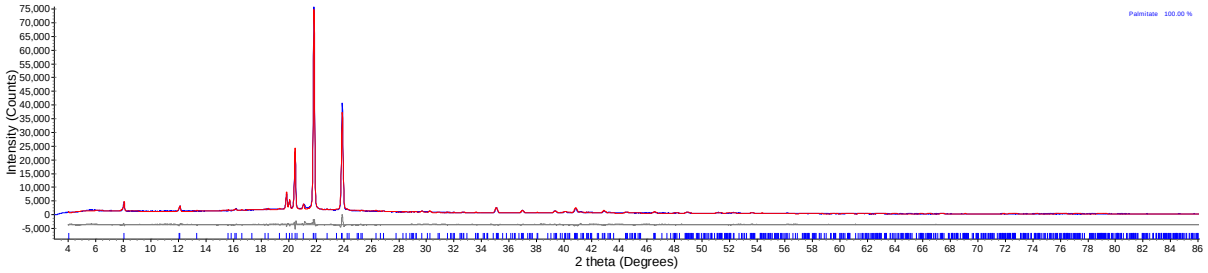


**Figure 7.144 Observed and calculated profiles for the Rietveld refinement of figure 5.48 line D with the MP-*C*2 structure. The bottom curve is the difference plot on the same intensity scale. ($R_{wp}$ = 8.21, $R_p$ = 6.23, $\chi$ = 2.77). The tick marks represent calculated peak positions.**

**Table 7.155 Refined lattice parameters for figure 5.48 line D Rietveld refinement with the MP-*C*2 structure.**

| Parameter | Value |
|---|---|
| **Phase / Space group** | MP-*C*2 / *C*2 |
| ***a* (Å)** | 43.881(4) |
| ***b* (Å)** | 7.4402(3) |
| ***c* (Å)** | 5.5996(3) |
| ***β* (°)** | 93.754(5) |
| **Volume (Å$^3$)** | 1824.3(2) |

## 5.12.5 Rietveld refinement of figure 5.48 line E

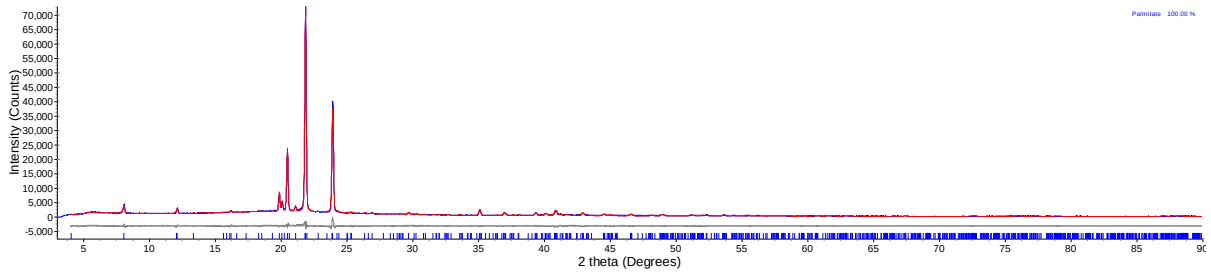


**Figure 7.145 Observed and calculated profiles for the Rietveld refinement of figure 5.48 line E with the MP-*C*2 structure. The bottom curve is the difference plot on the same intensity scale. ($R_{wp}$ = 7.56, $R_p$ = 5.79, $\chi$ = 2.59). The tick marks represent calculated peak positions.**

**Table 7.156 Refined lattice parameters for figure 5.48 line E Rietveld refinement with the MP-*C*2 structure.**

| Parameter | Value |
|---|---|
| **Phase / Space group** | MP-*C*2 / *C*2 |
| ***a* (Å)** | 43.893(4) |
| ***b* (Å)** | 7.4364(4) |
| ***c* (Å)** | 5.5997(4) |
| ***β* (°)** | 93.732(5) |
| **Volume (Å$^3$)** | 1823.9(2) |

## 5.12.6 Rietveld refinement of figure 5.48 line F

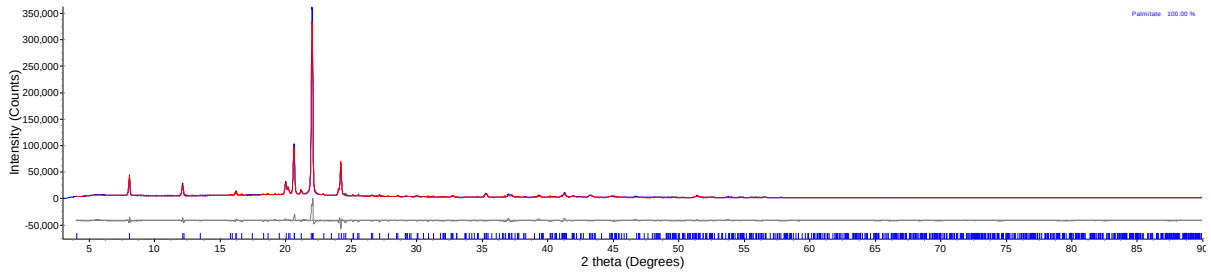


**Figure 7.146 Observed and calculated profiles for the Rietveld refinement of figure 5.48 line F with the MP-*C*2 structure. The bottom curve is the difference plot on the same intensity scale. ($R_{wp}$ = 13.06, $R_p$ = 9.85, $\chi$ = 8.97). The tick marks represent calculated peak positions.**

**Table 7.157 Refined lattice parameters for figure 5.48 line F Rietveld refinement with the MP-*C*2 structure.**

| Parameter | Value |
|---|---|
| **Phase / Space group** | MP-*C*2 / *C*2 |
| ***a* (Å)** | 43.771(6) |
| ***b* (Å)** | 7.340(1) |
| ***c* (Å)** | 5.5725(9) |
| ***β* (°)** | 93.369(6) |
| **Volume (Å$^3$)** | 1787.1(5) |

## 5.12.7 Rietveld refinement of figure 5.49 line D

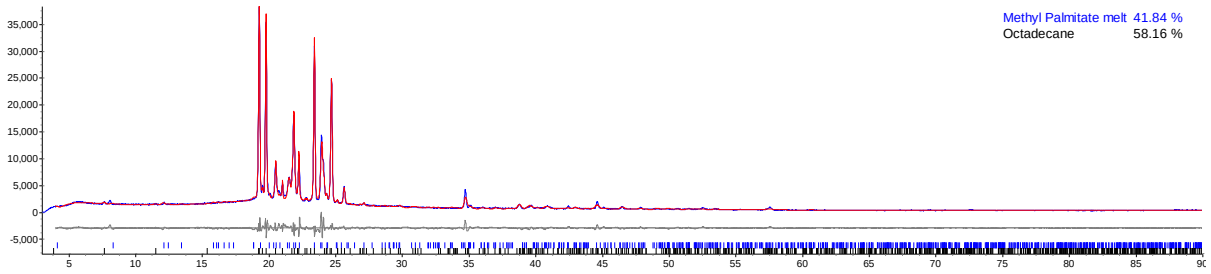


**Figure 7.147 Observed and calculated profiles for the mixed phase Rietveld refinement of figure 5.49 line D with the MP-*C*2 and octadecane structures. The bottom curve is the difference plot on the same intensity scale. ($R_{wp}$ = 8.15, $R_p$ = 5.85, $\chi$ = 2.96). The tick marks represent calculated peak positions.**

**Table 7.158 Refined lattice parameters for figure 5.49 line D mixed phase Rietveld refinement with the MP-*C*2 and octadecane structures.**

| Parameter | Value |
|---|---|
| **Phase / Space group** | MP-*C*2 / *C*2 |
| ***a* (Å)** | 42.84(1) |
| ***b* (Å)** | 7.4211(9) |
| ***c* (Å)** | 5.536(1) |
| ***β* (°)** | 95.82(1) |
| **Volume (Å$^3$)** | 1751.0(6) |
| **Phase / Space group** | Octadecane / *P*-1 |
| ***a* (Å)** | 4.2941(5) |
| ***b* (Å)** | 4.8320(6) |
| ***c* (Å)** | 24.950(5) |
| ***α* (°)** | 85.208(7) |
| ***β* (°)** | 67.690(7) |
| ***γ* (°)** | 72.409(3) |
| **Volume (Å$^3$)** | 456.3(1) |
| **Phase fractions** | MP-*C*2 41.84 : 58.16 Octadecane |

## 5.12.8 Rietveld refinement of figure 5.49 line E

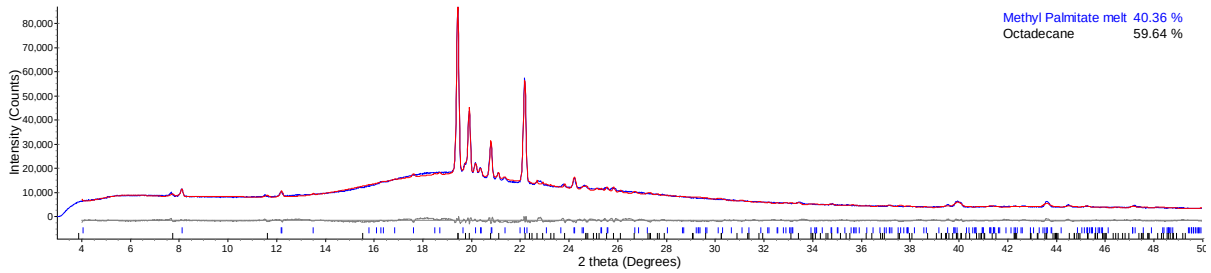


**Figure 7.148 Observed and calculated profiles for the mixed phase Rietveld refinement of figure 5.49 line E with the MP-*C*2 and octadecane structures. The bottom curve is the difference plot on the same intensity scale. ($R_{wp}$ = 3.32, $R_p$ = 2.65, $\chi$ = 3.20). The tick marks represent calculated peak positions.**

**Table 7.159 Refined lattice parameters for figure 5.49 line E mixed phase Rietveld refinement with the MP-*C*2 and octadecane structures.**

| Parameter | Value |
|---|---|
| **Phase / Space group** | MP-*C*2 / *C*2 |
| ***a* (Å)** | 43.60(1) |
| ***b* (Å)** | 7.341(1) |
| ***c* (Å)** | 5.508(1) |
| ***β* (°)** | 93.43(2) |
| **Volume (Å$^3$)** | 1760.0(6) |
| **Phase / Space group** | Octadecane / *P*-1 |
| ***a* (Å)** | 4.2004(7) |
| ***b* (Å)** | 4.7865(8) |
| ***c* (Å)** | 24.605(6) |
| ***α* (°)** | 84.635(9) |
| ***β* (°)** | 68.07(2) |
| ***γ* (°)** | 72.50(2) |
| **Volume (Å$^3$)** | 437.6(2) |
| **Phase fractions** | MP-*C*2 40.36 : 59.64 Octadecane |

## 5.12.9 Rietveld refinement of figure 5.49 line F

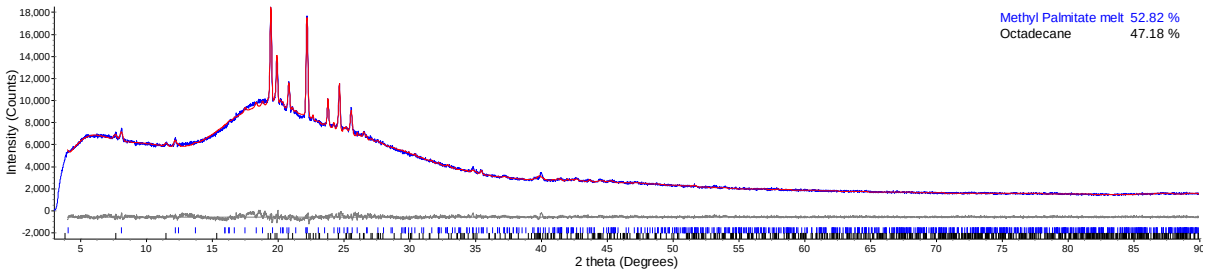


**Figure 7.149 Observed and calculated profiles for the mixed phase Rietveld refinement of figure 5.49 line F with the MP-*C*2 and octadecane structures. The bottom curve is the difference plot on the same intensity scale. ($R_{wp}$ = 2.22, $R_p$ = 1.73, $\chi$ = 1.38). The tick marks represent calculated peak positions.**

**Table 7.160 Refined lattice parameters for figure 5.49 line F mixed phase Rietveld refinement with the MP-*C*2 and octadecane structures.**

| Parameter | Value |
|---|---|
| **Phase / Space group** | MP-*C*2 / *C*2 |
| ***a* (Å)** | 43.62(2) |
| ***b* (Å)** | 7.217(1) |
| ***c* (Å)** | 5.562(1) |
| ***β* (°)** | 93.24(2) |
| **Volume (Å$^3$)** | 1748.2(8) |
| **Phase / Space group** | Octadecane / *P*-1 |
| ***a* (Å)** | 4.177(1) |
| ***b* (Å)** | 4.746(1) |
| ***c* (Å)** | 24.86(1) |
| ***α* (°)** | 85.26(2) |
| ***β* (°)** | 68.17(2) |
| ***γ* (°)** | 73.99(1) |
| **Volume (Å$^3$)** | 439.7(3) |
| **Phase fractions** | MP-*C*2 52.82 : 47.18 Octadecane |

## 5.12.10 Rietveld refinement of figure 5.50 line D

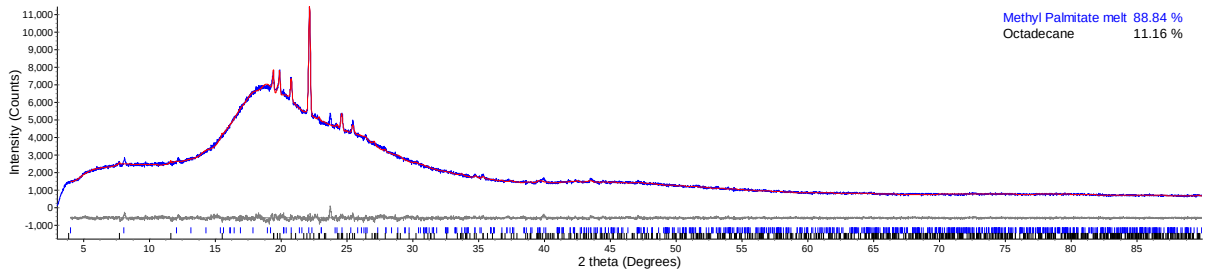


**Figure 7.150 Observed and calculated profiles for the mixed phase Rietveld refinement of figure 5.50 line D with the MP-*C*2 and octadecane structures. The bottom curve is the difference plot on the same intensity scale. ($R_{wp}$ = 2.76, $R_p$ = 2.10, $\chi$ = 1.24). The tick marks represent calculated peak positions.**

**Table 7.161 Refined lattice parameters for figure 5.50 line D mixed phase Rietveld refinement with the MP-*C*2 and octadecane structures.**

| Parameter | Value |
|---|---|
| **Phase / Space group** | MP-*C*2 / *C*2 |
| ***a* (Å)** | 44.1(1) |
| ***b* (Å)** | 6.82(7) |
| ***c* (Å)** | 5.77(1) |
| ***β* (°)** | 93.77(6) |
| **Volume (Å$^3$)** | 1732(7) |
| **Phase / Space group** | Octadecane / *P*-1 |
| ***a* (Å)** | 4.304(2) |
| ***b* (Å)** | 4.805(2) |
| ***c* (Å)** | 24.59(1) |
| ***α* (°)** | 84.46(2) |
| ***β* (°)** | 68.22(3) |
| ***γ* (°)** | 71.93(2) |
| **Volume (Å$^3$)** | 448.9(4) |
| **Phase fractions** | MP-*C*2 88.84 : 11.16 Octadecane |

# Appendix 5.13 Rietveld refinements of cocrystallisation experiments with Methyl Palmitate and Eicosane

## 5.13.1 Rietveld refinement of figure 5.51 line D

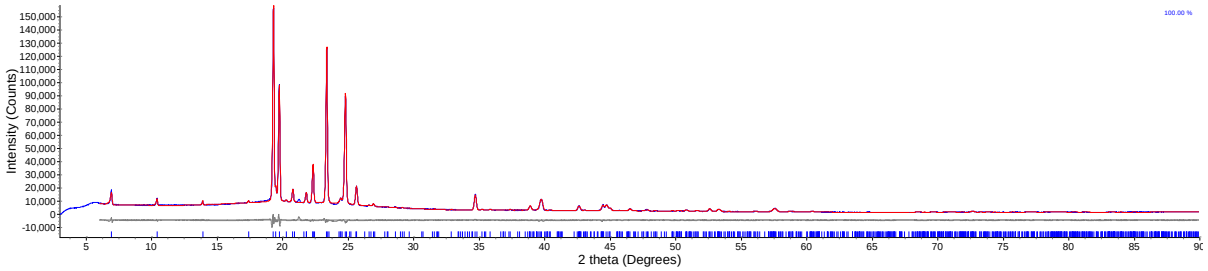


**Figure 7.151 Observed and calculated profiles for the Rietveld refinement of figure 5.51 line D with the eicosane structure. The bottom curve is the difference plot on the same intensity scale. ($R_{wp}$ = 3.68, $R_p$ = 2.67, $\chi$ = 2.61). The tick marks represent calculated peak positions.**

**Table 7.162 Refined lattice parameters for figure 5.51 line D Rietveld refinement with the eicosane structure.**

| Parameter | Value |
|---|---|
| **Phase / Space group** | Eicosane / *P*-1 |
| ***a* (Å)** | 4.2830(1) |
| ***b* (Å)** | 4.82310(6) |
| ***c* (Å)** | 27.428(1) |
| ***α* (°)** | 85.559(3) |
| ***β* (°)** | 68.340(4) |
| ***γ* (°)** | 72.560(1) |
| **Volume (Å$^3$)** | 502.02(3) |

## 5.13.2 Rietveld refinement of figure 5.51 line E

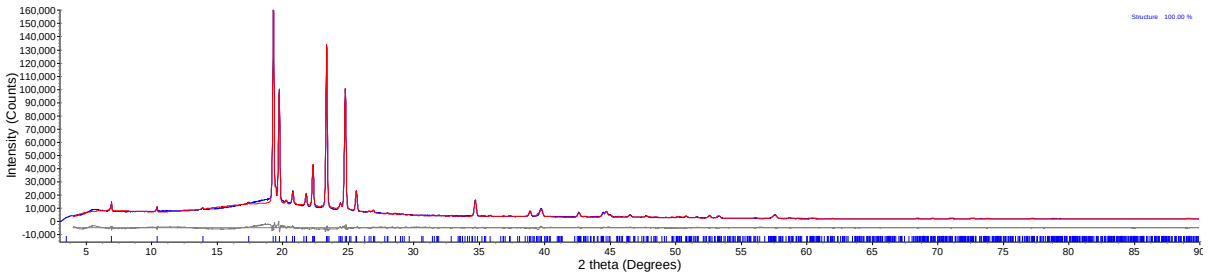


**Figure 7.152 Observed and calculated profiles for the Rietveld refinement of figure 5.51 line E with the eicosane structure. The bottom curve is the difference plot on the same intensity scale. ($R_{wp}$ = 5.81, $R_p$ = 4.49, $\chi$ = 4.43). The tick marks represent calculated peak positions.**

**Table 7.163 Refined lattice parameters for figure 5.51 line E Rietveld refinement with the eicosane structure.**

| Parameter | Value |
|---|---|
| **Phase / Space group** | Eicosane / *P*-1 |
| ***a* (Å)** | 4.2834(2) |
| ***b* (Å)** | 4.8224(2) |
| ***c* (Å)** | 27.426(2) |
| ***α* (°)** | 85.568(4) |
| ***β* (°)** | 68.330(7) |
| ***γ* (°)** | 72.545(2) |
| **Volume (Å$^3$)** | 501.88(5) |

## 5.13.3 Rietveld refinement of figure 5.51 line F

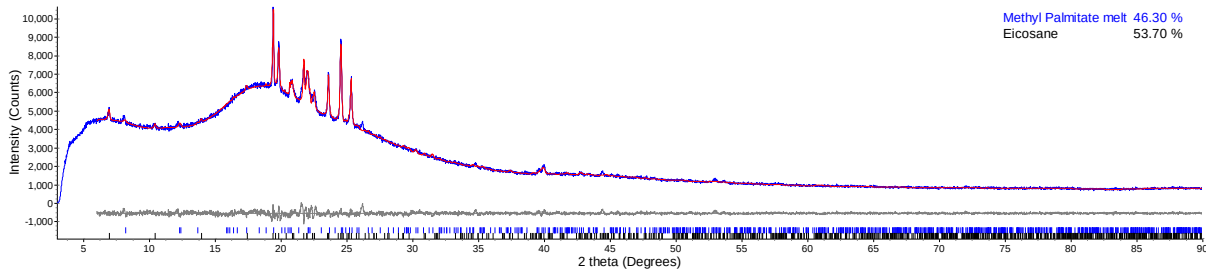


**Figure 7.153 Observed and calculated profiles for the mixed phase Rietveld refinement of figure 5.51 line F with the MP-*C*2 and eicosane structures. The bottom curve is the difference plot on the same intensity scale. ($R_{wp}$ = 2.72, $R_p$ = 2.05, $\chi$ = 1.31). The tick marks represent calculated peak positions.**

**Table 7.164 Refined lattice parameters for figure 5.51 line F mixed phase Rietveld refinement with the MP-*C*2 and eicosane structures.**

| Parameter | Value |
|---|---|
| **Phase / Space group** | MP-*C*2 / *C*2 |
| ***a* (Å)** | 43.34(1) |
| ***b* (Å)** | 7.2449(7) |
| ***c* (Å)** | 5.596(1) |
| ***β* (°)** | 93.87(1) |
| **Volume (Å$^3$)** | 1752.8(6) |
| **Phase / Space group** | Eicosane / *P*-1 |
| ***a* (Å)** | 4.2473(5) |
| ***b* (Å)** | 4.7951(6) |
| ***c* (Å)** | 27.429(8) |
| ***α* (°)** | 85.38(1) |
| ***β* (°)** | 67.94(3) |
| ***γ* (°)** | 72.68(1) |
| **Volume (Å$^3$)** | 494.0(2) |
| **Phase fractions** | MP-*C*2 46.30 : 53.70 Eicosane |

## 5.13.4 Rietveld refinement of figure 5.53 line D

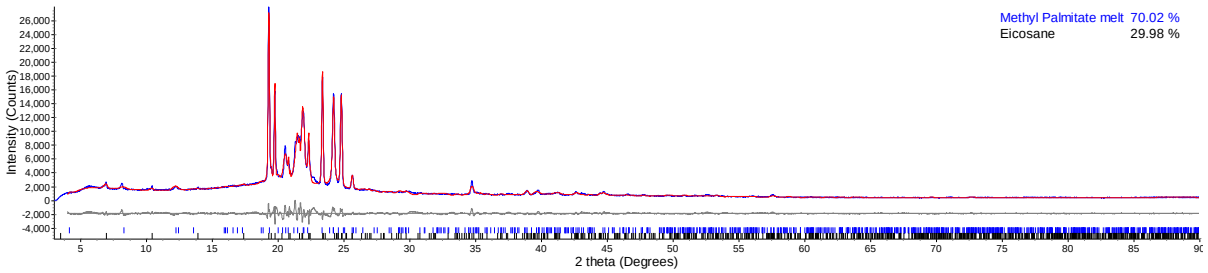


**Figure 7.154 Observed and calculated profiles for the mixed phase Rietveld refinement of figure 5.53 line D with the MP-*C*2 and eicosane structures. The bottom curve is the difference plot on the same intensity scale. ($R_{wp}$ = 7.57, $R_p$ = 5.76, $\chi$ = 2.76). The tick marks represent calculated peak positions.**

**Table 7.165 Refined lattice parameters for figure 5.53 line D mixed phase Rietveld refinement with the MP-*C*2 and eicosane structures.**

| Parameter | Value |
|---|---|
| **Phase / Space group** | MP-*C*2 / *C*2 |
| ***a* (Å)** | 42.96(2) |
| ***b* (Å)** | 7.346(1) |
| ***c* (Å)** | 5.564(1) |
| ***β* (°)** | 95.44(1) |
| **Volume (Å$^3$)** | 1749(1) |
| **Phase / Space group** | Eicosane / *P*-1 |
| ***a* (Å)** | 4.2777(7) |
| ***b* (Å)** | 4.8189(8) |
| ***c* (Å)** | 27.400(6) |
| ***α* (°)** | 85.59(1) |
| ***β* (°)** | 68.40(2) |
| ***γ* (°)** | 72.54(5) |
| **Volume (Å$^3$)** | 500.6(5) |
| **Phase fractions** | MP-*C*2 70.02 : 29.98 Eicosane |

## 5.13.5 Rietveld refinement of figure 5.53 line E

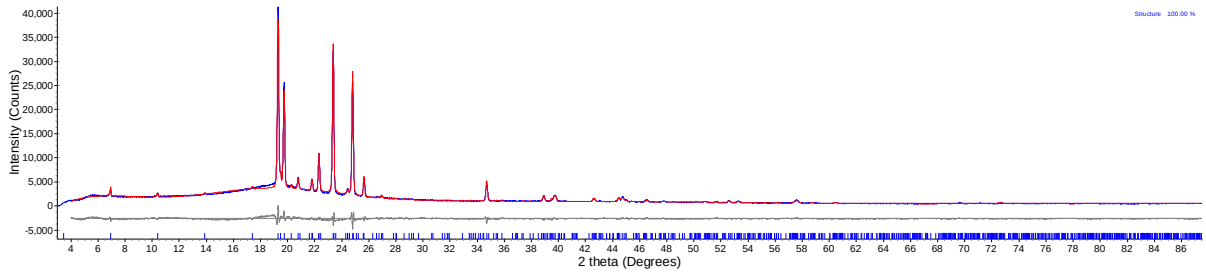


**Figure 7.155 Observed and calculated profiles for the Rietveld refinement of figure 5.53 line E with the eicosane structure. The bottom curve is the difference plot on the same intensity scale. ($R_{wp}$ = 6.50, $R_p$ = 5.21, $\chi$ = 2.53). The tick marks represent calculated peak positions.**

**Table 7.166 Refined lattice parameters for figure 5.53 line E Rietveld refinement with the eicosane structure.**

| Parameter | Value |
|---|---|
| **Phase / Space group** | Eicosane / *P*-1 |
| ***a* (Å)** | 4.2802(2) |
| ***b* (Å)** | 4.8205(3) |
| ***c* (Å)** | 27.425(2) |
| ***α* (°)** | 85.581(6) |
| ***β* (°)** | 68.346(8) |
| ***γ* (°)** | 72.593(2) |
| **Volume (Å$^3$)** | 501.47(6) |

## 5.13.6 Rietveld refinement of figure 5.53 line F

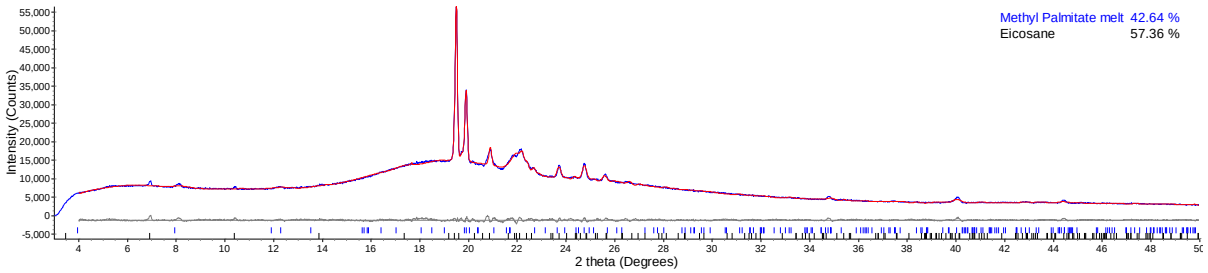


**Figure 7.156 Observed and calculated profiles for the mixed phase Rietveld refinement of figure 5.53 line F with the MP-*C*2 and eicosane structures. The bottom curve is the difference plot on the same intensity scale. ($R_{wp}$ = 2.36, $R_p$ = 1.78, $\chi$ = 2.09). The tick marks represent calculated peak positions.**

**Table 7.167 Refined lattice parameters for figure 5.53 line F mixed phase Rietveld refinement with the MP-*C*2 and eicosane structures.**

| Parameter | Value |
|---|---|
| **Phase / Space group** | MP-*C*2 / *C*2 |
| ***a* (Å)** | 44.66(5) |
| ***b* (Å)** | 7.287(7) |
| ***c* (Å)** | 5.681(2) |
| ***β* (°)** | 94.08(6) |
| **Volume (Å$^3$)** | 1844(3) |
| **Phase / Space group** | Eicosane / *P*-1 |
| ***a* (Å)** | 4.260(2) |
| ***b* (Å)** | 4.847(2) |
| ***c* (Å)** | 27.40(2) |
| ***α* (°)** | 85.09(1) |
| ***β* (°)** | 68.81(3) |
| ***γ* (°)** | 72.59(2) |
| **Volume (Å$^3$)** | 503.1(5) |
| **Phase fractions** | MP-*C*2 42.64 : 57.36 Eicosane |

## 5.13.7 Rietveld refinement of figure 5.53 line G

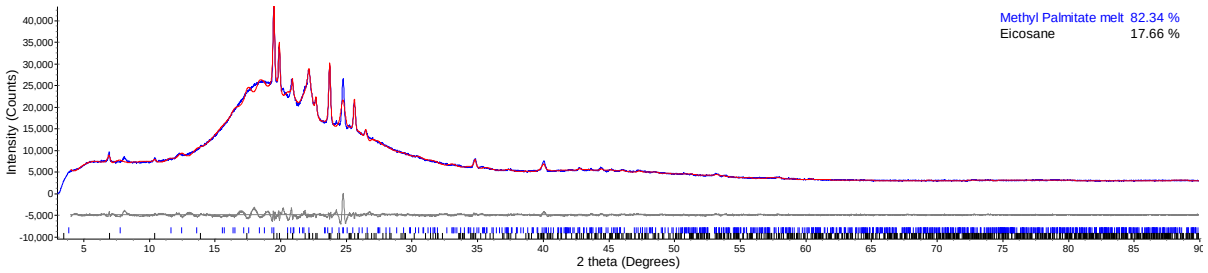


**Figure 7.157 Observed and calculated profiles for the mixed phase Rietveld refinement of figure 5.53 line G with the MP-*C*2 and eicosane structures. The bottom curve is the difference plot on the same intensity scale. ($R_{wp}$ = 2.86, $R_p$ = 2.05, $\chi$ = 2.46). The tick marks represent calculated peak positions.**

**Table 7.168 Refined lattice parameters for figure 5.53 line G mixed phase Rietveld refinement with the MP-*C*2 and eicosane structures.**

| Parameter | Value |
|---|---|
| **Phase / Space group** | MP-*C*2 / *C*2 |
| ***a* (Å)** | 45.72(5) |
| ***b* (Å)** | 7.190(2) |
| ***c* (Å)** | 5.423(3) |
| ***β* (°)** | 94.80(7) |
| **Volume (Å$^3$)** | 1777 (2) |
| **Phase / Space group** | Eicosane / *P*-1 |
| ***a* (Å)** | 4.179(1) |
| ***b* (Å)** | 4.733(1) |
| ***c* (Å)** | 27.380(9) |
| ***α* (°)** | 85.70(2) |
| ***β* (°)** | 68.40(3) |
| ***γ* (°)** | 74.11(9) |
| **Volume (Å$^3$)** | 484.1(2) |
| **Phase fractions** | MP-*C*2 82.34 : 17.66 Eicosane |

## 5.13.8 Rietveld refinement of figure 5.54 line D

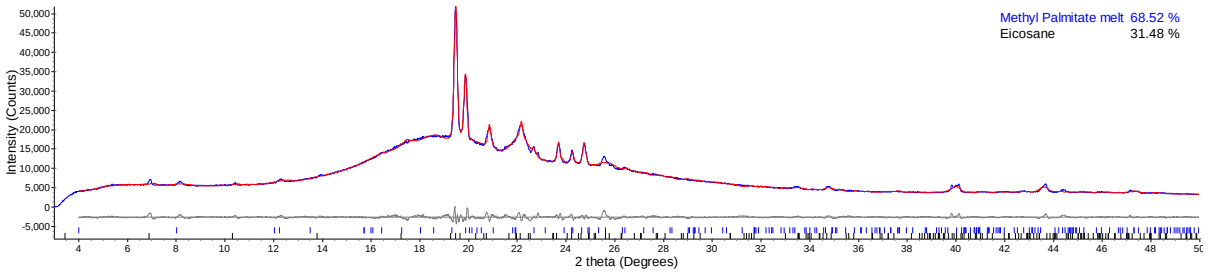


**Figure 7.158 Observed and calculated profiles for the mixed phase Rietveld refinement of figure 5.54 line D with the MP-*C*2 and eicosane structures. The bottom curve is the difference plot on the same intensity scale. ($R_{wp}$ = 2.90, $R_p$ = 2.10, $\chi$ = 2.63). The tick marks represent calculated peak positions.**

**Table 7.169 Refined lattice parameters for figure 5.54 line D mixed phase Rietveld refinement with the MP-*C*2 and eicosane structures.**

| Parameter | Value |
|---|---|
| **Phase / Space group** | MP-*C*2 / *C*2 |
| ***a* (Å)** | 44.13(8) |
| ***b* (Å)** | 7.32(1) |
| ***c* (Å)** | 5.648(8) |
| ***β* (°)** | 93.06(7) |
| **Volume (Å$^3$)** | 1822(5) |
| **Phase / Space group** | Eicosane / *P*-1 |
| ***a* (Å)** | 4.254(2) |
| ***b* (Å)** | 4.828(2) |
| ***c* (Å)** | 27.65(1) |
| ***α* (°)** | 85.0(2) |
| ***β* (°)** | 68.40(2) |
| ***γ* (°)** | 72.61(1) |
| **Volume (Å$^3$)** | 503.7(4) |
| **Phase fractions** | MP-*C*2 68.52 : 31.48 Eicosane |

# Appendix 5.14 Rietveld refinements of cocrystallisation experiments with Methyl Palmitate and Docosane

## 5.14.1 Rietveld refinement of figure 5.55 line D

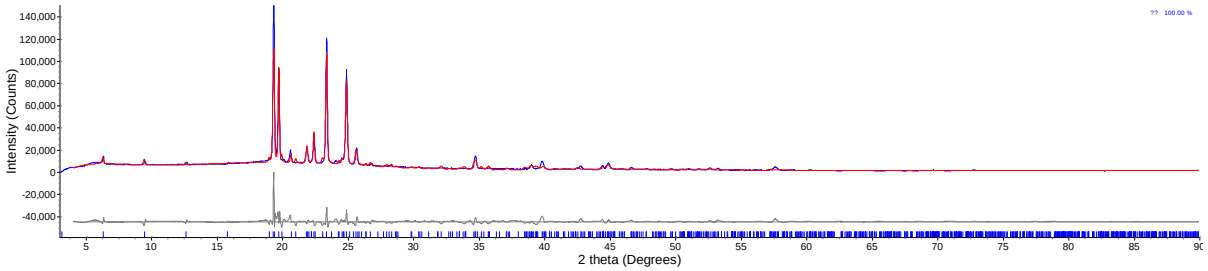


**Figure 7.159 Observed and calculated profiles for the Rietveld refinement of figure 5.55 line D with the docosane structure. The bottom curve is the difference plot on the same intensity scale. ($R_{wp}$ = 13.95, $R_p$ = 10.14, $\chi$ = 9.80). The tick marks represent calculated peak positions.**

**Table 7.170 Refined lattice parameters for figure 5.55 line D Rietveld refinement with the docosane structure.**

| Parameter | Value |
|---|---|
| **Phase / Space group** | Docosane / *P*-1 |
| ***a* (Å)** | 4.2640(5) |
| ***b* (Å)** | 4.8196(7) |
| ***c* (Å)** | 30.094(5) |
| ***α* (°)** | 86.89(1) |
| ***β* (°)** | 69.00(1) |
| ***γ* (°)** | 72.95(5) |
| **Volume (Å$^3$)** | 551.1(1) |

## 5.14.2 Rietveld refinement of figure 5.55 line E

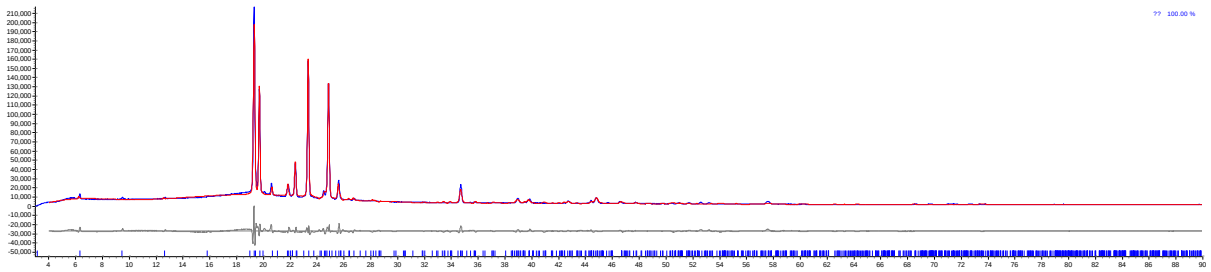

**Figure 7.160 Observed and calculated profiles for the Rietveld refinement of figure 5.55 line E with the docosane structure. The bottom curve is the difference plot on the same intensity scale. ($R_{wp}$ = 9.84, $R_p$ = 7.50, $\chi$ = 7.52). The tick marks represent calculated peak positions.**

**Table 7.171 Refined lattice parameters for figure 5.55 line E Rietveld refinement with the docosane structure.**

| Parameter | Value |
|---|---|
| **Phase / Space group** | Docosane / *P*-1 |
| ***a* (Å)** | 4.2672(5) |
| ***b* (Å)** | 4.8142(6) |
| ***c* (Å)** | 30.152(4) |
| ***α* (°)** | 86.890(7) |
| ***β* (°)** | 68.734(9) |
| ***γ* (°)** | 72.947(3) |
| **Volume (Å$^3$)** | 550.9(1) |

## 5.14.3 Rietveld refinement of figure 5.55 line F

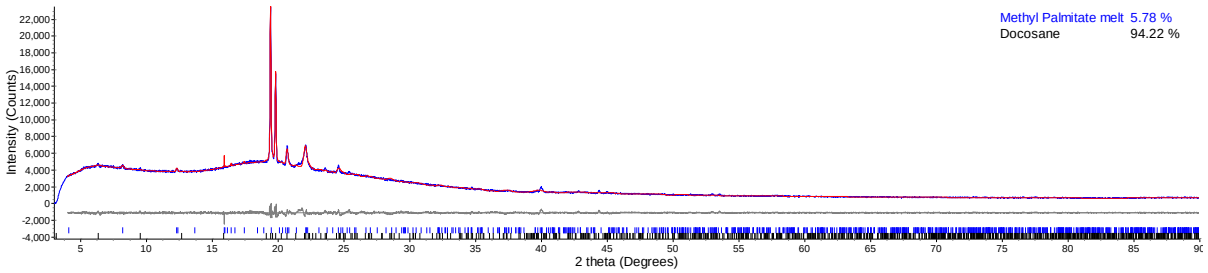


**Figure 7.161 Observed and calculated profiles for the mixed phase Rietveld refinement of figure 5.55 line F with the MP-*C*2 and docosane structures. The bottom curve is the difference plot on the same intensity scale. ($R_{wp}$ = 3.44, $R_p$ = 2.50, $\chi$ = 1.55). The tick marks represent calculated peak positions.**

**Table 7.172 Refined lattice parameters for figure 5.55 line F mixed phase Rietveld refinement with the MP-*C*2 and docosane structures.**

| Parameter | Value |
|---|---|
| **Phase / Space group** | MP-*C*2 / *C*2 |
| ***a* (Å)** | 43.24(3) |
| ***b* (Å)** | 7.246(6) |
| ***c* (Å)** | 5.577(2) |
| ***β* (°)** | 93.94(7) |
| **Volume (Å$^3$)** | 1743(2) |
| **Phase / Space group** | Docosane / *P*-1 |
| ***a* (Å)** | 4.239(2) |
| ***b* (Å)** | 4.793(2) |
| ***c* (Å)** | 29.99(2) |
| ***α* (°)** | 85.49(3) |
| ***β* (°)** | 68.52(5) |
| ***γ* (°)** | 72.39(6) |
| **Volume (Å$^3$)** | 540.1(5) |
| **Phase fractions** | MP-*C*2 5.78 : 94.22 Docosane |

## 5.14.4 Rietveld refinement of figure 5.55 line G

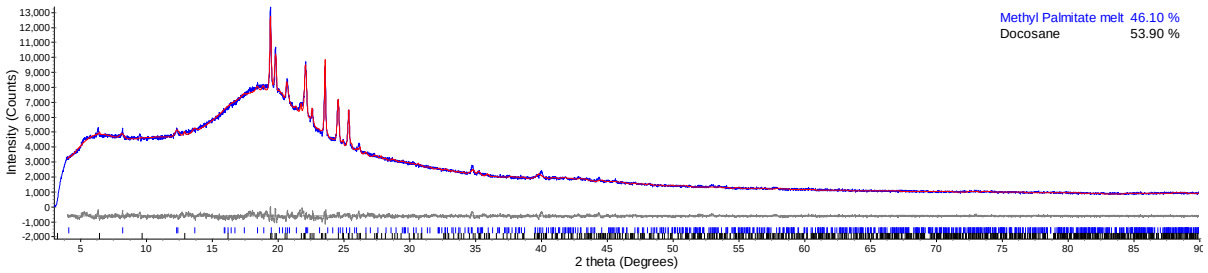


**Figure 7.162 Observed and calculated profiles for the mixed phase Rietveld refinement of figure 5.55 line G with the MP-*C*2 and docosane structures. The bottom curve is the difference plot on the same intensity scale. ($R_{wp}$ = 2.68, $R_p$ = 2.09, $\chi$ = 1.37). The tick marks represent calculated peak positions.**

**Table 7.173 Refined lattice parameters for figure 5.55 line G mixed phase Rietveld refinement with the MP-*C*2 and docosane structures.**

| Parameter | Value |
|---|---|
| **Phase / Space group** | MP-*C*2 / *C*2 |
| ***a* (Å)** | 43.26(3) |
| ***b* (Å)** | 7.2425(9) |
| ***c* (Å)** | 5.574(3) |
| ***β* (°)** | 93.98(4) |
| **Volume (Å$^3$)** | 1742(2) |
| **Phase / Space group** | Docosane / *P*-1 |
| ***a* (Å)** | 4.2240(4) |
| ***b* (Å)** | 4.7443(5) |
| ***c* (Å)** | 29.501(3) |
| ***α* (°)** | 84.366(2) |
| ***β* (°)** | 68.14(1) |
| ***γ* (°)** | 73.19(1) |
| **Volume (Å$^3$)** | 525.2(1) |
| **Phase fractions** | MP-*C*2 46.10 : 53.90 Docosane |

## 5.14.5 Rietveld refinement of figure 5.56 line D

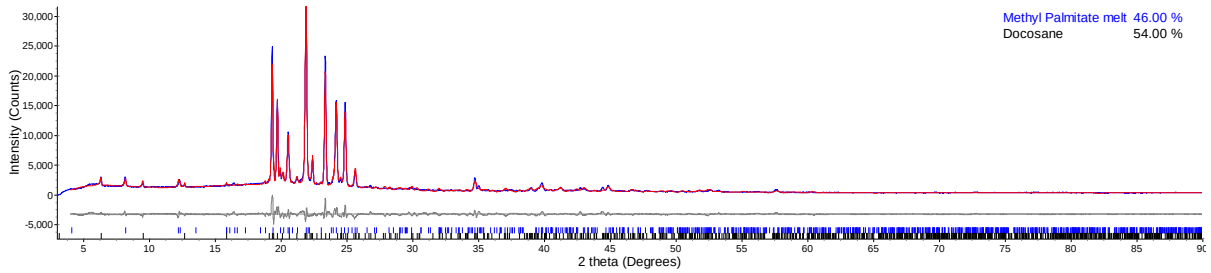


**Figure 7.163 Observed and calculated profiles for the mixed phase Rietveld refinement of figure 5.56 line D with the MP-*C*2 and docosane structures. The bottom curve is the difference plot on the same intensity scale. ($R_{wp}$ = 9.97, $R_p$ = 7.69, $\chi$ = 3.38). The tick marks represent calculated peak positions.**

**Table 7.174 Refined lattice parameters for figure 5.56 line D mixed phase Rietveld refinement with the MP-*C*2 and docosane structures.**

| Parameter | Value |
|---|---|
| **Phase / Space group** | MP-*C*2 / *C*2 |
| ***a* (Å)** | 43.176(9) |
| ***b* (Å)** | 7.3485(6) |
| ***c* (Å)** | 5.6011(8) |
| ***β* (°)** | 94.39(1) |
| **Volume (Å$^3$)** | 1771.9(5) |
| **Phase / Space group** | Docosane / *P*-1 |
| ***a* (Å)** | 4.2707(4) |
| ***b* (Å)** | 4.8104(5) |
| ***c* (Å)** | 29.965(4) |
| ***α* (°)** | 86.072(9) |
| ***β* (°)** | 68.68(1) |
| ***γ* (°)** | 72.709(4) |
| **Volume (Å$^3$)** | 547(1) |
| **Phase fractions** | MP-*C*2 46.00 : 54.00 Docosane |

## 5.14.6 Rietveld refinement of figure 5.56 line E

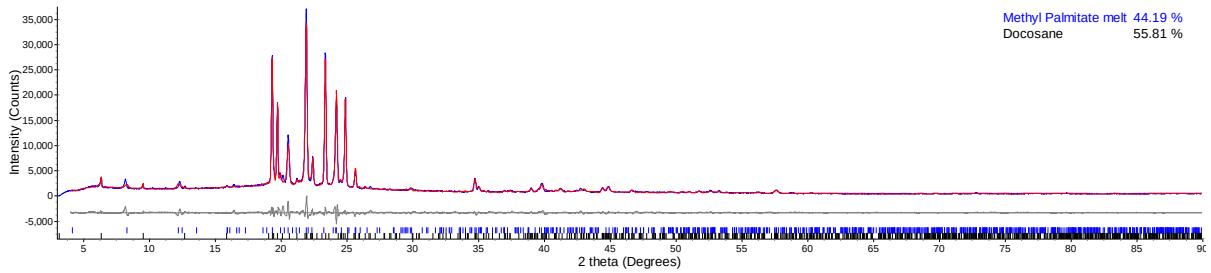


**Figure 7.164 Observed and calculated profiles for the mixed phase Rietveld refinement of figure 5.56 line E with the MP-*C*2 and docosane structures. The bottom curve is the difference plot on the same intensity scale. ($R_{wp}$ = 8.40, $R_p$ = 6.27, $\chi$ = 3.09). The tick marks represent calculated peak positions.**

**Table 7.175 Refined lattice parameters for figure 5.56 line E mixed phase Rietveld refinement with the MP-*C*2 and docosane structures.**

| Parameter | Value |
|---|---|
| **Phase / Space group** | MP-*C*2 / *C*2 |
| ***a* (Å)** | 42.772(8) |
| ***b* (Å)** | 7.3531(4) |
| ***c* (Å)** | 5.5852(8) |
| ***β* (°)** | 95.17(1) |
| **Volume (Å$^3$)** | 1749.4(4) |
| **Phase / Space group** | Docosane / *P*-1 |
| ***a* (Å)** | 4.2687(3) |
| ***b* (Å)** | 4.8128(3) |
| ***c* (Å)** | 29.950(3) |
| ***α* (°)** | 85.978(8) |
| ***β* (°)** | 68.803(9) |
| ***γ* (°)** | 72.675(3) |
| **Volume (Å$^3$)** | 547.15(8) |
| **Phase fractions** | MP-*C*2 44.19 : 55.81 Docosane |

## 5.14.7 Rietveld refinement of figure 5.57 line D

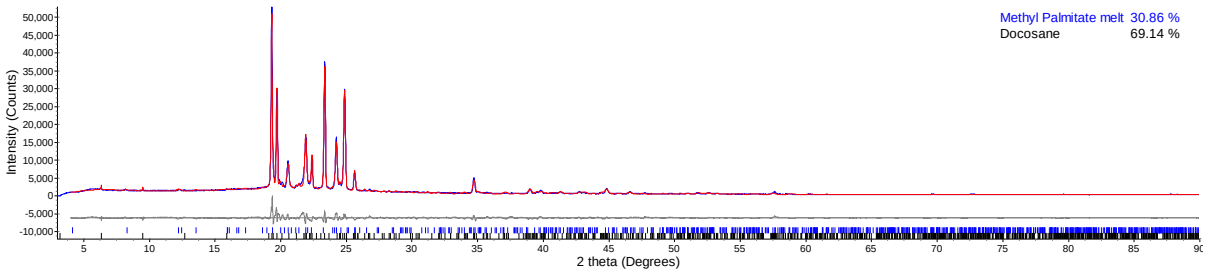


**Figure 7.165 Observed and calculated profiles for the mixed phase Rietveld refinement of figure 5.57 line D with the MP-*C*2 and docosane structures. The bottom curve is the difference plot on the same intensity scale. ($R_{wp}$ = 10.34, $R_p$ = 7.82, $\chi$ = 3.80). The tick marks represent calculated peak positions.**

**Table 7.176 Refined lattice parameters for figure 5.57 line D mixed phase Rietveld refinement with the MP-*C*2 and docosane structures.**

| Parameter | Value |
|---|---|
| **Phase / Space group** | MP-*C*2 / C2 |
| **a (Å)** | 42.77(1) |
| **b (Å)** | 7.3392(7) |
| **c (Å)** | 5.582(1) |
| **β (°)** | 95.06(2) |
| **Volume (Å$^3$)** | 1745.4(7) |
| **Phase / Space group** | Docosane / P-1 |
| **a (Å)** | 4.2741(3) |
| **b (Å)** | 4.8115(3) |
| **c (Å)** | 29.963(4) |
| **α (°)** | 86.026(8) |
| **β (°)** | 68.60(1) |
| **γ (°)** | 72.705(3) |
| **Volume (Å$^3$)** | 547.2(1) |
| **Phase fractions** | MP-*C*2 30.86 : 69.14 Docosane |

## 5.14.8 Rietveld refinement of figure 5.57 line E

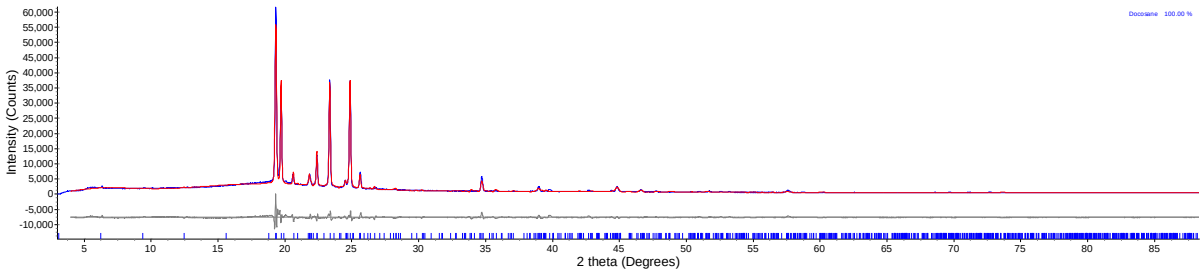


**Figure 7.166 Observed and calculated profiles for the Rietveld refinement of figure 5.57 line E with the docosane structure. The bottom curve is the difference plot on the same intensity scale. ($R_{wp}$ = 9.87, $R_p$ = 7.58, $\chi$ = 3.87). The tick marks represent calculated peak positions.**

**Table 7.177 Refined lattice parameters for figure 5.57 line E Rietveld refinement with the docosane structure.**

| Parameter | Value |
|---|---|
| **Phase / Space group** | Docosane / P-1 |
| **a (Å)** | 4.2716(5) |
| **b (Å)** | 4.8154(5) |
| **c (Å)** | 30.483(5) |
| **α (°)** | 86.952(8) |
| **β (°)** | 68.64(1) |
| **γ (°)** | 72.988(3) |
| **Volume (Å$^3$)** | 557.4(1) |

## 5.14.9 Rietveld refinement of figure 5.57 line G

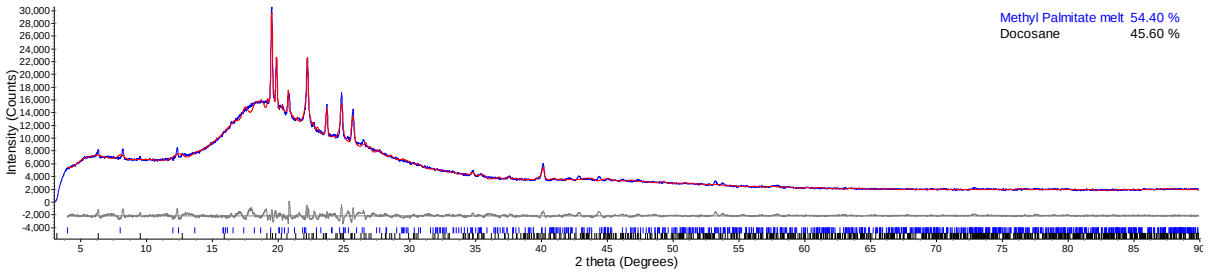


**Figure 7.167 Observed and calculated profiles for the mixed phase Rietveld refinement of figure 5.57 line G with the MP-*C*2 and docosane structures. The bottom curve is the difference plot on the same intensity scale. ($R_{wp}$ = 3.39, $R_p$ = 2.53, $\chi$ = 2.39). The tick marks represent calculated peak positions.**

**Table 7.178 Refined lattice parameters for figure 5.57 line G mixed phase Rietveld refinement with the MP-*C*2 and docosane structures.**

| Parameter | Value |
|---|---|
| **Phase / Space group** | MP-*C*2 / C2 |
| **a (Å)** | 44.31(3) |
| **b (Å)** | 7.219(3) |
| **c (Å)** | 5.586(2) |
| **β (°)** | 93.13(2) |
| **Volume (Å$^3$)** | 1784(1) |
| **Phase / Space group** | Docosane / P-1 |
| **a (Å)** | 4.242(2) |
| **b (Å)** | 4.822(2) |
| **c (Å)** | 29.78(1) |
| **α (°)** | 85.33(2) |
| **β (°)** | 69.23(2) |
| **γ (°)** | 71.47(2) |
| **Volume (Å$^3$)** | 539.6(4) |
| **Phase fractions** | MP-*C*2 54.40 : 45.60 Docosane |

## 5.14.10 Rietveld refinement of figure 5.58 line D

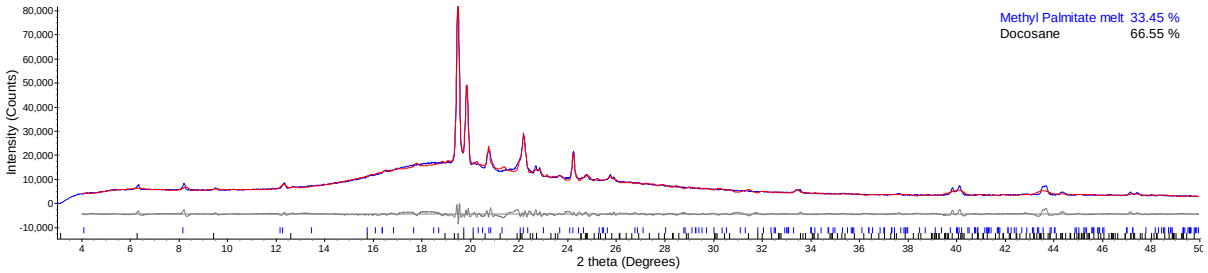


**Figure 7.168 Observed and calculated profiles for the mixed phase Rietveld refinement of figure 5.58 line D with the MP-*C*2 and docosane structures. The bottom curve is the difference plot on the same intensity scale. ($R_{wp}$ = 5.13, $R_p$ = 3.69, $\chi$ = 4.56). The tick marks represent calculated peak positions.**

**Table 7.179 Refined lattice parameters for figure 5.58 line D mixed phase Rietveld refinement with the MP-*C*2 and docosane structures.**

| Parameter | Value |
|---|---|
| **Phase / Space group** | MP-*C*2 / C2 |
| **a (Å)** | 43.38(1) |
| **b (Å)** | 7.384(2) |
| **c (Å)** | 5.515(2) |
| **β (°)** | 93.23(2) |
| **Volume (Å$^3$)** | 1763.6(9) |
| **Phase / Space group** | Docosane / P-1 |
| **a (Å)** | 4.224(1) |
| **b (Å)** | 4.800(1) |
| **c (Å)** | 30.04(1) |
| **α (°)** | 86.16(2) |
| **β (°)** | 69.41(3) |
| **γ (°)** | 72.94(3) |
| **Volume (Å$^3$)** | 544.6(4) |
| **Phase fractions** | MP-*C*2 33.45 : 66.55 Docosane |

# Appendix 5.15 Rietveld refinements of cocrystallisation experiments with Methyl Palmitate and Methyl Stearate

## 5.15.1 Rietveld refinement of figure 5.59 line E

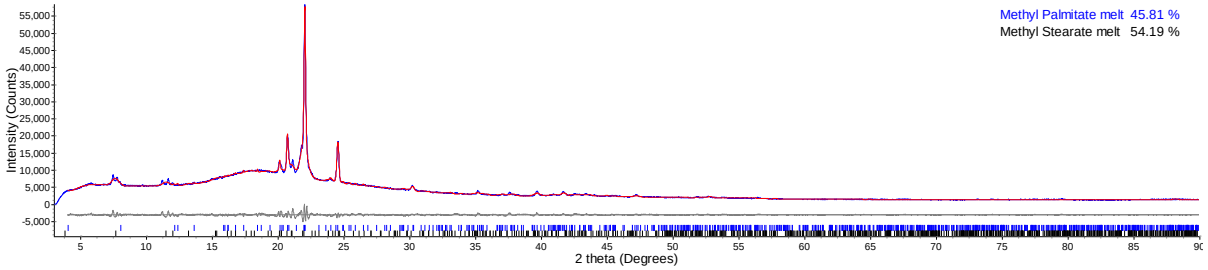


**Figure 7.169 Observed and calculated profiles for the mixed phase Rietveld refinement of figure 5.59 line E with the MP-*C*2 and MS-*C*2 structures. The bottom curve is the difference plot on the same intensity scale. ($R_{wp}$ = 3.86, $R_p$ = 2.87, $\chi$ = 2.37). The tick marks represent calculated peak positions.**

**Table 7.180 Refined lattice parameters for figure 5.59 line E mixed phase Rietveld refinement with the MP-*C*2 and MS-*C*2 structures.**

| Parameter | Value |
|---|---|
| **Phase / Space group** | MP-*C*2 / *C*2 |
| ***a* (Å)** | 43.90(1) |
| ***b* (Å)** | 7.2471(6) |
| ***c* (Å)** | 5.5621(9) |
| ***β* (°)** | 94.19(1) |
| **Volume (Å$^3$)** | 1764.7(5) |
| **Phase / Space group** | MS-*C*2 / *C*2 |
| ***a* (Å)** | 46.1707(2) |
| ***b* (Å)** | 7.469(7) |
| ***c* (Å)** | 5.494(5) |
| ***β* (°)** | 92.39(5) |
| **Volume (Å$^3$)** | 1893(3) |
| **Phase fractions** | MP-*C*2 45.81 : 54.19 MS-*C*2 |

## 5.15.2 Rietveld refinement of figure 5.59 line F

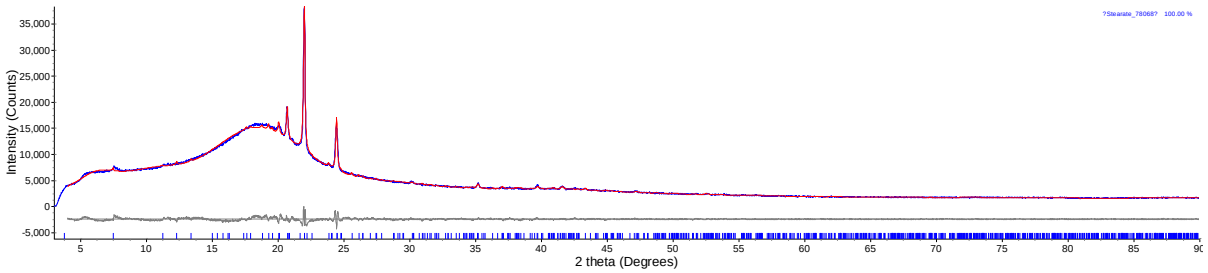


**Figure 7.170 Observed and calculated profiles for the Rietveld refinement of figure 5.59 line F with the MS-*C*2 structure. The bottom curve is the difference plot on the same intensity scale. ($R_{wp}$ = 2.92, $R_p$ = 2.28, $\chi$ = 1.96). The tick marks represent calculated peak positions.**

**Table 7.181 Refined lattice parameters for figure 5.59 line F Rietveld refinement with the MS-*C*2 structure.**

| Parameter | Value |
|---|---|
| **Phase / Space group** | MS-*C*2 / *C*2 |
| ***a* (Å)** | 47.20(1) |
| ***b* (Å)** | 7.2740(3) |
| ***c* (Å)** | 5.6073(7) |
| ***β* (°)** | 90.85(1) |
| **Volume (Å$^3$)** | 1924.9(5) |

## 5.15.3 Rietveld refinement of figure 5.60 line E

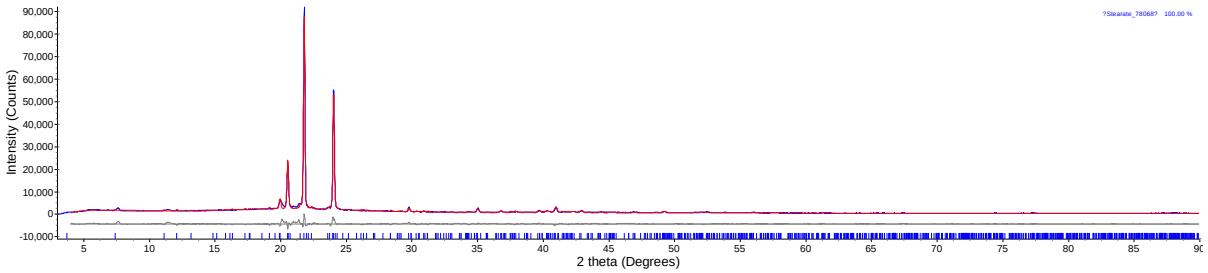


**Figure 7.171 Observed and calculated profiles for the Rietveld refinement of figure 5.60 line E with the MS-*C*2 structure. The bottom curve is the difference plot on the same intensity scale. ($R_{wp}$ = 10.11, $R_p$ = 7.41, $\chi$ = 3.75). The tick marks represent calculated peak positions.**

**Table 7.182 Refined lattice parameters for figure 5.60 line E Rietveld refinement with the MS-*C*2 structure.**

| Parameter | Value |
|---|---|
| **Phase / Space group** | MS-*C*2 / *C*2 |
| ***a* (Å)** | 47.753(6) |
| ***b* (Å)** | 7.4057(6) |
| ***c* (Å)** | 5.6129(7) |
| ***β* (°)** | 91.356(7) |
| **Volume (Å$^3$)** | 1984.4(4) |

## 5.15.4 Rietveld refinement of figure 5.60 line F

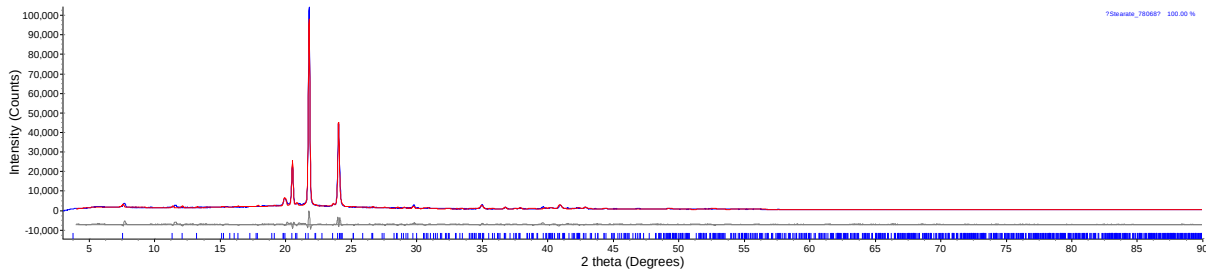


**Figure 7.172 Observed and calculated profiles for the Rietveld refinement of figure 5.60 line F with the MS-*C*2 structure. The bottom curve is the difference plot on the same intensity scale. ($R_{wp}$ = 10.58, $R_p$ = 7.71, $\chi$ = 4.02). The tick marks represent calculated peak positions.**

**Table 7.183 Refined lattice parameters for figure 5.60 line F Rietveld refinement with the MS-*C*2 structure.**

| Parameter | Value |
|---|---|
| **Phase / Space group** | MS-*C*2 / *C*2 |
| ***a* (Å)** | 46.842(7) |
| ***b* (Å)** | 734149(7) |
| ***c* (Å)** | 5.6245(7) |
| ***β* (°)** | 92.026(9) |
| **Volume (Å$^3$)** | 1952.3(4) |

## 5.15.5 Rietveld refinement of figure 5.60 line G

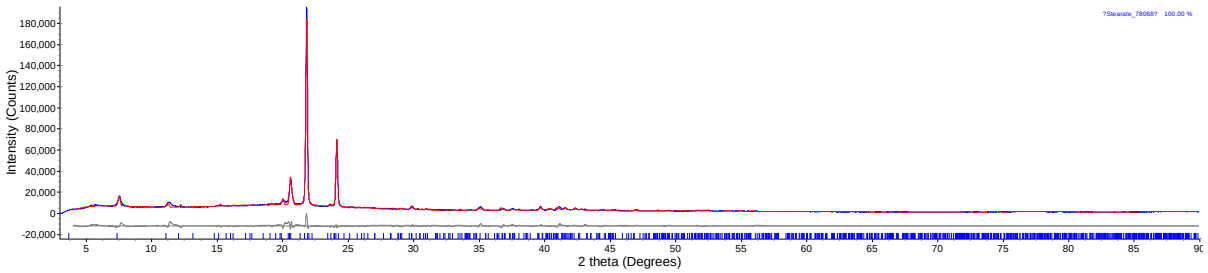


**Figure 7.173 Observed and calculated profiles for the Rietveld refinement of figure 5.60 line G with the MS-*C*2 structure. The bottom curve is the difference plot on the same intensity scale. ($R_{wp}$ = 8.96, $R_p$ = 6.48, $\chi$ = 5.84). The tick marks represent calculated peak positions.**

**Table 7.184 Refined lattice parameters for figure 5.60 line G Rietveld refinement with the MS-*C*2 structure.**

| Parameter | Value |
|---|---|
| **Phase / Space group** | MS-*C*2 / *C*2 |
| ***a* (Å)** | 47.897(7) |
| ***b* (Å)** | 7.4194(7) |
| ***c* (Å)** | 5.6465(7) |
| ***β* (°)** | 91.44(1) |
| **Volume (Å$^3$)** | 2006.0(4) |

## 5.15.6 Rietveld refinement of figure 5.61 line E

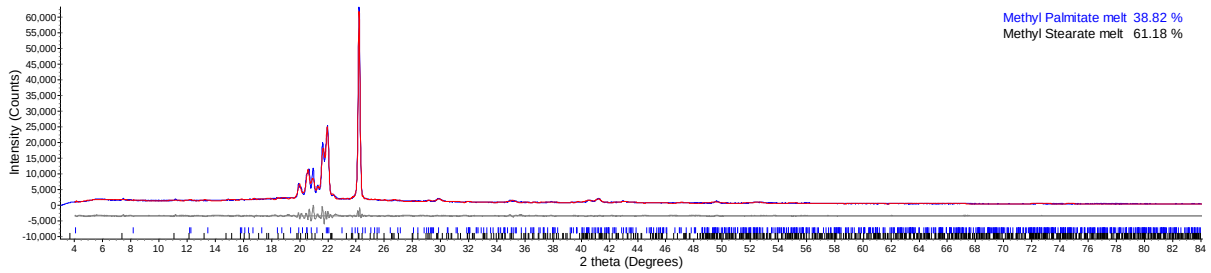


**Figure 7.174 Observed and calculated profiles for the mixed phase Rietveld refinement of figure 5.61 line E with the MP-*C*2 and MS-*C*2 structures. The bottom curve is the difference plot on the same intensity scale. ($R_{wp}$ = 8.60, $R_p$ = 6.57, $\chi$ = 3.21). The tick marks represent calculated peak positions.**

**Table 7.185 Refined lattice parameters for figure 5.61 line E mixed phase Rietveld refinement with the MP-*C*2 and MS-*C*2 structures.**

| Parameter | Value |
|---|---|
| **Phase / Space group** | MP-*C*2 / *C*2 |
| ***a* (Å)** | 43.43(1) |
| ***b* (Å)** | 7.371(2) |
| ***c* (Å)** | 5.595(1) |
| ***β* (°)** | 94.29(1) |
| **Volume (Å$^3$)** | 1786.0(8) |
| **Phase / Space group** | MS-*C*2 / *C*2 |
| ***a* (Å)** | 48.06(1) |
| ***b* (Å)** | 7.368(1) |
| ***c* (Å)** | 5.616(2) |
| ***β* (°)** | 92.93(1) |
| **Volume (Å$^3$)** | 1986.2(9) |
| **Phase fractions** | MP-*C*2 38.82 : 61.18 MS-*C*2 |

## 5.15.7 Rietveld refinement of figure 5.61 line F

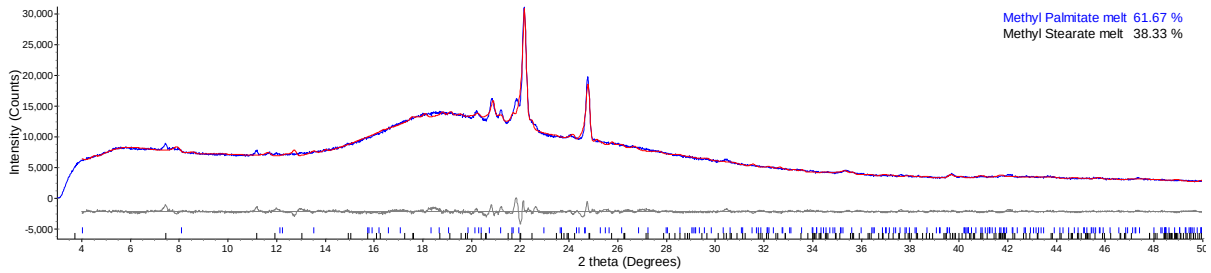


**Figure 7.175 Observed and calculated profiles for the mixed phase Rietveld refinement of figure 5.61 line F with the MP-*C*2 melt and MS-*C*2 structures. The bottom curve is the difference plot on the same intensity scale. ($R_{wp}$ = 2.84, $R_p$ = 2.07, $\chi$ = 2.46). The tick marks represent calculated peak positions.**

**Table 7.186 Refined lattice parameters for figure 5.61 line F mixed phase Rietveld refinement with the MP-*C*2 and MS-*C*2 structures.**

| Parameter | Value |
|---|---|
| **Phase / Space group** | MP-*C*2 / *C*2 |
| ***a* (Å)** | 43.88(2) |
| ***b* (Å)** | 7.321(2) |
| ***c* (Å)** | 5.650(3) |
| ***β* (°)** | 94.92(2) |
| **Volume (Å$^3$)** | 1808(1) |
| **Phase / Space group** | MS-*C*2 / *C*2 |
| ***a* (Å)** | 47.44(6) |
| ***b* (Å)** | 7.510(5) |
| ***c* (Å)** | 5.630(5) |
| ***β* (°)** | 91.40(6) |
| **Volume (Å$^3$)** | 2004(3) |
| **Phase fractions** | MP-*C*2 61.67 : 38.33 MS-*C*2 |

## 5.15.8 Rietveld refinement of figure 5.61 line G

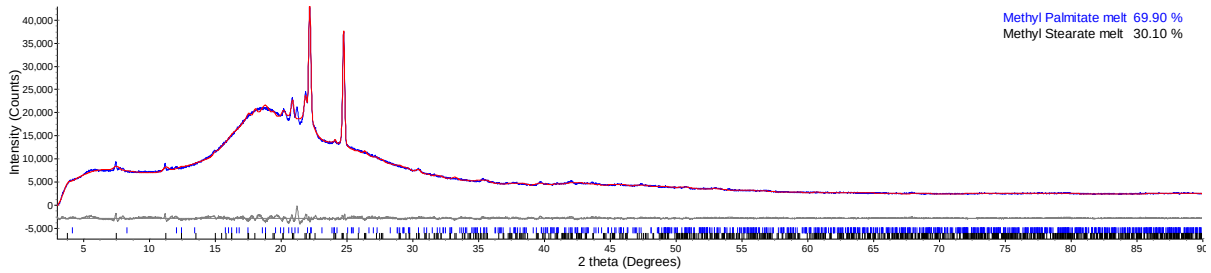


**Figure 7.176 Observed and calculated profiles for the mixed phase Rietveld refinement of figure 5.61 line G with the and MS-*C*2 structures. The bottom curve is the difference plot on the same intensity scale. ($R_{wp}$ = 2.68, $R_p$ = 1.94, $\chi$ = 2.12). The tick marks represent calculated peak positions.**

**Table 7.187 Refined lattice parameters for figure 5.61 line G mixed phase Rietveld refinement with the MP-*C*2 and MS-*C*2 structures.**

| Parameter | Value |
|---|---|
| **Phase / Space group** | MP-*C*2 / *C*2 |
| ***a* (Å)** | 42.8(3) |
| ***b* (Å)** | 7.45(4) |
| ***c* (Å)** | 5.55(3) |
| ***β* (°)** | 94.2(5) |
| **Volume (Å$^3$)** | 1763(2) |
| **Phase / Space group** | MS-*C*2 / *C*2 |
| ***a* (Å)** | 47.19(5) |
| ***b* (Å)** | 7.194(6) |
| ***c* (Å)** | 5.604(5) |
| ***β* (°)** | 90.19(4) |
| **Volume (Å$^3$)** | 1902(3) |
| **Phase fractions** | MP-*C*2 69.90 : 30.10 MS-*C*2 |

## 5.15.9 Rietveld refinement of figure 5.62 line E

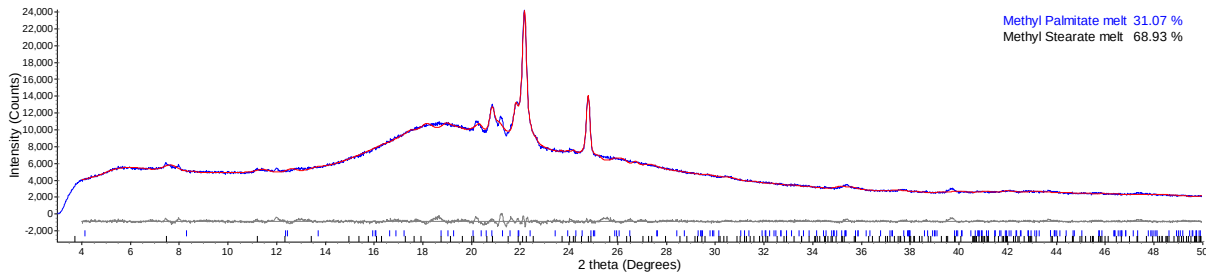


**Figure 7.177 Observed and calculated profiles for the mixed phase Rietveld refinement of figure 5.62 line E with the MP-*C*2 and MS-*C*2 structures. The bottom curve is the difference plot on the same intensity scale. ($R_{wp}$ = 2.30, $R_p$ = 1.74, $\chi$ = 1.71). The tick marks represent calculated peak positions.**

**Table 7.188 Refined lattice parameters for figure 5.62 line E mixed phase Rietveld refinement with the MP-*C*2 and MS-*C*2 structures.**

| Parameter | Value |
|---|---|
| **Phase / Space group** | MP-*C*2 / *C*2 |
| ***a* (Å)** | 42.85(5) |
| ***b* (Å)** | 7.248(6) |
| ***c* (Å)** | 5.580(6) |
| ***β* (°)** | 95.77(3) |
| **Volume (Å$^3$)** | 1724(3) |
| **Phase / Space group** | MS-*C*2 / *C*2 |
| ***a* (Å)** | 47.3(1) |
| ***b* (Å)** | 7.26(1) |
| ***c* (Å)** | 5.62(1) |
| ***β* (°)** | 91.5(2) |
| **Volume (Å$^3$)** | 1931(7) |
| **Phase fractions** | MP-*C*2 31.07 : 68.93 MS-*C*2 |