Supplementary Information

Synergistic influence of d^0 (Nb^{5+}) and d^{10} (Cd^{2+}) cations in stabilizing non-centrosymmetric Dion-Jacobson layered perovskites, $A'Cd_2Nb_3O_{10}$ (A′ = Rb, Cs)

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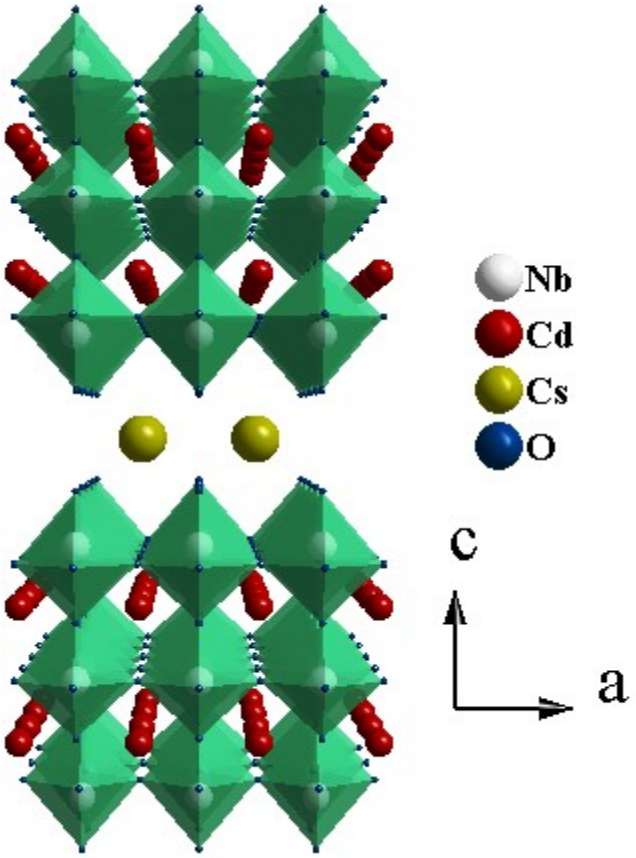

Figure S1 Crystal structure of $CsCd_2Nb_3O_{10}$ generated from the solution of single crystal X-ray diffraction measurements.

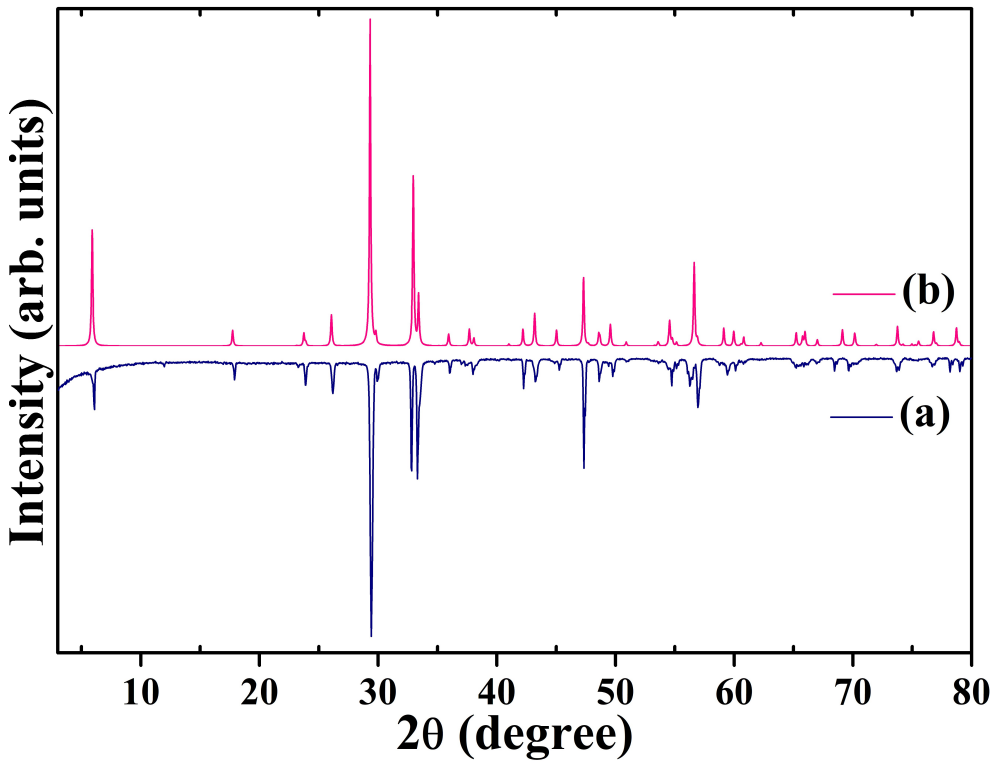

Figure S2 PXRD patterns (a) obtained for the bulk polycrystalline and (b) simulated using the SXRD solution of $CsCd_2Nb_3O_{10}$.

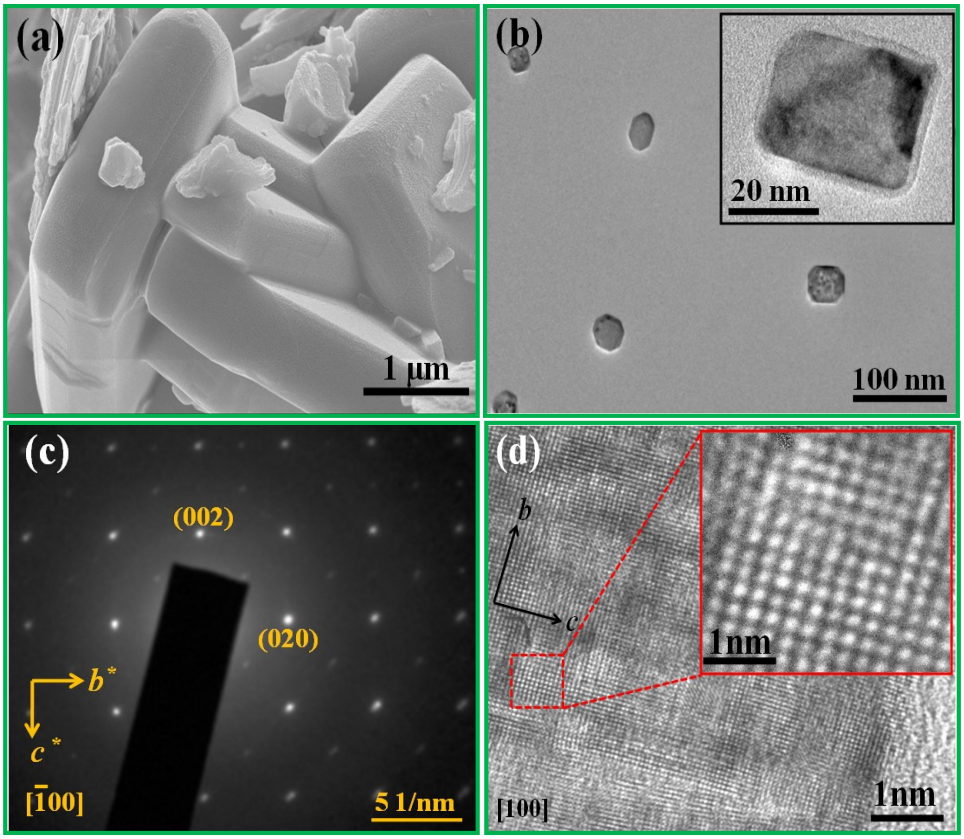

Figure S3 (a) FESEM, (b) TEM images, (c) SAED along [$\bar{1}$00] and (d) HRTEM pattern along [100] zone axes of $CsCd_2Nb_3O_{10}$ sample.

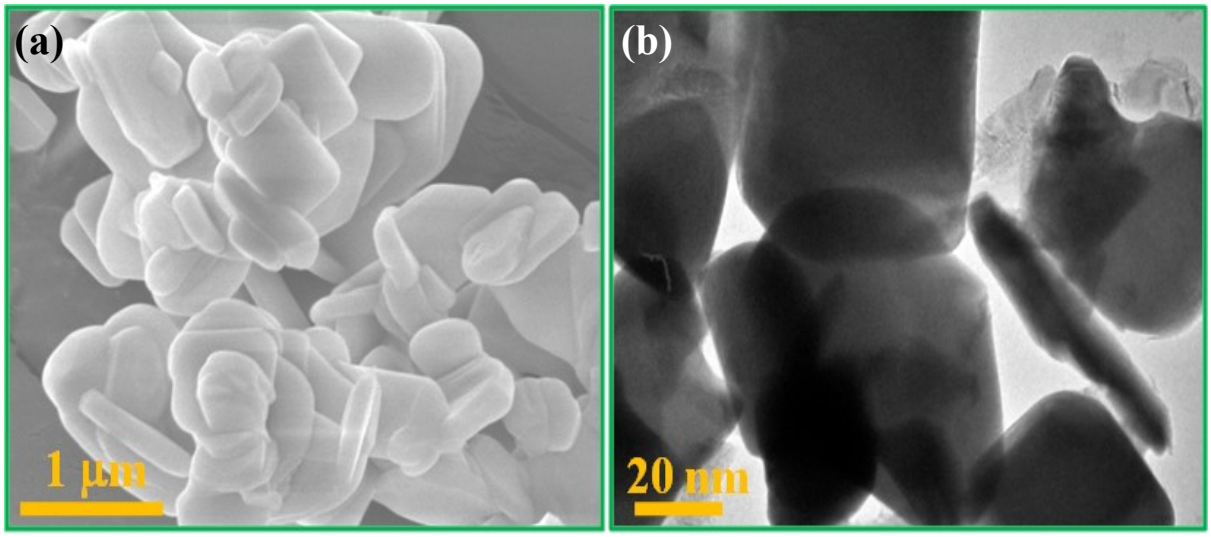

Figure S4 (a) FESEM and (b) TEM images of $RbCd_2Nb_3O_{10}$.

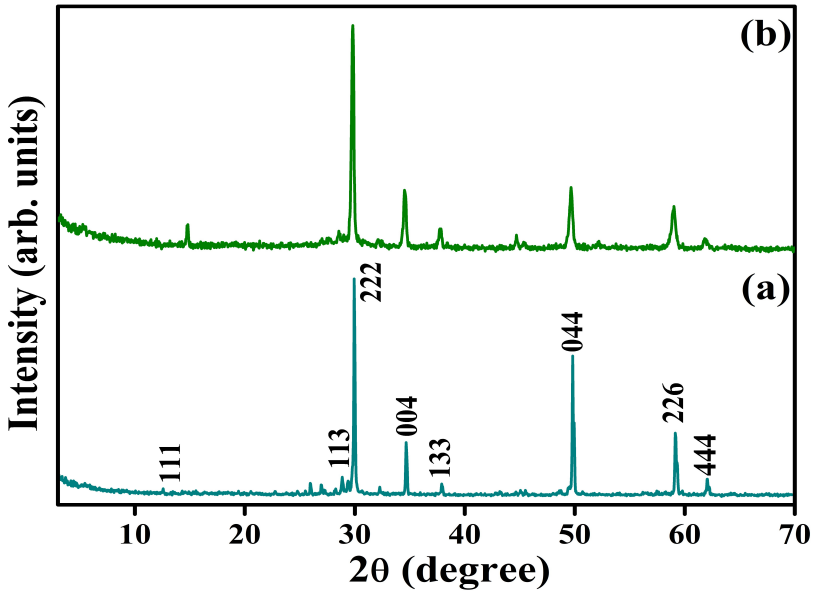

Figure S5 PXRD pattern of products obtained after calcination of (a) $RbCd_2Nb_3O_{10}$ and (b) $CsCd_2Nb_3O_{10}$ at 1075 °C.

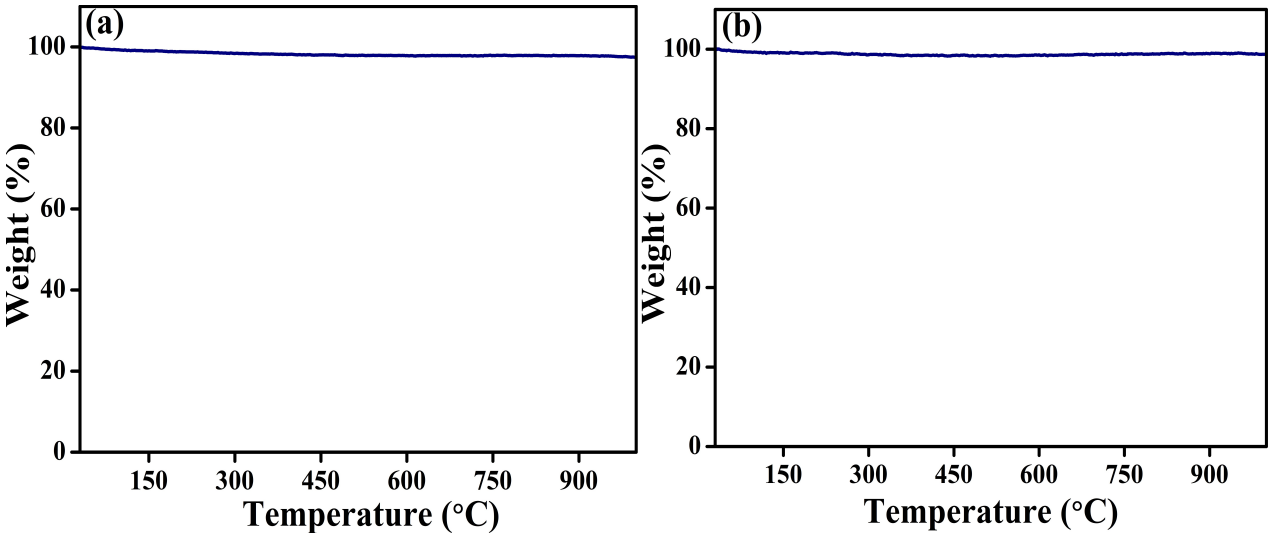

Figure S6 TG curves for the polycrystalline (a) $RbCd_2Nb_3O_{10}$ and (b) $CsCd_2Nb_3O_{10}$ samples.

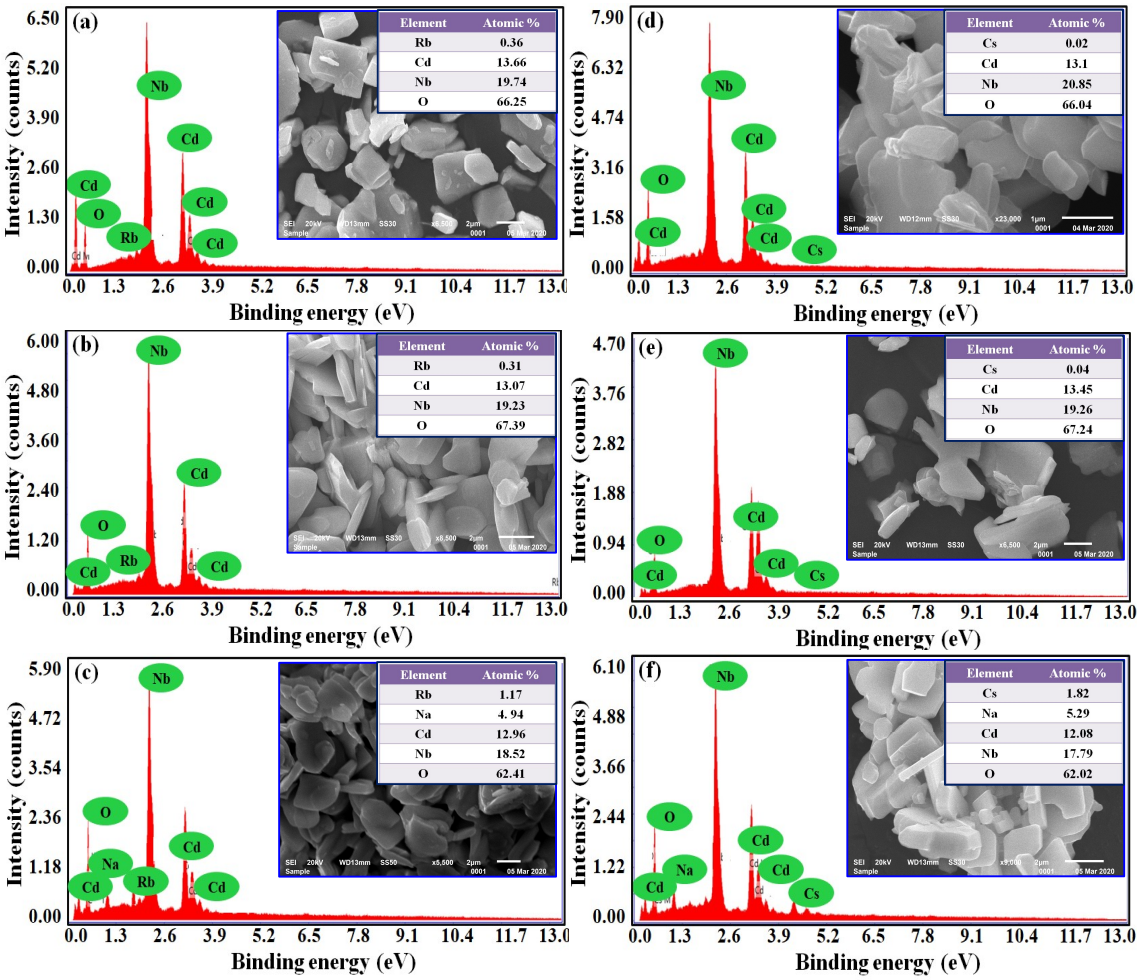

Figure S7 EDS spectra of (a) H^+, (b) Li^+ and (c) Na^+-exchanged products of $RbCd_2Nb_3O_{10}$. Inset shows their respective SEM image and elemental analysis table. The corresponding spectra for products obtained from $CsCd_2Nb_3O_{10}$ are shown in (d), (e) and (f).

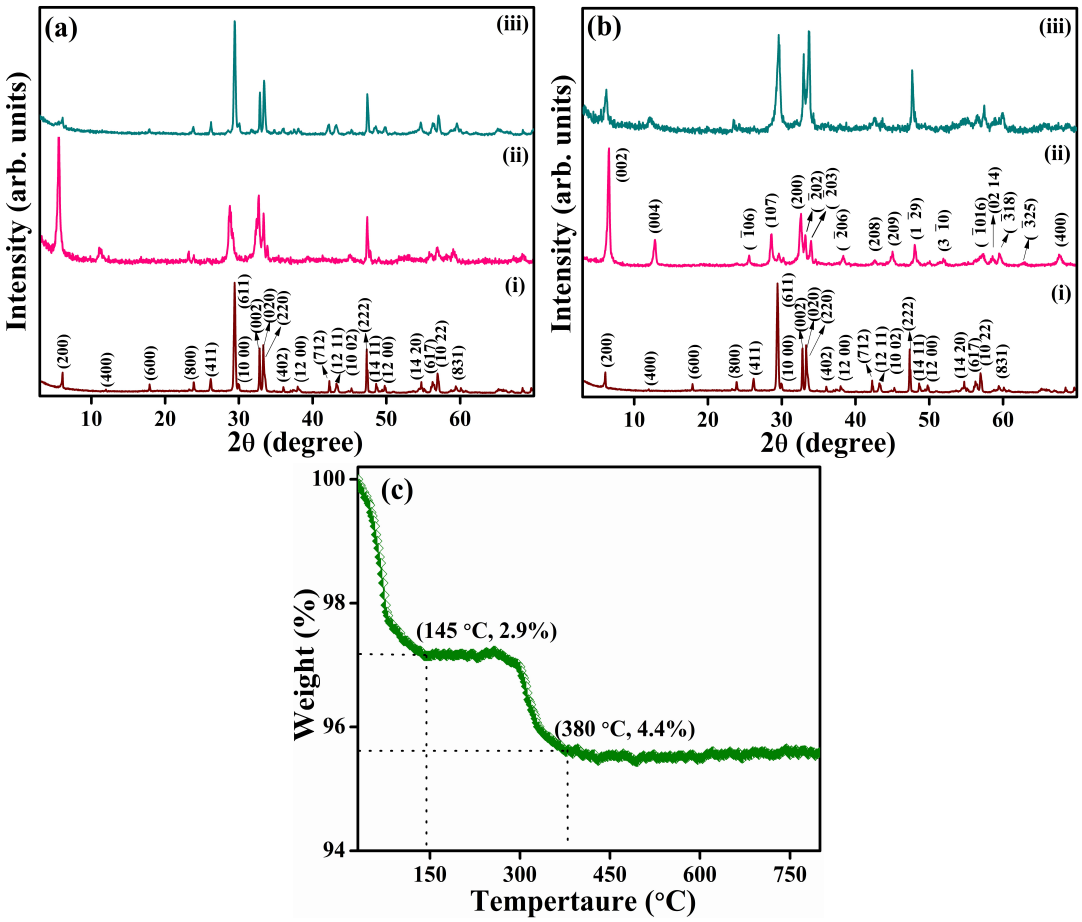

Figure S8 (a) PXRD patterns of (i) $CsCd_2Nb_3O_{10}$, (ii) H^+-exchanged and (iii) the regenerated product obtained after treatment of H^+-exchanged sample with a solution of 0.5 M $CsNO_3$. (b) PXRD patterns of (i) $CsCd_2Nb_3O_{10}$, (ii) Li^+-exchanged product and (iii) the regenerated product obtained after treatment of the Li^+-exchanged sample with a solution of 0.5 M $CsNO_3$. (c) TG curve for H^+-exchanged sample.

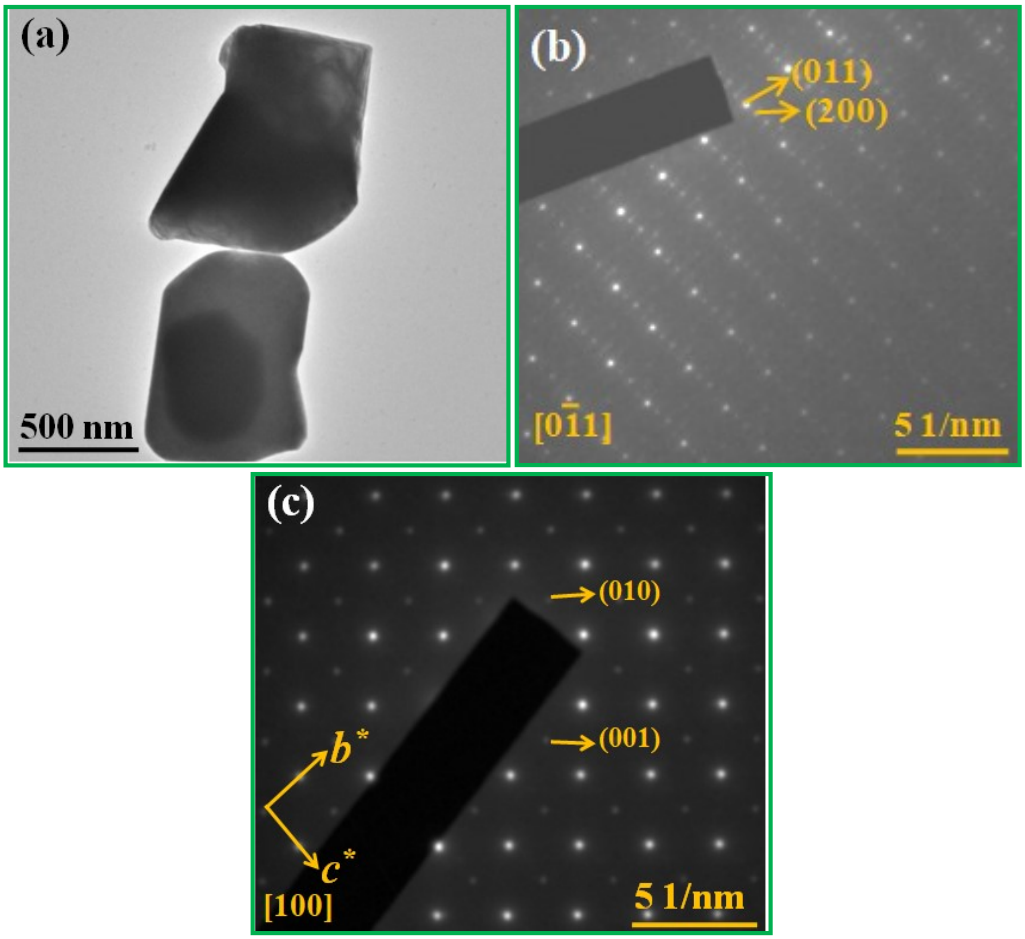

Figure S9 (a) TEM image and (b) & (c) represents SAED pattern along [0$\bar{1}$1] & [100] zone axes of $HCd_2Nb_3O_{10}$.

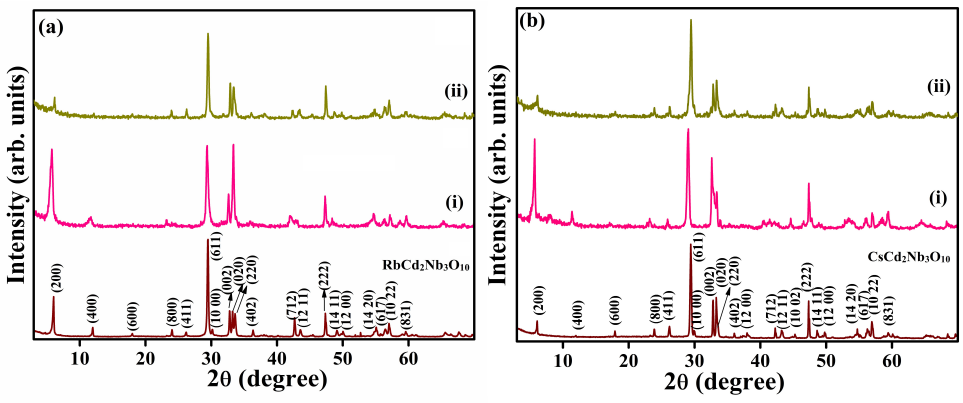

Figure S10 PXRD patterns of products of ion exchange reactions of (a) $RbCd_2Nb_3O_{10}$ and (b) $CsCd_2Nb_3O_{10}$ with (i) Na^+ ions and (ii) K^+ ions.

Table S1 Crystallographic parameters of $CsCd_2Nb_3O_{10}$ from SXRD

Crystal Data			
Formula	$CsCd_2Nb_3O_{10}$	**Largest diff. peak and hole [e /Å^3]**	3.22/-5.84
Crystal system	Tetragonal	**Scan mode**	ω scan
Space Group	*P4/mmm* (123)	**Min/Max Bragg angle [°]**	4.0783–29.2618
***a* [Å]**	3.8440(8)	***hkl* range**	-5 → 5, -4 → 4, -18→20
***b* [Å]**	3.8440(8)	**F(000)**	354
***c* [Å]**	14.990(5)	**μ (mm^{-1})**	12.576
V [Å^3]	221.51(12)	**R_{int}**	0.1068
Z	1	**R_{sigma}**	0.0531
ρ calc [g/cm^3]	5.971	**Refinement**	F2
Morphology	Rectangular	**No. of reflections used**	2817
Colour	Colorless	**Unique reflections**	234
Dimensions (mm)	0.08× 0.05 × 0.04	**Number of parameters**	19
Temperature [K]	150(2)	**R[F^2> 2σ(F^2)]**	0.0738
Wavelength [Mo K_α][Å]	0.71073	**wR_2**	0.1546
Monochromator	Graphite	**GOF**	1.237
Extinction Coefficient	0.007(3)		

Table S2 Positional and thermal parameters of $CsCd_2Nb_3O_{10}$ in S.G. *P4/mmm*.

Atom	***Wyckoff position***	***x/a***	***y/b***	***z/c***	**SOF**	$\mathbf{U_{(iso)}}$ **Å^2**
Cs	1*d*	0.5	0.5	0.5	1	0.017(1)
Cd	2*h*	-0.5	-0.5	0.1452(1)	1	0.0129(9)
Nb1	1*a*	0.0	0.0	0.0	1	0.008(1)
Nb2	2*g*	0.0	0.0	0.2803(2)	1	0.013 (1)
O1	2*g*	0.0	0.0	0.395(4)	1	0.062(14)
O2	4*i*	0.0	0.5	0.253(3)	1	0.10 (1)
O3	2*g*	0.0	0.0	0.123(6)	1	0.14 (3)
O4	2*f*	0.0	0.5	0.0	1	0.22(5)

Table S3 Selected bond distances (in Å) of $CsCd_2Nb_3O_{10}$ in S.G. *P4/mmm*.

Atoms	**Bond distance (Å)**
Cs–O1 × 8	3.14(3)
Nb1–O3 × 2	1.85(9)
Nb1–O4 × 4	1.9220(4)
Nb2–O1	1.72(5)
Nb2–O2 × 4	1.964(9)
Nb2–O3	2.36(9)
Cd–O2 × 4	2.51(3)
Cd–O3 × 4	2.73(1)
Cd–O4 × 4	2.90(1)