

**Table S2.** Atom coordinates and atom displacement parameters  $U_{ij}$  (Å<sup>2</sup>) of MgSi(OH)<sub>6</sub> crystal 7 at 100 K for refinements for space groups  $P2_1/n$  and  $P2_1$ .  
 \*Overall displacement parameter refined for H atoms. \*\* H atoms of the zigzag chains.

| $P2_1/n$ |           |           |           |           |           |           |            |            |            |                    |
|----------|-----------|-----------|-----------|-----------|-----------|-----------|------------|------------|------------|--------------------|
|          | $x$       | $y$       | $z$       | $U^{11}$  | $U^{22}$  | $U^{33}$  | $U^{23}$   | $U^{13}$   | $U^{12}$   | $U_{eq}/U_{iso}^*$ |
| Si       | 0         | 0         | 0         | 0.0039(2) | 0.0035(2) | 0.0034(2) | 0.0001(1)  | 0.0001(1)  | -0.0003(1) | 0.0036(1)          |
| Mg       | 0         | 0         | ½         | 0.0041(2) | 0.0041(2) | 0.0041(2) | -0.0001(2) | -0.003(2)  | 0.0000(2)  | 0.0043(1)          |
| O1       | 0.3520(2) | 0.7990(2) | 0.4393(1) | 0.0059(3) | 0.0040(3) | 0.0052(3) | 0.0001(3)  | 0.0003(2)  | 0.0005(3)  | 0.0050(2)          |
| O2       | 0.1161(2) | 0.0355(2) | 0.7708(1) | 0.0054(3) | 0.0049(3) | 0.0044(3) | 0.0003(3)  | 0.0002(2)  | -0.0015(3) | 0.0049(2)          |
| O3       | 0.1980(2) | 0.3383(2) | 0.4396(1) | 0.0047(3) | 0.0050(3) | 0.0049(3) | -0.0004(3) | -0.0006(2) | -0.0001(3) | 0.0049(2)          |
| H1A      | 0.438(8)  | 0.926(6)  | 0.472(6)  | -         | -         | -         | -          | -          | -          | 0.023(4)*          |
| H1B      | 0.338(8)  | 0.798(9)  | 0.327(3)  | -         | -         | -         | -          | -          | -          | 0.023(4)           |
| H2**     | 0.198(4)  | 0.173(3)  | 0.766(3)  | -         | -         | -         | -          | -          | -          | 0.023(4)           |
| H3A      | 0.078(7)  | 0.436(8)  | 0.472(6)  | -         | -         | -         | -          | -          | -          | 0.023(4)           |
| H3B      | 0.196(8)  | 0.347(9)  | 0.323(3)  | -         | -         | -         | -          | -          | -          | 0.023(4)           |

  

| $P2_1$ |           |           |            |           |           |           |           |            |            |                    |
|--------|-----------|-----------|------------|-----------|-----------|-----------|-----------|------------|------------|--------------------|
|        | $x$       | $y$       | $z$        | $U^{11}$  | $U^{22}$  | $U^{33}$  | $U^{23}$  | $U^{13}$   | $U^{12}$   | $U_{eq}/U_{iso}^*$ |
| Si     | 0.2475(2) | 0.0411(9) | 0.7496(2)  | 0.0040(2) | 0.0036(2) | 0.0035(2) | 0.0000(1) | 0.0001(1)  | 0.0001(1)  | 0.0037(1)          |
| Mg     | 0.2524(2) | 0.041(1)  | 0.2491(2)  | 0.0045(2) | 0.0042(2) | 0.0042(3) | 0.0000(2) | -0.0002(2) | 0.0002(2)  | 0.0043(1)          |
| O1     | 0.3651(4) | 0.0095(5) | 0.5199(3)  | 0.0062(7) | 0.005(1)  | 0.0034(9) | 0.000(1)  | 0.0015(6)  | 0.0023(9)  | 0.0050(5)          |
| O2     | 0.1327(4) | 0.0800(4) | -0.0217(4) | 0.0056(8) | 0.005(2)  | 0.006(1)  | 0.000(1)  | -0.0001(1) | 0.0013(9)  | 0.0054(5)          |
| O3     | 0.4531(4) | 0.7008(4) | 0.1889(3)  | 0.049(7)  | 0.003(1)  | 0.006(1)  | -0.002(1) | -0.0007(7) | -0.0007(8) | 0.0048(4)          |
| O4     | 0.0962(3) | 0.3390(5) | 0.6864(3)  | 0.0064(8) | 0.002(1)  | 0.004(1)  | 0.0011(9) | 0.0000(7)  | -0.0004(8) | 0.0042(5)          |
| O5     | 0.0573(4) | 0.3773(5) | 0.3096(3)  | 0.0042(7) | 0.007(1)  | 0.004(1)  | 0.0021(9) | -0.0001(6) | 0.0015(8)  | 0.0051(5)          |
| O6     | 0.6078(3) | 0.2409(5) | 0.1922(3)  | 0.0046(8) | 0.006(1)  | 0.006(1)  | 0.001(1)  | -0.0008(7) | -0.0006(8) | 0.0056(5)          |
| H1**   | 0.431(6)  | -0.134(5) | 0.494(5)   | -         | -         | -         | -         | -          | -          | 0.016(4)*          |
| H2**   | 0.042(6)  | 0.212(6)  | -0.036(5)  | -         | -         | -         | -         | -          | -          | 0.016(4)           |
| H3     | 0.16(1)   | 0.48(1)   | 0.260(9)   | -         | -         | -         | -         | -          | -          | 0.016(4)           |
| H4     | 0.61(1)   | 0.26(2)   | 0.079(4)   | -         | -         | -         | -         | -          | -          | 0.016(4)           |
| H5     | 0.42(1)   | 0.72(2)   | 0.076(4)   | -         | -         | -         | -         | -          | -          | 0.016(4)           |
| H6     | 0.06(1)   | 0.36(2)   | 0.578(4)   | -         | -         | -         | -         | -          | -          | 0.016(4)           |
| H7     | 0.04(1)   | 0.41(1)   | 0.421(4)   | -         | -         | -         | -         | -          | -          | 0.016(4)           |
| H8     | 0.71(1)   | 0.12(1)   | 0.208(9)   | -         | -         | -         | -         | -          | -          | 0.016(4)           |
| H9     | 0.17(1)   | 0.46(1)   | 0.745(8)   | -         | -         | -         | -         | -          | -          | 0.016(4)           |
| H10    | 0.313(8)  | 0.62(1)   | 0.192(9)   | -         | -         | -         | -         | -          | -          | 0.016(4)           |