# Supporting Information (SI) for
# Zigzag spin chains in the spin-5/2 antiferromagnet $Ba_2Mn(PO_4)_2$

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## SI-1: Ordered state (Magnetic structures determination):

Magnetic structures of $Ba_2Mn(PO_4)_2$ compatible with the crystallographic symmetry were determined by the representation analysis using the BASIREPS program of the Fullprof suite [1-9]. The symmetry analysis reveals four magnetic structures that can form upon the second-order phase transition at $T_N$. The magnetic reducible representation $\Gamma_{mag}$ for the Mn site can be decomposed as a direct sum of irreducible representations (IRs) as

$$\Gamma^{Mn}_{mag} = 3\Gamma^{1}_{1} + 3\Gamma^{1}_{2} + 3\Gamma^{1}_{3} + 3\Gamma^{1}_{4} \qquad (1)$$

**Table 1**: Basis vectors of the magnetic Mn site with the propagation vector **k** = $(\frac{1}{2}, 0, \frac{1}{2})$ for $Ba_2Mn(PO_4)_2$. Only the real components of the basis vectors are presented. The atoms of the non-primitive basis are defined according to Mn1: [(0.2628, 0.4911, 0.3596): $(x, y, z)$]; Mn2: [(0.2372, 0.9911, 0.1404): $(\bar{x}+\frac{1}{2}, y+\frac{1}{2}, \bar{z}+\frac{1}{2})$]; Mn3: [(−0.2628, −0.4911, −0.3596): $(\bar{x}, \bar{y}, \bar{z})$]; Mn4: [(0.7628, 0.0089, 0.8596) : $(x+\frac{1}{2}, \bar{y}+\frac{1}{2}, z+\frac{1}{2})$].

| IRs | | Basis Vectors | | | |
|---|---|---|---|---|---|
| | | Mn1 | Mn2 | Mn3 | Mn4 |
| $\Gamma^{1}_{1}$ | $\Psi_1$ | ( 1 0 0 ) | ( $\bar{1}$ 0 0 ) | ( 1 0 0 ) | ( $\bar{1}$ 0 0 ) |
| | $\Psi_2$ | ( 0 1 0 ) | ( 0 1 0 ) | ( 0 1 0 ) | ( 0 1 0 ) |
| | $\Psi_3$ | ( 0 0 1 ) | ( 0 0 $\bar{1}$ ) | ( 0 0 1 ) | ( 0 0 $\bar{1}$ ) |
| | | | | | |
| $\Gamma^{1}_{2}$ | $\Psi_1$ | ( 1 0 0 ) | ( $\bar{1}$ 0 0 ) | ( $\bar{1}$ 0 0 ) | ( 1 0 0 ) |
| | $\Psi_2$ | ( 0 1 0 ) | ( 0 1 0 ) | ( 0 $\bar{1}$ 0 ) | ( 0 $\bar{1}$ 0 ) |
| | $\Psi_3$ | ( 0 0 1 ) | ( 0 0 $\bar{1}$ ) | ( 0 0 $\bar{1}$ ) | ( 0 0 1 ) |
| | | | | | |
| $\Gamma^{1}_{3}$ | $\Psi_1$ | ( 1 0 0 ) | ( 1 0 0 ) | ( 1 0 0 ) | ( 1 0 0 ) |
| | $\Psi_2$ | ( 0 1 0 ) | ( 0 $\bar{1}$ 0 ) | ( 0 1 0 ) | ( 0 $\bar{1}$ 0 ) |
| | $\Psi_3$ | ( 0 0 1 ) | ( 0 0 1 ) | ( 0 0 1 ) | ( 0 0 1 ) |
| | | | | | |
| $\Gamma^{1}_{4}$ | $\Psi_1$ | ( 1 0 0 ) | ( 1 0 0 ) | ( $\bar{1}$ 0 0 ) | ( $\bar{1}$ 0 0 ) |

| | | | | | |
|---|---|---|---|---|---|
| | $\Psi_2$ | ( 0 1 0 ) | ( 0 $\bar{1}$ 0 ) | ( 0 $\bar{1}$ 0 ) | ( 0 1 0 ) |
| | $\Psi_3$ | ( 0 0 1 ) | ( 0 0 1 ) | ( 0 0 $\bar{1}$ ) | ( 0 0 $\bar{1}$ ) |

All the four Γ's are one-dimensional and appear three times in the $\Gamma_{mag}$. The basis vectors (Fourier components of the magnetization) for the magnetic Mn site 4*e* (*x, y, z*) are given in Table 1 for the four IRs. The basis vectors are calculated using the projection operator technique implemented in BASIREPS [1]. The refinement of the magnetic structure was tested for all the four Γ's. Only the $\Gamma_1$ produced a good fit of the observed diffraction patterns at 1.5 K. The fitted pattern is shown in the manuscript Fig. 6 (b). For further clarification, the pure magnetic pattern at 1.5 K (after subtraction of the nuclear background at 10 K) is shown in the manuscript Fig. 6 (c) along with the calculated magnetic pattern. The $R_{mag}$ factor was found to be 6.92 %. The basis vectors for $\Gamma_1$ [Table 1] indicate that all three components of the magnetic moment can be refined.

**References:**


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[2] A peak can be still seen in the magnetic susceptibility slightly above $T_N$, but this feature is common to Heisenberg antiferromagnets. Note also that the $T_{max}/T_N$ ratio for the magnetic susceptibility is 1.3 in $Ba_2Mn(PO_4)_2$ vs. 1.6 in $Ba_2Ni(PO_4)_2$, thus confirming the much stronger tendency of the Ni compound to the short-range order above TN.

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