

Supporting Information for “Optical Phonon Modes and Dielectric Behavior of $\text{Sr}_{1-3x/2}\text{Ce}_x\text{TiO}_3$ Microwave Ceramics”, by R.L. Moreira *et al.* (2007)

Tables – Fitting parameters obtained by using the four-parameter semi-quantum model [1] for the infrared reflectivity spectra of $\text{Sr}_{1-3x/2}\text{Ce}_x\text{TiO}_3$ ceramics and SrTiO_3 single crystal. Frequencies (Ω) and widths (γ) are in cm^{-1} . $\Delta\epsilon$ and $\Delta\eta$ measure, respectively, the amplitude of each TO and LO branch.

SrTiO₃(single crystal)

Ω_{TO}	γ_{TO}	Ω_{LO}	γ_{LO}	$\Delta\epsilon$	$\Delta\eta$
92.396	14.017	171.032	4.519	286.108489	0.000295
173.941	6.714	474.993	5.496	3.673827	0.030790
545.028	17.786	795.814	24.950	1.532589	0.149115
$\epsilon_\infty = 5.448$				$\epsilon_0 = 297$	

x = 0.133

Ω_{TO}	γ_{TO}	Ω_{LO}	γ_{LO}	$\Delta\epsilon$	$\Delta\eta$
112.766	24.190	175.238	12.000	158.026690	0.000566
180.970	12.928	471.181	8.656	6.537339	0.037300
549.902	21.274	780.379	26.462	1.472287	0.148834
$\epsilon_\infty = 5.194$				$\epsilon_0 = 171$	

x = 0.143

Ω_{TO}	γ_{TO}	Ω_{LO}	γ_{LO}	$\Delta\epsilon$	$\Delta\eta$
115.313	27.745	175.855	14.000	146.966876	0.000635
182.366	15.196	471.181	8.925	7.297565	0.037869
550.794	21.931	779.435	26.948	1.467924	0.148498
$\epsilon_\infty = 5.176$				$\epsilon_0 = 161$	

x = 0.154

Ω_{TO}	γ_{TO}	Ω_{LO}	γ_{LO}	$\Delta\epsilon$	$\Delta\eta$
114.585	34.918	175.955	17.000	143.283656	0.000742
183.274	19.236	471.326	9.733	7.741426	0.038468
549.782	22.726	778.164	28.597	1.415062	0.152829
$\epsilon_\infty = 5.041$				$\epsilon_0 = 157$	

x = 0.167

Ω_{TO}	γ_{TO}	Ω_{LO}	γ_{LO}	$\Delta\epsilon$	$\Delta\eta$
118.301	34.561	175.212	17.000	132.315721	0.000763
183.265	20.346	471.292	9.952	8.951070	0.038309
550.604	21.926	776.927	28.447	1.436789	0.149560
$\epsilon_\infty = 5.118$				$\epsilon_0 = 148$	

x = 0.182

Ω_{TO}	γ_{TO}	Ω_{LO}	γ_{LO}	$\Delta\epsilon$	$\Delta\eta$
119.735	32.586	176.071	16.000	130.420782	0.000743
184.057	18.599	471.390	10.475	8.948010	0.037905
550.664	21.611	776.012	29.863	1.448517	0.147433
$\epsilon_\infty = 5.183$				$\epsilon_0 = 146$	

x = 0.200

Ω_{TO}	γ_{TO}	Ω_{LO}	γ_{LO}	$\Delta\varepsilon$	$\Delta\eta$
121.583	38.019	177.186	19.000	120.700462	0.000844
186.055	22.280	471.510	11.184	9.377360	0.039132
551.325	22.743	774.251	29.828	1.410006	0.149681
$\varepsilon_\infty = 5.077$			$\varepsilon_0 = 137$		

x = 0.222

Ω_{TO}	γ_{TO}	Ω_{LO}	γ_{LO}	$\Delta\varepsilon$	$\Delta\eta$
124.687	32.928	176.277	16.000	115.310675	0.000755
184.834	19.569	471.648	11.996	9.833714	0.038661
551.412	22.969	772.956	32.097	1.421909	0.147143
$\varepsilon_\infty = 5.151$			$\varepsilon_0 = 132$		

x = 0.250

Ω_{TO}	γ_{TO}	Ω_{LO}	γ_{LO}	$\Delta\varepsilon$	$\Delta\eta$
127.110	33.251	180.556	17.000	108.004461	0.000844
189.555	18.091	471.923	13.165	9.222710	0.039772
552.285	23.078	770.736	32.884	1.388069	0.148211
$\varepsilon_\infty = 5.078$			$\varepsilon_0 = 124$		

x = 0.286

Ω_{TO}	γ_{TO}	Ω_{LO}	γ_{LO}	$\Delta\varepsilon$	$\Delta\eta$
128.090	39.507	179.823	20.000	101.854744	0.000904
189.471	22.829	472.575	17.845	9.772044	0.040532
551.827	28.100	768.512	41.813	1.330195	0.151754
$\varepsilon_\infty = 4.959$			$\varepsilon_0 = 118$		

x = 0.333

Ω_{TO}	γ_{TO}	Ω_{LO}	γ_{LO}	$\Delta\varepsilon$	$\Delta\eta$
131.549	32.977	178.273	16.000	96.664487	0.000798
187.743	19.402	473.445	15.911	10.713089	0.040422
552.917	25.020	761.697	33.564	1.320746	0.144701
$\varepsilon_\infty = 5.136$			$\varepsilon_0 = 114$		

x = 0.400

Ω_{TO}	γ_{TO}	Ω_{LO}	γ_{LO}	$\Delta\varepsilon$	$\Delta\eta$
139.823	34.670	177.424	17.000	76.315460	0.000829
189.061	22.740	475.827	21.354	14.156426	0.040023
551.894	27.095	756.196	39.761	1.235329	0.146701
$\varepsilon_\infty = 5.053$			$\varepsilon_0 = 97$		

[1] Gervais, F.; Echegut, P., in *Incommensurate phases in dielectrics*; Blinc, R., Levanyuk, A. P., Eds.; North-Holland: Amsterdam, 1986; p 337.

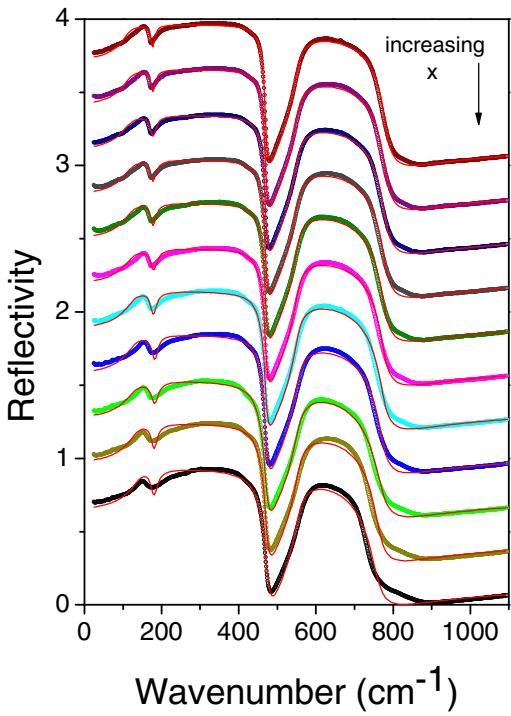


Figure S1. Infrared reflectivity spectra (circles) with their corresponding fitting (solid curves) by the four-parameter semi-quantum model, for $\text{Sr}_{1-3x/2}\text{Ce}_x\text{TiO}_3$ ceramics. The spectra were vertically shifted for clarity. The fittings were done using the three cubic phonon modes.

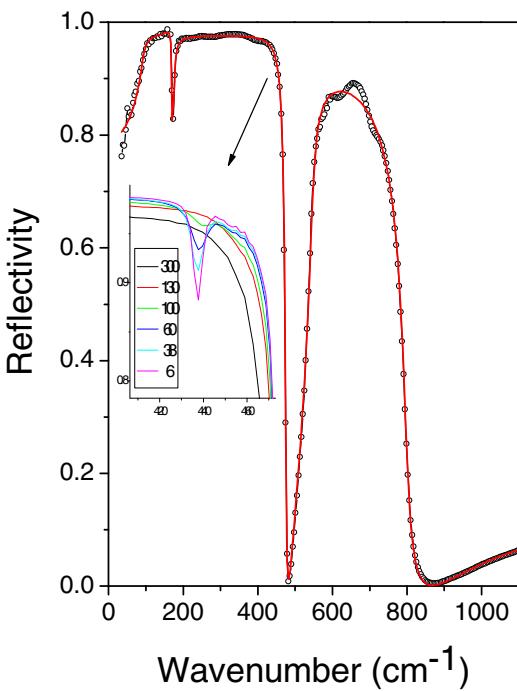


Figure S2. Experimental (circles) and adjusted (solid red line) infrared spectra of a ST single crystal. The inset shows a zoom of low-temperature spectra around the dip appearing below 120K (at the cubic-to-tetragonal transition).

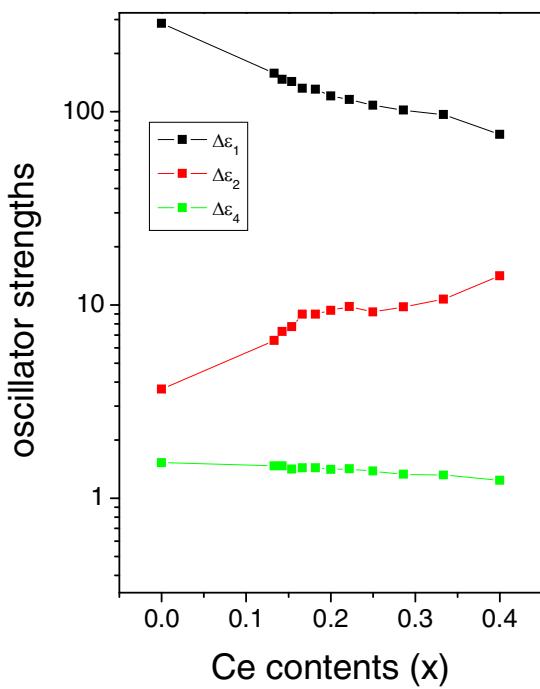


Figure S3. Ce-contents exponential dependences of the oscillator strengths ($\Delta\epsilon$) of the three adjusted modes for the $\text{Sr}_{1-3x/2}\text{Ce}_x\text{TiO}_3$ (SCT) ceramics and ST single crystal.

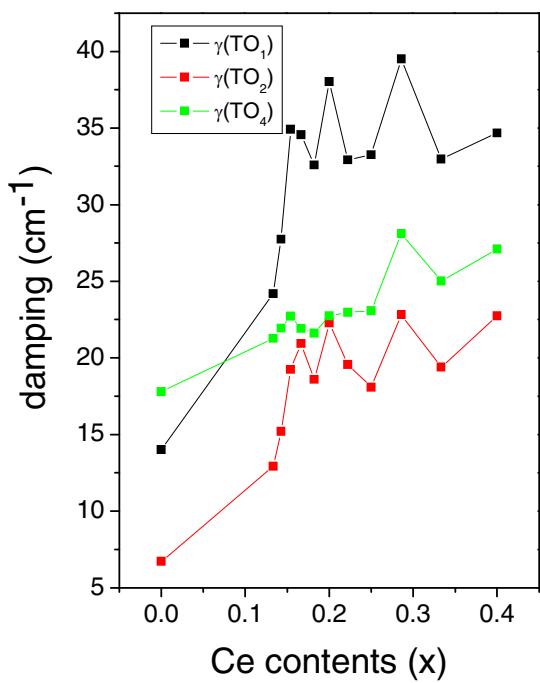


Figure S4. Increasing of the adjusted transverse-mode phonon widths of the SCT ceramics and ST single crystal with x . Note the large fluctuations (low accuracy) of the damping values because of using only three modes for the fittings.