

Database of Ruddlesden-Popper perovskites: lattice parameters a ($= b$) and c [\AA], conventional cell volume V [\AA^3], density ρ [g/cm^3], elastic constants c_{ij} [GPa], Young's modulus E [GPa], bulk modulus B [GPa], shear modulus G [GPa], Pugh's ratio G/B , Poisson's ratio ν , Debye temperature θ_D [K], theoretical minimum thermal conductivity κ_{\min} [$\text{W}/(\text{m}\cdot\text{K})$], and band gap E_g [eV].

No.	Material	a	c	V	ρ	c_{11}	c_{33}	c_{44}	c_{66}	c_{12}	c_{13}	E	B	G	G/B	ν	θ_D^*	κ_{\min}	E_g
1	Ca_2MnO_4	3.692	11.708	160	4.143	301.0	299.0	86.2	76.4	77.5	85.8	231	156	92	0.594	0.252	693.3	1.43	1.2
2	Sr_2TiO_4	3.876	12.522	188	5.068	251.0	226.1	69.8	101.2	83.0	75.4	201	133	80	0.606	0.248	553.3	1.08	3.6
3	Sr_2VO_4	3.792	12.556	181	5.337	259.6	244.4	75.5	89.6	86.0	89.7	205	144	81	0.564	0.263	550.3	1.09	0.0
4	Sr_2CrO_4	3.753	12.556	177	5.468	271.6	244.4	76.7	96.4	95.1	83.7	213	146	85	0.582	0.256	558.6	1.11	0.0
5	Sr_2MnO_4	3.783	12.376	177	5.517	254.8	247.4	72.6	90.3	88.0	76.6	203	138	81	0.589	0.254	544.1	1.08	0.9
6	Sr_2FeO_4	3.787	12.324	177	5.545	223.0	231.2	70.7	84.4	73.8	91.5	185	132	73	0.552	0.267	515.7	1.03	0.0
7	Sr_2CoO_4	3.751	12.452	175	5.653	237.3	213.5	72.6	46.7	65.3	90.5	171	131	66	0.506	0.283	489.9	0.98	0.0
8	Sr_2CuO_4	3.832	12.215	179	5.606	204.4	225.3	58.8	50.9	67.9	76.1	156	119	61	0.511	0.282	467.2	0.93	0.0
9	Sr_2MoO_4	3.900	12.735	194	5.748	305.7	254.9	64.0	49.8	83.3	80.7	190	150	74	0.492	0.289	495.6	0.96	0.0
10	Sr_2TcO_4	3.851	12.740	189	5.927	320.9	258.3	67.4	58.6	79.5	79.7	204	152	80	0.523	0.277	510.8	1.00	0.7
11	Sr_2RhO_4	3.866	12.568	188	6.050	230.5	263.1	67.8	56.7	153.1	68.6	167	145	64	0.443	0.307	455.5	0.89	0.0
12	Sr_2SnO_4	4.064	12.554	207	5.735	226.8	244.1	61.1	56.0	45.2	78.1	171	122	68	0.556	0.266	463	0.87	4.6
13	Sr_2IrO_4	3.908	12.581	192	7.457	263.2	277.9	62.6	41.6	143.7	67.2	170	151	65	0.431	0.312	410.3	0.80	0.0
14	Y_2CuO_4	3.825	11.553	169	5.999	313.4	258.7	32.4	142.9	175.1	57.1	179	158	68	0.429	0.312	488.8	0.99	1.0
15	Ba_2CuO_4	3.996	12.887	206	6.49	174.7	180.3	42.1	65.3	71.8	60.4	132	102	52	0.507	0.283	381.6	0.72	0.0
16	Ba_2ZrO_4	4.180	13.435	235	6.078	232.1	205.0	51.0	61.1	57.4	69.5	160	118	63	0.533	0.274	416.3	0.75	4.4
17	Ba_2RuO_4	3.943	13.443	209	6.987	221.9	201.8	54.9	78.3	110.7	73.4	162	128	63	0.489	0.29	403.8	0.76	0.0
18	Ba_2SnO_4	4.163	13.272	230	6.603	193.0	204.5	48.7	63.1	52.7	70.0	148	108	58	0.536	0.273	386.2	0.70	0.0

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19	Ba ₂ IrO ₄	4.002	13.319	213	8.265	217.3	218.9	52.1	61.1	152.0	65.2	145	134	55	0.409	0.32	346.1	0.65	0.0
20	Ba ₂ PbO ₄	4.324	13.252	248	7.318	169.9	192.6	46.9	40.8	40.3	65.0	129	96	50	0.523	0.277	333.7	0.59	0.0
21	La ₂ CoO ₄	3.770	12.622	180	7.401	285.0	272.6	67.3	51.0	102.9	113.3	184	167	70	0.419	0.316	437.5	0.87	0.0
22	La ₂ NiO ₄	3.770	12.710	181	7.363	246.9	218.5	47.2	101.1	136.1	74.9	167	141	64	0.455	0.302	418.7	0.83	0.7
23	La ₂ PdO ₄	4.030	12.451	203	7.351	263.0	189.2	40.5	89.5	158.7	71.1	153	141	58	0.412	0.319	384.1	0.73	0.3
24	La ₂ CuO ₄	3.961	12.501	196	6.866	241.8	219.1	46.8	102.4	139.9	73.9	165	140	63	0.450	0.304	418.9	0.81	0.5
25	Pr ₂ CuO ₄	3.944	12.321	192	7.096	251.7	235.5	47.4	110.5	148.8	69.2	173	144	67	0.461	0.3	425.4	0.83	0.0
26	Nd ₂ CuO ₄	3.921	12.175	187	7.381	263.6	241.5	46.3	115.9	154.5	68.5	177	148	68	0.459	0.301	425.3	0.83	0.1
27	Sm ₂ CuO ₄	3.884	11.934	180	7.902	278.4	246.6	42.3	125.4	155.9	59.4	181	148	70	0.472	0.296	421.1	0.83	0.1
28	Eu ₂ CuO ₄	3.866	11.822	177	8.112	294.7	256.5	36.5	130.3	173.1	66.1	176	159	67	0.422	0.315	411	0.82	0.3
29	Gd ₂ CuO ₄	3.848	11.711	173	8.466	303.6	260.3	36.2	135.4	177.6	64.9	179	161	68	0.424	0.314	408.7	0.82	0.2
30	Dy ₂ CuO ₄	3.821	11.544	169	8.917	318.5	270.9	31.5	143.1	185.7	61.7	178	166	67	0.407	0.321	399.6	0.81	0.0
31	Eu ₂ TiO ₄	3.823	12.057	176	7.845	308.2	369.2	38.9	31.3	88.4	104.7	158	175	59	0.335	0.349	393.4	0.78	0.0
32	Ca ₃ Ti ₂ O ₇	3.828	19.401	285	3.822	317.9	297.9	88.0	83.9	78.9	95.5	240	164	95	0.583	0.256	724.4	1.47	3.2
33	Ca ₃ Mn ₂ O ₇	3.713	19.074	263	4.325	316.4	313.7	89.8	87.6	87.8	94.8	245	167	97	0.584	0.256	706.9	1.48	0.9
34	Ca ₂ LaMn ₂ O ₇	3.814	19.114	278	5.268	232.9	321.0	88.0	84.7	118.0	82.5	212	150	84	0.559	0.264	583.7	1.20	0.0
35	Ba ₃ Zr ₂ O ₇	4.188	20.779	385	6.101	259.8	234.4	57.1	73.4	66.1	70.7	183	130	72	0.557	0.265	452.1	0.83	4.5
36	Sr ₃ Ti ₂ O ₇	3.890	20.254	307	5.099	293.0	273.2	85.5	95.2	80.1	89.5	232	153	93	0.607	0.247	603.4	1.20	3.3
37	Sr ₃ V ₂ O ₇	3.816	20.026	292	5.43	312.9	288.9	88.3	107.7	96.6	89.8	247	163	99	0.608	0.247	613.6	1.24	0.0
38	Sr ₃ Cr ₂ O ₇	3.770	20.195	287	5.542	245.4	251.7	87.5	105.7	126.2	106.9	209	158	82	0.516	0.28	556.2	1.13	0.0
39	Sr ₃ Mn ₂ O ₇	3.792	19.867	286	5.634	218.0	265.3	81.4	109.9	167.9	88.8	180	155	69	0.445	0.306	509.3	1.03	0.7
40	Sr ₃ Fe ₂ O ₇	3.800	19.835	287	5.641	213.2	254.4	82.1	93.4	67.0	89.4	199	129	80	0.619	0.243	544.3	1.10	0.3
41	Sr ₃ Mo ₂ O ₇	3.876	21.004	316	5.966	403.0	295.7	65.1	73.2	77.7	77.4	234	172	92	0.534	0.273	551.4	1.08	0.0
42	Sr ₃ Zr ₂ O ₇	4.144	20.758	357	5.192	291.1	260.5	63.4	62.8	57.4	74.6	197	140	78	0.557	0.265	521.2	0.98	4.6
43	Sr ₃ Ru ₂ O ₇	3.871	20.715	310	6.175	264.1	270.3	66.0	68.2	154.8	87.1	183	161	70	0.433	0.311	477.1	0.94	0.0

No.	Material	a	c	V	ρ	c_{11}	c_{33}	c_{44}	c_{66}	c_{12}	c_{13}	E	B	G	G/B	ν	θ_D^*	κ_{\min}	E_g
44	Sr ₃ Sn ₂ O ₇	4.069	20.602	682	5.962	255.4	255.9	68.7	67.7	59.0	80.0	193	134	77	0.573	0.259	489.9	0.94	3.7
45	Sr ₃ Hf ₂ O ₇	4.105	20.697	349	6.969	313.1	281.4	71.4	71.4	56.0	68.5	219	144	88	0.610	0.246	480.1	0.91	5.0
46	Sr ₂ LaMn ₂ O ₇	3.856	19.799	294	6.048	246.0	295.6	80.0	91.5	136.4	89.2	205	157	80	0.508	0.283	523.3	1.05	0.0
47	Sr ₂ NdMn ₂ O ₇	3.840	19.732	291	6.18	249.2	298.0	81.7	93.0	133.0	86.2	210	156	82	0.527	0.276	526.8	1.06	0.0
48	La ₂ SrMn ₂ O ₇	3.852	20.268	301	6.486	208.1	234.2	80.3	73.3	59.6	95.7	183	127	73	0.574	0.259	477.1	0.95	0.0
49	La ₂ SrFe ₂ O ₇	3.824	20.109	588	6.668	258.0	235.7	82.6	75.1	95.2	112.3	197	155	76	0.494	0.288	487.8	0.98	0.7
50	La ₃ Ni ₂ O ₇	3.793	20.002	288	7.456	319.9	268.1	78.9	66.5	97.0	140.7	207	185	79	0.426	0.314	472.9	0.96	0.0
51	La ₂ SrAl ₂ O ₇	3.740	20.456	286	6.166	288.4	238.8	115.1	129.5	115.3	131.5	246	174	97	0.557	0.265	575.3	1.17	4.4
52	Nd ₂ SrAl ₂ O ₇	3.721	20.168	272	6.612	307.2	273.1	123.0	133.8	106.3	134.5	269	182	107	0.589	0.2538	623.784	1.36	5.0
53	Sm ₂ SrAl ₂ O ₇	3.707	19.799	272	6.767	314.8	289.3	126.1	133.8	103.0	135.2	278	185	111	0.601	0.2497	612.504	1.30	5.3
54	Eu ₂ SrAl ₂ O ₇	3.705	19.681	270	6.854	309.0	299.1	126.9	133.1	104.5	136.5	278	186	111	0.598	0.251	593.7	1.23	5.1
55	Gd ₂ SrAl ₂ O ₇	3.700	19.551	268	7.047	314.4	307.0	128.1	133.2	102.6	136.2	283	187	113	0.605	0.248	592.9	1.23	5.2
56	Dy ₂ SrAl ₂ O ₇	3.687	19.379	263	7.294	324.6	315.4	129.4	133.4	98.0	135.2	290	189	117	0.617	0.244	610.14	1.31	5.4
57	Nd ₂ BaMn ₂ O ₇	3.883	20.215	305	7.056	243.1	246.8	87.5	79.6	79.5	108.1	202	147	80	0.541	0.271	476.6	0.95	0.0
58	Eu ₂ BaMn ₂ O ₇	3.860	19.901	298	7.403	241.2	249.7	84.5	79.6	75.8	106.4	200	145	79	0.544	0.27	467.1	0.94	0.0
59	Tb ₂ BaMn ₂ O ₇	3.855	19.708	294	7.659	240.8	249.2	64.4	78.4	76.1	105.3	182	145	71	0.489	0.29	437.6	0.88	0.0
60	Ca ₄ Mn ₃ O ₁₀	3.700	26.494	216	4.398	372.0	251.6	91.7	91.9	156.8	158.4	233	212	88	0.417	0.317	676.2	1.42	0.7
61	Sr ₄ Ti ₃ O ₁₀	3.917	27.891	428	5.075	307.1	290.5	93.5	100.5	85.7	92.4	248	161	100	0.620	0.243	628.8	1.25	3.0
62	Sr ₄ V ₃ O ₁₀	3.820	27.569	402	5.476	319.4	296.5	97.1	107.0	97.1	105.2	255	172	102	0.592	0.253	625.9	1.27	0.0
63	Sr ₄ Cr ₃ O ₁₀	3.778	27.789	397	5.579	264.5	266.1	94.0	109.8	149.1	140.7	213	184	81	0.442	0.307	560.4	1.15	0.0
64	La ₄ Ni ₃ O ₁₀	3.795	27.501	396	7.476	337.4	304.3	80.7	73.2	107.3	127.7	226	189	87	0.459	0.301	500.3	1.02	0.0