Electronic Supplementary Material (ESI) for Journal of Materials Chemistry A.
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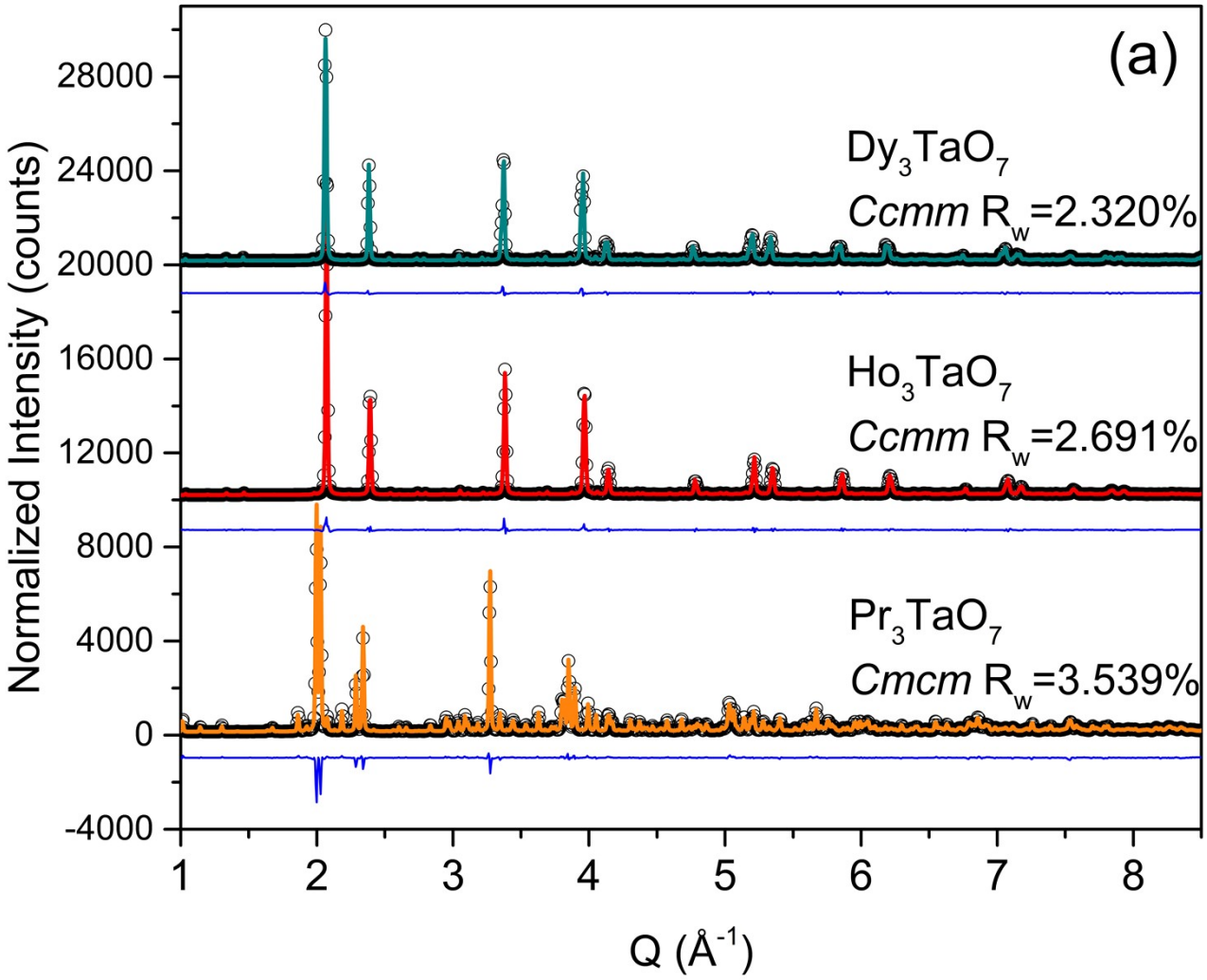
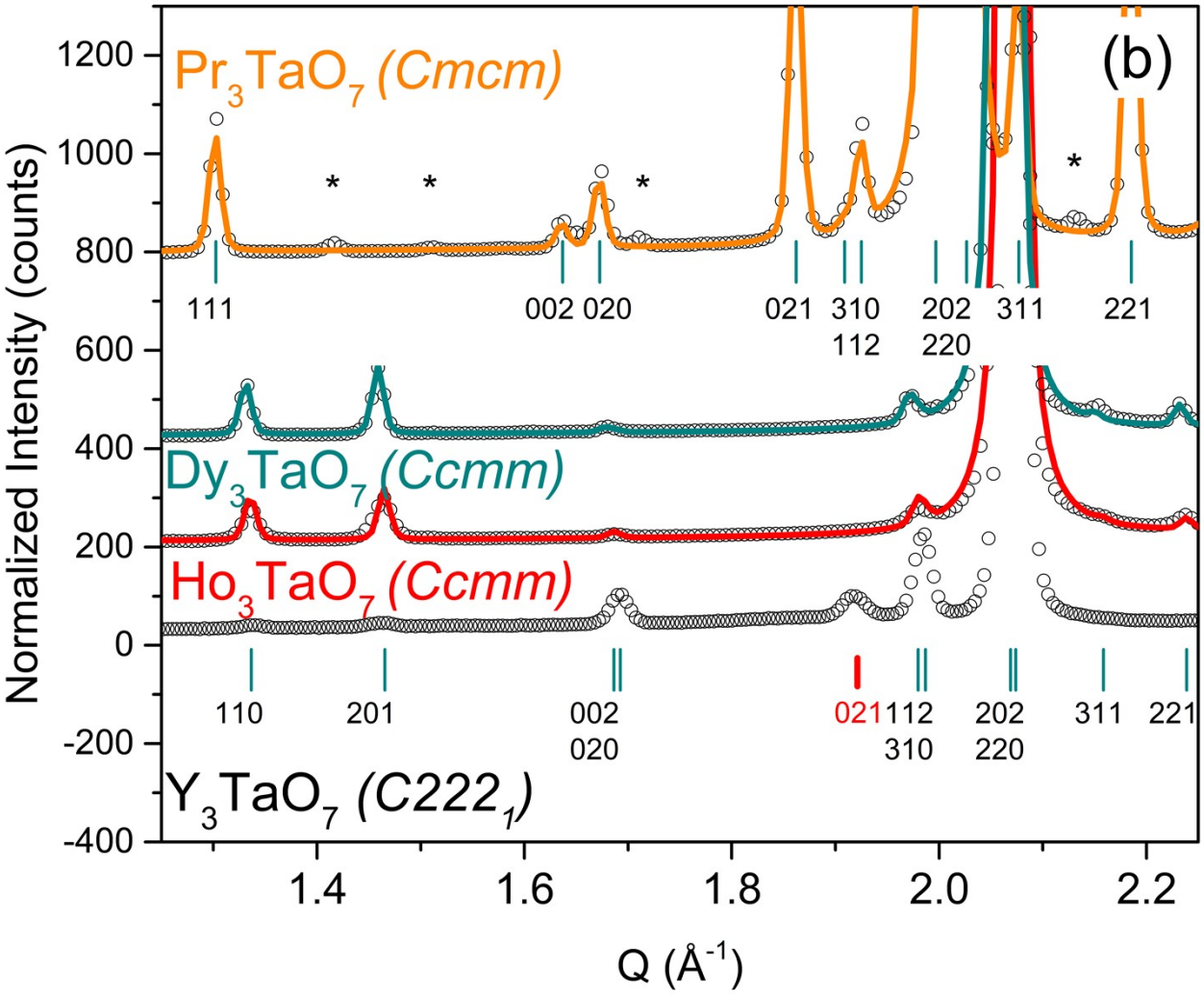
**Supplementary information:**

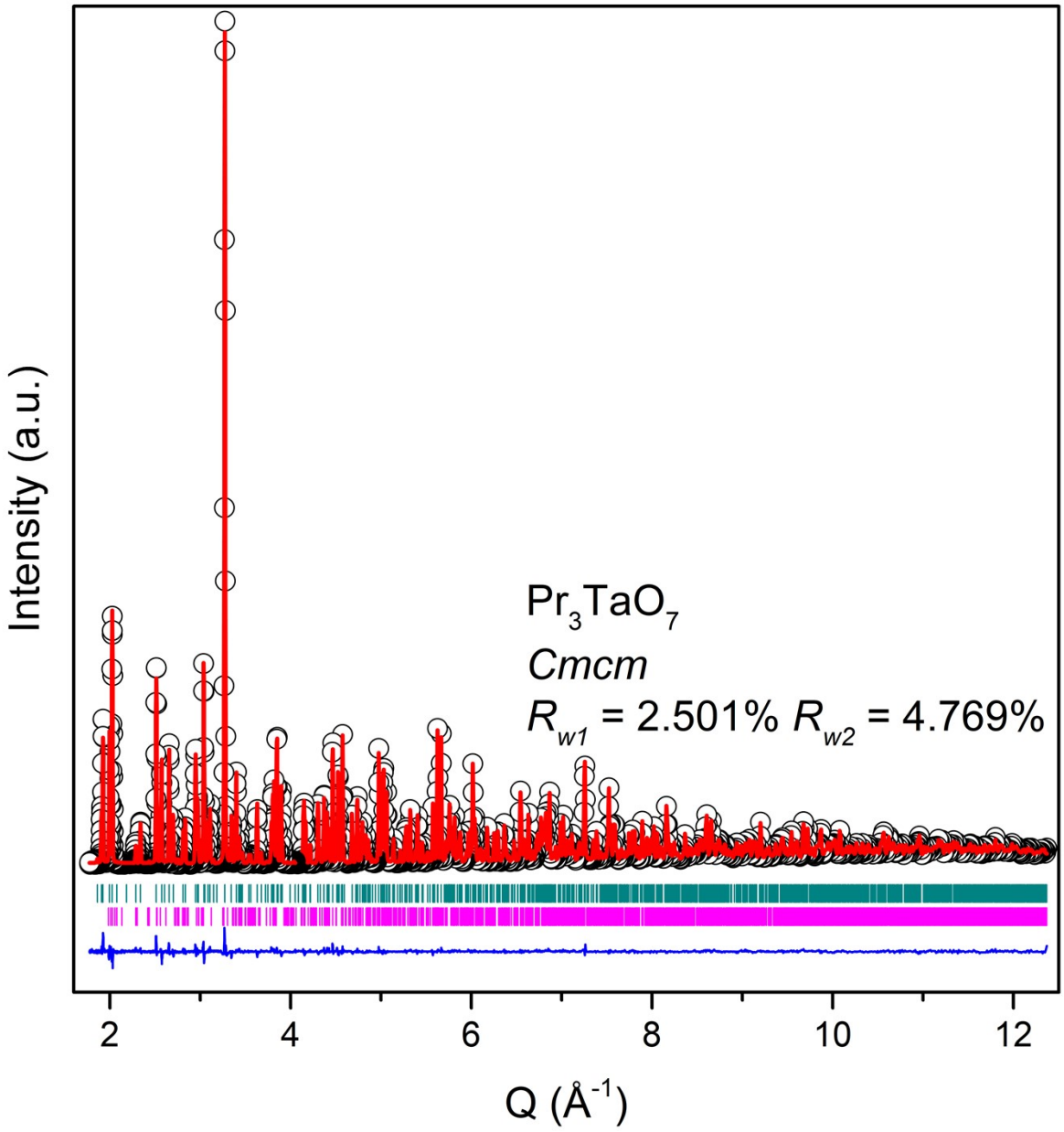
**Supplementary Table 1**: Starting values for the $Ln_3TaO_7$ prototype *Cmmm* (65) structure.

| **$Ln_3TbO_7$** | | **a (Å)** | **b (Å)** | **c (Å)** |
|---|---|---|---|---|
| *Cmmm* | | 10.49940 | 7.42422 | 3.71211 |
| **Atom** | **Wyckoff Site** | **x** | **y** | **z** |
| Ta1 | 2a | 0 | 0 | 0 |
| Ln1 | 2b | 0 | 0.5 | 0 |
| Ln2 | 4f | 0.25 | 0.25 | 0.5 |
| O1 | 8p | 0.37388 | 0.29953 | 0 |
| O2 | 2d | 0 | 0 | 0.5 |
| O3 | 4h | 0.125 | 0.5 | 0.5 |

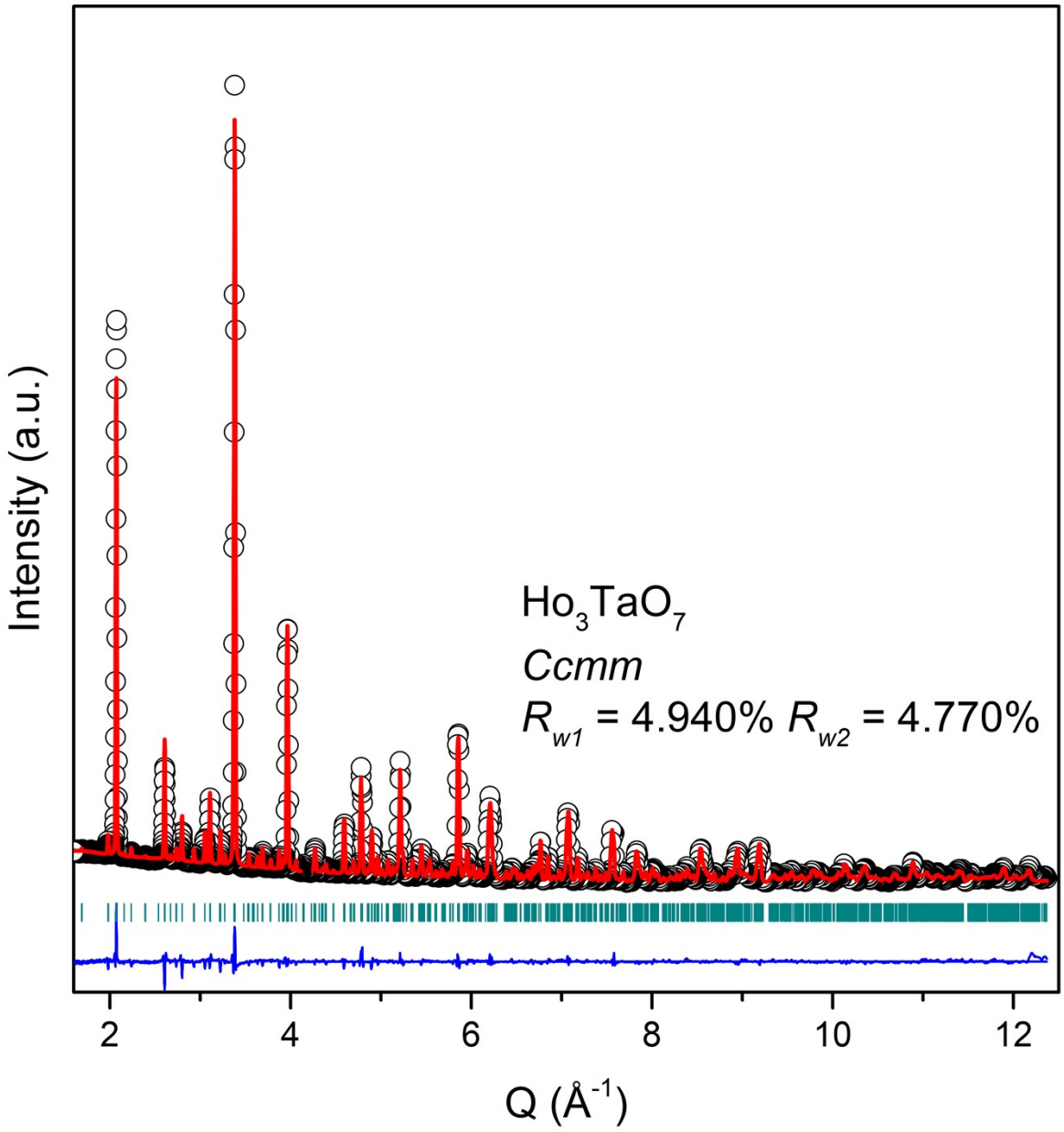

(a)
Dy3TaO7
Ccmm Rw=2.320%
Ho3TaO7
Ccmm Rw=2.691%
Pr3TaO7
Cmcm Rw=3.539%
Normalized Intensity (counts)
28000
24000
20000
16000
12000
8000
4000
0
-4000
1
2
3
4
5
6
7
8
Q (Å-1)



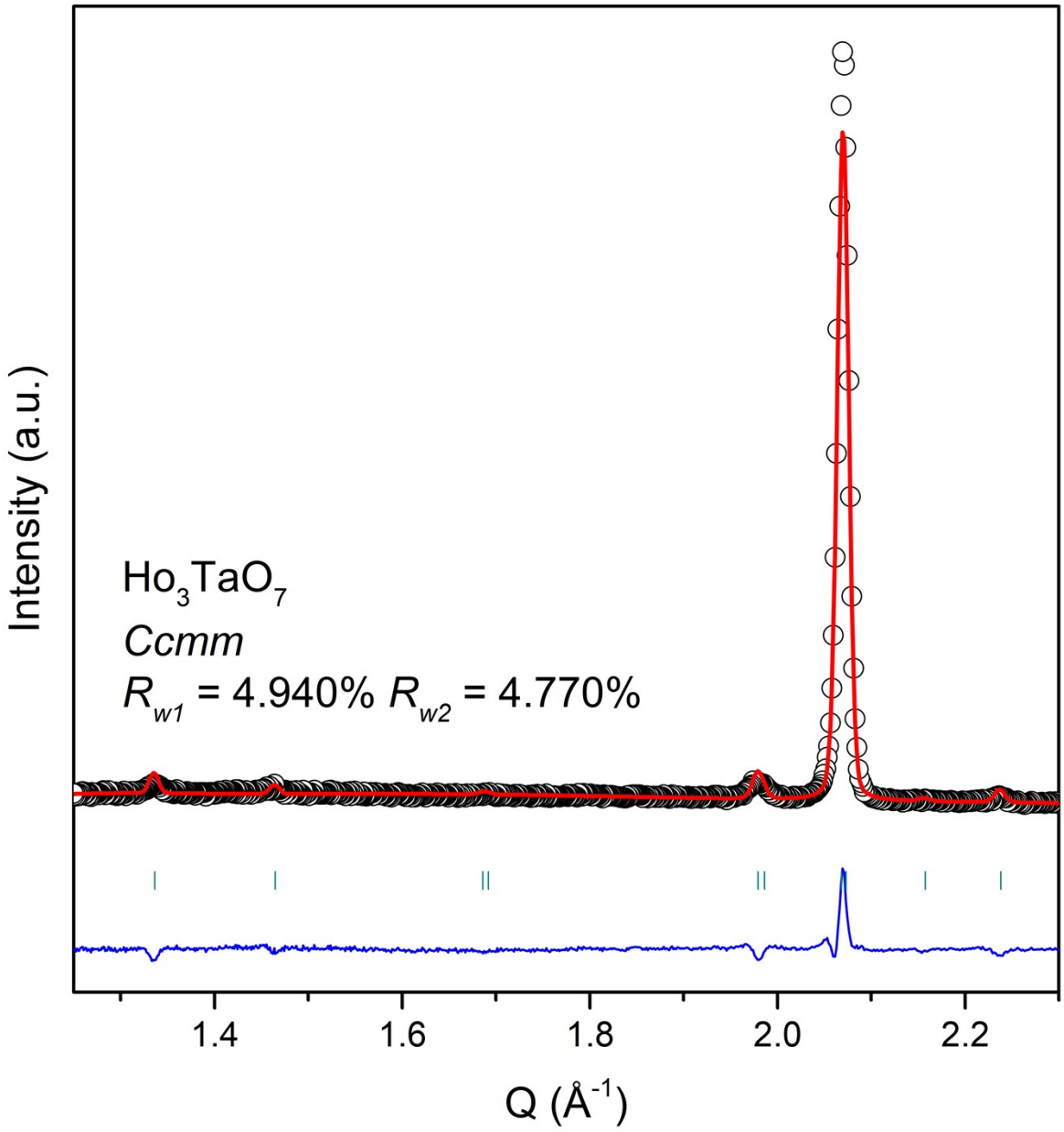

**Enlarged version of Figure 2:** (a) Stacked high-energy synchrotron X-ray diffraction patterns for $A_3TaO_7$ (A = Pr, Dy, Ho) as measured (black circles) and modeled (orange, cyan and red curves). Blue curves represent the difference between measurement and calculated model (space groups *Cmcm* and *Ccmm*). The reliability factor (*Rw*) is reported for every sample. Diffraction patterns are offset by values of 10'000 and 20'000 respectively. (b) Expanded view of the low-Q range of (a) using the same color labeling, along with diffraction data of $Y_3TaO_7$ (black circles), which serves as reference measurement. Cyan ticks represent diffraction conditions allowed in (top) *Cmcm* and (bottom) *Ccmm* space groups. Asterisks (*) mark the $PrTaO_4$ impurity phase reflections for $Pr_3TaO_7$. The red tick mark at ~1.93 $Å^{-1}$ indicates the location of the (021) diffraction peak, which serves as space group distinction between $C222_1$ and *Ccmm* (and it is only allowed for $C222_1$). Diffraction patterns are offset by values of 200, 400 and 800 respectively. Enlarged version of this figure is available in the supplementary section.



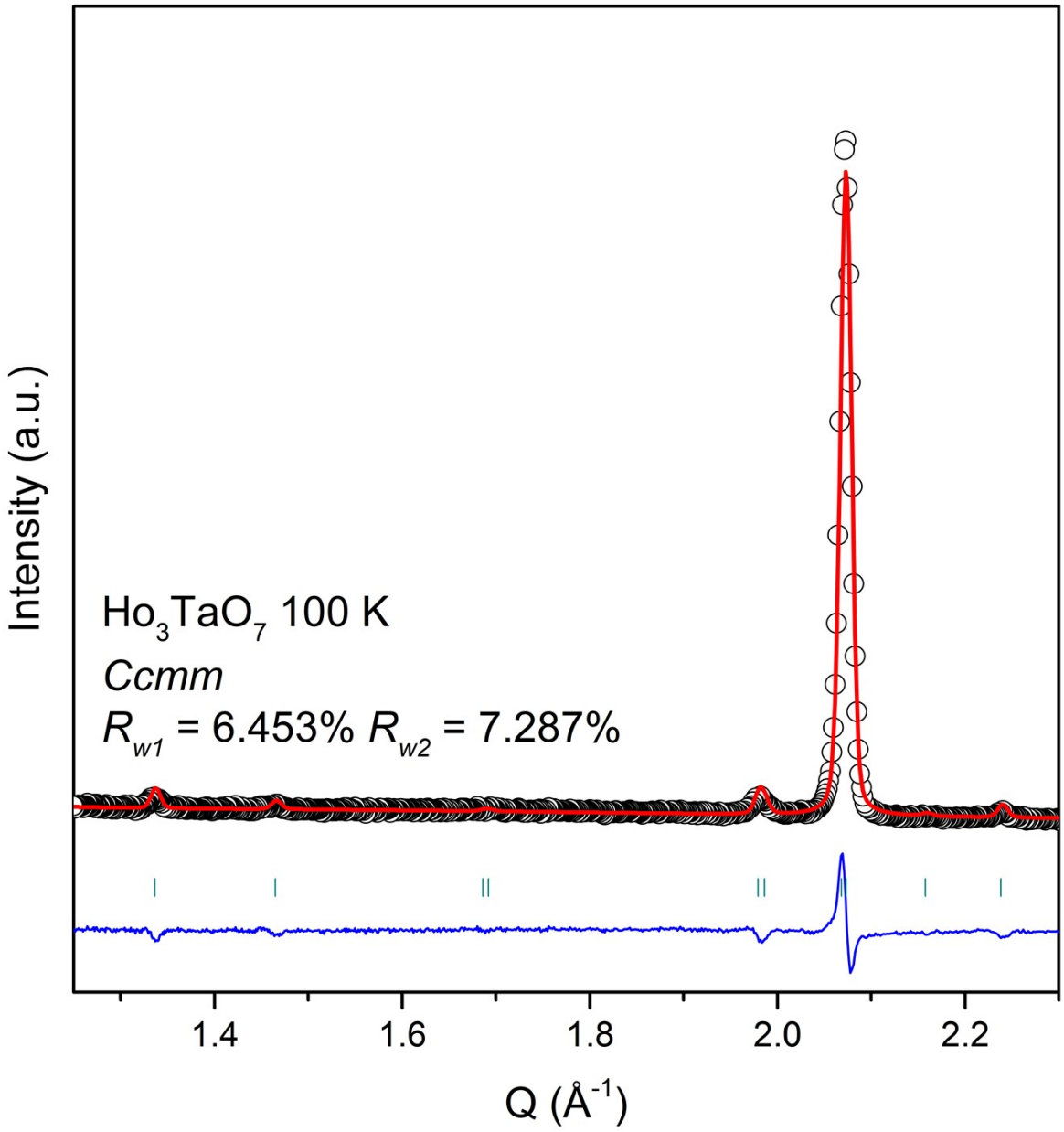

**Supplementary Figure 1:** POWGEN' high-resolution neutron diffraction pattern of $Pr_3TaO_7$ measured at room temperature (black circles) and modeled (red curve) using *Cmcm* space group. The blue curve represents the difference curve between measurement and the model fit, with *Rw1* and *Rw2* being the fit reliability factors. Cyan and Magenta ticks indicate the expected Bragg peak positions according to the crystal structure models of $Pr_3TaO_7$ and $PrTaO_4$ impurity phase respectively.




**Supplementary Figure 2:** POWGEN' high-resolution neutron diffraction pattern of $Ho_3TaO_7$ measured at room temperature (black circles) and modeled (red curve) using *Ccmm* space group. The blue curve represents the difference curve between measurement and the model fit, with *Rw1* and *Rw2* being the fit reliability factors. Cyan ticks indicate the expected Bragg peak positions according to the crystal structure model.




**Supplementary Figure 3:** An expanded view of low-Q region of POWGEN' high-resolution neutron diffraction pattern of $Ho_3TaO_7$ measured at room temperature (black circles) and modeled (red curve) using *Ccmm* space group. The blue curve represents the difference curve between measurement and the model fit, with *Rw1* and *Rw2* being the fit reliability factors. Cyan ticks indicate the expected Bragg peak positions according to the crystal structure model.




**Supplementary Figure 4:** Low-Q region of POWGEN' high-resolution neutron diffraction pattern of $Ho_3TaO_7$ measured at 100 K (black circles) and modeled (red curve) using *Ccmm* space group. The blue curve represents the difference curve between measurement and the model fit, with *Rw1* and *Rw2* being the fit reliability factors. Cyan ticks indicate the expected Bragg peak positions according to the crystal structure model.

**Supplementary Table 2:** Structural information for long-range diffraction data refinements. Unit cell parameters, fractional positional coordinates and thermal factors are followed by sigma values. NOMAD and POWGEN denote neutron diffraction data collected at respective neutron total scattering instruments while SXRD denotes synchrotron X-ray diffraction data. Uiso denote isotropic thermal factors. When applicable, harmonic thermal factors (Uij) are shown with first row denoting $U_{11}$, $U_{22}$ and $U_{33}$ factors while $U_{12}$, $U_{13}$ and $U_{23}$ are shown in the second below.

| **$Pr_3TaO_7$** (NOMAD) | | **a (Å)** | **b (Å)** | **c (Å)** | |
|---|---|---|---|---|---|
| *Cmcm* (63) | | 10.98712(17) | 7.51112(13) | 7.67928(16) | |
| **Atom** | **Wyckoff Site** | **x** | **y** | **z** | **Uiso** |
| Pr1 | 4b | 0 | 0.5 | 0 | 0.0086(5) |
| Pr2 | 8g | 0.22948(16) | 0.7943(3) | 0.25 | 0.0016(3) |
| Ta1 | 4a | 0 | 0 | 0 | 0.0008(3) |
| O1 | 16h | 0.37393(11) | 0.68544(14) | 0.03476(16) | 0.0089(3) |
| O2 | 8g | 0.13001(16) | 0.5250(2) | 0.25 | 0.0033(3) |
| O3 | 4c | 0 | 0.9332(3) | 0.25 | 0.0073(4) |

| **$Tb_3TaO_7$** (NOMAD) | | **a (Å)** | **b (Å)** | **c (Å)** | |
|---|---|---|---|---|---|
| *Ccmm* (63) | | 10.5716(2) | 7.46997(16) | 7.51362(14) | |
| **Atom** | **Wyckoff Site** | **x** | **y** | **z** | **Uiso** |
| Tb1 | 4b | 0.5 | 0 | 0 | 0.0075(3) |
| Tb2 | 8g | 0.23511(15) | 0.2357(2) | 0.75 | 0.0030(2) |
| Ta1 | 4a | 0 | 0 | 0 | 0.0015(3) |
| O1 | 16h | 0.37637(16) | 0.30011(18) | 0.9717(2) | 0.0149(4) |
| O2 | 4c | 0.0614(4) | 0 | 0.75 | 0.0163(7) |
| O3 | 4c | 0.6283(3) | 0 | 0.75 | 0.0018(4) |
| O4 | 4c | 0.3625(4) | 0 | 0.75 | 0.0086(6) |

| **$Ho_3TaO_7$** (NOMAD) | | **a (Å)** | **b (Å)** | **c (Å)** | | |
|---|---|---|---|---|---|---|
| *Ccmm* (63) | | 10.4933(3) | 7.4250(2) | 7.4553(2) | | |
| **Atom** | **Wyckoff Site** | **x** | **y** | **z** | **Uiso** | |
| Ho1 | 4b | 0.5 | 0 | 0 | 0.0247(8) | |
| Ho2 | 8g | 0.2404(2) | 0.2386(3) | 0.75 | 0.0013(3) | |
| Ta1 | 4a | 0 | 0 | 0 | 0.0171(6) | |
| O1 | 16h | 0.3766(4) | 0.2891(4) | 0.9745(5) | 0.0294(8) | |
| O2 | 4c | 0.0622(7) | 0 | 0.75 | 0.0227(13) | |
| O3 | 4c | 0.6281(6) | 0 | 0.75 | 0.0129(9) | |
| O4 | 4c | 0.3621(7) | 0 | 0.75 | 0.0218(14) | |

| **$Ho_3TaO_7$** (NOMAD) | | **a (Å)** | **b (Å)** | **c (Å)** | | |
|---|---|---|---|---|---|---|
| *Fm-3m* (225) | | 5.25850(11) | 5.25850(11) | 5.25850(11) | | |
| **Atom** | **Wyckoff Site** | **x** | **y** | **z** | **Occupancy** | **Uiso** |
| Ho1 | 4a | 0 | 0 | 0 | 0.75 | 0.0212(5) |
| Ta1 | 4a | 0 | 0 | 0 | 0.25 | 0.0212(5) |
| O1 | 8c | 0.25 | 0.25 | 0.25 | 0.875 | 0.0681(8) |

| **$Tm_3TaO_7$** (NOMAD) | | **a (Å)** | **b (Å)** | **c (Å)** | | |
|---|---|---|---|---|---|---|
| *Fm-3m* (225) | | 5.21362(5) | 5.21362(5) | 5.21362(5) | | |
| **Atom** | **Wyckoff Site** | **x** | **y** | **z** | **Occupancy** | **Uiso** |
| Tm1 | 4a | 0 | 0 | 0 | 0.75 | 0.0179(3) |
| Ta1 | 4a | 0 | 0 | 0 | 0.25 | 0.0179(3) |
| O1 | 8c | 0.25 | 0.25 | 0.25 | 0.875 | 0.0595(5) |

| **$Yb_3TaO_7$** (NOMAD) | | **a (Å)** | **b (Å)** | **c (Å)** | | |
|---|---|---|---|---|---|---|
| *Fm-3m* (225) | | 5.19453(5) | 5.19453(5) | 5.19453(5) | | |
| **Atom** | **Wyckoff Site** | **x** | **y** | **z** | **Occupancy** | **Uiso** |
| Ho1 | 4a | 0 | 0 | 0 | 0.75 | 0.0214(3) |
| Ta1 | 4a | 0 | 0 | 0 | 0.25 | 0.0214(3) |
| O1 | 8c | 0.25 | 0.25 | 0.25 | 0.875 | 0.0577(5) |

| **$Pr_3TaO_7$** (SXRD) | | **a (Å)** | **b (Å)** | **c (Å)** | |
|---|---|---|---|---|---|
| *Cmcm* (63) | | 10.98488(18) | 7.51246(12) | 7.67712(13) | |
| **Atom** | **Wyckoff Site** | **x** | **y** | **z** | **Uiso** |
| Pr1 | 4b | 0 | 0.5 | 0 | 0.0087(5) |
| Pr2 | 8g | 0.22797(11) | 0.79573(15) | 0.25000 | 0.0031(4) |
| Ta1 | 4a | 0 | 0 | 0 | 0.0014(4) |
| O1 | 16h | 0.3740(9) | 0.6822(12) | 0.0361(12) | 0.002(3) |
| O2 | 8g | 0.1285(16) | 0.528(2) | 0.25 | 0.012(4) |
| O3 | 4c | 0 | 0.9421(27) | 0.25 | 0.003(6) |

| **$Dy_3TaO_7$** (SXRD) | | **a (Å)** | **b (Å)** | **c (Å)** | |
|---|---|---|---|---|---|
| *Ccmm* (63) | | 10.52150(19) | 7.43849(13) | 7.48792(10) | |
| **Atom** | **Wyckoff Site** | **x** | **y** | **z** | **Uiso** |
| Dy1 | 4b | 0.5 | 0 | 0 | 0.0109(6) |
| Dy2 | 8g | 0.23408(9) | 0.23493(13) | 0.75 | 0.0069(3) |
| Ta1 | 4a | 0 | 0 | 0 | 0.0044(5) |
| O1 | 16h | 0.3778(12) | 0.3046(15) | 0.9685(13) | 0.002(3) |
| O2 | 4c | 0.058(3) | 0 | 0.75 | 0.018(7) |
| O3 | 4c | 0.630(3) | 0 | 0.75 | 0.003(6) |
| O4 | 4c | 0.357(3) | 0 | 0.75 | 0.009(7) |

| **$Ho_3TaO_7$** (SXRD) | | **a (Å)** | **b (Å)** | **c (Å)** | |
|---|---|---|---|---|---|
| *Ccmm* (63) | | 10.4852(3) | 7.4241(2) | 7.45141(17) | |
| **Atom** | **Wyckoff Site** | **x** | **y** | **z** | **Uiso** |
| Ho1 | 4b | 0.5 | 0 | 0 | 0.0131(9) |
| Ho2 | 8g | 0.23721(14) | 0.23741(19) | 0.75 | 0.0111(4) |
| Ta1 | 4a | 0 | 0 | 0 | 0.0074(8) |
| O1 | 16h | 0.377(2) | 0.298(3) | 0.971(2) | 0.007(6) |
| O2 | 4c | 0.060(4) | 0 | 0.75 | 0.018(11) |
| O3 | 4c | 0.631(5) | 0 | 0.75 | 0.027(13) |
| O4 | 4c | 0.358(5) | 0 | 0.75 | 0.026(14) |

| **$Pr_3TaO_7$** (POWGEN, RT) | | **a (Å)** | **b (Å)** | **c (Å)** | | | |
|---|---|---|---|---|---|---|---|
| *Cmcm* (63) | | 10.98883(4) | 7.51223(3) | 7.68015(3) | | | |
| **Atom** | **Wyckoff Site** | **x** | **y** | **z** | $\frac{U_{11}}{U_{12}}$ | $\frac{U_{22}}{U_{13}}$ | $\frac{U_{33}}{U_{23}}$ |
| Pr1 | 4b | 0 | 0.5 | 0 | 0.0062(5)<br>0 | 0.0249(8)<br>0 | 0.0027(5)<br>-0.0022(10) |
| Pr2 | 8g | 0.22838(8) | 0.79583(12) | 0.25 | 0.0056(4)<br>-0.0007(6) | 0.0083(5)<br>0 | 0.0037(3)<br>0 |
| Ta1 | 4a | 0 | 0 | 0 | 0.0017(3)<br>0 | 0.0062(4)<br>0 | 0.0009(3)<br>0.0000(5) |
| O1 | 16h | 0.37429(5) | 0.68615(9) | 0.03461(7) | 0.0116(3)<br>0.0126(5) | 0.0239(3)<br>-0.0009(4) | 0.0056(2)<br>-0.0035(4) |
| O2 | 8g | 0.13092(7) | 0.52372(11) | 0.25 | 0.0053(3)<br>-0.0003(6) | 0.0086(4)<br>0 | 0.0065(3)<br>0 |
| O3 | 4c | 0 | 0.93200(15) | 0.25 | 0.0125(5)<br>0 | 0.0110(5)<br>0 | 0.0006(4)<br>0 |

| **$Ho_3TaO_7$** (POWGEN, RT) | | **a (Å)** | **b (Å)** | **c (Å)** | | | |
|---|---|---|---|---|---|---|---|
| *Ccmm* (63) | | 10.48914(18) | 7.42688(14) | 7.45209(13) | | | |
| **Atom** | **Wyckoff Site** | **x** | **y** | **z** | $\frac{U_{11}}{U_{12}}$ | $\frac{U_{22}}{U_{13}}$ | $\frac{U_{33}}{U_{23}}$ |
| Ho1 | 4b | 0.5 | 0 | 0 | 0.0055(13)<br>0 | 0.0122(14)<br>-0.0031(17) | 0.0077(12)<br>0 |
| Ho2 | 8g | 0.23578(15) | 0.2354(2) | 0.75 | 0.0053(7)<br>0.0016(11) | 0.0036(7)<br>0 | 0.0039(8)<br>0 |
| Ta1 | 4a | 0 | 0 | 0 | 0.0006(12)<br>0 | 0.0031(13)<br>0.0032(18) | 0.0026(11)<br>0 |
| O1 | 16h | 0.3761(2) | 0.2999(3) | 0.9711 (3) | 0.0116(9)<br>-0.0057(15) | 0.0191(9)<br>0.0035(15) | 0.0171(10)<br>-0.0063(13) |
| O2 | 4c | 0.0675(4) | 0 | 0.75 | 0.0180(18)<br>0 | 0.0106(19)<br>0 | 0.0058(16)<br>0 |
| O3 | 4c | 0.6306(4) | 0 | 0.75 | 0.0015(15)<br>0 | 0.0033(14)<br>0 | 0.0069(15)<br>0 |
| O4 | 4c | 0.3620(4) | 0 | 0.75 | 0.0047(17)<br>0 | 0.0089(17)<br>0 | 0.0111(16)<br>0 |

**Supplementary Table 3:** Structural information for room temperature (RT) short-range PDF data refinements. Unit cell parameters, fractional positional coordinates and thermal factors are followed by sigma values.

| **$Pr_3TaO_7$** (PDF, RT) | | **a (Å)** | **b (Å)** | **c (Å)** | | | |
|---|---|---|---|---|---|---|---|
| *Cmcm* (63) | | 10.995(4) | 7.523(3) | 7.6858(18) | | | |
| **Atom** | **Wyckoff Site** | **x** | **y** | **z** | $\frac{U_{11}}{U_{12}}$ | $\frac{U_{22}}{U_{13}}$ | $\frac{U_{33}}{U_{23}}$ |
| Pr1 | 4b | 0 | 0.5 | 0 | 0.0094(18)<br>0 | 0.044(4)<br>0 | 0.001(1)<br>-0.003(2) |
| Pr2 | 8g | 0.2290(3) | 0.2041(5) | 0.25 | 0.0061(9)<br>-0.0018(6) | 0.008(1)<br>0 | 0.0072(9)<br>0 |
| Ta1 | 4a | 0 | 0 | 0 | 0.0019(6)<br>0 | 0.0071(11)<br>0 | 0.0055(8)<br>-0.0005(6) |
| O1 | 16h | 0.37592(18) | 0.3116(4) | 0.0367(3) | 0.0119(9)<br>-0.013(1) | 0.0279(17)<br>-0.0025(5) | 0.0066(5)<br>0.0043(7) |
| O2 | 8g | 0.1306(3) | 0.4767(5) | 0.25 | 0.0074(8)<br>0.0004(8) | 0.0061(8)<br>0 | 0.0080(7)<br>0 |
| O3 | 4c | 0 | 0.0646(5) | 0.25 | 0.0157(14)<br>0 | 0.003(1)<br>0 | 0.0042(7)<br>0 |

| **$Tb_3TaO_7$** (PDF, RT) | | **a (Å)** | **b (Å)** | **c (Å)** | | | |
|---|---|---|---|---|---|---|---|
| *Ccmm* (63) | | 10.529(6) | 7.492(3) | 7.514(3) | | | |
| **Atom** | **Wyckoff Site** | **x** | **y** | **z** | $\frac{U_{11}}{U_{12}}$ | $\frac{U_{22}}{U_{13}}$ | $\frac{U_{33}}{U_{23}}$ |
| Tb1 | 4b | 0.5 | 0 | 0 | 0.0073(19)<br>0 | 0.049(4)<br>0.0068(9) | 0.0083(14)<br>0 |
| Tb2 | 8g | 0.2324(2) | 0.2378(5) | 0.75 | 0.0086(6)<br>0.0022(5) | 0.0045(6)<br>0 | 0.0094(7)<br>0 |
| Ta1 | 4a | 0 | 0 | 0 | 0.0152(19)<br>0 | 0.005(1)<br>0.0044(11) | 0.0108(15)<br>0 |
| O1 | 16h | 0.3766(3) | 0.3029(5) | 0.9680(5) | 0.0178(12)<br>-0.020(1) | 0.0358(15)<br>0.0067(7) | 0.0108(8)<br>-0.0072(9) |
| O2 | 4c | 0.0641(6) | 0 | 0.75 | 0.0132(18)<br>0 | 0.0066(14)<br>0 | 0.0102(15)<br>0 |
| O3 | 4c | 0.6308(5) | 0 | 0.75 | 0.0020(9)<br>0 | 0.0120(14)<br>0 | 0.0107(16)<br>0 |
| O4 | 4c | 0.3641(5) | 0 | 0.75 | 0.0071(11)<br>0 | 0.0081(13)<br>0 | 0.0028(9)<br>0 |

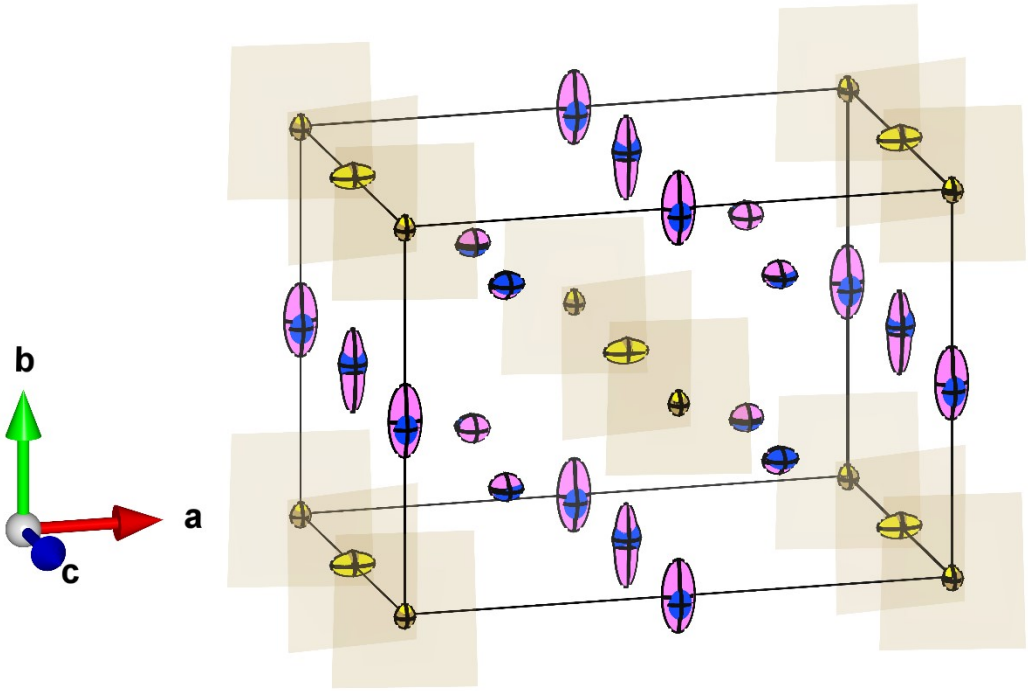
| **$Ho_3TaO_7$** (PDF, RT) | | **a (Å)** | **b (Å)** | **c (Å)** | | | |
|---|---|---|---|---|---|---|---|
| *Ccmm* (63) | | 10.458(7) | 7.440(4) | 7.457(4) | | | |
| **Atom** | **Wyckoff Site** | **x** | **y** | **z** | $\frac{U_{11}}{U_{12}}$ | $\frac{U_{22}}{U_{13}}$ | $\frac{U_{33}}{U_{23}}$ |
| Ho1 | 4b | 0.5 | 0 | 0 | 0.0056(17)<br>0 | 0.083(7)<br>-0.0054(14) | 0.0045(12)<br>0 |
| Ho2 | 8g | 0.2313(4) | 0.2412(6) | 0.75 | 0.0109(9)<br>0.0030(8) | 0.0041(6)<br>0 | 0.01476(13)<br>0 |
| Ta1 | 4a | 0 | 0 | 0 | 0.014(2)<br>0 | 0.0054(16)<br>0.0065(15) | 0.010(3)<br>0 |
| O1 | 16h | 0.3778(3) | 0.2965(7) | 0.9709(8) | 0.0139(14)<br>-0.0158(14) | 0.028(2)<br>0.0015(13) | 0.0137(13)<br>0.0002(18) |
| O2 | 4c | 0.0619(9) | 0 | 0.75 | 0.017(3)<br>0 | 0.009(3)<br>0 | 0.009(3)<br>0 |
| O3 | 4c | 0.6276(9) | 0 | 0.75 | 0.009(3)<br>0 | 0.0078(15)<br>0 | 0.011(3)<br>0 |

| | | | | | | | |
|---|---|---|---|---|---|---|---|
| O4 | 4c | 0.3624(8) | 0 | 0.75 | 0.002(1)<br>0 | 0.012(3)<br>0 | 0.0077(19)<br>0 |

| **$Ho_3TaO_7$** (PDF) | | **a (Å)** | **b (Å)** | **c (Å)** | | |
|---|---|---|---|---|---|---|
| *Fm-3m* (225) | | 5.2708(6) | 5.2708(6) | 5.2708(6) | | |
| **Atom** | **Wyckoff Site** | **x** | **y** | **z** | **Occupancy** | **Uiso** |
| Ho1 | 4a | 0 | 0 | 0 | 0.75 | 0.0201(3) |
| Ta1 | 4a | 0 | 0 | 0 | 0.25 | 0.0201(3) |
| O1 | 8c | 0.25 | 0.25 | 0.25 | 0.875 | 0.0590(5) |

| **$Tm_3TaO_7$** (PDF) | | **a (Å)** | **b (Å)** | **c (Å)** | | |
|---|---|---|---|---|---|---|
| *Fm-3m* (225) | | 5.2267(5) | 5.2267(5) | 5.2267(5) | | |
| **Atom** | **Wyckoff Site** | **x** | **y** | **z** | **Occupancy** | **Uiso** |
| Tm1 | 4a | 0 | 0 | 0 | 0.75 | 0.0215(3) |
| Ta1 | 4a | 0 | 0 | 0 | 0.25 | 0.0215(3) |
| O1 | 8c | 0.25 | 0.25 | 0.25 | 0.875 | 0.0627(5) |

| **$Yb_3TaO_7$** (PDF) | | **a (Å)** | **b (Å)** | **c (Å)** | | |
|---|---|---|---|---|---|---|
| *Fm-3m* (225) | | 5.2093(3) | 5.2093(3) | 5.2093(3) | | |
| **Atom** | **Wyckoff Site** | **x** | **y** | **z** | **Occupancy** | **Uiso** |
| Yb1 | 4a | 0 | 0 | 0 | 0.75 | 0.0234(3) |
| Ta1 | 4a | 0 | 0 | 0 | 0.25 | 0.0234(3) |
| O1 | 8c | 0.25 | 0.25 | 0.25 | 0.875 | 0.0623(3) |




**Supplementary Figure 5:** Overlayed $C222_1$ **(**$\Gamma_1$-) and C2/m ($\Gamma_3$+) $Ho_3TaO_7$ structural models from short-range PDF refinement performed at 100 K. Solid black lines indicate the respective unit cell while shaded brown regions represent $TaO_6$ octahedra. Ta and Ho cations in respective atomic sites in the $C222_1$ structure are indicated as solid dark brown and blue ellipsoids, while Ta and Ho cations in respective atomic sites in the C2/m structure are indicated as solid yellow and pink ellipsoids. The ellipsoids represent the extent of anisotropic thermal vibrations, $U_{11}$, $U_{22}$ and $U_{33}$.

**Supplementary Table 4:** Structural information for localized 100 K temperature short-range PDF data refinements. Unit cell parameters, fractional positional coordinates and thermal factors are followed by sigma values.

| **$Pr_3TaO_7$** (PDF, 100K) | | **a (Å)** | **b (Å)** | **c (Å)** | |
|---|---|---|---|---|---|
| *C2cm* (40) | | 10.988(4) | 7.490(3) | 7.681(3) | |
| **Atom** | **Wyckoff Site** | **x** | **y** | **z** | **Uiso** |
| Pr1 | 4a | 0.5042(14) | 0 | 0 | 0.0109(9) |
| Pr2 | 4b | 0.2300(7) | 0.2015(11) | 0.25 | 0.0042(8) |
| Pr3 | 4b | 0.2758(7) | 0.705(1) | 0.25 | 0.0034(6) |
| Ta1 | 4a | 0.0054(7) | 0 | 0 | 0.0047(3) |
| O1 | 8c | 0.8709(5) | 0.8254(7) | 0.037(1) | 0.0090(6) |
| O2 | 8c | 0.625 | 0.3059(6) | 0.4632(8) | 0.0053(4) |
| O3 | 4b | 0.1337(7) | 0.4686(9) | 0.25 | 0.0057(6) |
| O4 | 4b | 0.3751(6) | 0.9833(8) | 0.25 | 0.0046(6) |
| O5 | 4b | 0.9982(8) | 0.0716(6) | 0.25 | 0.0049(5) |

| **$Ho_3TaO_7$** (PDF, 100K) | | **a (Å)** | **b (Å)** | **c (Å)** | |
|---|---|---|---|---|---|
| *$C222_1$* (20) | | 10.486(5) | 7.419(3) | 7.445(2) | |
| **Atom** | **Wyckoff Site** | **x** | **y** | **z** | **Uiso** |
| Ho1 | 4a | 0 | 0.4810(7) | 0 | 0.0080(5) |
| Ho2 | 8c | 0.2349(3) | 0.2362(4) | 0.7451(7) | 0.0062(3) |
| Ta1 | 4a | 0 | 0.9960(7) | | 0.0029(4) |
| O1 | 8c | 0.3726(5) | 0.3122(7) | 0.9639(8) | 0.0098(7) |
| O2 | 8c | 0.3775(4) | 0.2899(5) | 0.5230(7) | 0.0060(6) |
| O3 | 4b | 0.0667(5) | 0 | 0.75 | 0.0073(5) |
| O4 | 4b | 0.6281(8) | 0 | 0.75 | 0.0076(5) |
| O5 | 4b | 0.3628(7) | 0 | 0.75 | 0.0084(8) |

| **$Ybr_3TaO_7$** (PDF, 100K) | | **a (Å)** | **b (Å)** | **c (Å)** | |
|---|---|---|---|---|---|
| *C2mm* (38) | | 10.558(4) | 7.171(3) | 7.443(3) | |
| **Atom** | **Wyckoff Site** | **x** | **y** | **z** | **Uiso** |
| Yb1 | 4c | 0.4799(5) | 0 | 0.7210(4) | 0.0104(4) |
| Yb2 | 4d | 0.2166(5) | 0.7499(8) | 0 | 0.0124(5) |
| Yb3 | 4e | 0.2289(5) | 0.2508(6) | 0.5 | 0.0077(5) |
| Ta1 | 4c | 0.9996(6) | 0 | 0.7328(6) | 0.0037(4) |
| O1 | 8f | 0.5929(6) | 0.2684(4) | 0.2656(5) | 0.0072(5) |
| O2 | 8f | 0.875000 | 0.7589(8) | 0.1839(5) | 0.0116(6) |
| O3 | 2a | 0.0379(11) | 0 | 0 | 0.012(2) |
| O4 | 2b | 0.9520(8) | 0 | 0.5 | 0.007(1) |
| O5 | 2a | 0.6156(13) | 0 | 0 | 0.019(1) |
| O6 | 2b | 0.3598(13) | 0 | 0.5 | 0.019(1) |
| O7 | 2a | 0.3755(18) | 0 | 0 | 0.019(1) |
| O8 | 2b | 0.6089(16) | 0 | 0.5 | 0.019(1) |