Supplementary material for the article: The tolerance factor for pyrochlores and related structures

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Table 1
Crystallographic data used in this work. The superscript in compound names describes: [a] lone pair (Bi^{3+}); [b] lone pair (Pb^{2+}); [c] lone pair (Te^{4+}); [d] compounds synthesized at high pressure. The symbols used to describe as the structural data were obtained are: n=neutron; e=electron; x=x-ray; s=synchrotron; ?=non-specified. The abbreviations BS is related to the Brik and Srivastava's work, while TW means "This Work".

Item	Compound	t	R_A/R_B	a (exp.) / Å	x	Measure-ment	Absolute error / Å		Relative error / %		ICSD	Refer-ences
							BS	TW	BS	TW		
1a	$Bi_2Ru_2O_7$[a]	0.88636	1.887096774	10.293	0.31500	x	-0.1320	0.1465	-1.28	1.42	73787	(?)
1b	$Bi_2Ru_2O_7$[a]	0.88636	1.887096774	10.294	0.33000	x	-0.1310	0.1455	-1.27	1.41	166566	(?)
2a	$Ca_2Nb_2O_7$	0.90241	1.75	10.444	0.32140	x	0.0059	-0.0239	0.06	-0.23	72206	(?)
2b	$Ca_2Nb_2O_7$	0.90241	1.75	10.348	0.33000	x	-0.0901	0.0721	-0.87	0.70	22411	(?)
3	$Ca_2Ru_2O_7$[d]	0.88192	1.982300885	10.197	0.32190	x	-0.0053	-0.0135	-0.05	-0.13	156409	(?)
4	$Ca_2Ta_2O_7$	0.90241	1.75	10.37	0.32500	?	-0.0743	0.0501	-0.72	0.48	27121	(?)
5a	$Cd_2Nb_2O_7$	0.90666	1.71875	10.375	0.31864	x	-0.0077	0.0104	-0.07	0.10	75601	(?)
5b	$Cd_2Nb_2O_7$	0.90666	1.71875	10.372	0.31510	x	-0.0107	0.0134	-0.10	0.13	9714	(?)
5c	$Cd_2Nb_2O_7$	0.90666	1.71875	10.372	0.32000	x	-0.0107	0.0134	-0.10	0.13	33672	(?)
6	$Cd_2Os_2O_7$	0.88913	1.913043478	10.171	0.32017	n	-0.0023	0.0137	-0.02	0.13	155773	(?)
7	$Cd_2Ru_2O_7$[d]	0.88633	1.946902655	10.129	0.31940	x	-0.0179	0.0236	-0.18	0.23	86773	(?)
8	$Cd_2Sb_2O_7$	0.89601	1.833333333	10.257	0.32360	x	0.0081	0.0064	0.08	0.06	165168	(?)
9	$Cd_2Ta_2O_7$	0.90666	1.71875	10.375	0.31540	x	-0.0139	0.0104	-0.13	0.10	9715	(?)
10	$Dy_2Sn_2O_7$	0.93453	1.488405797	10.398	0.33720	n	0.0406	-0.0084	0.39	-0.08	82960	(?)
11	$Dy_2Tc_2O_7$	0.92343	1.592248062	10.246	0.31500	x	0.0040	0.0202	0.04	0.20	109080	(?)
12	$Dy_2V_2O_7$	0.90651	1.770689655	10.039	0.32858	x	-0.0477	0.0391	-0.47	0.39	160863	(?)
13	$Er_2Mn_2O_7$	0.89788	1.894339623	9.875	0.32810	x	-0.0378	0.0118	-0.38	0.12	202517	(?)
14	$Er_2Ru_2O_7$	0.92199	1.619354839	10.106	0.33580	n	-0.0047	0.0463	-0.05	0.46	97533	(?)
15	$Er_2Sn_2O_7$	0.9393	1.455072464	10.35	0.33750	n	0.0390	-0.0072	0.38	-0.07	82962	(?)
16	$Er_2Tc_2O_7$	0.92831	1.556589147	10.194	0.32900	x	-0.0016	0.0278	-0.02	0.27	109081	(?)
17a	$Er_2Ti_2O_7$	0.91813	1.659504132	10.074	0.33100	e	-0.0380	0.0357	-0.38	0.35	150211	(?)
17b	$Er_2Ti_2O_7$	0.91813	1.659504132	10.087	0.33060	x	-0.0250	0.0227	-0.25	0.22	24209	(?)
18	$Er_2V_2O_7$	0.91155	1.731034483	9.9924	0.33430	x	-0.0479	0.0449	-0.48	0.45	160866	(?)
19	$Eu_2Hf_2O_7$	0.93129	1.501408451	10.56	0.34200	x	0.0303	-0.0386	0.29	-0.37	173953	(?)
20a	$Eu_2Ir_2O_7$	0.90999	1.7056	10.302	0.33200	x	0.0533	-0.0213	0.52	-0.21	173948	(?)
20b	$Eu_2Ir_2O_7$	0.90999	1.7056	10.274	0.33900	x	0.0253	0.0067	0.25	0.07	156437	(?)
21	$Eu_2Mo_2O_7$	0.91644	1.64	10.375	0.33200	x	0.0576	-0.0214	0.56	-0.21	173946	(?)
22	$Eu_2Pb_2O_7$	0.94645	1.375483871	10.742	0.34500	x	0.1042	-0.0494	0.97	-0.46	173951	(?)
23	$Eu_2Pt_2O_7$	0.90999	1.7056	10.293	0.32900	x	0.0492	-0.0123	0.48	-0.12	173952	(?)
24	$Eu_2Ru_2O_7$	0.90868	1.719354839	10.252	0.32900	x	0.0165	0.0139	0.16	0.14	109306	(?)
25a	$Eu_2Sn_2O_7$	0.92644	1.544927536	10.475	0.33380	x	0.0392	-0.0085	0.37	-0.08	84754	(?)
25b	$Eu_2Sn_2O_7$	0.92644	1.544927536	10.482	0.33350	x	0.0462	-0.0155	0.44	-0.15	165931	(?)
26a	$Eu_2Ti_2O_7$	0.90472	1.761983471	10.197	0.32700	x	-0.0398	0.0241	-0.39	0.24	173945	(?)
26b	$Eu_2Ti_2O_7$	0.90472	1.761983471	10.205	0.32800	x	-0.0318	0.0161	-0.31	0.16	92767	(?)
27	$Eu_2Zr_2O_7$	0.93369	1.480555556	10.588	0.34400	x	0.0337	-0.0396	0.32	-0.37	173950	(?)
28	$Gd_2Mo_2O_7$	0.91919	1.62	10.34	0.32400	s	0.0486	-0.0105	0.47	-0.10	159775	(?)
29	$Gd_2Ru_2O_7$	0.91147	1.698387097	10.228	0.33200	x	0.0185	0.0147	0.18	0.14	79332	(?)
30	$Gd_2Sn_2O_7$	0.92914	1.526086957	10.454	0.33480	x	0.0442	-0.0128	0.42	-0.12	84753	(?)

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Table 2
Crystallographic data used in this work. The superscript in compound names describes: [a] lone pair (Bi^{3+}); [b] lone pair (Pb^{2+}); [c] lone pair (Te^{4+}); [d] compounds synthesized at high pressure. The symbols used to describe as the structural data were obtained are: n=neutron; e=electron; x=x-ray; s=synchrotron; ?=non-specified. The abbreviations BS is related to the Brik and Srivastava's work, while TW means "This Work".

Item	Compound	t	R_A/R_B	a (exp.) / Å	x	Measure-ment	Absolute error / Å		Relative error / %		ICSD	References
							BS	TW	BS	TW		
31a	$Gd_2Ti_2O_7$	0.90753	1.740495868	10.185	0.32370	x	-0.0258	0.0134	-0.25	0.13	24207	(?)
31b	$Gd_2Ti_2O_7$	0.90753	1.740495868	10.182	0.32700	e	-0.0288	0.0164	-0.28	0.16	150210	(?)
32	$Gd_2Zr_2O_7$	0.93634	1.4625	10.541	0.34400	x	0.0126	-0.0188	0.12	-0.18	160158	(?)
33	$Hg_2Ru_2O_7$[d]	0.8775	2.017699115	10.201	0.31700	x	-0.0189	0.0126	-0.18	0.12	420818	(?)
34	$Hg_2Sb_2O_7$	0.88734	1.9	10.352	0.32300	x	0.0302	-0.0240	0.29	-0.23	160088	(?)
35	$Ho_2Ru_2O_7$	0.91963	1.637096774	10.142	0.33900	x	0.0091	0.0310	0.09	0.31	96730	(?)
36	$Ho_2Sn_2O_7$	0.93702	1.471014493	10.373	0.33660	n	0.0398	-0.0077	0.38	-0.07	84748	(?)
37	$In_2Mn_2O_7$	0.91676	1.735849057	9.7079	0.33090	x	-0.0250	0.0311	-0.26	0.32	56517	(?)
38	$In_2Si_2O_7$[d]	0.879	2.3	9.413	0.32280	x	0.0460	-0.0751	0.49	-0.80	1458	(?)
39	$La_2Hf_2O_7$	0.91198	1.633802817	10.773	0.32980	n	0.0532	-0.0738	0.49	-0.69	173790	(?)
40a	$La_2Sn_2O_7$	0.90694	1.68115942	10.703	0.32943	n	0.0772	-0.0630	0.72	-0.59	82956	(?)
40b	$La_2Sn_2O_7$	0.90694	1.68115942	10.7	0.32840	n	0.0742	-0.0600	0.69	-0.56	24195	(?)
40c	$La_2Sn_2O_7$	0.90694	1.68115942	10.685	0.32827	x	0.0592	-0.0450	0.55	-0.42	167144	(?)
41a	$La_2Zr_2O_7$	0.91447	1.611111111	10.8	0.33070	s	0.0556	-0.0717	0.51	-0.66	51573	(?)
41b	$La_2Zr_2O_7$	0.91447	1.611111111	10.786	0.33000	?	0.0416	-0.0577	0.39	-0.53	15165	(?)
41c	$La_2Zr_2O_7$	0.91447	1.611111111	10.805	0.33100	n	0.0606	-0.0767	0.56	-0.71	153222	(?)
41d	$La_2Zr_2O_7$	0.91447	1.611111111	10.802	0.33300	e	0.0576	-0.0737	0.53	-0.68	150206	(?)
42	$Lu_2Mn_2O_7$	0.90395	1.843396226	9.8268	0.32980	x	-0.0314	0.0140	-0.32	0.14	56518	(?)
43	$Lu_2Ru_2O_7$	0.92779	1.575806452	10.075	0.33800	n	0.0189	0.0254	0.19	0.25	109308	(?)
44	$Lu_2Ti_2O_7$	0.92396	1.614876033	10.018	0.32990	x	-0.0394	0.0408	-0.39	0.41	24205	(?)
45a	$Lu_2V_2O_7$	0.91746	1.684482759	9.9401	0.32300	x	-0.0455	0.0479	-0.46	0.48	159290	(?)
45b	$Lu_2V_2O_7$	0.91746	1.684482759	9.9368	0.32400	x	-0.0488	0.0512	-0.49	0.51	159286	(?)
45c	$Lu_2V_2O_7$	0.91746	1.684482759	9.933	0.33710	x	-0.0526	0.0550	-0.53	0.55	160599	(?)
45d	$Lu_2V_2O_7$	0.91746	1.684482759	9.928	0.33120	n	-0.0576	0.0600	-0.58	0.60	32688	(?)
46	$Sc_2Mn_2O_7$	0.928	1.641509434	9.5965	0.33420	x	-0.0459	0.0475	-0.48	0.50	83277	(?)
47	$Nd_2Pt_2O_7$	0.90079	1.7744	10.404	0.33310	x	0.0730	-0.0484	0.70	-0.47	402456	(?)
48a	$Nd_2Ru_2O_7$	0.89945	1.788709677	10.344	0.33010	n	0.0212	-0.0037	0.21	-0.04	82304	(?)
48b	$Nd_2Ru_2O_7$	0.89945	1.788709677	10.336	0.32800	x	0.0132	0.0043	0.13	0.04	78133	(?)
48c	$Nd_2Ru_2O_7$	0.89945	1.788709677	10.342	0.32890	x	0.0192	-0.0017	0.19	-0.02	161572	(?)
49	$Nd_2Sn_2O_7$	0.91752	1.607246377	10.567	0.33220	n	0.0440	-0.0190	0.42	-0.18	82958	(?)
50a	$Nd_2Zr_2O_7$	0.9249	1.540277778	10.676	0.33400	x	0.0344	-0.0432	0.32	-0.40	62794	(?)
50b	$Nd_2Zr_2O_7$	0.9249	1.540277778	10.68	0.33200	x	0.0384	-0.0472	0.36	-0.44	160164	(?)
50c	$Nd_2Zr_2O_7$	0.9249	1.540277778	10.666	0.33000	x	0.0244	-0.0332	0.23	-0.31	174187	(?)
51	$Pb_2Sb_2O_7$[b]	0.85481	2.15	10.4	0.32500	?	-0.2142	0.1417	-2.06	1.36	27120	(?)
52	$Pr_2Ir_2O_7$	0.89715	1.8016	10.396	0.32900	x	0.0258	-0.0118	0.25	-0.11	156436	(?)
53a	$Pr_2Ru_2O_7$	0.8958	1.816129032	10.377	0.32950	n	0.0200	-0.0083	0.19	-0.08	82303	(?)
53b	$Pr_2Ru_2O_7$	0.8958	1.816129032	10.373	0.33100	x	0.0160	-0.0043	0.15	-0.04	163397	(?)
53c	$Pr_2Ru_2O_7$	0.8958	1.816129032	10.371	0.32600	x	0.0140	-0.0023	0.14	-0.02	78123	(?)
54	$Pr_2Sn_2O_7$	0.914	1.631884058	10.6	0.33148	n	0.0428	-0.0208	0.40	-0.20	82957	(?)
55	$Pr_2Te_2O_7$[c]	0.97592	1.160824742	10.672	0.33360	x	-0.6178	0.6240	-5.79	5.85	92444	(?)
56	$Pr_2Zr_2O_7$	0.92142	1.563888889	10.692	0.33500	e	0.0162	-0.0268	0.15	-0.25	150207	(?)
57	$Sc_2Si_2O_7$[d]	0.89106	2.175	9.287	0.31870	x	0.0105	-0.0268	0.11	-0.29	1457	(?)
58	$Sm_2Mo_2O_7$	0.91369	1.66	10.4	0.34300	x	0.0559	-0.0226	0.54	-0.22	108769	(?)
59	$Sm_2Sn_2O_7$	0.92374	1.563768116	10.51	0.33330	x	0.0476	-0.0185	0.45	-0.18	24194	(?)
60	$Sm_2Tc_2O_7$	0.91241	1.672868217	10.352	0.32700	x	0.0050	0.0108	0.05	0.10	109079	(?)
61a	$Sm_2Ti_2O_7$	0.9019	1.783471074	10.231	0.32700	e	-0.0325	0.0125	-0.32	0.12	150209	(?)
61b	$Sm_2Ti_2O_7$	0.9019	1.783471074	10.233	0.32700	x	-0.0305	0.0105	-0.30	0.10	24208	(?)
62	$Sm_2Zr_2O_7$	0.93103	1.498611111	10.587	0.34200	e	0.0060	-0.0127	0.06	-0.12	150208	(?)

Table 3
Crystallographic data used in this work. The superscript in compound names describes: [a] lone pair (Bi^{3+}); [b] lone pair (Pb^{2+}); [c] lone pair (Te^{4+}); [d] compounds synthesized at high pressure. The symbols used to describe as the structural data were obtained are: n=neutron; e=electron; x=x-ray; s=synchrotron; ?=non-specified. The abbreviations BS is related to the Brik and Srivastava's work, while TW means "This Work".

Item	Compound	t	R_A/R_B	a (exp.) / Å	x	Measurement	Absolute error / Å		Relative error / %		ICSD	References
							BS	TW	BS	TW		
63	$Tb_2Mo_2O_7$	0.92194	1.6	10.312	0.33400	s	0.0443	-0.0070	0.43	-0.07	159770	(?)
64	$Tb_2Ru_2O_7$	0.91426	1.677419355	10.206	0.33530	n	0.0202	0.0132	0.20	0.13	82305	(?)
65	$Tb_2Sn_2O_7$	0.93183	1.507246377	10.424	0.33560	n	0.0380	-0.0085	0.36	-0.08	82959	(?)
66a	$Tl_2Mn_2O_7$	0.90327	1.849056604	9.8909	0.32600	x	0.0345	-0.0449	0.35	-0.45	56515	(?)
66b	$Tl_2Mn_2O_7$	0.90327	1.849056604	9.8927	0.32500	n	0.0363	-0.0467	0.37	-0.47	83269	(?)
67	$Tl_2Pt_2O_7$[d]	0.92841	1.568	10.132	0.35500	x	0.0695	-0.0120	0.69	-0.12	22215	(?)
68	$Tm_2Ru_2O_7$	0.92414	1.603225806	10.096	0.33600	x	0.0055	0.0372	0.05	0.37	109307	(?)
69	$Tm_2Sn_2O_7$	0.94137	1.44057971	10.326	0.33820	n	0.0352	-0.0038	0.34	-0.04	84750	(?)
70	$Tm_2V_2O_7$	0.91374	1.713793103	9.973	0.33040	n	-0.0470	0.0462	-0.47	0.46	32690	(?)
71a	Y_2Mn_2O7[d]	0.89451	1.922641509	9.9127	0.32740	x	-0.0306	-0.0011	-0.31	-0.01	56516	(?)
71b	$Y_2Mn_2O_7$[d]	0.89451	1.922641509	9.902	0.32800	x	-0.0413	0.0096	-0.42	0.10	202516	(?)
72	$Y_2Mo_2O_7$	0.92638	1.567692308	10.23	0.33820	n	0.0069	0.0348	0.07	0.34	202522	(?)
73a	$Y_2Ru_2O_7$	0.91877	1.643548387	10.143	0.33536	n	0.0019	0.0375	0.02	0.37	79733	(?)
73b	$Y_2Ru_2O_7$	0.91877	1.643548387	10.134	0.33300	x	-0.0071	0.0465	-0.07	0.46	73799	(?)
74a	$Y_2Sn_2O_7$	0.93619	1.476811594	10.373	0.33800	x	0.0316	0.0004	0.30	0.00	24193	(?)
74b	$Y_2Sn_2O_7$	0.93619	1.476811594	10.372	0.33694	n	0.0306	0.0014	0.30	0.01	74706	(?)
74c	$Y_2Sn_2O_7$	0.93619	1.476811594	10.375	0.33500	x	0.0336	-0.0016	0.32	-0.02	157673	(?)
75a	$Y_2Ti_2O_7$	0.91488	1.684297521	10.099	0.32770	x	-0.0435	0.0384	-0.43	0.38	157666	(?)
75b	$Y_2Ti_2O_7$	0.91488	1.684297521	10.095	0.32990	x	-0.0475	0.0424	-0.47	0.42	24206	(?)
76a	$Y_2V_2O_7$	0.90826	1.756896552	10.014	0.32980	x	-0.0567	0.0500	-0.57	0.50	160865	(?)
76b	$Y_2V_2O_7$	0.90826	1.756896552	10.014	0.32980	x	-0.0567	0.0500	-0.57	0.50	160600	(?)
77	$Yb_2Ru_2O_7$	0.92607	1.588709677	10.075	0.33780	n	-0.0009	0.0409	-0.01	0.41	82306	(?)
78	$Yb_2Sn_2O_7$	0.94324	1.427536232	10.305	0.33908	n	0.0289	-0.0016	0.28	-0.02	82964	(?)
79	$Yb_2Ti_2O_7$	0.92223	1.628099174	10.09	0.32990	n	0.0128	-0.0160	0.13	-0.16	173750	(?)

Table 4
Compounds used to calculate the data of Figure 7 according to the tolerance factor.

Tolerance factor		$\Delta\varepsilon_n$	Compound
Cai et al.	This work		
0.897	0.8946	5.758	$Bi_{1.65}Zn_{0.35}Ti_{1.65}Nb_{0.35}O_7$
0.903	0.89961	5.742	$Bi_{1.50}Zn_{0.50}Nb_{0.50}Ti_{1.50}O_7$
0.908	0.90411	5.107	$Bi_{1.50}Zn_{0.667}Nb_{0.833}TiO_7$
0.914	0.90852	4.719	$Bi_{1.50}Zn_{0.833}Nb_{1.167}Ti_{0.50}O_7$
0.916	0.9107	4.269	$Bi_{1.50}Zn_{0.9167}Nb_{1.3333}Ti_{0.25}O_7$
0.917	0.91216	3.913	$Bi_{1.50}Zn_{0.92}Nb_{1.50}O_{6.92}$
0.92	0.91286	3.742	$Bi_{1.50}ZnNbTa_{0.50}O_7$
0.921	0.91339	3.573	$Bi_{1.50}Zn_{0.9167}Sn_{0.25}Nb_{1.3333}O_7$
0.925	0.91624	3.37	$BiZnNbTiO_7$
0.922	0.91391	2.813	$Bi_{1.50}Zn_{0.833}Sn_{0.5}Nb_{1.167}O_7$
0.928	0.92154	2.426	$Bi_{1.50}Zn_{0.50}Nb_{0.5}Zr_{1.5}O_7$
0.923	0.91496	1.867	$Bi_{1.50}Zn_{0.667}SnNd_{0.833}O_7$
0.919	0.91286	1.728	$Bi_{1.50}ZnNb_{0.5}0TaO_7$
0.924	0.91599	1.605	$Bi_{1.50}Zn_{0.50}Nb_{0.50}Sn_{1.5}O_7$
0.947	0.94754	0.644	$Bi_{1.50}Zn_{0.50}Nb_{0.50}Ce_{1.5}O_7$