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Verification of the de Wolff hypothesis concerning the symmetry of β-MnO2

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SUPPLEMENTING INFO FOR Verification of deWolff hypothesis concerning the symmetry of β-MnO_2

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Table S1a. Symmetry operations of the superspace group $P4_2/mnm(00\gamma)$ are given in the Seitz notation [1].

$P4_2/mnm(00\gamma)$				
$\{1\|0000\}$	x_1	x_2	x_3	x_4
$\{2_{[001]}\|0000\}$	$-x_1$	$-x_2$	x_3	x_4
$\{4^+_{[001]}\|\frac{1}{2}\frac{1}{2}\frac{1}{2}0\}$	$-x_2+\frac{1}{2}$	$x_1+\frac{1}{2}$	$x_3+\frac{1}{2}$	x_4
$\{4^-_{[001]}\|\frac{1}{2}\frac{1}{2}\frac{1}{2}0\}$	$x_2+\frac{1}{2}$	$-x_1+\frac{1}{2}$	$x_3+\frac{1}{2}$	x_4
$\{2_{[010]}\|\frac{1}{2}\frac{1}{2}\frac{1}{2}0\}$	$-x_1+\frac{1}{2}$	$x_2+\frac{1}{2}$	$-x_3+\frac{1}{2}$	$-x_4$
$\{2_{[100]}\|\frac{1}{2}\frac{1}{2}\frac{1}{2}0\}$	$x_1+\frac{1}{2}$	$-x_2+\frac{1}{2}$	$-x_3+\frac{1}{2}$	$-x_4$
$\{2_{[110]}\|0000\}$	x_2	x_1	$-x_3$	$-x_4$
$\{2_{[1\bar{1}0]}\|0000\}$	$-x_2$	$-x_1$	$-x_3$	$-x_4$
$\{\bar{1}\|0000\}$	$-x_1$	$-x_2$	$-x_3$	$-x_4$
$\{m_{[001]}\|0000\}$	x_1	x_2	$-x_3$	$-x_4$
$\{\bar{4}^+_{[001]}\|\frac{1}{2}\frac{1}{2}\frac{1}{2}0\}$	$x_2+\frac{1}{2}$	$-x_1+\frac{1}{2}$	$-x_3+\frac{1}{2}$	$-x_4$
$\{\bar{4}^-_{[001]}\|\frac{1}{2}\frac{1}{2}\frac{1}{2}0\}$	$-x_2+\frac{1}{2}$	$x_1+\frac{1}{2}$	$-x_3+\frac{1}{2}$	$-x_4$
$\{m_{[010]}\|\frac{1}{2}\frac{1}{2}\frac{1}{2}0\}$	$x_1+\frac{1}{2}$	$-x_2+\frac{1}{2}$	$x_3+\frac{1}{2}$	x_4
$\{m_{[100]}\|\frac{1}{2}\frac{1}{2}\frac{1}{2}0\}$	$-x_1+\frac{1}{2}$	$x_2+\frac{1}{2}$	$x_3+\frac{1}{2}$	x_4
$\{m_{[110]}\|0000\}$	$-x_2$	$-x_1$	x_3	x_4
$\{m_{[1\bar{1}0]}\|0000\}$	x_2	x_1	x_3	x_4

Table S1b. Symmetry operations of the superspace group $P4_2/mnm(00\gamma)00ss$ are given in the Seitz notation [1].

$P4_2/mnm(00\gamma)00ss$				
$\{1\|0000\}$	x_1	x_2	x_3	x_4
$\{2_{[001]}\|0000\}$	$-x_1$	$-x_2$	x_3	x_4
$\{4^+_{[001]}\|\frac{1}{2}\frac{1}{2}\frac{1}{2}0\}$	$-x_2+\frac{1}{2}$	$x_1+\frac{1}{2}$	$x_3+\frac{1}{2}$	x_4
$\{4^-_{[001]}\|\frac{1}{2}\frac{1}{2}\frac{1}{2}0\}$	$x_2+\frac{1}{2}$	$-x_1+\frac{1}{2}$	$x_3+\frac{1}{2}$	x_4
$\{2_{[010]}\|\frac{1}{2}\frac{1}{2}\frac{1}{2}\frac{1}{2}\}$	$-x_1+\frac{1}{2}$	$x_2+\frac{1}{2}$	$-x_3+\frac{1}{2}$	$-x_4+\frac{1}{2}$
$\{2_{[100]}\|\frac{1}{2}\frac{1}{2}\frac{1}{2}\frac{1}{2}\}$	$x_1+\frac{1}{2}$	$-x_2+\frac{1}{2}$	$-x_3+\frac{1}{2}$	$-x_4+\frac{1}{2}$
$\{2_{[110]}\|000\frac{1}{2}\}$	x_2	x_1	$-x_3$	$-x_4+\frac{1}{2}$
$\{2_{[1\bar{1}0]}\|000\frac{1}{2}\}$	$-x_2$	$-x_1$	$-x_3$	$-x_4+\frac{1}{2}$
$\{\bar{1}\|0000\}$	$-x_1$	$-x_2$	$-x_3$	$-x_4$
$\{m_{[001]}\|0000\}$	x_1	x_2	$-x_3$	$-x_4$
$\{\bar{4}^+_{[001]}\|\frac{1}{2}\frac{1}{2}\frac{1}{2}0\}$	$x_2+\frac{1}{2}$	$-x_1+\frac{1}{2}$	$-x_3+\frac{1}{2}$	$-x_4$
$\{\bar{4}^-_{[001]}\|\frac{1}{2}\frac{1}{2}\frac{1}{2}0\}$	$-x_2+\frac{1}{2}$	$x_1+\frac{1}{2}$	$-x_3+\frac{1}{2}$	$-x_4$
$\{m_{[010]}\|\frac{1}{2}\frac{1}{2}\frac{1}{2}\frac{1}{2}\}$	$x_1+\frac{1}{2}$	$-x_2+\frac{1}{2}$	$x_3+\frac{1}{2}$	$x_4+\frac{1}{2}$
$\{m_{[100]}\|\frac{1}{2}\frac{1}{2}\frac{1}{2}\frac{1}{2}\}$	$-x_1+\frac{1}{2}$	$x_2+\frac{1}{2}$	$x_3+\frac{1}{2}$	$x_4+\frac{1}{2}$
$\{m_{[110]}\|000\frac{1}{2}\}$	$-x_2$	$-x_1$	x_3	$x_4+\frac{1}{2}$
$\{m_{[1\bar{1}0]}\|000\frac{1}{2}\}$	x_2	x_1	x_3	$x_4+\frac{1}{2}$

Table S2. Magnetic space groups, called also as Black-and-white space groups or Shubnikov groups [4] associated with $P4_2/mnm$. The enumeration of magnetic space groups based on the OG notation [2] taken from [3] is used. The symbol (+) refers to standard 'unprimed' symmetry operations (i.e. without antisymmetry). The symbol (−) refers to 'primed' symmetry operations (including antisymmetry).

	$P4_2/mnm$ 136.1	$P4_2/m'nm$ 136.3	$P4_2'/mn'm$ 136.4	$P4_2'/mnm'$ 136.5	$P4_2'/m'n'm$ 136.6	$P4_2/mn'm'$ 136.7	$P4_2'/m'nm'$ 136.8	$P4_2/m'n'm'$ 136.9
$\{1\|0000\}$	+	+	+	+	+	+	+	+
$\{2_{[001]}\|000\}$	+	+	+	+	+	+	+	+
$\{4^+_{[001]}\|\frac{1}{2}\frac{1}{2}\frac{1}{2}\}$	+	+	−	−	−	+	−	+
$\{4^-_{[001]}\|\frac{1}{2}\frac{1}{2}\frac{1}{2}\}$	+	+	−	−	−	+	−	+
$\{2_{[010]}\|\frac{1}{2}\frac{1}{2}\frac{1}{2}\}$	+	−	−	+	+	−	−	+
$\{2_{[100]}\|\frac{1}{2}\frac{1}{2}\frac{1}{2}\}$	+	−	−	+	+	−	−	+
$\{2_{[110]}\|000\}$	+	−	+	−	−	−	+	+
$\{2_{[1\bar{1}0]}\|000\}$	+	−	+	−	−	−	+	+
$\{\bar{1}\|000\}$	+	−	+	+	−	+	−	−
$\{m_{[001]}\|000\}$	+	−	+	+	−	+	−	−
$\{\bar{4}^+_{[001]}\|\frac{1}{2}\frac{1}{2}\frac{1}{2}\}$	+	−	−	−	+	+	+	−
$\{\bar{4}^-_{[001]}\|\frac{1}{2}\frac{1}{2}\frac{1}{2}\}$	+	−	−	−	+	+	+	−
$\{m_{[010]}\|\frac{1}{2}\frac{1}{2}\frac{1}{2}\}$	+	+	−	+	−	−	+	−
$\{m_{[100]}\|\frac{1}{2}\frac{1}{2}\frac{1}{2}\}$	+	+	−	+	−	−	+	−
$\{m_{[110]}\|000\}$	+	+	+	−	+	−	−	−
$\{m_{[1\bar{1}0]}\|000\frac{1}{2}\}$	+	+	+	−	+	−	−	−

Table S3a. Magnetic superspace group $P4_2/mnm.1'(00\gamma)00sss$. For Mn ions in position (2a) this superspace group describes a ferromagnetic type longitudinal spin-density-wave along [001] as explained below the Table. Please note that the shifts of x_4 by 1/2 occur at operations which are primed in the Shubnikov group $P4_2/mn'm'$ (No. 136.7), see Table S2.

$P4_2/mnm.1'(00\gamma)00sss$					
$\{1\|0000\}$	x_1	x_2	x_3	x_4	m
$\{2_{[001]}\|0000\}$	$-x_1$	$-x_2$	x_3	x_4	m
$\{4^+_{[001]}\|\frac{1}{2}\frac{1}{2}\frac{1}{2}0\}$	$-x_2+\frac{1}{2}$	$x_1+\frac{1}{2}$	$x_3+\frac{1}{2}$	x_4	m
$\{4^-_{[001]}\|\frac{1}{2}\frac{1}{2}\frac{1}{2}0\}$	$x_2+\frac{1}{2}$	$-x_1+\frac{1}{2}$	$x_3+\frac{1}{2}$	x_4	m
$\{2_{[010]}\|\frac{1}{2}\frac{1}{2}\frac{1}{2}\frac{1}{2}\}$	$-x_1+\frac{1}{2}$	$x_2+\frac{1}{2}$	$-x_3+\frac{1}{2}$	$-x_4+\frac{1}{2}$	m
$\{2_{[100]}\|\frac{1}{2}\frac{1}{2}\frac{1}{2}\frac{1}{2}\}$	$x_1+\frac{1}{2}$	$-x_2+\frac{1}{2}$	$-x_3+\frac{1}{2}$	$-x_4+\frac{1}{2}$	m
$\{2_{[110]}\|000\frac{1}{2}\}$	x_2	x_1	$-x_3$	$-x_4+\frac{1}{2}$	m
$\{2_{[1\bar{1}0]}\|000\frac{1}{2}\}$	$-x_2$	$-x_1$	$-x_3$	$-x_4+\frac{1}{2}$	m
$\{\bar{1}\|0000\}$	$-x_1$	$-x_2$	$-x_3$	$-x_4$	m
$\{m_{[001]}\|0000\}$	x_1	x_2	$-x_3$	$-x_4$	m
$\{\bar{4}^+_{[001]}\|\frac{1}{2}\frac{1}{2}\frac{1}{2}0\}$	$x_2+\frac{1}{2}$	$-x_1+\frac{1}{2}$	$-x_3+\frac{1}{2}$	$-x_4$	m
$\{\bar{4}^-_{[001]}\|\frac{1}{2}\frac{1}{2}\frac{1}{2}0\}$	$-x_2+\frac{1}{2}$	$x_1+\frac{1}{2}$	$-x_3+\frac{1}{2}$	$-x_4$	m
$\{m_{[010]}\|\frac{1}{2}\frac{1}{2}\frac{1}{2}\frac{1}{2}\}$	$x_1+\frac{1}{2}$	$-x_2+\frac{1}{2}$	$x_3+\frac{1}{2}$	$x_4+\frac{1}{2}$	m
$\{m_{[100]}\|\frac{1}{2}\frac{1}{2}\frac{1}{2}\frac{1}{2}\}$	$-x_1+\frac{1}{2}$	$x_2+\frac{1}{2}$	$x_3+\frac{1}{2}$	$x_4+\frac{1}{2}$	m
$\{m_{[110]}\|000\frac{1}{2}\}$	$-x_2$	$-x_1$	x_3	$x_4+\frac{1}{2}$	m
$\{m_{[1\bar{1}0]}\|000\frac{1}{2}\}$	x_2	x_1	x_3	$x_4+\frac{1}{2}$	m
$\ldots \times \{1'\|000\frac{1}{2}\}$					

For ions in sublattice 1: $(0,0,0)$ $\quad M = [0, 0, M_0 \cos(2\pi x_4)]$

For ions in sublattice 2: $(\frac{1}{2}, \frac{1}{2}, \frac{1}{2})$ $\quad M = [0, 0, M_0 \cos(2\pi x_4)]$

Table S3b. Magnetic superspace group $P4_2/mnm.1'(00\gamma)s00ss$. For Mn ions in position (2a) this superspace group describes an antiferromagnetic type longitudinal spin-density-wave along [001] as explained below the Table. Please note that the shifts of x_4 by 1/2 occur at operations which are primed in the Shubnikov group $P4_2'/mnm'$ (No. 136.5), see Table S2.

$P4_2/mnm.1'(00\gamma)s00ss$					
$\{1\|0000\}$	x_1	x_2	x_3	x_4	m
$\{2_{[001]}\|0000\}$	$-x_1$	$-x_2$	x_3	x_4	m
$\{4^+_{[001]}\|\frac{1}{2}\frac{1}{2}\frac{1}{2}\frac{1}{2}\}$	$-x_2+\frac{1}{2}$	$x_1+\frac{1}{2}$	$x_3+\frac{1}{2}$	$x_4+\frac{1}{2}$	m
$\{4^-_{[001]}\|\frac{1}{2}\frac{1}{2}\frac{1}{2}\frac{1}{2}\}$	$x_2+\frac{1}{2}$	$-x_1+\frac{1}{2}$	$x_3+\frac{1}{2}$	$x_4+\frac{1}{2}$	m
$\{2_{[010]}\|\frac{1}{2}\frac{1}{2}\frac{1}{2}0\}$	$-x_1+\frac{1}{2}$	$x_2+\frac{1}{2}$	$-x_3+\frac{1}{2}$	$-x_4$	m
$\{2_{[100]}\|\frac{1}{2}\frac{1}{2}\frac{1}{2}0\}$	$x_1+\frac{1}{2}$	$-x_2+\frac{1}{2}$	$-x_3+\frac{1}{2}$	$-x_4$	m
$\{2_{[110]}\|000\frac{1}{2}\}$	x_2	x_1	$-x_3$	$-x_4+\frac{1}{2}$	m
$\{2_{[1\bar{1}0]}\|000\frac{1}{2}\}$	$-x_2$	$-x_1$	$-x_3$	$-x_4+\frac{1}{2}$	m
$\{\bar{1}\|0000\}$	$-x_1$	$-x_2$	$-x_3$	$-x_4$	m
$\{m_{[001]}\|000\}$	x_1	x_2	$-x_3$	$-x_4$	m
$\{\bar{4}^+_{[001]}\|\frac{1}{2}\frac{1}{2}\frac{1}{2}\frac{1}{2}\}$	$x_2+\frac{1}{2}$	$-x_1+\frac{1}{2}$	$-x_3+\frac{1}{2}$	$-x_4+\frac{1}{2}$	m
$\{\bar{4}^-_{[001]}\|\frac{1}{2}\frac{1}{2}\frac{1}{2}\frac{1}{2}\}$	$-x_2+\frac{1}{2}$	$x_1+\frac{1}{2}$	$-x_3+\frac{1}{2}$	$-x_4+\frac{1}{2}$	m
$\{m_{[010]}\|\frac{1}{2}\frac{1}{2}\frac{1}{2}0\}$	$x_1+\frac{1}{2}$	$-x_2+\frac{1}{2}$	$x_3+\frac{1}{2}$	x_4	m
$\{m_{[100]}\|\frac{1}{2}\frac{1}{2}\frac{1}{2}0\}$	$-x_1+\frac{1}{2}$	$x_2+\frac{1}{2}$	$x_3+\frac{1}{2}$	x_4	m
$\{m_{[110]}\|000\frac{1}{2}\}$	$-x_2$	$-x_1$	x_3	$x_4+\frac{1}{2}$	m
$\{m_{[1\bar{1}0]}\|000\frac{1}{2}\}$	x_2	x_1	x_3	$x_4+\frac{1}{2}$	m
$\ldots\times\{1'\|000\frac{1}{2}\}$					

For ions in sublattice 1: $(0,0,0)$ $\quad M=[0,0,M_0\cos(2\pi x_4)]$

For ions in sublattice 2: $(\frac{1}{2},\frac{1}{2},\frac{1}{2})$ $\quad M=[0,0,-M_0\cos(2\pi x_4)]$

Table S3c. Magnetic superspace group $P4_2/mnm.1'(00\gamma)0000s$. For Mn ions at position (2a) all magnetic moment amplitudes are zero by symmetry. Please note that there are no shifts of x_4 by 1/2 as there is no primed operations in the group $P4_2/mnm$ (No. 136.1), see Table S2.

$P4_2/mnm.1'(00\gamma)0000s$					
$\{1\|0000\}$	x_1	x_2	x_3	x_4	m
$\{2_{[001]}\|0000\}$	$-x_1$	$-x_2$	x_3	x_4	m
$\{4^+_{[001]}\|\frac{1}{2}\frac{1}{2}\frac{1}{2}0\}$	$-x_2+\frac{1}{2}$	$x_1+\frac{1}{2}$	$x_3+\frac{1}{2}$	x_4	m
$\{4^-_{[001]}\|\frac{1}{2}\frac{1}{2}\frac{1}{2}0\}$	$x_2+\frac{1}{2}$	$-x_1+\frac{1}{2}$	$x_3+\frac{1}{2}$	x_4	m
$\{2_{[010]}\|\frac{1}{2}\frac{1}{2}\frac{1}{2}0\}$	$-x_1+\frac{1}{2}$	$x_2+\frac{1}{2}$	$-x_3+\frac{1}{2}$	$-x_4$	m
$\{2_{[100]}\|\frac{1}{2}\frac{1}{2}\frac{1}{2}0\}$	$x_1+\frac{1}{2}$	$-x_2+\frac{1}{2}$	$-x_3+\frac{1}{2}$	$-x_4$	m
$\{2_{[110]}\|0000\}$	x_2	x_1	$-x_3$	$-x_4$	m
$\{2_{[1\bar{1}0]}\|0000\}$	$-x_2$	$-x_1$	$-x_3$	$-x_4$	m
$\{\bar{1}\|0000\}$	$-x_1$	$-x_2$	$-x_3$	$-x_4$	m
$\{m_{[001]}\|0000\}$	x_1	x_2	$-x_3$	$-x_4$	m
$\{\bar{4}^+_{[001]}\|\frac{1}{2}\frac{1}{2}\frac{1}{2}0\}$	$x_2+\frac{1}{2}$	$-x_1+\frac{1}{2}$	$-x_3+\frac{1}{2}$	$-x_4$	m
$\{\bar{4}^-_{[001]}\|\frac{1}{2}\frac{1}{2}\frac{1}{2}0\}$	$-x_2+\frac{1}{2}$	$x_1+\frac{1}{2}$	$-x_3+\frac{1}{2}$	$-x_4$	m
$\{m_{[010]}\|\frac{1}{2}\frac{1}{2}\frac{1}{2}0\}$	$x_1+\frac{1}{2}$	$-x_2+\frac{1}{2}$	$x_3+\frac{1}{2}$	x_4	m
$\{m_{[100]}\|\frac{1}{2}\frac{1}{2}\frac{1}{2}0\}$	$-x_1+\frac{1}{2}$	$x_2+\frac{1}{2}$	$x_3+\frac{1}{2}$	x_4	m
$\{m_{[110]}\|000\frac{1}{2}0\}$	$-x_2$	$-x_1$	x_3	x_4	m
$\{m_{[110]}\|000\frac{1}{2}0\}$	x_2	x_1	x_3	x_4	m
$\ldots \times \{1'\|000\frac{1}{2}\}$					

Table S3d. Magnetic superspace group $P4_2/mnm.1'(00\gamma)s0s0s$. For Mn ions at position (2a) all magnetic moment amplitudes are zero by symmetry. Please note that the shifts of x_4 by 1/2 occur at operations which are primed in the Shubnikov group $P4_2'/mn'm'$ (No. 136.4), see Table S2.

$P4_2/mnm.1'(00\gamma)s0s0s$					
$\{1\|0000\}$	x_1	x_2	x_3	x_4	m
$\{2_{[001]}\|0000\}$	$-x_1$	$-x_2$	x_3	x_4	m
$\{4^+_{[001]}\|\frac{1}{2}\frac{1}{2}\frac{1}{2}\}$	$-x_2+\frac{1}{2}$	$x_1+\frac{1}{2}$	$x_3+\frac{1}{2}$	$x_4+\frac{1}{2}$	m
$\{4^-_{[001]}\|\frac{1}{2}\frac{1}{2}\frac{1}{2}\}$	$x_2+\frac{1}{2}$	$-x_1+\frac{1}{2}$	$x_3+\frac{1}{2}$	$x_4+\frac{1}{2}$	m
$\{2_{[010]}\|\frac{1}{2}\frac{1}{2}\frac{1}{2}\frac{1}{2}\}$	$-x_1+\frac{1}{2}$	$x_2+\frac{1}{2}$	$-x_3+\frac{1}{2}$	$-x_4+\frac{1}{2}$	m
$\{2_{[100]}\|\frac{1}{2}\frac{1}{2}\frac{1}{2}\frac{1}{2}\}$	$x_1+\frac{1}{2}$	$-x_2+\frac{1}{2}$	$-x_3+\frac{1}{2}$	$-x_4+\frac{1}{2}$	m
$\{2_{[110]}\|0000\}$	x_2	x_1	$-x_3$	$-x_4$	m
$\{2_{[1\bar{1}0]}\|0000\}$	$-x_2$	$-x_1$	$-x_3$	$-x_4$	m
$\{\bar{1}\|0000\}$	$-x_1$	$-x_2$	$-x_3$	$-x_4$	m
$\{m_{[001]}\|0000\}$	x_1	x_2	$-x_3$	$-x_4$	m
$\{\bar{4}^+_{[001]}\|\frac{1}{2}\frac{1}{2}\frac{1}{2}\frac{1}{2}\}$	$x_2+\frac{1}{2}$	$-x_1+\frac{1}{2}$	$-x_3+\frac{1}{2}$	$-x_4+\frac{1}{2}$	m
$\{\bar{4}^-_{[001]}\|\frac{1}{2}\frac{1}{2}\frac{1}{2}\frac{1}{2}\}$	$-x_2+\frac{1}{2}$	$x_1+\frac{1}{2}$	$-x_3+\frac{1}{2}$	$-x_4+\frac{1}{2}$	m
$\{m_{[010]}\|\frac{1}{2}\frac{1}{2}\frac{1}{2}\frac{1}{2}\}$	$x_1+\frac{1}{2}$	$-x_2+\frac{1}{2}$	$x_3+\frac{1}{2}$	$x_4+\frac{1}{2}$	m
$\{m_{[100]}\|\frac{1}{2}\frac{1}{2}\frac{1}{2}\frac{1}{2}\}$	$-x_1+\frac{1}{2}$	$x_2+\frac{1}{2}$	$x_3+\frac{1}{2}$	$x_4+\frac{1}{2}$	m
$\{m_{[110]}\|0000\}$	$-x_2$	$-x_1$	x_3	x_4	m
$\{m_{[1\bar{1}0]}\|0000\}$	x_2	x_1	x_3	x_4	m
$\ldots \times \{1'\|000\frac{1}{2}\}$					

Table S4a. Superspace group $Pnnm(00\gamma)$.

$Pnnm(00\gamma)$				
$\{1\|0000\}$	x_1	x_2	x_3	x_4
$\{2_{001}\|0000\}$	$-x_1$	$-x_2$	x_3	x_4
$\{2_{010}\|\frac{1}{2}\frac{1}{2}\frac{1}{2}0\}$	$-x_1+\frac{1}{2}$	$x_2+\frac{1}{2}$	$-x_3+\frac{1}{2}$	$-x_4$
$\{2_{100}\|\frac{1}{2}\frac{1}{2}\frac{1}{2}0\}$	$x_1+\frac{1}{2}$	$-x_2+\frac{1}{2}$	$-x_3+\frac{1}{2}$	$-x_4$
$\{\bar{1}\|0000\}$	$-x_1$	$-x_2$	$-x_3$	$-x_4$
$\{m_{001}\|0000\}$	x_1	x_2	$-x_3$	$-x_4$
$\{m_{010}\|\frac{1}{2}\frac{1}{2}\frac{1}{2}0\}$	$x_1+\frac{1}{2}$	$-x_2+\frac{1}{2}$	$x_3+\frac{1}{2}$	x_4
$\{m_{001}\|\frac{1}{2}\frac{1}{2}\frac{1}{2}0\}$	$-x_1+\frac{1}{2}$	$x_2+\frac{1}{2}$	$x_3+\frac{1}{2}$	x_4

Table S4b. Superspace group $Pnnm(00\gamma)s00$.

$Pnnm'(00\gamma)s0$				
$\{1\|0000\}$	x_1	x_2	x_3	x_4
$\{2_{001}\|000\frac{1}{2}\}$	$-x_1$	$-x_2$	x_3	$x_4+\frac{1}{2}$
$\{2_{010}\|\frac{1}{2}\frac{1}{2}\frac{1}{2}0\}$	$-x_1+\frac{1}{2}$	$x_2+\frac{1}{2}$	$-x_3+\frac{1}{2}$	$-x_4$
$\{2_{100}\|\frac{1}{2}\frac{1}{2}\frac{1}{2}\frac{1}{2}\}$	$x_1+\frac{1}{2}$	$-x_2+\frac{1}{2}$	$-x_3+\frac{1}{2}$	$-x_4+\frac{1}{2}$
$\{\bar{1}\|0000\}$	$-x_1$	$-x_2$	$-x_3$	$-x_4$
$\{m_{001}\|000\frac{1}{2}\}$	x_1	x_2	$-x_3$	$-x_4+\frac{1}{2}$
$\{m_{010}\|\frac{1}{2}\frac{1}{2}\frac{1}{2}0\}$	$x_1+\frac{1}{2}$	$-x_2+\frac{1}{2}$	$x_3+\frac{1}{2}$	x_4
$\{m_{100}\|\frac{1}{2}\frac{1}{2}\frac{1}{2}\frac{1}{2}\}$	$-x_1+\frac{1}{2}$	$x_2+\frac{1}{2}$	$x_3+\frac{1}{2}$	$x_4+\frac{1}{2}$

Table S5a. Magnetic superspace group $Pnnm.1'(00\gamma)000s$.

$Pnnm.1'(00\gamma)000s$					
$\{1\|0000\}$	x_1	x_2	x_3	x_4	m
$\{2_{001}\|0000\}$	$-x_1$	$-x_2$	x_3	x_4	m
$\{2_{010}\|\frac{1}{2}\frac{1}{2}\frac{1}{2}0\}$	$-x_1+\frac{1}{2}$	$x_2+\frac{1}{2}$	$-x_3+\frac{1}{2}$	$-x_4$	m
$\{2_{100}\|\frac{1}{2}\frac{1}{2}\frac{1}{2}0\}$	$x_1+\frac{1}{2}$	$-x_2+\frac{1}{2}$	$-x_3+\frac{1}{2}$	$-x_4$	m
$\{\bar{1}\|0000\}$	$-x_1$	$-x_2$	$-x_3$	$-x_4$	m
$\{m_{001}\|0000\}$	x_1	x_2	$-x_3$	$-x_4$	m
$\{m_{010}\|\frac{1}{2}\frac{1}{2}\frac{1}{2}0\}$	$x_1+\frac{1}{2}$	$-x_2+\frac{1}{2}$	$x_3+\frac{1}{2}$	x_4	m
$\{m_{001}\|\frac{1}{2}\frac{1}{2}\frac{1}{2}0\}$	$-x_1+\frac{1}{2}$	$x_2+\frac{1}{2}$	$x_3+\frac{1}{2}$	x_4	m
$\{1'\|000\frac{1}{2}\}$	x_1	x_2	x_3	$x_4+\frac{1}{2}$	$-m$
$\{2'_{001}\|000\frac{1}{2}\}$	$-x_1$	$-x_2$	x_3	$x_4+\frac{1}{2}$	$-m$
$\{2'_{010}\|\frac{1}{2}\frac{1}{2}\frac{1}{2}\frac{1}{2}\}$	$-x_1+\frac{1}{2}$	$x_2+\frac{1}{2}$	$-x_3+\frac{1}{2}$	$-x_4+\frac{1}{2}$	$-m$
$\{2'_{100}\|\frac{1}{2}\frac{1}{2}\frac{1}{2}\frac{1}{2}\}$	$x_1+\frac{1}{2}$	$-x_2+\frac{1}{2}$	$-x_3+\frac{1}{2}$	$-x_4+\frac{1}{2}$	$-m$
$\{\bar{1}'\|000\frac{1}{2}\}$	$-x_1$	$-x_2$	$-x_3$	$-x_4+\frac{1}{2}$	$-m$
$\{m'_{001}\|000\frac{1}{2}\}$	x_1	x_2	$-x_3$	$-x_4+\frac{1}{2}$	$-m$
$\{m'_{010}\|\frac{1}{2}\frac{1}{2}\frac{1}{2}\frac{1}{2}\}$	$x_1+\frac{1}{2}$	$-x_2+\frac{1}{2}$	$x_3+\frac{1}{2}$	$x_4+\frac{1}{2}$	$-m$
$\{m'_{100}\|\frac{1}{2}\frac{1}{2}\frac{1}{2}\frac{1}{2}\}$	$-x_1+\frac{1}{2}$	$x_2+\frac{1}{2}$	$x_3+\frac{1}{2}$	$x_4+\frac{1}{2}$	$-m$

Antiferromagnetic longitudinal spin density wave along [001]

For ions in sublattice 1: $(0,0,0)$ $(0,0,m^0_{001}cos(2\pi x_4))$

For ions in sublattice 2: $(\frac{1}{2},\frac{1}{2},\frac{1}{2})$ $(0,0,-m^0_{001}cos(2\pi x_4))$

Table S5b. Magnetic superspace group $Pnnm.1'(00\gamma)ss0s$.

$Pnnm.1'(00\gamma)ss0s$					
$\{1\|0000\}$	x_1	x_2	x_3	x_4	m
$\{2_{001}\|0000\}$	$-x_1$	$-x_2$	x_3	x_4	m
$\{2_{010}\|\frac{1}{2}\frac{1}{2}\frac{1}{2}\frac{1}{2}\}$	$-x_1+\frac{1}{2}$	$x_2+\frac{1}{2}$	$-x_3+\frac{1}{2}$	$-x_4+\frac{1}{2}$	m
$\{2_{100}\|\frac{1}{2}\frac{1}{2}\frac{1}{2}\frac{1}{2}\}$	$x_1+\frac{1}{2}$	$-x_2+\frac{1}{2}$	$-x_3+\frac{1}{2}$	$-x_4+\frac{1}{2}$	m
$\{\bar{1}\|0000\}$	$-x_1$	$-x_2$	$-x_3$	$-x_4$	m
$\{m_{001}\|0000\}$	x_1	x_2	$-x_3$	$-x_4$	m
$\{m_{010}\|\frac{1}{2}\frac{1}{2}\frac{1}{2}\frac{1}{2}\}$	$x_1+\frac{1}{2}$	$-x_2+\frac{1}{2}$	$x_3+\frac{1}{2}$	$x_4+\frac{1}{2}$	m
$\{m_{100}\|\frac{1}{2}\frac{1}{2}\frac{1}{2}\frac{1}{2}\}$	$-x_1+\frac{1}{2}$	$x_2+\frac{1}{2}$	$x_3+\frac{1}{2}$	$x_4+\frac{1}{2}$	m
$\{1'\|000\frac{1}{2}\}$	x_1	x_2	x_3	$x_4+\frac{1}{2}$	$-m$
$\{2'_{001}\|000\frac{1}{2}\}$	$-x_1$	$-x_2$	x_3	$x_4+\frac{1}{2}$	$-m$
$\{2'_{010}\|\frac{1}{2}\frac{1}{2}\frac{1}{2}0\}$	$-x_1+\frac{1}{2}$	$x_2+\frac{1}{2}$	$-x_3+\frac{1}{2}$	$-x_4$	$-m$
$\{2'_{100}\|\frac{1}{2}\frac{1}{2}\frac{1}{2}0\}$	$x_1+\frac{1}{2}$	$-x_2+\frac{1}{2}$	$-x_3+\frac{1}{2}$	$-x_4$	$-m$
$\{\bar{1}'\|000\frac{1}{2}\}$	$-x_1$	$-x_2$	$-x_3$	$-x_4+\frac{1}{2}$	$-m$
$\{m'_{001}\|000\frac{1}{2}\}$	x_1	x_2	$-x_3$	$-x_4+\frac{1}{2}$	$-m$
$\{m'_{010}\|\frac{1}{2}\frac{1}{2}\frac{1}{2}0\}$	$x_1+\frac{1}{2}$	$-x_2+\frac{1}{2}$	$x_3+\frac{1}{2}$	x_4	$-m$
$\{m'_{100}\|\frac{1}{2}\frac{1}{2}\frac{1}{2}0\}$	$-x_1+\frac{1}{2}$	$x_2+\frac{1}{2}$	$x_3+\frac{1}{2}$	x_4	$-m$

Ferromagnetic longitudinal spin density wave along [001]

For ions in sublattice 1: $(0,0,0)$ $(0,0,m^0_{001}cos(2\pi x_4))$

For ions in sublattice 2: $(\frac{1}{2},\frac{1}{2},\frac{1}{2})$ $(0,0,m^0_{001}cos(2\pi x_4))$

Table S5c. Magnetic superspace group $Pnnm.1'(00\gamma)s00s$.

$Pnnm.1'(00\gamma)s00s$					
$\{1\|0000\}$	x_1	x_2	x_3	x_4	m
$\{2_{001}\|000\frac{1}{2}\}$	$-x_1$	$-x_2$	x_3	$x_4+\frac{1}{2}$	m
$\{2_{010}\|\frac{1}{2}\frac{1}{2}\frac{1}{2}0\}$	$-x_1+\frac{1}{2}$	$x_2+\frac{1}{2}$	$-x_3+\frac{1}{2}$	$-x_4$	m
$\{2_{100}\|\frac{1}{2}\frac{1}{2}\frac{1}{2}\frac{1}{2}\}$	$x_1+\frac{1}{2}$	$-x_2+\frac{1}{2}$	$-x_3+\frac{1}{2}$	$-x_4+\frac{1}{2}$	m
$\{\bar{1}\|0000\}$	$-x_1$	$-x_2$	$-x_3$	$-x_4$	m
$\{m_{001}\|000\frac{1}{2}\}$	x_1	x_2	$-x_3$	$-x_4+\frac{1}{2}$	m
$\{m_{010}\|\frac{1}{2}\frac{1}{2}\frac{1}{2}0\}$	$x_1+\frac{1}{2}$	$-x_2+\frac{1}{2}$	$x_3+\frac{1}{2}$	x_4	m
$\{m_{100}\|\frac{1}{2}\frac{1}{2}\frac{1}{2}\frac{1}{2}\}$	$-x_1+\frac{1}{2}$	$x_2+\frac{1}{2}$	$x_3+\frac{1}{2}$	$x_4+\frac{1}{2}$	m
$\{1'\|000\frac{1}{2}\}$	x_1	x_2	x_3	$x_4+\frac{1}{2}$	$-m$
$\{2'_{001}\|0000\}$	$-x_1$	$-x_2$	x_3	x_4	$-m$
$\{2'_{010}\|\frac{1}{2}\frac{1}{2}\frac{1}{2}\frac{1}{2}\}$	$-x_1+\frac{1}{2}$	$x_2+\frac{1}{2}$	$-x_3+\frac{1}{2}$	$-x_4+\frac{1}{2}$	$-m$
$\{2'_{100}\|\frac{1}{2}\frac{1}{2}\frac{1}{2}0\}$	$x_1+\frac{1}{2}$	$-x_2+\frac{1}{2}$	$-x_3+\frac{1}{2}$	$-x_4$	$-m$
$\{\bar{1}'\|000\frac{1}{2}\}$	$-x_1$	$-x_2$	$-x_3$	$-x_4+\frac{1}{2}$	$-m$
$\{m'_{001}\|0000\}$	x_1	x_2	$-x_3$	$-x_4$	$-m$
$\{m'_{010}\|\frac{1}{2}\frac{1}{2}\frac{1}{2}\frac{1}{2}\}$	$x_1+\frac{1}{2}$	$-x_2+\frac{1}{2}$	$x_3+\frac{1}{2}$	$x_4+\frac{1}{2}$	$-m$
$\{m'_{100}\|\frac{1}{2}\frac{1}{2}\frac{1}{2}0\}$	$-x_1+\frac{1}{2}$	$x_2+\frac{1}{2}$	$x_3+\frac{1}{2}$	x_4	$-m$

Antiferromagnetic transverse spin density wave along [100] and ferromagnetic transverse spin density wave along [010]

For ions in sublattice 1: $(0,0,0)$ $(m^0_{100}cos(2\pi x_4), m^0_{010}cos(2\pi x_4), 0)$

For ions in sublattice 2: $(\frac{1}{2},\frac{1}{2},\frac{1}{2})$ $(-m^0_{100}cos(2\pi x_4), m^0_{010}cos(2\pi x_4), 0)$

Table S5d. Magnetic superspace group $Pnnm.1'(00\gamma)0s0s$.

$Pnnm.1'(00\gamma)0s0s$					
$\{1\|0000\}$	x_1	x_2	x_3	x_4	m
$\{2_{001}\|000\frac{1}{2}\}$	$-x_1$	$-x_2$	x_3	$x_4+\frac{1}{2}$	m
$\{2_{010}\|\frac{1}{2}\frac{1}{2}\frac{1}{2}\frac{1}{2}\}$	$-x_1+\frac{1}{2}$	$x_2+\frac{1}{2}$	$-x_3+\frac{1}{2}$	$-x_4+\frac{1}{2}$	m
$\{2_{100}\|\frac{1}{2}\frac{1}{2}\frac{1}{2}0\}$	$x_1+\frac{1}{2}$	$-x_2+\frac{1}{2}$	$-x_3+\frac{1}{2}$	$-x_4$	m
$\{\bar{1}\|0000\}$	$-x_1$	$-x_2$	$-x_3$	$-x_4$	m
$\{m_{001}\|000\frac{1}{2}\}$	x_1	x_2	$-x_3$	$-x_4+\frac{1}{2}$	m
$\{m_{010}\|\frac{1}{2}\frac{1}{2}\frac{1}{2}\frac{1}{2}\}$	$x_1+\frac{1}{2}$	$-x_2+\frac{1}{2}$	$x_3+\frac{1}{2}$	$x_4+\frac{1}{2}$	m
$\{m_{100}\|\frac{1}{2}\frac{1}{2}\frac{1}{2}0\}$	$-x_1+\frac{1}{2}$	$x_2+\frac{1}{2}$	$x_3+\frac{1}{2}$	x_4	m
$\{1'\|000\frac{1}{2}\}$	x_1	x_2	x_3	$x_4+\frac{1}{2}$	$-m$
$\{2'_{001}\|0000\}$	$-x_1$	$-x_2$	x_3	x_4	$-m$
$\{2'_{010}\|\frac{1}{2}\frac{1}{2}\frac{1}{2}0\}$	$-x_1+\frac{1}{2}$	$x_2+\frac{1}{2}$	$-x_3+\frac{1}{2}$	$-x_4$	$-m$
$\{2'_{100}\|\frac{1}{2}\frac{1}{2}\frac{1}{2}\frac{1}{2}\}$	$x_1+\frac{1}{2}$	$-x_2+\frac{1}{2}$	$-x_3+\frac{1}{2}$	$-x_4+\frac{1}{2}$	$-m$
$\{\bar{1}'\|000\frac{1}{2}\}$	$-x_1$	$-x_2$	$-x_3$	$-x_4+\frac{1}{2}$	$-m$
$\{m'_{001}\|0000\}$	x_1	x_2	$-x_3$	$-x_4$	$-m$
$\{m'_{010}\|\frac{1}{2}\frac{1}{2}\frac{1}{2}0\}$	$x_1+\frac{1}{2}$	$-x_2+\frac{1}{2}$	$x_3+\frac{1}{2}$	x_4	$-m$
$\{m'_{100}\|\frac{1}{2}\frac{1}{2}\frac{1}{2}\frac{1}{2}\}$	$-x_1+\frac{1}{2}$	$x_2+\frac{1}{2}$	$x_3+\frac{1}{2}$	$x_4+\frac{1}{2}$	$-m$

Ferromagnetic transverse spin density wave along [100] and antiferromagnetic transverse spin density wave along [010]

For ions in sublattice 1: $(0,0,0)(m^0_{100}cos(2\pi x_4), m^0_{010}cos(2\pi x_4), 0)$

For ions in sublattice 2: $(\frac{1}{2},\frac{1}{2},\frac{1}{2})(m^0_{100}cos(2\pi x_4), -m^0_{010}cos(2\pi x_4), 0)$

References

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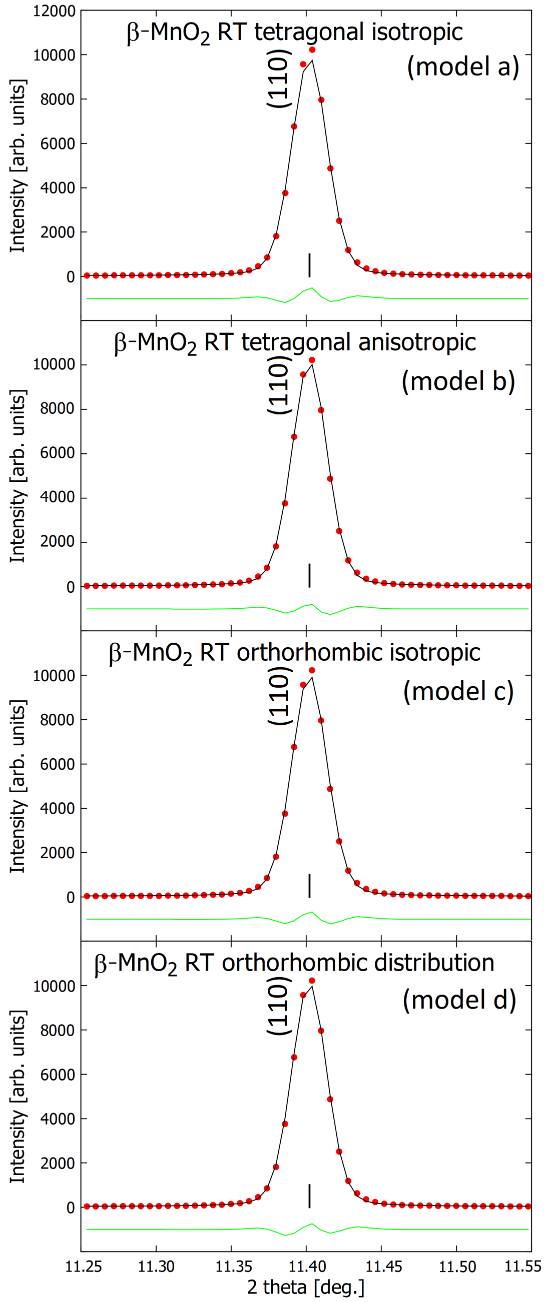

Figure 1: [Fig. S1] Selected region of the SR powder diffraction data of β-MnO_2 at RT near the position of (110) Bragg peak. Solid symbols denote the same experimental data in panels (a-d). The solid line represent the refined pattern obtained with the tetragonal phase with isotropic broadening (model a), tetragonal phase with anisotropic broadening (model b), orthorhombic phase with isotropic broadening (model c) and a gaussian distribution of orthorhmobic phases (model d), see text. The solid lines below the plots show the difference between experimental and refined data (shifted down for clarity). Vertical ticks denote the position of Bragg peaks in each structural model.

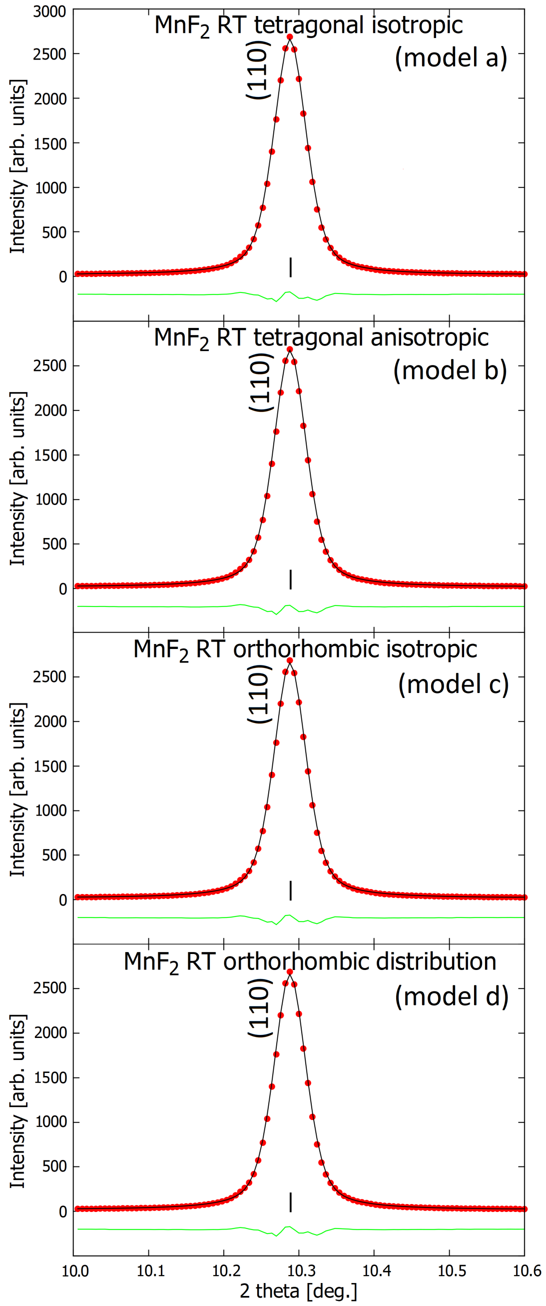

Figure 2: [Fig. S2] Selected region of the SR powder diffraction data of MnF_2 at RT near the position of (110) Bragg peak. Solid symbols denote the same experimental data in panels (a-d). The solid line represent the refined pattern obtained with the tetragonal phase with isotropic broadening (model a), tetragonal phase with anisotropic broadening (model b), orthorhombic phase with isotropic broadening (model c) and a gaussian distribution of orthorhmobic phases (model d), see text. The solid lines below the plots show the difference between experimental and refined data (shifted down for clarity). Vertical ticks denote the position of Bragg peaks in each structural model.

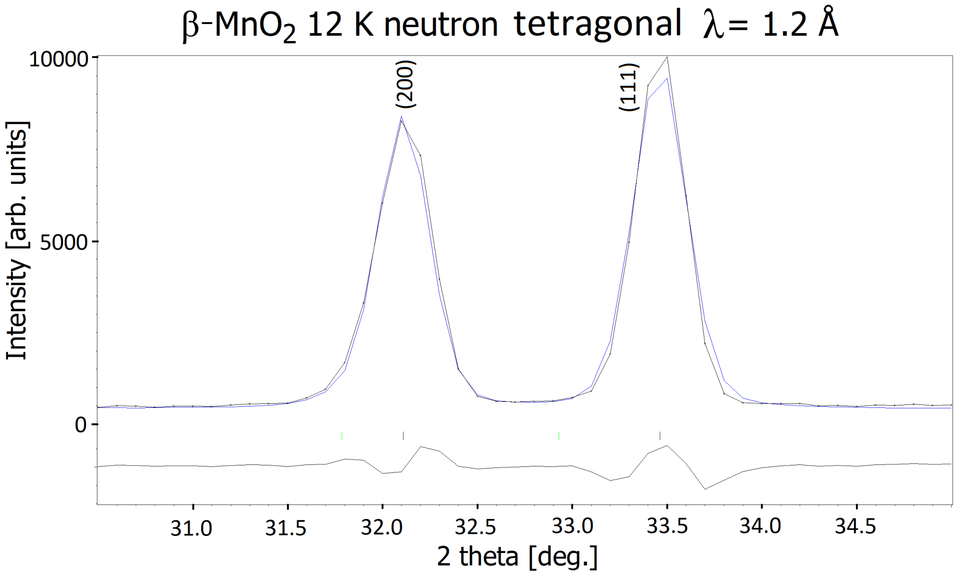

Figure 3: [Fig. S3] Observed and calculated β-MnO_2 part of powder neutron diffraction pattern obtained at 12 K and λ=1.2 Å. Tetragonal isotropic model used.

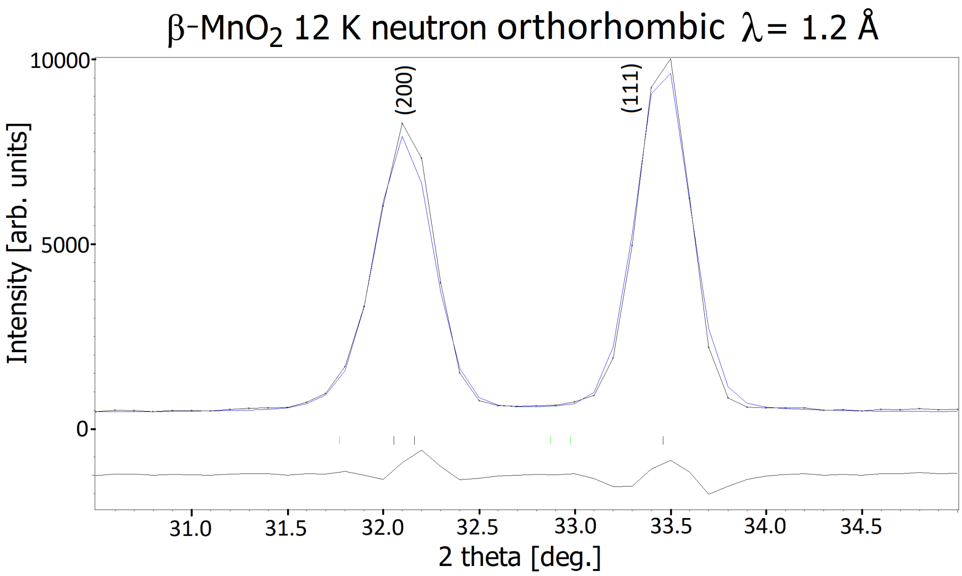

Figure 4: [Fig. S4] Observed and calculated β-MnO_2 part of powder neutron diffraction pattern obtained at 12 K and λ=1.2 Å. Orthorhombic isotropic model used.

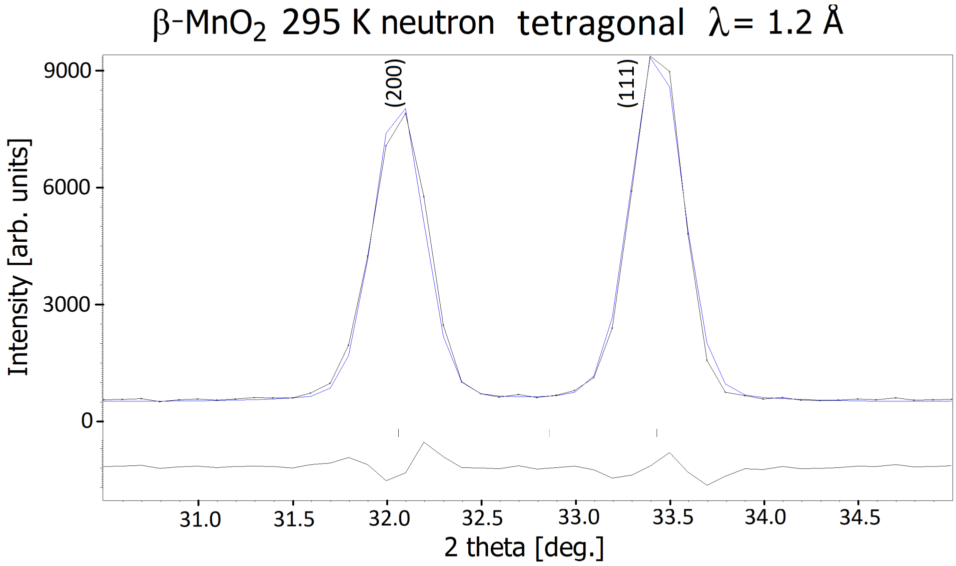

Figure 5: [Fig. S5] Observed and calculated β-MnO_2 part of powder neutron diffraction pattern obtained at 295 K and λ=1.2 Å. Tetragonal isotropic model used.

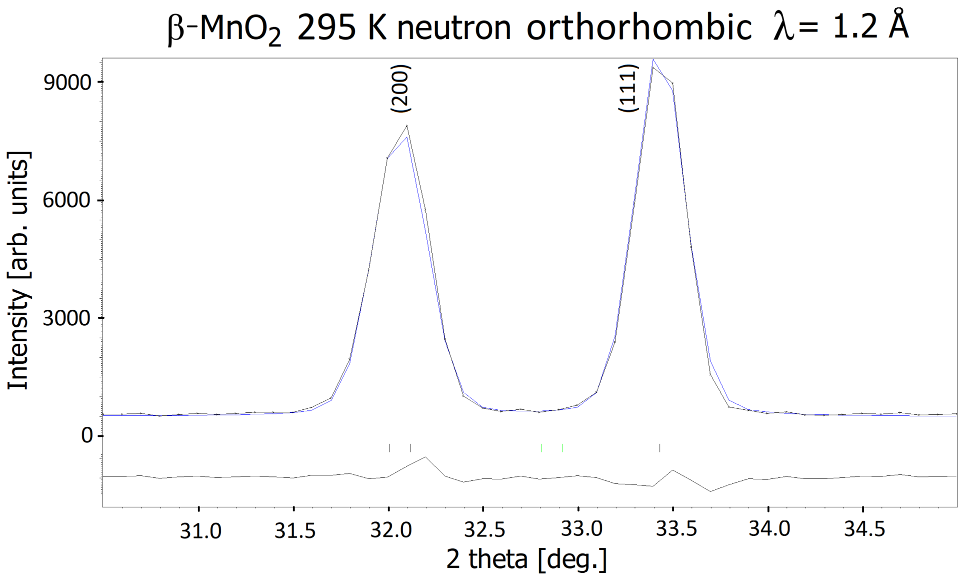

Figure 6: [Fig. S6] Observed and calculated β-MnO_2 part of powder neutron diffraction pattern obtained at 295 K and λ=1.2 Å. Orthorhombic isotropic model used.

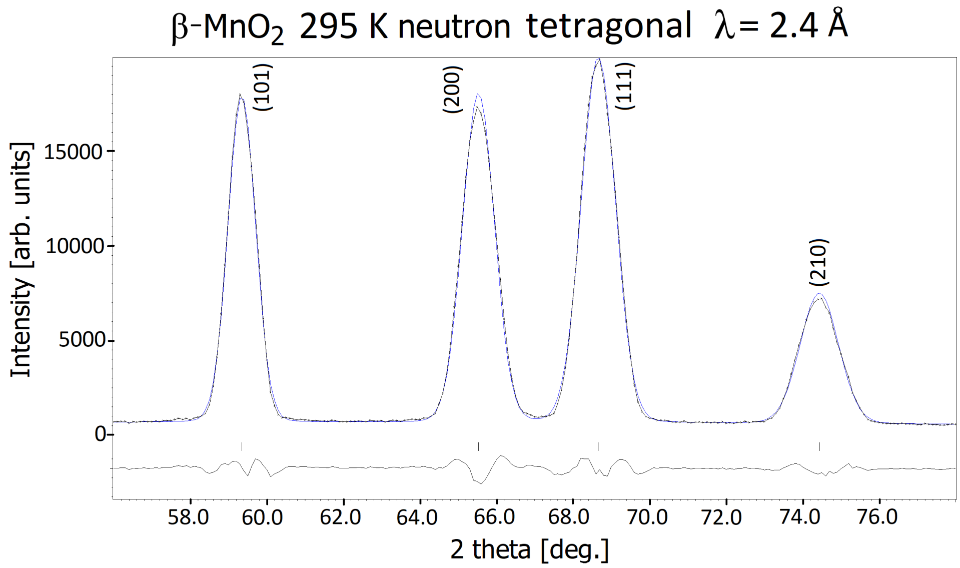

Figure 7: [Fig. S7] Observed and calculated β-MnO_2 part of powder neutron diffraction pattern obtained at 295 K and λ=2.4 Å. Tetragonal isotropic model used.

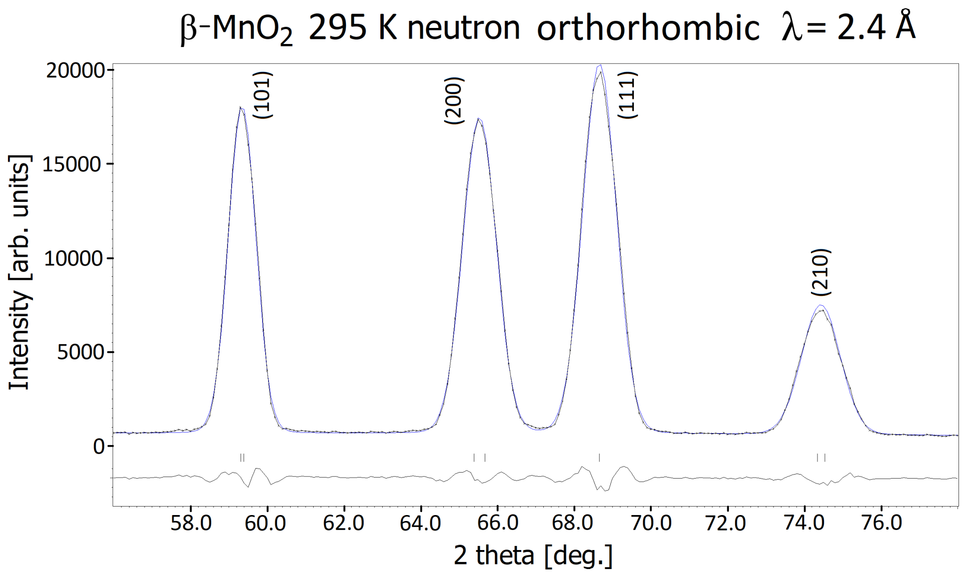

Figure 8: [Fig. S8] Observed and calculated β-MnO_2 part of powder neutron diffraction pattern obtained at 295 K and λ=2.4 Å. Orthorhombic isotropic model used.