Spin Quenching Assisted by a Strongly Anisotropic Compression Behavior in MnP

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SUPPORTING INFORMATION

Rietveld refinement results for APS 16-BM-D data

1) Pressure: 0.1 GPa

Space group: \textit{Pnma}

Cell parameters: \( a = 5.2595(2) \) Å, \( b = 3.1706(1) \) Å, \( c = 5.9156(2) \) Å, \( Z = 4 \)

| Atom | Site | \( x \) | \( y \) | \( x \) | Uiso |
|------|------|-------|------|-------|------|
| Mn   | 4c   | 0.0086(4) | 0.250000 | 0.19705(19) | 0.0276 |
| P    | 4c   | 0.1912(5)  | 0.250000 | 0.5582(4)   | 0.0132 |

2) Pressure: 0.8 GPa

Space group: \textit{Pnma}

Cell parameters: \( a = 5.2543(1) \) Å, \( b = 3.1654(1) \) Å, \( c = 5.9104(2) \) Å, \( Z = 4 \)

| Atom | Site | \( x \) | \( y \) | \( x \) | Uiso |
|------|------|-------|------|-------|------|
| Mn   | 4c   | 0.00358(28) | 0.250000 | 0.19669(14) | 0.0204 |
| P    | 4c   | 0.18952(31) | 0.250000 | 0.57260(27) | 0.0169 |

3) Pressure: 1.7 GPa

Space group: \textit{Pnma}

Cell parameters: \( a = 5.2472(4) \) Å, \( b = 3.1499(3) \) Å, \( c = 5.8963(6) \) Å, \( Z = 4 \)

| Atom | Site | \( x \) | \( y \) | \( x \) | Uiso |
|------|------|-------|------|-------|------|
| Mn   | 4c   | 0.0056(8)  | 0.250000 | 0.1913(4)  | 0.0204 |
| P    | 4c   | 0.1852(9)  | 0.250000 | 0.5768(8)  | 0.0169 |

4) Pressure: 3.2 GPa

Space group: \textit{Pnma}

Cell parameters: \( a = 5.2306(2) \) Å, \( b = 3.1365(1) \) Å, \( c = 5.8854(2) \) Å, \( Z = 4 \)
| Atom | Site | x       | y       | x       | Uiso  |
|------|------|---------|---------|---------|-------|
| Mn   | 4c   | 0.0044(4) | 0.250000 | 0.19644(18) | 0.0381 |
| P    | 4c   | 0.1855(4) | 0.250000 | 0.5675(4)    | 0.0116 |

5) Pressure: 4.8 GPa

Space group: *Pnma*

Cell parameters: $a = 5.2247(4)$ Å, $b = 3.1131(3)$ Å, $c = 5.8743(5)$ Å, $Z = 4$

| Atom | Site | x       | y       | x       | Uiso  |
|------|------|---------|---------|---------|-------|
| Mn   | 4c   | 0.0066(8) | 0.250000 | 0.1939(4) | 0.0055 |
| P    | 4c   | 0.1840(9) | 0.250000 | 0.5721(7) | 0.0062 |

6) Pressure: 6.8 GPa

Space group: *Pnma*

Cell parameters: $a = 5.2117(3)$ Å, $b = 3.0906(2)$ Å, $c = 5.8634(4)$ Å, $Z = 4$

| Atom | Site | x       | y       | x       | Uiso  |
|------|------|---------|---------|---------|-------|
| Mn   | 4c   | 0.0082(6) | 0.250000 | 0.19471(28) | 0.0044 |
| P    | 4c   | 0.1870(6) | 0.250000 | 0.5663(5) | 0.0268 |

7) Pressure: 8.7 GPa

Space group: *Pnma*

Cell parameters: $a = 5.1989(3)$ Å, $b = 3.0602(2)$ Å, $c = 5.8564(4)$ Å, $Z = 4$

| Atom | Site | x       | y       | x       | Uiso  |
|------|------|---------|---------|---------|-------|
| Mn   | 4c   | 0.0057(5) | 0.250000 | 0.19516(24) | 0.0046 |
| P    | 4c   | 0.1820(6) | 0.250000 | 0.5636(5) | 0.0089 |

8) Pressure: 10.2 GPa

Space group: *Pnma*
Cell parameters: \(a = 5.1936(5) \, \text Å, \ b = 3.0497(3) \, \text Å, \ c = 5.8612(5) \, \text Å, \ Z = 4\)

| Atom | Site | \(x\)   | \(y\)   | \(x\)   | \(U_{\text{iso}}\) |
|------|------|---------|---------|---------|------------------|
| Mn   | 4c   | 0.0035(6)| 0.250000| 0.19439(28)| 0.0065          |
| P    | 4c   | 0.1778(7)| 0.250000| 0.5650(6) | 0.0148          |

9) Pressure: 12.3 GPa

Space group: \(Pnma\)

Cell parameters: \(a = 5.1959(4) \, \text Å, \ b = 3.0152(3) \, \text Å, \ c = 5.8602(3) \, \text Å, \ Z = 4\)

| Atom | Site | \(x\)   | \(y\)   | \(x\)   | \(U_{\text{iso}}\) |
|------|------|---------|---------|---------|------------------|
| Mn   | 4c   | 0.0068(4)| 0.250000| 0.19508(27)| 0.0085          |
| P    | 4c   | 0.1832(6)| 0.250000| 0.5637(4) | 0.0286          |

10) Pressure: 14.7 GPa

Space group: \(Pnma\)

Cell parameters: \(a = 5.1903(5) \, \text Å, \ b = 2.9935(4) \, \text Å, \ c = 5.8476(5) \, \text Å, \ Z = 4\)

| Atom | Site | \(x\)   | \(y\)   | \(x\)   | \(U_{\text{iso}}\) |
|------|------|---------|---------|---------|------------------|
| Mn   | 4c   | 0.0088(6)| 0.250000| 0.1947(4) | 0.0315          |
| P    | 4c   | 0.1813(10)| 0.250000| 0.5621(7) | 0.0073          |

11) Pressure: 18.3 GPa

Space group: \(Pnma\)

Cell parameters: \(a = 5.1896(8) \, \text Å, \ b = 2.9645(5) \, \text Å, \ c = 5.8441(6) \, \text Å, \ Z = 4\)

| Atom | Site | \(x\)   | \(y\)   | \(x\)   | \(U_{\text{iso}}\) |
|------|------|---------|---------|---------|------------------|
| Mn   | 4c   | 0.0094(6)| 0.250000| 0.1969(5) | 0.0049          |
| P    | 4c   | 0.1863(10)| 0.250000| 0.5598(7) | 0.0053          |

12) Pressure: 22.3 GPa
Space group: \textit{Pnma}

Cell parameters: $a = 5.1885(11) \, \text{Å}, \quad b = 2.9305(7) \, \text{Å}, \quad c = 5.8374(8) \, \text{Å}, \quad Z = 4$

| Atom | Site | x      | y      | x       | Uiso |
|------|------|--------|--------|---------|------|
| Mn   | 4c   | 0.0052(6) | 0.250000 | 0.1972(4) | 0.0049 |
| P    | 4c   | 0.1876(9)  | 0.250000 | 0.5576(7) | 0.0053 |

13) Pressure: 26.3 GPa

Space group: \textit{Pnma}

Cell parameters: $a = 5.1911(9) \, \text{Å}, \quad b = 2.9122(6) \, \text{Å}, \quad c = 5.8284(7) \, \text{Å}, \quad Z = 4$

| Atom | Site | x      | y      | x       | Uiso |
|------|------|--------|--------|---------|------|
| Mn   | 4c   | 0.0039(6) | 0.250000 | 0.19644(30) | 0.0180 |
| P    | 4c   | 0.1865(8)  | 0.250000 | 0.5559(7) | 0.0083 |

14) Pressure: 30.3 GPa

Space group: \textit{Pnma}

Cell parameters: $a = 5.1714(8) \, \text{Å}, \quad b = 2.8609(7) \, \text{Å}, \quad c = 5.7840(8) \, \text{Å}, \quad Z = 4$

| Atom | Site | x      | y      | x       | Uiso |
|------|------|--------|--------|---------|------|
| Mn   | 4c   | 0.0046(6) | 0.250000 | 0.19665(30) | 0.0180 |
| P    | 4c   | 0.1851(8)  | 0.250000 | 0.5547(7) | 0.0083 |

15) Pressure: 34.9 GPa

Space group: \textit{Pnma}

Cell parameters: $a = 5.1758(9) \, \text{Å}, \quad b = 2.8629(8) \, \text{Å}, \quad c = 5.7924(8) \, \text{Å}, \quad Z = 4$

| Atom | Site | x      | y      | x       | Uiso |
|------|------|--------|--------|---------|------|
| Mn   | 4c   | 0.0040(6) | 0.250000 | 0.19656(30) | 0.0180 |
| P    | 4c   | 0.1842(8)  | 0.250000 | 0.5533(7) | 0.0083 |
16) Pressure: 40.3 GPa

Space group: *Pnma*

Cell parameters: $a = 5.1678(9)$ Å, $b = 2.8393(9)$ Å, $c = 5.7737(12)$ Å, $Z = 4$

| Atom | Site | $x$     | $y$     | $x$     | $U_{iso}$ |
|------|------|---------|---------|---------|-----------|
| Mn   | 4c   | 0.0045(8)| 0.250000| 0.1963(4)| 0.0116    |
| P    | 4c   | 0.1866(9)| 0.250000| 0.5552(10)| 0.0182   |