# Deposit Items

## Table 1 – Statistic agreement factors for all the structural refinements performed with the Jana2006 software

| | R(obs) | wR(obs) | R(all) | wR(all) |
|---|---|---|---|---|
| run1-p0 | 6.57 | 7.49 | 7.07 | 7.51 |
| run1-p1 | 6.02 | 6.51 | 7.48 | 6.59 |
| run1-p2 | 6.33 | 7.09 | 6.99 | 7.16 |
| run1-p3 | 5.67 | 6.65 | 6.07 | 6.66 |
| run1-p4 | 4.68 | 5.43 | 5.24 | 5.45 |
| run1-p5 | 4.87 | 6.16 | 5.62 | 6.2 |
| run1-p6 | 4.44 | 5.08 | 4.93 | 5.09 |
| run1-p7 | 4.73 | 5.44 | 5.06 | 5.46 |
| run1-p8 | 5.29 | 6.22 | 5.41 | 6.22 |
| run1-p9 | 4 | 5.54 | 4.33 | 5.56 |
| run1-p10 | 5.64 | 5.65 | 7.74 | 5.93 |
| run1-p11 | 6.48 | 6.84 | 8.46 | 7.05 |
| run1-p11* | 7.65 | 7.99 | 8.53 | 8.03 |
| run1-p12 | 7.22 | 8.55 | 8.21 | 8.77 |
| run1-p13 | 7.8 | 9.11 | 8.64 | 9.24 |
| run1-p14 | 8.84 | 9.96 | 9.52 | 9.99 |
| run2-p0 | 4.4 | 5.15 | 5.04 | 5.17 |
| run2-p1 | 2.56 | 3.83 | 2.86 | 3.84 |
| run2-p2 | 3.12 | 3.84 | 3.33 | 3.85 |
| run2-p3 | 3.14 | 3.37 | 3.68 | 3.44 |
| run2-p4 | 2.86 | 3.16 | 3.22 | 3.19 |
| run2-p5 | 3.62 | 4.07 | 3.91 | 4.08 |
| run2-p6 | 5.11 | 4.93 | 5.37 | 4.94 |
| run2-p7 | 3.69 | 4.07 | 4.57 | 4.09 |
| run2-p8 | 5.5 | 5.75 | 6.78 | 6.13 |
| run2-p9 | 4.32 | 4.8 | 4.71 | 4.81 |
| run2-p10 | 5.41 | 5.97 | 5.78 | 6 |
| run2-p11 | 2.77 | 3.43 | 3.04 | 3.44 |
| run2-p12 | 3.46 | 4.08 | 3.66 | 4.09 |
| run2-p13 | 4.26 | 4.85 | 4.67 | 4.87 |
| run2-p14 | 3.51 | 4.17 | 3.76 | 4.18 |
| run2-p15 | 2.79 | 3.55 | 2.95 | 3.55 |
| run2-p16 | 2.09 | 2.85 | 2.24 | 2.86 |
| run2-p17 | 3.53 | 4.34 | 3.65 | 4.34 |
| run2-p18 | 2.74 | 3.5 | 3.36 | 3.7 |
| run2-p19 | 4.58 | 5.59 | 4.73 | 5.59 |
| run2-p20 | 5.53 | 5.87 | 6.47 | 5.94 |
| run2-p21 | 5.15 | 5.04 | 7.07 | 5.33 |
| run2-p22 | 4.11 | 4.78 | 4.6 | 4.8 |
| run2-p23 | 3.51 | 4.13 | 3.92 | 4.15 |

Table 2 – Crystallographic data of $MnCO_3$-II

| P step | P (Gpa) | atom | x | y | z | Uiso (Å $^2$) |
|---|---|---|---|---|---|---|
| run1-p11 | 44.46(5) | Mn1 | 0.197(2) | 0.3078(13) | 0.7281(9) | 0.017(3) |
| | | O1 | 0.734(8) | 0.064(5) | 0.825(3) | 0.009(2) |
| | | O2 | 0.721(8) | 0.614(6) | 0.875(4) | 0.014(3) |
| | | O3 | -0.295(9) | 0.253(5) | 0.420(4) | 0.015(3) |
| | | C1 | 0.567(10) | 0.800(7) | 0.770(5) | 0.007(3) |
| run1-p11* | 46.79(5) | Mn1 | 0.199(2) | 0.3067(14) | 0.7244(10) | 0.012(5) |
| | | O1 | 0.697(13) | 0.045(8) | 0.849(5) | 0.021(4) |
| | | O2 | 0.716(9) | 0.595(6) | 0.880(4) | 0.002(2) |
| | | O3 | -0.335(11) | 0.236(7) | 0.436(4) | 0.015(4) |
| | | C1 | 0.575(15) | 0.788(10) | 0.760(6) | 0.010(4) |
| run1-p12 | 44.01(5) | Mn1 | 0.193(4) | 0.303(2) | 0.7264(12) | 0.026(5) |
| | | O1 | 0.693(17) | 0.042(10) | 0.855(6) | 0.022(4) |
| | | O2 | 0.719(9) | 0.608(5) | 0.867(4) | 0.004(3) |
| | | O3 | -0.350(12) | 0.233(6) | 0.436(5) | 0.024(4) |
| | | C1 | 0.589(18) | 0.804(10) | 0.766(8) | 0.032(6) |
| run1-p13 | 41.55(5) | Mn1 | 0.195(4) | 0.306(2) | 0.7257(13) | 0.037(6) |
| | | O1 | 0.70(2) | 0.048(12) | 0.846(8) | 0.030(6) |
| | | O2 | 0.729(9) | 0.617(5) | 0.863(4) | 0.006(3) |
| | | O3 | -0.337(11) | 0.242(6) | 0.431(4) | 0.018(3) |
| | | C1 | 0.635(15) | 0.846(9) | 0.735(7) | 0.022(5) |
| run1-p14 | 35.67(5) | Mn1 | 0.199(4) | 0.307(2) | 0.7262(14) | 0.036(6) |
| | | O1 | 0.68(2) | 0.038(12) | 0.845(8) | 0.025(5) |
| | | O2 | 0.704(11) | 0.599(7) | 0.866(5) | 0.004(3) |
| | | O3 | -0.313(18) | 0.266(10) | 0.434(6) | 0.013(4) |
| | | C1 | 0.59(3) | 0.812(18) | 0.780(12) | 0.030(8) |

Table 3 – Axial compressibility of $MnCO_3$, calculated using the cube of a and c lattice parameters

| | |
|---|---|
| $K_0a$ 227(7) GPa | $a_0^3$ 108.92(13) Å$^3$ |
| $K_0c$ 39(1) | $c_{03}$ 3948(15) Å$^3$ |

Figure 1 – f-F plot (Angel 2000) for $MnCO_3$ in the pressure range 0-40 GPa. The plot suggest that a 2nd or a 3rd (with K'<4 and close to 4) order Birch-Murnagham Equation of State is appropriate for fitting the volume data at various pressures.