Structural characterisation of ferroelectric $Ag_2Nb_4O_{11}$ and dielectric $Ag_2Ta_4O_{11}$

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Electronic Supplementary Information

Table S1. R_{wp} and R_p (background subtracted); χ^2, $R(F^2)$ for space groups *R*3*c*, *R*32 and *R*3 as a function of temperature.

Temp (K)	*R*3*c* (N° 161)				*R*32 (N° 155)				*R*3 (N° 146)			
	R_{wp}	R_p	$R(F^2)$	χ^2	R_{wp}	R_p	$R(F^2)$	χ^2	R_{wp}	R_p	$R(F^2)$	χ^2
343	4.55	3.56	3.08	3.429	4.51	3.50	2.90	3.363	–	–	–	–
298	4.85	3.85	3.48	4.359	4.86	3.86	3.41	4.419	–	–	–	–
223	4.69	3.76	3.22	4.449	4.76	3.83	4.64	4.750	–	–	–	–
198	4.23	3.34	3.35	3.724	4.51	3.64	6.68	4.505	–	–	–	–
173	4.29	3.41	3.84	3.926	4.63	3.78	6.03	4.838	4.34	3.47	3.69	3.914
123	4.48	3.63	3.76	4.240	4.85	4.02	6.50	5.318	4.55	3.68	3.74	4.231
10	4.64	3.77	3.87	4.679	5.08	4.21	5.74	5.933	4.66	3.78	3.77	4.606

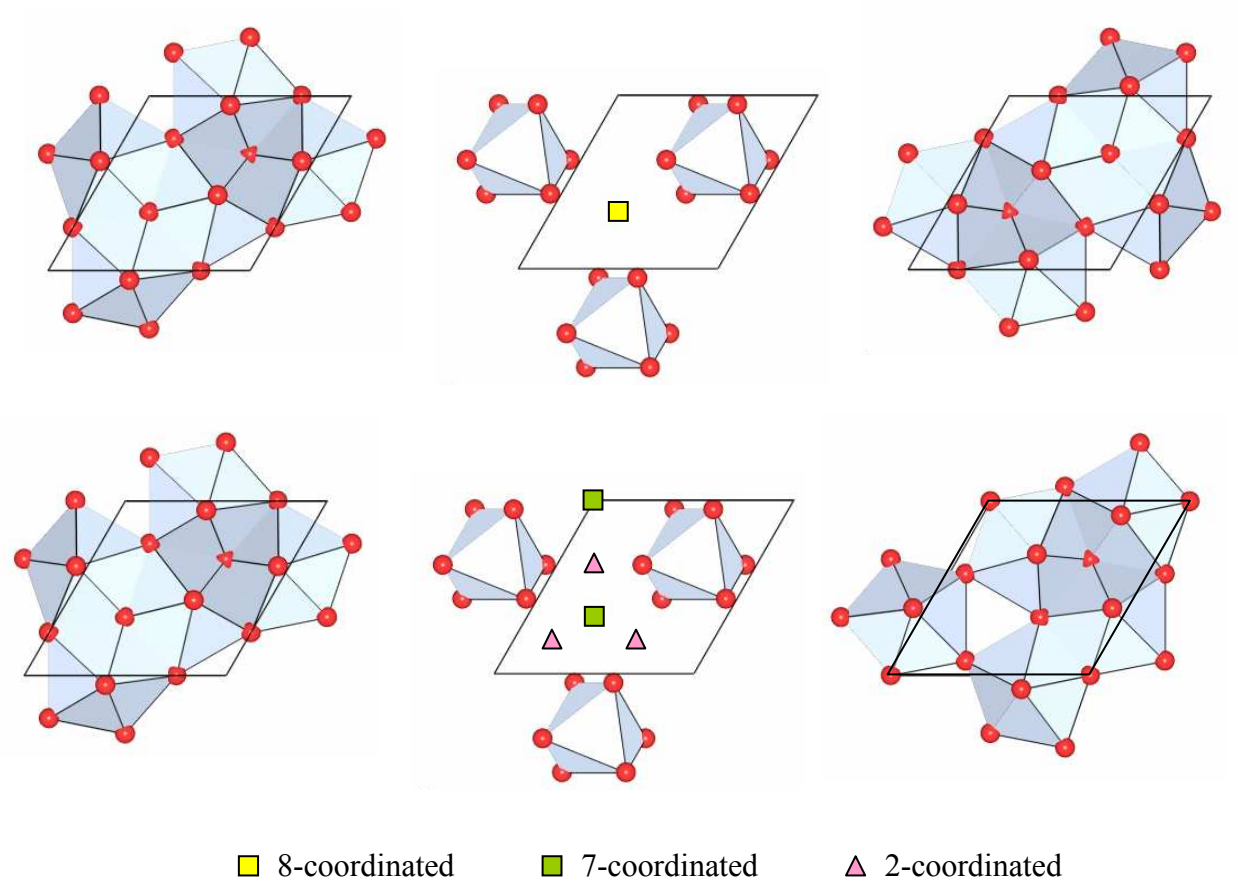

Fig S1. Successive pentagonal bipyramid layers forming octahedral sites suitable for Nb/Ta atoms and a range of coordination sites (2, 7 and 8) for extra metal atoms.
Eight coordinated sites are created if two consecutive MO_7 layers are not shifted whereas two and seven coordinated sites are created by a translation of the upper layer relative to the lower one.

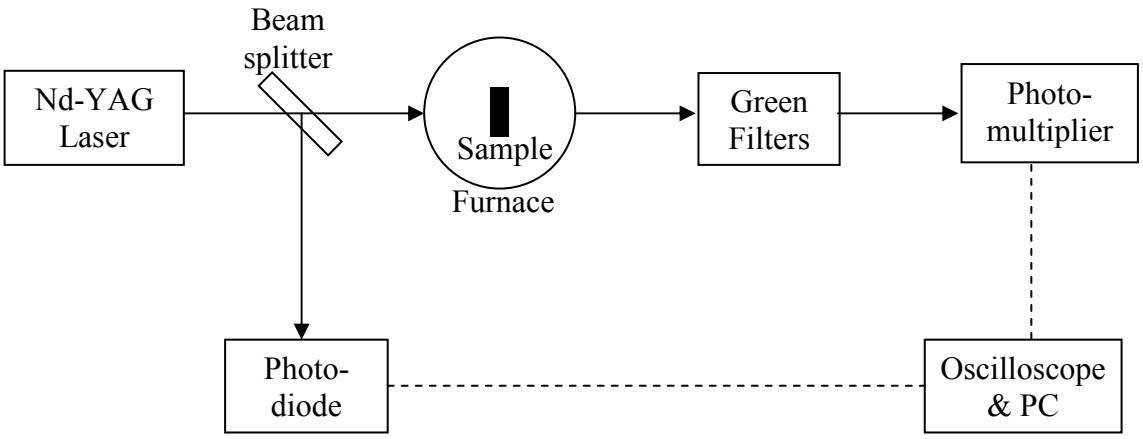

Fig S2. Experimental set-up for second harmonic generation.

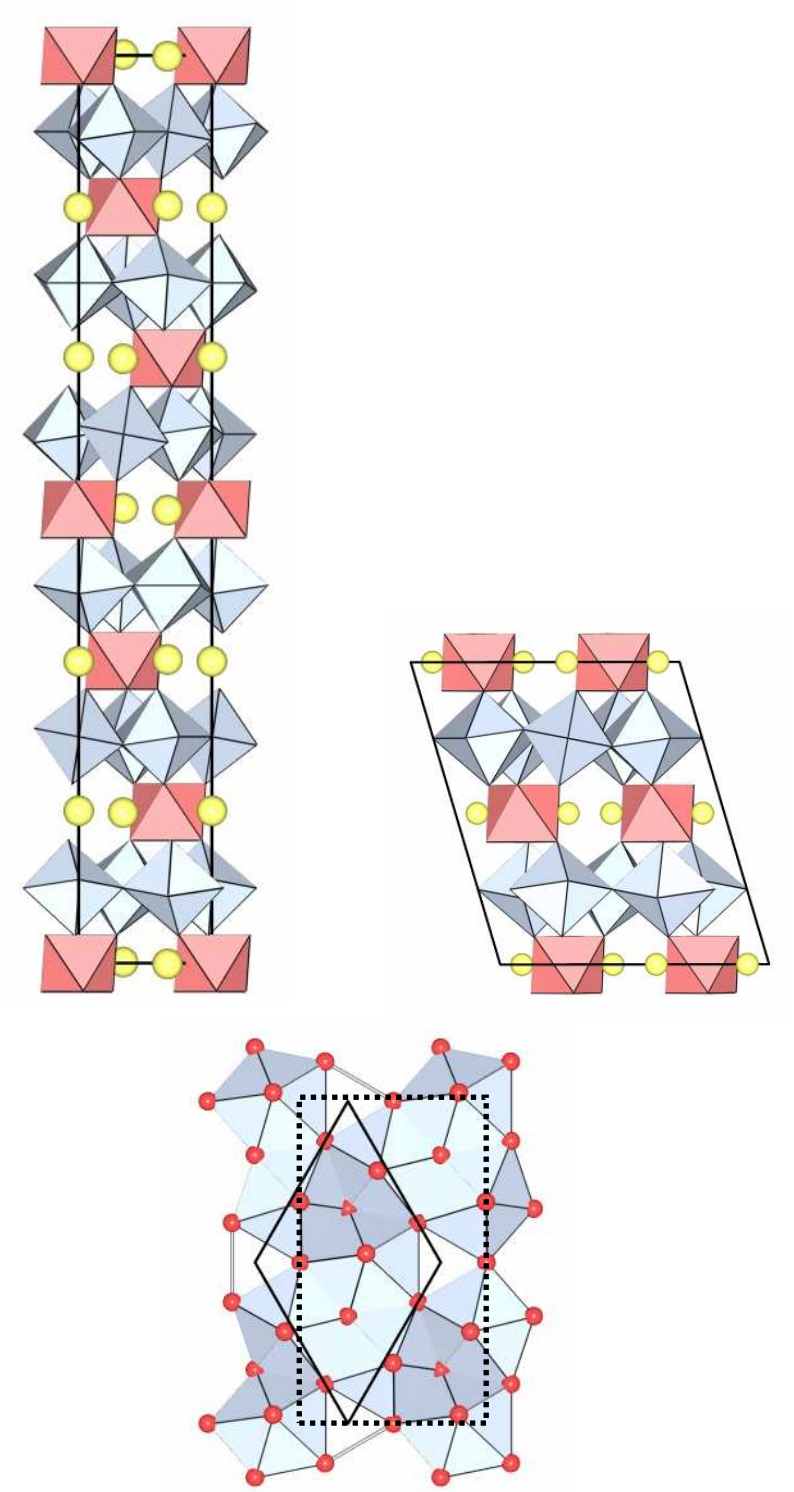

Fig S3. Projection of the hexagonal–*R* (on to the *yz* plane) and monoclinic (on to the *xz* plane) unit cells (top). Octahedra and pentagonal bypyramids are shown in red and blue, respectively, and Ag atoms in yellow. (Bottom) Hexagonal–*R* (solid line) and monoclinic (dashed line) unit cells are shown within a layer of pentagonal bipyramids.

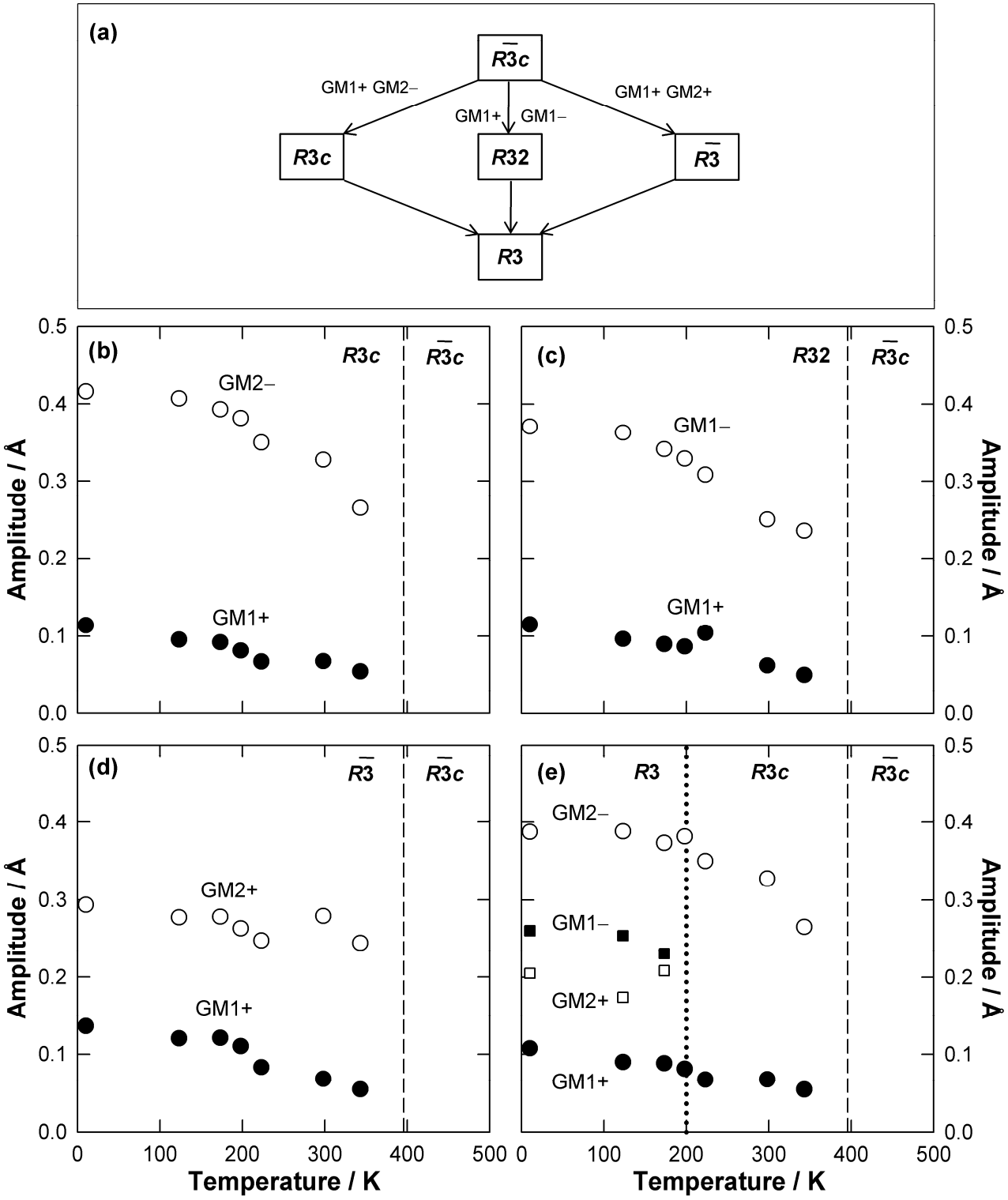

Fig S4. (a) Maximal subgroups and distortion modes of *R*–3*c*. Global amplitude of the distortion modes *vs* temperature for maximal subgroups (b) *R*3*c*, (c) *R*32, (d) *R*–3 and (e) *R*3.

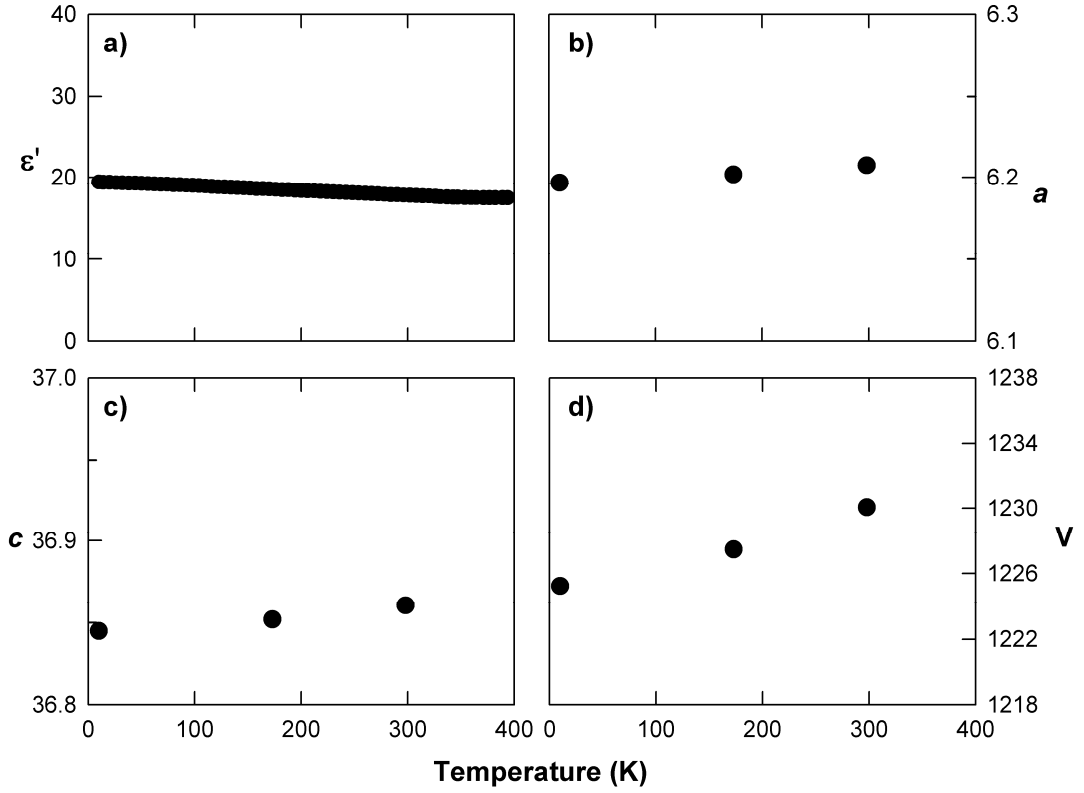

Fig S5. (a) Permittivity ε' at 1 MHz, (b,c) lattice parameters (in Å) and (d) unit cell volume (in $Å^3$) *vs* temperature for $Ag_2Ta_4O_{11}$.

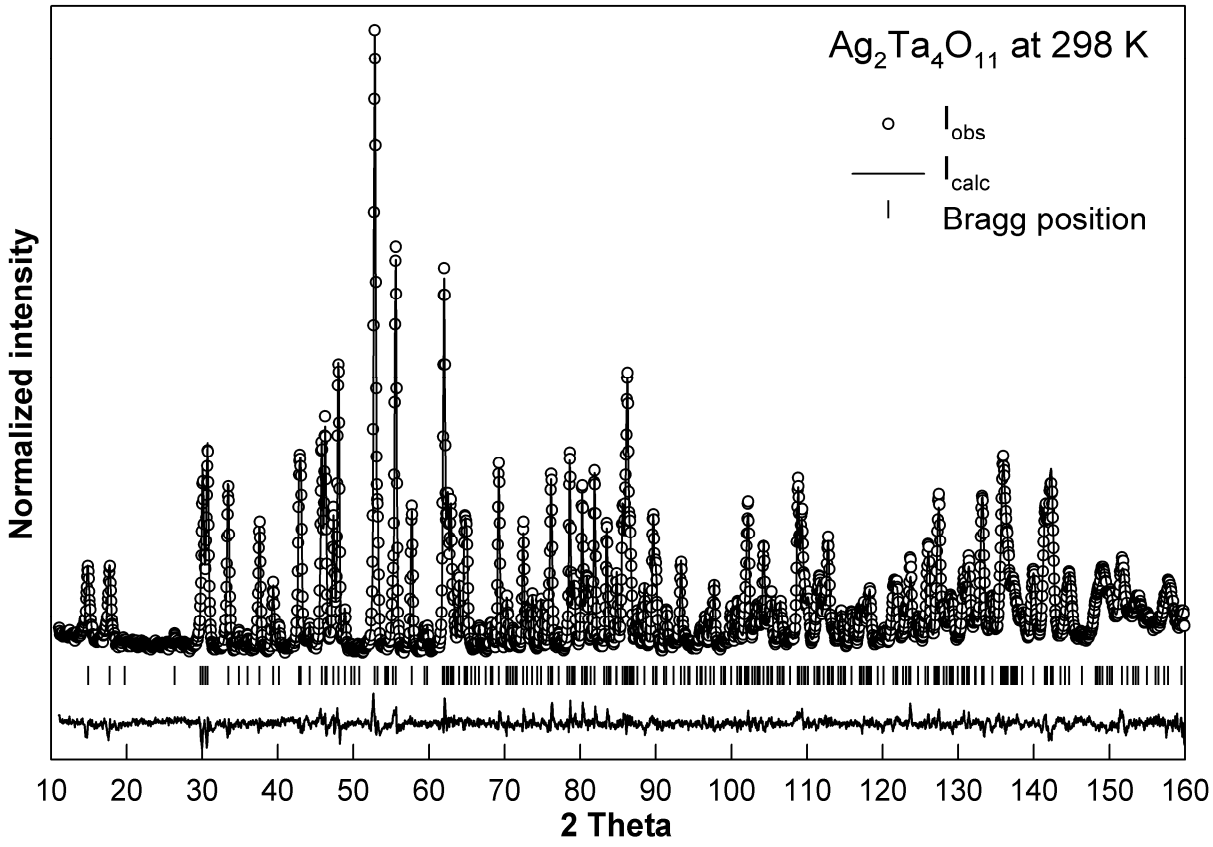

Fig S6. Experimental, calculated and difference ND patterns for $Ag_2Ta_4O_{11}$ at 298 K.