

Table 1. Refined lattice parameters of Cs₂NaScCl₆ obtained from CELREF3.

Parameter	Value	Standard error
Zero shift (°)	0.000	0.0000
Wavelength λ (Å)	1.54060	0.00000
a (Å)	10.4871	0.0207
b (Å)	10.4871	0.0000
c (Å)	10.4871	0.0000
α (°)	90.00	0.000
β (°)	90.00	0.000
γ (°)	90.00	0.000
Unit cell volume (Å ³)	1153.37	2.280
RMS deviation (2 θ)	0.0267	—
RMS deviation / Nref	0.0252	—

Table 2. Gaussian fitting parameters of the room-temperature PL spectra.

Parameter	Dark	Under illumination	Physical meaning
Amplitude (A)	0.944	0.755	Peak intensity of the STE emission band
Peak position, λ_0 (nm)	453.1	453.1	Maximum of the STE emission (no spectral shift)
σ (nm)	31.41	31.41	Standard deviation of the Gaussian profile
FWHM (nm)	73.97	73.98	Band broadening due to exciton–phonon coupling
Baseline (C)	0.0308	0.0246	Residual background intensity

Table 3. Pseudo-Voigt fitting parameters of the Raman modes.

Mode (cm ⁻¹)	Condition	Position (cm ⁻¹)	FWHM (cm ⁻¹)	Amplitude (a.u.)	Lorentzian Fraction g	Notes
F _{2g} (lattice)	Dark	51.00	6.21	1123	0.42	Bulk lattice vibration
	Light	51.00	6.19	1032	0.41	Slight amplitude decrease
A _{1g} (sym. breathing)	Dark	147.02	8.54	2015	0.57	Strongest mode
	Light	147.02	8.53	1854	0.57	8–10% amplitude drop
E _g (bending)	Dark	209.01	7.80	1543	0.48	No shift observed
	Light	209.01	7.78	1421	0.48	Stable under illumination
F _{2g} (stretching)	Dark	292.05	9.10	980	0.51	Octahedral stretching
	Light	292.05	9.09	905	0.50	Fully invariant frequency

Table 4. Equivalent-circuit ($R_1 \parallel CPE_1$) fitting parameters extracted from Nyquist plots.

Temperature (K)	R_1 (Ω)	CPE_1 -T ($F \cdot s^{(P-1)}$)	CPE_1 -P
300 K	3.84×10^4	8.65×10^{-7}	0.942
325 K	3.76×10^3	1.08×10^{-6}	0.927
350 K	1.55×10^3	5.82×10^{-7}	1.022
375 K	2.40×10^2	6.55×10^{-7}	1.017