**The complete set of planes delivered through the prediction of the BFDH morphology for methyl stearate crystals using three different sets of unit cell parameters**

* Complete set of planes delivered by the prediction of the BFDH morphology for orthorhombic methyl stearate crystals according to C.H. MacGillavry and M. Wolthuis-Spuy, 1970. These planes are organised innine different groups defined by zone axis analysis.

**Group 1/Zone axis [100]**

|  |  |  |  |
| --- | --- | --- | --- |
| hkl | Mult | dhkl | Distance |
| { 0 1 1} | 4 | 7.33 | 13.64 |
| { 0 1 3} | 4 | 7.16 | 13.96 |
| { 0 2 0} | 2 | 3.68 | 27.20 |
| { 0 2 4} | 4 | 3.63 | 27.52 |
| { 0 3 1} | 4 | 2.45 | 40.81 |
| { 0 4 2} | 4 | 1.84 | 54.43 |
| { 0 4 6} | 4 | 1.83 | 54.76 |
| { 0 6 4} | 4 | 1.22 | 81.70 |

**Group 2/Zone axis [1-10]**

|  |  |  |  |
| --- | --- | --- | --- |
| hkl | Mult | dhkl | Distance |
| { 1 1 1} | 8 | 4.46 | 22.44 |
| { 1 1 2} | 8 | 4.44 | 22.51 |
| { 1 1 3} | 8 | 4.42 | 22.63 |
| { 2 2 0} | 4 | 2.23 | 44.82 |
| { 2 2 1} | 8 | 2.23 | 44.84 |
| { 2 2 3} | 8 | 2.23 | 44.94 |
| { 3 3 1} | 8 | 1.49 | 67.24 |
| { 3 3 2} | 8 | 1.49 | 67.27 |

**Group 3/Zone axis [2-10]**

|  |  |  |  |
| --- | --- | --- | --- |
| hkl | Mult | dhkl | Distance |
| { 1 2 0} | 4 | 3.08 | 32.51 |
| { 1 2 1} | 8 | 3.07 | 32.53 |
| { 1 2 2} | 8 | 3.07 | 32.58 |
| { 1 2 3} | 8 | 3.06 | 32.66 |

**Group 4/Zone axis [3-10]**

|  |  |  |  |
| --- | --- | --- | --- |
| hkl | Mult | dhkl | Distance |
| { 1 3 1} | 8 | 2.25 | 44.53 |
| { 1 3 2} | 8 | 2.24 | 44.56 |
| { 1 3 3} | 8 | 2.24 | 44.63 |
| { 2 6 0} | 4 | 1.12 | 89.03 |

**Group 5/Zone axis [0-10]**

|  |  |  |  |
| --- | --- | --- | --- |
| hkl | Mult | dhkl | Distance |
| { 2 0 0} | 2 | 2.81 | 35.63 |
| { 2 0 1} | 4 | 2.81 | 35.65 |
| { 2 0 2} | 4 | 2.80 | 35.69 |
| { 2 0 3} | 4 | 2.80 | 35.77 |
| { 2 0 4} | 4 | 2.79 | 35.88 |
| { 2 0 6} | 4 | 2.76 | 36.19 |
| { 6 0 2} | 4 | 0.94 | 106.92 |
| { 6 0 4} | 4 | 0.93 | 106.98 |

**Group 6/Zone axis [1-20]**

|  |  |  |  |
| --- | --- | --- | --- |
| hkl | Mult | dhkl | Distance |
| { 2 1 1} | 8 | 2.62 | 38.15 |
| { 2 1 2} | 8 | 2.62 | 38.20 |
| { 2 1 3} | 8 | 2.61 | 38.27 |
| { 4 2 0} | 4 | 1.31 | 76.28 |

**Group 7/Zone axis [3-20]**

|  |  |  |  |
| --- | --- | --- | --- |
| hkl | Mult | dhkl | Distance |
| { 2 3 1} | 8 | 1.85 | 54.17 |
| { 2 3 2} | 8 | 1.84 | 54.21 |
| { 2 3 3} | 8 | 1.84 | 54.26 |
| { 4 6 0} | 4 | 0.92 | 108.33 |

**Group 8/Zone axis [1-30]**

|  |  |  |  |
| --- | --- | --- | --- |
| hkl | Mult | dhkl | Distance |
| { 3 1 1} | 8 | 1.81 | 55.16 |
| { 3 1 2} | 8 | 1.81 | 55.19 |
| { 3 1 3} | 8 | 1.81 | 55.24 |
| { 6 2 0} | 4 | 0.91 | 110.30 |

**Group 9/Zone axis [2-30]**

|  |  |  |  |
| --- | --- | --- | --- |
| hkl | Mult | dhkl | Distance |
| { 3 2 0} | 4 | 1.67 | 59.97 |
| { 3 2 1} | 8 | 1.67 | 59.98 |
| { 3 2 2} | 8 | 1.67 | 60.01 |
| { 3 2 3} | 8 | 1.67 | 60.05 |

* Complete set of planes delivered by the prediction of the BFDH morphology for monoclinic methyl stearate crystals according to S. Aleby, E. von Sydow, 1960. These planes are organised innine different groups defined by zone axis analysis.

**Group 1/Zone axis [100]**

|  |  |  |  |
| --- | --- | --- | --- |
| hkl | Mult | dhkl | Distance |
| { 0 1 1} | 4 | 7.31 | 13.68 |
| { 0 1 3} | 4 | 7.14 | 14.00 |
| { 0 2 0} | 2 | 3.67 | 27.29 |
| { 0 2 4} | 4 | 3.62 | 27.61 |
| { 0 3 1} | 4 | 2.44 | 40.94 |
| { 0 4 2} | 4 | 1.83 | 54.61 |
| { 0 4 6} | 4 | 1.82 | 54.93 |
| { 0 6 4} | 4 | 1.22 | 81.96 |

**Group 2/Zone axis [1-10]**

|  |  |  |  |
| --- | --- | --- | --- |
| hkl | Mult | dhkl | Distance |
| { 1 1 1} | 4 | 4.07 | 24.59 |
| { 1 1 3} | 4 | 3.92 | 25.52 |
| { 1 1 -1} | 4 | 4.20 | 23.81 |
| { 1 1 -3} | 4 | 4.31 | 23.20 |
| { 2 2 0} | 4 | 2.07 | 48.37 |
| { 2 2 4} | 4 | 2.00 | 50.08 |
| { 2 2 -4} | 4 | 2.13 | 46.96 |
| { 3 3 1} | 4 | 1.37 | 72.95 |
| { 3 3 -1} | 4 | 1.39 | 72.16 |
| { 4 4 2} | 4 | 1.03 | 97.53 |
| { 4 4 6} | 4 | 1.01 | 99.25 |
| { 4 4 -2} | 4 | 1.04 | 95.97 |
| { 4 4 -6} | 4 | 1.06 | 94.57 |
| { 6 6 4} | 4 | 0.68 | 146.71 |
| { 6 6 -4} | 4 | 0.70 | 143.58 |

**Group 3/Zone axis [2-10]**

|  |  |  |  |
| --- | --- | --- | --- |
| hkl | Mult | dhkl | Distance |
| { 1 2 0} | 4 | 2.96 | 33.81 |
| { 1 2 2} | 4 | 2.90 | 34.43 |
| { 1 2 -2} | 4 | 3.00 | 33.31 |
| { 2 4 2} | 4 | 1.47 | 68.21 |
| { 2 4 6} | 4 | 1.44 | 69.56 |
| { 2 4 -2} | 4 | 1.49 | 67.09 |
| { 2 4 -6} | 4 | 1.51 | 66.22 |

**Group 4/Zone axis [3-10]**

|  |  |  |  |
| --- | --- | --- | --- |
| hkl | Mult | dhkl | Distance |
| { 1 3 1} | 4 | 2.19 | 45.76 |
| { 1 3 3} | 4 | 2.16 | 46.26 |
| { 1 3 -1} | 4 | 2.21 | 45.34 |
| { 1 3 -3} | 4 | 2.22 | 45.02 |
| { 2 6 0} | 4 | 1.10 | 91.08 |
| { 2 6 4} | 4 | 1.09 | 92.00 |
| { 2 6 -4} | 4 | 1.11 | 90.34 |

**Group 5/Zone axis [0-10]**

|  |  |  |  |
| --- | --- | --- | --- |
| hkl | Mult | dhkl | Distance |
| { 2 0 0} | 2 | 2.50 | 39.93 |
| { 2 0 2} | 2 | 2.44 | 40.92 |
| { 2 0 4} | 2 | 2.38 | 42.00 |
| { 2 0 6} | 2 | 2.32 | 43.14 |
| { 2 0 -2} | 2 | 2.56 | 39.03 |
| { 2 0 -4} | 2 | 2.62 | 38.22 |
| { 2 0 -6} | 2 | 2.67 | 37.52 |
| { 4 0 2} | 2 | 1.24 | 80.84 |
| { 4 0 6} | 2 | 1.21 | 82.90 |
| { 4 0 -2} | 2 | 1.27 | 78.94 |
| { 4 0 -6} | 2 | 1.29 | 77.23 |
| { 6 0 2} | 2 | 0.83 | 120.76 |
| { 6 0 4} | 2 | 0.82 | 121.75 |
| { 6 0 -2} | 2 | 0.84 | 118.87 |
| { 6 0 -4} | 2 | 0.85 | 117.97 |

**Group 6/Zone axis [1-20]**

|  |  |  |  |
| --- | --- | --- | --- |
| hkl | Mult | dhkl | Distance |
| { 2 1 1} | 4 | 2.34 | 42.66 |
| { 2 1 3} | 4 | 2.29 | 43.64 |
| { 2 1 -1} | 4 | 2.39 | 41.76 |
| { 2 1 -3} | 4 | 2.44 | 40.96 |
| { 4 2 0} | 4 | 1.18 | 84.40 |
| { 4 2 4} | 4 | 1.16 | 86.28 |
| { 4 2 -4} | 4 | 1.21 | 82.70 |

**Group 7/Zone axis [3-20]**

|  |  |  |  |
| --- | --- | --- | --- |
| hkl | Mult | dhkl | Distance |
| { 2 3 1} | 4 | 1.74 | 57.52 |
| { 2 3 3} | 4 | 1.72 | 58.25 |
| { 2 3 -1} | 4 | 1.76 | 56.86 |
| { 2 3 -3} | 4 | 1.78 | 56.27 |
| { 4 6 0} | 4 | 0.87 | 114.36 |
| { 4 6 4} | 4 | 0.86 | 115.76 |
| { 4 6 -4} | 4 | 0.88 | 113.11 |

**Group 8/Zone axis [1-30]**

|  |  |  |  |
| --- | --- | --- | --- |
| hkl | Mult | dhkl | Distance |
| { 3 1 1} | 4 | 1.62 | 61.90 |
| { 3 1 3} | 4 | 1.59 | 62.88 |
| { 3 1 -1} | 4 | 1.64 | 60.98 |
| { 3 1 -3} | 4 | 1.66 | 60.12 |
| { 6 2 0} | 4 | 0.81 | 122.87 |
| { 6 2 4} | 4 | 0.80 | 124.77 |
| { 6 2 -4} | 4 | 0.83 | 121.08 |

**Group 9/Zone axis [2-30]**

|  |  |  |  |
| --- | --- | --- | --- |
| hkl | Mult | dhkl | Distance |
| { 3 2 0} | 4 | 1.52 | 65.82 |
| { 3 2 2} | 4 | 1.50 | 66.71 |
| { 3 2 -2} | 4 | 1.54 | 64.99 |
| { 6 4 2} | 4 | 0.75 | 132.52 |
| { 6 4 6} | 4 | 0.74 | 134.35 |
| { 6 4 -2} | 4 | 0.76 | 130.80 |
| { 6 4 -6} | 4 | 0.77 | 129.19 |

* Complete set of planes delivered by the prediction of the BFDH morphology for monoclinic methyl stearate crystals (I. More/Infineum UK, personal communication, July 25, 2014). These planes are organised innine different groups defined by zone axis analysis.

**Group 1/Zone axis [100]**

|  |  |  |  |
| --- | --- | --- | --- |
| hkl | Mult | dhkl | Distance |
| { 0 2 0} | 1 | 3.70 | 27.03 |
| { 0 2 1} | 2 | 3.69 | 27.13 |
| { 0 2 2} | 2 | 3.65 | 27.43 |
| { 0 2 3} | 2 | 3.58 | 27.92 |
| { 0 2 4} | 2 | 3.50 | 28.60 |
| { 0 2 6} | 2 | 3.28 | 30.44 |
| { 0 6 2} | 2 | 1.23 | 81.22 |
| { 0 6 4} | 2 | 1.23 | 81.62 |

**Group 2/Zone axis [-100]**

|  |  |  |  |
| --- | --- | --- | --- |
| hkl | Mult | dhkl | Distance |
| { 0 -2 0} | 1 | 3.70 | 27.03 |
| { 0 -2 1} | 2 | 3.69 | 27.13 |
| { 0 -2 2} | 2 | 3.65 | 27.43 |
| { 0 -2 3} | 2 | 3.58 | 27.92 |
| { 0 -2 4} | 2 | 3.50 | 28.60 |
| { 0 -2 6} | 2 | 3.28 | 30.44 |
| { 0 -6 2} | 2 | 1.23 | 81.22 |
| { 0 -6 4} | 2 | 1.23 | 81.62 |

**Group 3/Zone axis [1-10]**

|  |  |  |  |
| --- | --- | --- | --- |
| hkl | Mult | dhkl | Distance |
| { 1 1 -3} | 2 | 4.45 | 22.48 |
| { 1 1 -2} | 2 | 4.39 | 22.80 |
| { 1 1 -1} | 2 | 4.28 | 23.36 |
| { 1 1 0} | 2 | 4.14 | 24.13 |
| { 1 1 1} | 2 | 3.98 | 25.10 |
| { 1 1 2} | 2 | 3.81 | 26.24 |
| { 1 1 3} | 2 | 3.63 | 27.53 |
| { 2 2 -3} | 2 | 2.17 | 46.11 |
| { 2 2 -1} | 2 | 2.11 | 47.44 |
| { 2 2 1} | 2 | 2.03 | 49.18 |
| { 2 2 3} | 2 | 1.95 | 51.29 |
| { 3 3 -2} | 2 | 1.41 | 70.78 |
| { 3 3 -1} | 2 | 1.40 | 71.56 |
| { 3 3 1} | 2 | 1.36 | 73.30 |
| { 3 3 2} | 2 | 1.35 | 74.27 |

**Group 4/Zone axis [-1-10]**

|  |  |  |  |
| --- | --- | --- | --- |
| hkl | Mult | dhkl | Distance |
| { 1 -1 -3} | 2 | 4.45 | 22.48 |
| { 1 -1 -2} | 2 | 4.39 | 22.80 |
| { 1 -1 -1} | 2 | 4.28 | 23.36 |
| { 1 -1 0} | 2 | 4.14 | 24.13 |
| { 1 -1 1} | 2 | 3.98 | 25.10 |
| { 1 -1 2} | 2 | 3.81 | 26.24 |
| { 1 -1 3} | 2 | 3.63 | 27.53 |
| { 2 -2 -3} | 2 | 2.17 | 46.11 |
| { 2 -2 -1} | 2 | 2.11 | 47.44 |
| { 2 -2 1} | 2 | 2.03 | 49.18 |
| { 2 -2 3} | 2 | 1.95 | 51.29 |
| { 3 -3 -2} | 2 | 1.41 | 70.78 |
| { 3 -3 -1} | 2 | 1.40 | 71.56 |
| { 3 -3 1} | 2 | 1.36 | 73.30 |
| { 3 -3 2} | 2 | 1.35 | 74.27 |

**Group 5/Zone axis [3-10]**

|  |  |  |  |
| --- | --- | --- | --- |
| hkl | Mult | dhkl | Distance |
| { 1 3 -3} | 2 | 2.26 | 44.34 |
| { 1 3 -2} | 2 | 2.25 | 44.51 |
| { 1 3 -1} | 2 | 2.23 | 44.80 |
| { 1 3 0} | 2 | 2.21 | 45.20 |
| { 1 3 1} | 2 | 2.19 | 45.73 |
| { 1 3 2} | 2 | 2.16 | 46.36 |
| { 1 3 3} | 2 | 2.12 | 47.10 |

**Group 6/Zone axis [-3-10]**

|  |  |  |  |
| --- | --- | --- | --- |
| hkl | Mult | dhkl | Distance |
| { 1 -3 -3} | 2 | 2.26 | 44.34 |
| { 1 -3 -2} | 2 | 2.25 | 44.51 |
| { 1 -3 -1} | 2 | 2.23 | 44.80 |
| { 1 -3 0} | 2 | 2.21 | 45.20 |
| { 1 -3 1} | 2 | 2.19 | 45.73 |
| { 1 -3 2} | 2 | 2.16 | 46.36 |
| { 1 -3 3} | 2 | 2.12 | 47.10 |

**Group 7/Zone axis [0-10]**

|  |  |  |  |
| --- | --- | --- | --- |
| hkl | Mult | dhkl | Distance |
| { 2 0 -6} | 2 | 2.78 | 35.92 |
| { 2 0 -4} | 2 | 2.72 | 36.74 |
| { 2 0 -3} | 2 | 2.68 | 37.36 |
| { 2 0 -2} | 2 | 2.62 | 38.11 |
| { 2 0 -1} | 2 | 2.56 | 38.99 |
| { 2 0 0} | 2 | 2.50 | 39.99 |
| { 2 0 1} | 2 | 2.43 | 41.09 |
| { 2 0 2} | 2 | 2.36 | 42.30 |
| { 2 0 3} | 2 | 2.29 | 43.59 |
| { 2 0 4} | 2 | 2.22 | 44.98 |
| { 2 0 6} | 2 | 2.09 | 47.96 |
| { 6 0 -4} | 2 | 0.86 | 116.05 |
| { 6 0 -2} | 2 | 0.85 | 117.93 |
| { 6 0 2} | 2 | 0.82 | 122.14 |
| { 6 0 4} | 2 | 0.80 | 124.45 |

**Group 8/Zone axis [2-10]**

|  |  |  |  |
| --- | --- | --- | --- |
| hkl | Mult | dhkl | Distance |
| { 2 4 -6} | 2 | 1.54 | 64.90 |
| { 2 4 -4} | 2 | 1.53 | 65.36 |
| { 2 4 -2} | 2 | 1.51 | 66.14 |
| { 2 4 0} | 2 | 1.49 | 67.24 |
| { 2 4 2} | 2 | 1.46 | 68.64 |
| { 2 4 4} | 2 | 1.42 | 70.32 |
| { 2 4 6} | 2 | 1.38 | 72.26 |

**Group 9/Zone axis [-2-10]**

|  |  |  |  |
| --- | --- | --- | --- |
| hkl | Mult | dhkl | Distance |
| { 2 -4 -6} | 2 | 1.54 | 64.90 |
| { 2 -4 -4} | 2 | 1.53 | 65.36 |
| { 2 -4 -2} | 2 | 1.51 | 66.14 |
| { 2 -4 0} | 2 | 1.49 | 67.24 |
| { 2 -4 2} | 2 | 1.46 | 68.64 |
| { 2 -4 4} | 2 | 1.42 | 70.32 |
| { 2 -4 6} | 2 | 1.38 | 72.26 |

**Group 10/Zone axis [1-30]**

|  |  |  |  |
| --- | --- | --- | --- |
| hkl | Mult | dhkl | Distance |
| { 3 1 -3} | 2 | 1.70 | 58.74 |
| { 3 1 -2} | 2 | 1.68 | 59.58 |
| { 3 1 -1} | 2 | 1.65 | 60.49 |
| { 3 1 0} | 2 | 1.63 | 61.48 |
| { 3 1 1} | 2 | 1.60 | 62.55 |
| { 3 1 2} | 2 | 1.57 | 63.68 |
| { 3 1 3} | 2 | 1.54 | 64.87 |

**Group 11/Zone axis [-1-30]**

|  |  |  |  |
| --- | --- | --- | --- |
| hkl | Mult | dhkl | Distance |
| { 3 -1 -3} | 2 | 1.70 | 58.74 |
| { 3 -1 -2} | 2 | 1.68 | 59.58 |
| { 3 -1 -1} | 2 | 1.65 | 60.49 |
| { 3 -1 0} | 2 | 1.63 | 61.48 |
| { 3 -1 1} | 2 | 1.60 | 62.55 |
| { 3 -1 2} | 2 | 1.57 | 63.68 |
| { 3 -1 3} | 2 | 1.54 | 64.87 |

**Group 12/Zone axis [1-20]**

|  |  |  |  |
| --- | --- | --- | --- |
| hkl | Mult | dhkl | Distance |
| { 4 2 -6} | 2 | 1.26 | 79.45 |
| { 4 2 -4} | 2 | 1.24 | 80.87 |
| { 4 2 -2} | 2 | 1.21 | 82.53 |
| { 4 2 0} | 2 | 1.18 | 84.42 |
| { 4 2 2} | 2 | 1.16 | 86.51 |
| { 4 2 4} | 2 | 1.13 | 88.81 |
| { 4 2 6} | 2 | 1.10 | 91.28 |

**Group 13/Zone axis [-1-20]**

|  |  |  |  |
| --- | --- | --- | --- |
| hkl | Mult | dhkl | Distance |
| { 4 -2 -6} | 2 | 1.26 | 79.45 |
| { 4 -2 -4} | 2 | 1.24 | 80.87 |
| { 4 -2 -2} | 2 | 1.21 | 82.53 |
| { 4 -2 0} | 2 | 1.18 | 84.42 |
| { 4 -2 2} | 2 | 1.16 | 86.51 |
| { 4 -2 4} | 2 | 1.13 | 88.81 |
| { 4 -2 6} | 2 | 1.10 | 91.28 |

**Group 14/Zone axis [3-20]**

|  |  |  |  |
| --- | --- | --- | --- |
| hkl | Mult | dhkl | Distance |
| { 4 6 -6} | 2 | 0.91 | 110.26 |
| { 4 6 -4} | 2 | 0.90 | 111.28 |
| { 4 6 -2} | 2 | 0.89 | 112.50 |
| { 4 6 0} | 2 | 0.88 | 113.89 |
| { 4 6 2} | 2 | 0.87 | 115.45 |
| { 4 6 4} | 2 | 0.85 | 117.18 |
| { 4 6 6} | 2 | 0.84 | 119.06 |

**Group 15/Zone axis [-3-20]**

|  |  |  |  |
| --- | --- | --- | --- |
| hkl | Mult | dhkl | Distance |
| { 4 -6 -6} | 2 | 0.91 | 110.26 |
| { 4 -6 -4} | 2 | 0.90 | 111.28 |
| { 4 -6 -2} | 2 | 0.89 | 112.50 |
| { 4 -6 0} | 2 | 0.88 | 113.89 |
| { 4 -6 2} | 2 | 0.87 | 115.45 |
| { 4 -6 4} | 2 | 0.85 | 117.18 |
| { 4 -6 6} | 2 | 0.84 | 119.06 |

**Group 16/Zone axis [2-30]**

|  |  |  |  |
| --- | --- | --- | --- |
| hkl | Mult | dhkl | Distance |
| { 6 4 -6} | 2 | 0.79 | 126.47 |
| { 6 4 -4} | 2 | 0.78 | 128.02 |
| { 6 4 -2} | 2 | 0.77 | 129.73 |
| { 6 4 0} | 2 | 0.76 | 131.58 |
| { 6 4 2} | 2 | 0.75 | 133.56 |
| { 6 4 4} | 2 | 0.74 | 135.68 |
| { 6 4 6} | 2 | 0.73 | 137.93 |

**Group 17/Zone axis [-2-30]**

|  |  |  |  |
| --- | --- | --- | --- |
| hkl | Mult | dhkl | Distance |
| { 6 -4 -6} | 2 | 0.79 | 126.47 |
| { 6 -4 -4} | 2 | 0.78 | 128.02 |
| { 6 -4 -2} | 2 | 0.77 | 129.73 |
| { 6 -4 0} | 2 | 0.76 | 131.58 |
| { 6 -4 2} | 2 | 0.75 | 133.56 |
| { 6 -4 4} | 2 | 0.74 | 135.68 |
| { 6 -4 6} | 2 | 0.73 | 137.93 |