

Supplementary material for “Si-compatible candidates for high-K dielectrics with the Pbnm perovskite structure”

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In this supplemental material we present the results of our calculations of the zone-center phonon frequencies, as well as the infrared activities for those modes that are infrared-active, for the compounds considered in the main article.

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I. SUPPLEMENT: PHONON PROPERTIES

As stated in the main text, in the frequency range of the lattice vibrations, the dielectric tensor $\epsilon_{\alpha\beta}$ can be decomposed as

$$\epsilon_{\alpha\beta}(\omega) = \epsilon_{\alpha\beta}^{\text{el}} + \epsilon_{\alpha\beta}^{\text{ion}}(\omega), \quad (1)$$

where $\epsilon_{\alpha\beta}^{\text{el}}$ is the purely electronic contribution (assumed to be independent of frequency in this range) and $\epsilon_{\alpha\beta}^{\text{ion}}(\omega)$ is the ionic (or lattice) contribution. The values of the electronic contributions are given in the main text, and also repeated in this Supplement in Table I for completeness.

The ionic contribution can be reconstructed from the information given in Tables II, III and IV using the relation

$$\epsilon_{\alpha\beta}^{\text{ion}}(\omega) = \Omega_0^2 \sum_n \frac{Z_{\alpha}^{\star n} Z_{\beta}^{\star n}}{\omega_n^2 - \omega^2}, \quad (2)$$

where

$$Z_{\alpha}^{\star n} = \sum_{i\beta} \frac{1}{\sqrt{M_i}} Z_{i,\alpha\beta} \zeta_{i\beta}^n \quad (3)$$

is the dimensionless mode dynamical charge and

$$\Omega_0 = \sqrt{\frac{4\pi e^2}{Vm_0}} \quad (4)$$

has units of a plasma frequency. Here ω_n is the phonon frequency, $Z_{i,\alpha\beta}$ is the atomic Born effective-charge tensor, $\zeta_{i\beta}^n$ is the dimensionless eigenvector of the dynamical matrix normalized to unity, M_i is the mass of i -th ion in atomic mass units, e is the electron charge, V is the unit cell volume, and m_0 is the atomic mass unit.

The values of Ω_0 are reported in Table II. The results for the frequencies ω_n and for the activities of the infrared-active modes are presented in Tables III and

IV for simple perovskites and double perovskites respectively. For the infrared-active modes, note that only the non-zero elements of the $Z_{\alpha}^{\star n}$ tensor are reported.

TABLE I: Electronic part of the dielectric tensors for the compounds considered.

	Electronic part				Electronic part			
	$\epsilon_{xx}^{\text{el}}$	$\epsilon_{yy}^{\text{el}}$	$\epsilon_{zz}^{\text{el}}$		$\epsilon_{xx}^{\text{el}}$	$\epsilon_{yy}^{\text{el}}$	$\epsilon_{zz}^{\text{el}}$	
LaScO ₃	5.0	5.0	4.8	LaTmO ₃	4.6	4.6	4.3	
PrScO ₃	5.0	5.0	4.8	LaYbO ₃	4.6	4.5	4.3	
NdScO ₃	5.0	4.9	4.7	LaLuO ₃	4.6	4.5	4.3	
SmScO ₃	4.9	4.9	4.7	CeTmO ₃	4.6	4.6	4.3	
GdScO ₃	4.9	4.8	4.6	CeYbO ₃	4.6	4.6	4.3	
TbScO ₃	4.8	4.8	4.6	CeLuO ₃	4.6	4.5	4.3	
DyScO ₃	4.8	4.8	4.5	PrYbO ₃	4.6	4.5	4.3	
LaYO ₃	4.7	4.6	4.3	PrLuO ₃	4.6	4.5	4.3	
CaZrO ₃	4.6	4.7	4.6	NdLuO ₃	4.6	4.5	4.3	
SrZrO ₃	4.6	4.6	4.6	La ₂ MgZrO ₆	4.8	4.6	4.5	-0.06
SrHfO ₃	4.3	4.3	4.3	La ₂ MgHfO ₆	4.6	4.5	4.4	-0.05
LaHoO ₃	4.7	4.6	4.3	La ₂ CaZrO ₆	4.7	4.6	4.4	-0.06
LaErO ₃	4.7	4.6	4.3	La ₂ CaHfO ₆	4.6	4.5	4.3	-0.04

TABLE II: Values of Ω_0 (in cm^{-1}) for all compounds considered (see Eq. 4).

LaScO ₃	PrScO ₃	NdScO ₃	SmScO ₃	GdScO ₃	TbScO ₃	DyScO ₃
425.80	429.94	431.89	436.40	440.32	442.13	443.82
LaYO ₃	CaZrO ₃	SrZrO ₃	SrHfO ₃	LaHoO ₃	LaErO ₃	LaTmO ₃
398.31	434.61	419.11	426.55	397.40	399.3	401.19
LaYbO ₃	LaLuO ₃	CeTmO ₃	CeYbO ₃	CeLuO ₃	PrYbO ₃	PrLuO ₃
402.93	404.35	403.17	404.94	406.36	406.97	408.41
NdLuO ₃	La ₂ MgZrO ₆	La ₂ MgHfO ₆	La ₂ CaZrO ₆	La ₂ CaHfO ₆		
410.28	427.70	431.74	407.17	410.54		

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TABLE III: Γ -point phonon frequencies for $Pbnm$ perovskites we considered. Phonon frequencies are given in cm^{-1} . For infrared-active modes, the non-zero values of the dimensionless mode charges Z_α^* are given (see Eq. 3). B_{3u} modes are active along x -axis, B_{2u} along y , and B_{1u} along z .

	Infrared active						Raman active				Inactive
	B_{1u}		B_{2u}		B_{3u}		A_g	B_{1g}	B_{2g}	B_{3g}	A_u
	ω	Z_z^*	ω	Z_y^*	ω	Z_x^*	ω	ω	ω	ω	ω
LaScO ₃	145.6	1.16	104.1	0.20	107.5	0.17	101.6	111.2	124.7	144.1	90.0
	182.3	0.23	175.1	1.27	159.9	1.37	121.6	144.8	283.7	174.4	162.9
	279.9	1.66	222.2	0.40	255.9	0.66	204.7	226.0	402.9	334.3	219.7
	304.1	1.17	266.9	1.27	267.9	1.27	280.2	322.1	450.6	456.6	241.4
	349.4	0.79	308.9	1.56	314.7	1.17	339.8	401.3	648.7	588.4	299.8
	440.6	0.03	320.0	0.67	348.4	1.42	407.6	475.8			348.0
	457.0	0.97	403.2	0.56	371.4	0.44	462.5	631.5			424.6
			455.1	0.99	427.8	0.10					461.4
		510.0	0.20	484.7	0.77						
PrScO ₃	144.2	1.11	102.5	0.18	109.9	0.17	108.7	113.5	121.9	137.9	88.8
	183.3	0.14	187.1	1.13	163.8	1.31	124.2	151.5	286.7	194.0	161.7
	281.1	1.55	227.8	0.55	266.7	1.38	220.5	253.7	416.1	346.0	219.9
	316.4	1.15	271.8	1.23	277.2	0.49	295.9	329.3	452.1	458.4	241.8
	352.1	1.01	317.7	1.70	316.6	0.83	365.6	421.1	647.1	590.2	309.0
	442.0	0.02	335.6	0.52	357.3	1.53	419.9	488.8			352.2
	459.4	0.95	407.6	0.75	382.5	0.69	467.1	630.8			426.0
			461.0	0.87	446.0	0.13					466.0
		517.5	0.25	492.0	0.73						
NdScO ₃	142.1	1.09	101.2	0.17	109.9	0.16	110.0	113.4	119.3	133.6	86.9
	183.3	0.10	190.5	1.06	165.1	1.28	124.3	152.8	287.5	200.6	160.9
	280.8	1.52	229.6	0.64	268.4	1.44	226.1	264.4	421.6	350.5	219.7
	321.0	1.09	274.3	1.16	282.9	0.32	301.7	332.2	452.4	459.9	241.4
	354.3	1.12	321.1	1.75	317.3	0.72	377.0	430.0	646.6	590.2	312.5
	442.9	0.02	341.7	0.52	360.8	1.52	425.3	494.9			354.9
	459.8	0.93	410.2	0.84	387.8	0.81	470.5	631.3			425.6
			464.7	0.81	454.4	0.15					468.9
		520.9	0.27	496.3	0.72						

	Infrared active						Raman active				Inactive
	B _{1u}		B _{2u}		B _{3u}		A _g	B _{1g}	B _{2g}	B _{3g}	A _u
	ω	Z_z^*	ω	Z_y^*	ω	Z_x^*	ω	ω	ω	ω	ω
SmScO ₃	133.3	1.08	98.1	0.18	109.0	0.19	110.2	112.6	112.3	125.2	83.5
	183.5	0.05	191.7	1.02	165.0	1.25	123.3	153.5	287.1	208.0	157.4
	278.6	1.48	230.7	0.69	271.4	1.43	233.7	280.2	428.6	356.4	218.9
	326.6	1.00	276.8	1.03	288.8	0.26	308.0	335.7	452.1	464.0	240.1
	360.1	1.24	326.2	1.76	319.9	0.59	396.0	441.6	646.0	589.0	317.0
	445.2	0.01	349.2	0.59	364.0	1.49	432.7	506.8			361.2
	458.7	0.87	415.2	0.98	399.3	0.96	477.9	634.4			422.5
			471.2	0.76	467.8	0.10					475.4
		528.3	0.31	505.7	0.73						
GdScO ₃	Infrared active						Raman active				Inactive
	B _{1u}		B _{2u}		B _{3u}		A _g	B _{1g}	B _{2g}	B _{3g}	A _u
	ω	Z_z^*	ω	Z_y^*	ω	Z_x^*	ω	ω	ω	ω	ω
	124.1	1.08	95.8	0.18	107.9	0.21	109.2	111.3	105.7	118.4	79.7
	183.7	0.004	192.1	0.98	165.7	1.21	122.2	153.3	286.6	211.6	154.3
	275.3	1.46	231.8	0.73	274.6	1.41	239.0	292.5	434.0	361.3	217.4
	330.5	0.92	278.4	0.92	290.9	0.26	312.0	339.0	451.8	469.1	239.6
	366.3	1.32	330.1	1.73	324.2	0.49	411.9	451.5	646.5	586.9	320.6
	448.3	0.11	355.0	0.66	366.1	1.46	440.0	517.1			368.1
	457.4	0.78	420.4	1.11	410.7	1.05	486.0	638.8			418.4
		478.4	0.73	479.1	0.05					482.8	
		535.3	0.33	515.3	0.75						
TbScO ₃	Infrared active						Raman active				Inactive
	B _{1u}		B _{2u}		B _{3u}		A _g	B _{1g}	B _{2g}	B _{3g}	A _u
	ω	Z_z^*	ω	Z_y^*	ω	Z_x^*	ω	ω	ω	ω	ω
	119.3	1.08	95.2	0.19	107.8	0.22	108.8	111.2	103.0	115.7	78.5
	183.7	0.02	192.3	0.97	166.5	1.20	122.2	153.7	286.4	212.6	153.0
	273.2	1.45	231.9	0.74	276.3	1.39	241.4	297.8	436.0	363.8	215.8
	332.4	0.89	279.0	0.87	291.1	0.29	313.4	340.8	451.9	471.7	239.6
	369.6	1.34	331.5	1.71	326.7	0.44	419.3	456.0	647.0	585.7	322.2
	449.6	0.20	357.7	0.69	366.9	1.45	443.4	522.0			371.7
	457.0	0.71	422.9	1.17	416.4	1.08	490.1	641.4			416.0
		481.9	0.72	484.2	0.02					486.7	
		538.7	0.34	520.2	0.76						
DyScO ₃	Infrared active						Raman active				Inactive
	B _{1u}		B _{2u}		B _{3u}		A _g	B _{1g}	B _{2g}	B _{3g}	A _u
	ω	Z_z^*	ω	Z_y^*	ω	Z_x^*	ω	ω	ω	ω	ω
	113.6	1.09	94.0	0.20	107.3	0.23	107.7	110.5	99.6	112.3	76.8
	183.6	0.05	192.0	0.96	166.8	1.18	121.5	153.2	285.9	212.7	151.2
	271.1	1.44	232.0	0.74	277.7	1.38	242.9	302.2	437.3	366.2	214.1
	333.6	0.87	279.5	0.83	290.7	0.32	314.6	342.4	452.3	474.2	239.6
	372.8	1.37	332.6	1.68	329.2	0.40	425.9	460.3	647.6	584.5	323.6
	450.5	0.31	359.9	0.72	367.6	1.44	446.9	526.5			375.1
	457.2	0.62	425.3	1.23	421.8	1.10	493.6	643.9			413.7
		485.3	0.71	489.0	0.01					490.5	
		542.0	0.36	524.8	0.77						

	Infrared active						Raman active				Inactive
	B _{1u}		B _{2u}		B _{3u}		A _g	B _{1g}	B _{2g}	B _{3g}	A _u
	ω	Z_z^*	ω	Z_y^*	ω	Z_x^*	ω	ω	ω	ω	ω
LaYO ₃	79.6	0.96	76.2	0.37	91.6	0.39	99.1	110.4	92.3	98.3	75.2
	138.0	0.29	150.4	0.96	132.9	1.19	106.8	145.2	244.5	164.6	120.3
	194.4	0.97	171.3	0.22	197.2	0.28	208.1	247.9	378.4	336.1	145.9
	245.6	0.25	221.9	0.56	216.9	1.10	257.8	305.1	417.5	454.1	175.1
	306.3	1.75	239.7	1.59	253.2	0.51	365.9	379.3	592.7	529.3	229.4
	391.1	0.57	276.9	0.17	299.9	0.72	398.6	473.4			304.2
	411.5	0.19	347.9	0.94	335.5	1.69	461.1	593.5			363.9
			421.3	1.17	426.1	0.39					433.7
		467.3	0.56	466.5	0.65						
CaZrO ₃	Infrared active						Raman active				Inactive
	B _{1u}		B _{2u}		B _{3u}		A _g	B _{1g}	B _{2g}	B _{3g}	A _u
	ω	Z_z^*	ω	Z_y^*	ω	Z_x^*	ω	ω	ω	ω	ω
	85.6	1.18	118.4	0.58	125.5	0.57	134.0	185.0	153.3	169.7	99.6
	133.3	0.59	184.5	1.19	174.2	1.23	178.3	204.3	297.0	220.6	136.7
	196.8	1.61	204.7	0.56	201.1	1.50	252.6	231.2	413.9	342.2	165.0
	267.4	0.45	232.0	1.14	260.7	0.06	281.5	337.9	517.1	524.2	182.5
	328.8	1.37	260.0	1.70	274.0	0.00	354.6	409.1	747.5	685.5	242.9
	447.2	0.29	308.0	0.38	335.6	1.69	420.5	454.6			327.6
	472.6	1.44	399.2	0.36	369.3	0.33	532.1	728.2			433.0
		469.6	1.62	396.1	0.20					476.8	
		475.9	0.25	495.9	1.35						
SrZrO ₃	Infrared active						Raman active				Inactive
	B _{1u}		B _{2u}		B _{3u}		A _g	B _{1g}	B _{2g}	B _{3g}	A _u
	ω	Z_z^*	ω	Z_y^*	ω	Z_x^*	ω	ω	ω	ω	ω
	109.0	0.94	99.9	0.52	91.6	0.35	94.7	116.2	124.4	140.0	93.1
	128.9	0.60	136.0	1.05	146.7	0.88	105.9	132.4	280.8	153.0	122.7
	197.0	1.92	187.2	1.27	192.4	1.92	170.2	144.6	390.1	306.6	138.9
	226.9	0.63	203.3	1.23	205.2	0.58	250.3	315.7	518.5	517.5	192.9
	312.5	0.98	239.9	1.17	253.9	0.61	277.2	378.3	762.4	694.7	235.7
	454.9	0.16	262.0	0.55	308.3	1.08	398.5	425.8			307.3
	477.8	1.61	373.5	0.04	315.7	0.60	525.3	735.6			443.8
		447.8	0.30	356.7	0.26					471.4	
		471.2	1.65	488.4	1.51						
SrHfO ₃	Infrared active						Raman active				Inactive
	B _{1u}		B _{2u}		B _{3u}		A _g	B _{1g}	B _{2g}	B _{3g}	A _u
	ω	Z_z^*	ω	Z_y^*	ω	Z_x^*	ω	ω	ω	ω	ω
	94.5	0.23	97.8	0.43	87.9	0.24	83.7	110.4	128.3	123.2	86.1
	123.8	0.77	123.5	0.79	139.3	0.49	105.9	114.9	296.3	161.4	108.5
	187.2	1.60	165.5	0.43	179.3	0.84	162.6	137.4	405.4	314.8	109.8
	214.1	0.62	200.8	1.68	192.2	1.32	234.5	325.5	556.9	556.8	202.8
	259.3	1.27	223.0	0.14	230.7	1.13	278.6	393.9	793.4	721.8	216.3
	490.7	0.08	230.9	1.09	277.6	1.18	414.6	438.9			264.8
509.9	1.47	352.8	0.12	293.8	0.46	564.1	766.2			476.7	
		426.8	0.21	332.5	0.07					504.6	
		505.7	1.52	521.0	1.41						

	Infrared active						Raman active				Inactive
	B _{1u}		B _{2u}		B _{3u}		A _g	B _{1g}	B _{2g}	B _{3g}	A _u
	ω	Z_z^*	ω	Z_y^*	ω	Z_x^*	ω	ω	ω	ω	ω
LaHoO ₃	68.9	0.85	67.9	0.33	83.0	0.32	98.2	110.5	91.3	97.7	65.6
	109.6	0.44	133.3	0.72	121.3	0.99	107.6	145.4	244.4	164.5	103.5
	155.1	0.82	139.8	0.01	149.7	0.35	209.3	248.0	382.8	345.9	119.0
	193.4	0.58	197.4	0.69	189.8	1.15	259.5	309.9	436.5	474.6	146.4
	305.3	1.71	221.0	1.63	218.2	0.72	368.5	380.9	601.2	537.3	173.7
	396.7	0.59	244.3	0.18	290.3	0.31	402.6	475.2			301.5
	416.0	0.14	342.1	0.90	329.8	1.75	480.8	602.2			369.3
			426.4	1.14	428.9	0.34					439.1
		456.9	0.63	469.9	0.64						
LaErO ₃	75.1	0.80	70.8	0.31	84.4	0.29	100.5	110.9	94.6	101.3	68.2
	110.9	0.48	134.7	0.71	122.9	0.97	107.6	145.7	247.2	166.3	104.2
	157.8	0.83	139.9	0.00	150.6	0.36	209.4	248.2	384.4	346.4	119.5
	194.0	0.63	200.1	0.67	192.4	1.16	261.4	311.3	442.3	478.0	151.1
	306.0	1.68	223.4	1.66	218.2	0.74	369.1	382.8	605.8	542.5	174.8
	404.1	0.62	245.0	0.20	291.2	0.27	401.6	475.0			302.3
	421.7	0.15	344.3	0.88	330.6	1.74	483.8	605.9			377.4
			431.9	1.12	430.8	0.28					444.3
		457.2	0.61	472.2	0.66						
LaTmO ₃	79.7	0.75	73.1	0.29	85.8	0.26	101.8	111.1	97.7	104.9	70.4
	112.1	0.51	136.0	0.70	124.2	0.95	107.6	146.0	249.9	168.1	105.2
	160.6	0.83	140.3	0.04	152.0	0.36	209.7	248.1	386.0	347.2	120.0
	195.0	0.68	202.7	0.63	194.9	1.16	263.3	312.8	448.5	481.5	155.4
	307.0	1.65	225.8	1.68	218.4	0.76	369.4	384.5	610.5	547.9	176.4
	412.1	0.65	246.0	0.23	292.1	0.24	400.2	474.9			303.5
	427.8	0.17	346.3	0.85	331.5	1.73	487.0	609.6			386.1
			437.7	1.11	432.4	0.22					449.9
		457.6	0.59	475.4	0.68						
LaYbO ₃	83.2	0.69	75.1	0.27	86.7	0.23	103.5	111.3	100.3	108.0	71.9
	112.9	0.55	136.6	0.68	125.0	0.93	107.8	146.2	252.6	169.6	105.5
	162.3	0.81	140.0	0.08	152.2	0.36	209.8	247.8	387.7	347.8	119.7
	195.3	0.75	204.3	0.60	196.7	1.15	265.0	314.0	454.2	484.7	158.6
	308.1	1.63	227.8	1.71	217.9	0.80	368.8	386.2	614.9	553.2	177.2
	419.7	0.67	246.5	0.26	292.7	0.20	399.8	474.9			304.5
	433.6	0.19	348.2	0.83	332.2	1.73	489.8	613.0			394.3
			443.3	1.10	433.5	0.17					455.2
		458.0	0.56	478.9	0.69						

	Infrared active						Raman active				Inactive
	B _{1u}		B _{2u}		B _{3u}		A _g	B _{1g}	B _{2g}	B _{3g}	A _u
	ω	Z_z^*	ω	Z_y^*	ω	Z_x^*	ω	ω	ω	ω	ω
LaLuO ₃	85.7	0.65	76.9	0.26	87.7	0.22	104.6	111.4	102.2	110.6	72.9
	113.9	0.58	137.2	0.66	125.8	0.91	108.1	146.3	254.6	170.7	106.1
	164.2	0.79	140.4	0.17	153.2	0.37	209.9	247.3	389.2	348.4	119.8
	196.4	0.80	206.0	0.56	198.6	1.13	266.5	315.2	459.5	487.9	161.3
	309.3	1.61	229.8	1.73	218.2	0.84	368.5	387.7	619.1	558.0	178.9
	427.1	0.69	247.5	0.28	293.6	0.18	400.0	475.0			305.9
	439.8	0.21	350.2	0.81	333.2	1.72	492.8	616.4			402.4
			449.2	1.10	434.6	0.13					461.0
		458.7	0.52	483.2	0.70						
CeTmO ₃	Infrared active						Raman active				Inactive
	B _{1u}		B _{2u}		B _{3u}		A _g	B _{1g}	B _{2g}	B _{3g}	A _u
	ω	Z_z^*	ω	Z_y^*	ω	Z_x^*	ω	ω	ω	ω	ω
	76.5	0.78	72.5	0.29	86.6	0.25	102.3	111.8	95.9	101.7	67.2
	111.5	0.46	137.4	0.66	125.9	0.92	109.7	148.8	250.9	171.4	104.8
	159.0	0.82	140.7	0.01	151.1	0.33	214.9	256.6	394.4	354.0	121.6
	196.2	0.66	203.4	0.66	195.7	1.18	270.0	317.3	447.7	485.1	153.4
	316.4	1.67	230.6	1.64	222.2	0.75	379.5	395.0	612.1	547.4	176.6
411.9	0.59	250.1	0.29	298.3	0.32	410.6	482.6			313.0	
430.8	0.15	356.6	0.95	342.3	1.73	491.6	612.6			384.6	
		442.4	1.06	440.8	0.21					455.6	
		463.8	0.65	482.9	0.66						
CeYbO ₃	Infrared active						Raman active				Inactive
	B _{1u}		B _{2u}		B _{3u}		A _g	B _{1g}	B _{2g}	B _{3g}	A _u
	ω	Z_z^*	ω	Z_y^*	ω	Z_x^*	ω	ω	ω	ω	ω
	80.4	0.72	74.5	0.27	87.4	0.23	103.9	112.0	98.4	104.7	68.8
	112.4	0.50	138.0	0.64	126.7	0.90	110.0	149.0	253.5	173.2	105.1
	160.8	0.81	140.3	0.03	151.4	0.34	215.2	256.7	396.1	354.7	121.3
	196.3	0.72	205.1	0.63	197.6	1.18	272.1	318.8	453.6	488.2	156.7
	317.5	1.64	232.7	1.66	221.7	0.78	379.7	396.8	616.4	552.7	177.1
419.6	0.62	251.0	0.35	299.2	0.29	410.3	482.6			314.0	
436.3	0.16	358.6	0.93	343.0	1.73	494.2	615.9			393.0	
		448.1	1.06	442.3	0.16					460.7	
		464.3	0.62	486.0	0.67						
CeLuO ₃	Infrared active						Raman active				Inactive
	B _{1u}		B _{2u}		B _{3u}		A _g	B _{1g}	B _{2g}	B _{3g}	A _u
	ω	Z_z^*	ω	Z_y^*	ω	Z_x^*	ω	ω	ω	ω	ω
	83.1	0.68	76.3	0.26	88.5	0.21	105.1	112.2	100.4	107.2	70.0
	113.3	0.53	138.8	0.62	127.5	0.88	110.4	149.2	255.6	174.7	105.8
	162.9	0.80	140.7	0.14	152.6	0.33	215.5	256.5	397.6	355.4	121.4
	197.2	0.77	206.9	0.60	199.6	1.17	273.7	320.1	458.9	491.2	159.7
	318.9	1.62	234.7	1.68	221.9	0.80	379.5	398.3	620.3	557.4	178.6
427.0	0.64	252.3	0.39	300.1	0.27	410.4	482.6			315.4	
442.4	0.18	360.4	0.91	344.0	1.72	497.0	619.1			401.2	
		453.8	1.05	443.8	0.12					466.2	
		464.8	0.60	489.8	0.68						

TABLE IV: Γ -point phonon frequencies for the $\text{La}_2\text{BB}'\text{O}_6$ perovskites considered. Phonon frequencies are given in cm^{-1} . For infrared-active modes, non-zero components of mode charges Z_α^* are given (see Eq. 3). B_u modes are active in x - z plane and A_u modes along y -axis.

	Infrared active					Raman active	
	A_u		B_u			A_g	B_g
	ω	Z_y^*	ω	Z_x^*	Z_z^*	ω	ω
$\text{La}_2\text{MgZrO}_6$	85.6	0.08	99.2	0.11	0.02	98.9	110.0
	99.5	0.08	146.8	0.20	1.10	122.0	139.8
	160.7	0.69	159.2	1.26	-0.22	126.8	152.9
	173.1	0.95	174.9	0.18	0.18	203.0	172.0
	189.1	0.25	252.1	-0.35	0.56	269.0	219.7
	236.9	0.59	260.7	1.18	-0.003	296.4	304.4
	246.7	0.12	274.8	0.002	1.19	328.0	350.0
	265.7	1.15	309.4	-0.09	1.22	399.9	402.6
	294.2	0.75	318.1	0.50	-0.18	406.6	455.1
	311.9	0.03	331.4	0.37	0.72	466.7	492.3
	314.9	0.88	336.5	1.54	-0.15	477.8	580.1
	337.4	0.82	355.8	0.61	0.39	657.7	648.7
	385.6	0.63	425.5	0.05	0.19		
	430.8	0.23	482.0	0.22	0.30		
	490.8	0.85	494.6	0.39	0.71		
	503.4	0.19	519.7	0.69	-0.42		
540.1	0.19						
$\text{La}_2\text{MgHfO}_6$	Infrared active					Raman active	
	A_u		B_u			A_g	B_g
	ω	Z_y^*	ω	Z_x^*	Z_z^*	ω	ω
	81.7	0.08	92.0	0.06	-0.03	96.3	110.2
	97.9	0.03	142.8	0.45	0.82	124.8	141.5
	140.0	0.41	146.8	0.52	-0.31	130.1	157.2
	151.4	0.65	155.4	0.70	-0.35	200.9	167.3
	165.6	0.44	237.5	1.41	-0.53	268.2	210.6
	229.0	1.08	243.0	0.49	1.26	305.5	308.2
	249.6	0.31	254.8	0.21	0.18	326.1	363.4
	254.5	1.20	308.7	-0.03	1.03	410.8	410.1
	288.4	0.33	318.4	0.08	0.35	417.7	468.1
	305.8	0.15	330.9	-0.37	0.95	486.3	504.8
	320.6	0.56	339.1	1.51	0.10	496.4	594.3
	340.4	1.00	355.7	0.58	0.39	675.0	665.3
	387.2	0.55	425.6	0.10	0.15		
448.2	0.20	488.5	0.18	0.12			
499.0	0.72	502.5	0.33	0.67			
506.8	0.26	527.0	0.59	-0.34			
530.5	0.19						

		Infrared active			Raman active			
		A _u		B _u			A _g	B _g
		ω	Z_y^*	ω	Z_x^*	Z_z^*	ω	ω
La ₂ CaZrO ₆		71.4	0.23	94.6	0.39	0.47	94.0	96.7
		91.3	0.15	101.5	0.23	0.87	106.9	120.1
		131.9	0.27	144.1	1.21	-0.14	110.2	148.8
		155.5	0.81	157.4	-0.23	0.31	207.5	173.1
		167.4	0.73	229.8	0.30	0.68	235.6	247.0
		191.0	0.47	236.2	0.50	0.38	287.8	283.1
		211.5	0.17	239.7	0.93	-0.88	353.8	359.0
		243.2	0.69	278.0	0.10	0.002	385.5	394.3
		272.4	0.63	282.4	0.13	-0.02	399.1	449.5
		273.9	1.20	313.6	1.00	-1.00	446.7	495.2
		295.8	0.20	318.3	0.51	1.25	475.5	538.3
		316.8	0.70	343.9	1.49	0.35	635.4	638.0
		363.5	0.98	413.3	0.16	0.04		
		402.2	0.04	424.6	0.40	0.81		
		431.8	0.87	455.7	-0.08	0.28		
		460.2	0.82	481.9	0.87	-0.32		
		504.2	0.27					
		Infrared active			Raman active			
		A _u		B _u			A _g	B _g
		ω	Z_y^*	ω	Z_x^*	Z_z^*	ω	ω
La ₂ CaHfO ₆		69.1	0.16	89.9	-0.08	0.21	97.3	99.9
		93.5	0.13	105.8	0.44	0.82	108.7	124.4
		121.8	0.14	135.8	0.34	0.19	113.7	149.7
		135.4	0.39	140.9	0.91	-0.31	208.4	175.0
		152.2	0.66	213.8	0.97	0.65	237.0	245.9
		187.0	0.76	219.8	-0.60	0.67	297.1	284.7
		209.8	0.43	233.9	-0.65	0.84	354.7	371.4
		244.8	0.19	264.2	0.43	-0.12	394.2	402.9
		251.0	1.12	275.0	-0.11	0.19	407.6	458.9
		275.3	1.14	307.9	0.78	-0.77	464.9	505.0
		288.2	0.21	316.7	0.10	1.30	490.5	550.7
		311.0	0.45	338.2	1.56	0.41	649.6	651.5
		356.5	0.97	412.6	0.18	-0.07		
		417.7	0.06	437.7	0.36	0.71		
		441.4	0.63	463.9	-0.04	0.28		
		461.7	0.86	486.5	0.73	-0.26		
		496.2	0.25					