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# Pressure induced octahedral tilting distortion in $Ba_2YTaO_6$

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Crystallographic data for $Ba_2YTaO_6$.

Table 1 – Pressure dependence of the full width at half max of the peak(s) near 27° 2θ. Up to 4.3 GPa a single peak was used, above this pressure two peaks were used.

| Pressure (GPa) | FWHM (°) |
|---|---|
| 0.9 | 0.0555 |
| 2.2 | 0.0567 |
| 3.1 | 0.0617 |
| 4.3 | 0.0697 |
| 5.6 | 0.0573, 0.0663 |
| 6.3 | 0.0627, 0.0730 |

Table 2 – Pressure dependence of the Rietveld refinements of $Ba_2YTaO_6$ in space group $Fm\bar{3}m$. The atoms positions are Ba (¼, ¼, ¼), Y (0, 0, 0), Ta (½, ½, ½), O ($x$, 0, 0).

| Pressure (GPa) | 0.9 | 2.2 | 3.1 | 4.3 |
|---|---|---|---|---|
| O ($x$) | 0.260(2) | 0.257(2) | 0.259(2) | 0.267(2) |
| Ba $U_{iso}$ Å$^2$ (×100) | 1.3(2) | 1.5(2) | 1.7(2) | 1.3(2) |
| Y $U_{iso}$ Å$^2$ (×100) | 0.8(3) | 2.0(3) | 1.4(3) | 1.3(3) |
| Ta $U_{iso}$ Å$^2$ (×100) | 1.5(2) | 1.7(1) | 1.6(2) | 1.0(2) |
| O $U_{iso}$ Å$^2$ (×100) | 4.3(6) | 2.7(5) | 2.8(5) | 4.4(6) |
| $R_{wp}$ (%) | 10.51 | 10.09 | 9.95 | 9.21 |
| $R_p$ (%) | 8.21 | 8.01 | 7.83 | 7.20 |
| $\chi^2$ | 1.85 | 2.18 | 1.76 | 2.75 |

Table 3 – Rietveld refinement results for $Ba_2YTaO_6$ at 6.3 GPa in space group *I*4/*m*. The fit statistics are $R_{wp}$ 7.92%, $R_p$ 5.76%, and $\chi^2$ 2.75.

| Atom | x | y | z | $U_{iso}$ Å$^2$ (×100) |
|---|---|---|---|---|
| Ba | 0 | ½ | ¼ | 1.5(2) |
| Y | 0 | 0 | 0 | 1.8(3) |
| Ta | ½ | ½ | 0 | 1.6(2) |
| O1 | 0 | 0 | 0.269(8) | 4.7(10) |
| O2 | 0.242(15) | 0.278(16) | 0 | 4.7(10) |

Table 4 – Selected interatomic distances and bond angles for $Ba_2YTaO_6$ at 6.3 GPa in space group *I*4/*m*.

| (6.3 GPa) | $Ba_2YTaO_6$ |
|---|---|
| Ba-O1 (×4) Å | 2.947(3) |
| Ba-OX (×4) Å | 2.84(4) |
| Ba-OX (×4) Å | 3.06(9) |
| Y-O1 (×2) Å | 2.24(6) |
| Y-O2 (×4) Å | 2.18(4) |
| Ta-O1 (×2) Å | 1.93(6) |
| Ta-O2 (×4) Å | 1.99(3) |
| Y-O2-Ta (°) | 172(7) |