Structural Stability and Formability of ABO_3-type Perovskite Compounds

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Supplementary

232 perovskite compounds and 144 non-perovskite compounds are respectively compiled and classified into three groups: $A^{1+}B^{5+}O_3$-type, $A^{2+}B^{4+}O_3$-type and $A^{3+}B^{3+}O_3$-type on the basis of the different combinations of oxidation states of A and B cations. Of all the 376 ABO_3-type compounds, their ideal A–O and B–O bond distances (d_{A-O} and d_{B-O}), ionic radii calculated tolerance factors (t_{IR} if possible), bond valence calculated tolerance factors (t_{BV}) and GII values are listed in Table S1 (for $A^{1+}B^{5+}O_3$-type), Table S2 (for $A^{2+}B^{4+}O_3$-type) and Table S3 (for $A^{3+}B^{3+}O_3$-type), respectively. Table S1(a), S2(a) and S3(a) are for the non-

perovskite compounds and Table S1(b), S2(b) and S3(b) are for the perovskite compounds.

Table S1
(a) Non-perovskites in $A^{1+}B^{5+}O_3$-type compounds

Compound	Citation†	d_{A-O} (Å)	d_{B-O} (Å)	t_{BV}	t_{IR}	GII (v.u.)
$AgBiO_3$	89432	2.761	2.127	0.918	–	0.252
$AgBrO_3$	31109	2.761	1.907	1.024	–	0.097
$AgClO_3$	30227	2.761	1.737	1.124	–	0.659
$AgNO_3$	1685	2.761	1.499	1.302	–	2.402
$AgPO_3$	15436	2.761	1.684	1.159	–	0.923
$CsBrO_3$	74769	3.336	1.907	1.237	–	2.387
$CsNbO_3$	1266	3.336	1.978	1.192	1.137	1.697
$CsVO_3$	1489	3.336	1.870	1.261	1.196	2.823
$KBrO_3$	47173	3.051	1.907	1.131	–	0.827
$KClO_3$	26409	3.051	1.737	1.242	–	2.057
KNO_3	10289	3.051	1.499	1.439	1.405	5.875
KPO_3	26146	3.051	1.684	1.281	1.208	2.635
$KSbO_3$	33546	3.051	2.009	1.074	1.075	0.394
KVO_3	33706	3.051	1.870	1.154	1.108	1.032
$LiAsO_3$	16617	2.385	1.834	0.919	–	0.223
$LiBiO_3$	82277	2.385	2.127	0.793	–	0.421
$LiIO_3$	46025	2.385	2.070	0.815	–	0.397
$LiNbO_3$	94493	2.385	1.978	0.853	–	0.347
$LiNO_3$	67981	2.385	1.499	1.125	–	0.540
$LiPO_3$	51630	2.385	1.684	1.001	–	0.005
$LiReO_3$	200998	2.385	1.927	0.875	–	0.311
$LiSbO_3$	39574	2.385	2.009	0.839	–	0.366
$LiTaO_3$	84226	2.385	1.987	0.849	–	0.353
$LiVO_3$	51443	2.385	1.870	0.902	–	0.261
$NaAsO_3$	16654	2.722	1.834	1.049	1.061	0.214
$NaBiO_3$	91776	2.722	2.127	0.905	0.913	0.278
$NaBrO_3$	47174	2.722	1.907	1.009	–	0.036
$NaClO_3$	80340	2.722	1.737	1.108	–	0.541
$NaNO_3$	31011	2.722	1.499	1.284	1.289	2.110
$NaPO_3$	35198	2.722	1.684	1.143	1.108	0.779
$RbBrO_3$	74768	3.182	1.907	1.180	–	1.398
$RbClO_3$	36260	3.182	1.737	1.295	–	3.150
$RbNO_3$	66709	3.182	1.499	1.501	1.442	8.590

$RbPO_3$	74738	3.182	1.684	1.336	1.239	3.974
$RbVO_3$	1488	3.182	1.870	1.203	1.137	1.689
$TlBrO_3$	76966	3.043	1.907	1.128	–	0.799
$TlNO_3$	50295	3.043	1.499	1.435	1.433	5.738
$TlSbO_3$	10142	3.043	2.009	1.071	1.096	0.374
$AgSbO_3$	9043	2.761	2.009	0.972	–	0.101
$AgVO_3$	56861	2.761	1.870	1.044	–	0.191
$KBiO_3$	73746	3.051	2.127	1.014	0.995	0.063
$NaVO_3$	29450	2.722	1.870	1.029	1.017	0.120
$TlVO_3$	6108	3.043	1.870	1.151	1.130	0.998

† Notation of the column: Muller refers to (Muller, O. & Roy, R. 1974), the codes indicate the collection codes in ICSD and P refers to (Mizoguchi *et al.*, 2004; Ito *et al.*, 2001; Belik *et al.*, 2006), respectively.

(b) Perovskites in $A^{1+}B^{5+}O_3$-type compounds

Compound	Citation†	d_{A-O} (Å)	d_{B-O} (Å)	t_{BV}	t_{IR}	GII (v.u.)
$AgNbO_3$	Muller	2.761	1.978	0.987	–	0.049
$AgTaO_3$	40831	2.761	1.987	0.982	–	0.064
$NaIO_3$	20168	2.722	2.070	0.930	–	0.220
$CsIO_3$	33665	3.336	2.070	1.139	0.987	1.041
$KNbO_3$	9534	3.051	1.978	1.091	1.054	0.508
$KTaO_3$	280424	3.051	1.987	1.086	1.054	0.473
KUO_3	71241	3.051	2.142	1.007	0.995	0.031
$NaNbO_3$	89317	2.722	1.978	0.973	0.967	0.095
$NaTaO_3$	88375	2.722	1.987	0.969	0.967	0.110
$NaUO_3$	202889	2.722	2.142	0.899	0.913	0.291
$RbUO_3$	45171	3.182	2.142	1.050	1.021	0.263
$RbPaO_3$	Muller	3.182	2.174	1.035	1.012	0.175
$NaPaO_3$	Muller	2.722	2.174	0.886	0.905	0.317
$KPaO_3$	Muller	3.051	2.174	0.993	0.986	0.031
$NaWO_3$	26688	2.722	1.957	0.983	0.977	0.060
$RbIO_3$	2825	3.182	2.070	1.087	0.939	0.510
KIO_3	200759	3.051	2.070	1.042	0.915	0.204
$TlIO_3$	62106	3.043	2.070	1.039	0.933	0.189
$NaSbO_3$	P	2.722	2.009	0.958	0.986	0.142
$RbNbO_3$	200854	3.182	1.978	1.137	1.081	0.943
$RbTaO_3$	14149	3.182	1.987	1.132	1.081	0.894

† Notation of the column: Muller refers to (Muller, O. & Roy, R. 1974), the codes indicate the collection codes in ICSD and P refers to (Mizoguchi *et al.*, 2004; Ito *et al.*, 2001; Belik *et al.*, 2006), respectively.

Table S2
(a) Non-perovskites in $A^{2+}B^{4+}O_3$-type compounds

Compound	Citation†	d_{A-O} (Å)	d_{B-O} (Å)	t_{BV}	t_{IR}	GII (v.u.)
$BaCO_3$	56101	2.948	1.540	1.354	1.364	7.244
$BaCoO_3$	88670	2.948	1.870	1.115	1.103	1.312
$BaCrO_3$	32524	2.948	1.960	1.064	1.091	0.629
$BaGeO_3$	23925	2.948	1.898	1.098	1.103	1.074
$BaMnO_3$	89994	2.948	1.903	1.095	1.103	1.034
$BaNiO_3$	175	2.948	1.922	1.085	1.132	0.890
$BaRuO_3$	84652	2.948	1.984	1.051	1.054	0.484
$BaSiO_3$	6245	2.948	1.790	1.165	1.182	2.150
$CaCO_3$	80869	2.630	1.540	1.208	1.242	2.471
$CdCO_3$	33662	2.567	1.540	1.179	1.228	1.923
$CdPbO_3$	9213	2.567	2.192	0.828	0.881	0.788
$CdSO_3$	62641	2.567	1.794	1.012	1.083	0.087
$CdTeO_3$	60067	2.567	2.127	0.853	0.809	0.719
$CoCO_3$	52377	2.355	1.540	1.081	–	0.634
$CoGeO_3$	26814	2.355	1.898	0.877	–	0.609
$CoMnO_3$	31854	2.355	1.903	0.875	–	0.617
$CoSiO_3$	17054	2.355	1.790	0.930	–	0.392
$CoTiO_3$	48107	2.355	1.965	0.847	–	0.704
$CuCO_3$	6179	2.342	1.540	1.075	–	0.576
$CuGeO_3$	411018	2.342	1.898	0.872	–	0.623
$CuNbO_3$	201899	2.342	2.030	0.816	–	0.786
$CuSiO_3$	89669	2.342	1.790	0.925	–	0.414
$CuTeO_3$	202451	2.342	2.127	0.779	–	0.862
$CuVO_3$	19046	2.342	1.934	0.856	–	0.676
$FeMnO_3$	33561	2.397	1.903	0.891	–	0.567
$FeSiO_3$	34858	2.397	1.790	0.947	–	0.315
$FeSO_3$	14190	2.397	1.794	0.945	–	0.326
$FeTiO_3$	30664	2.397	1.965	0.863	–	0.665
$HgTeO_3$	61673	2.635	2.127	0.876	–	0.656
$MgCO_3$	94588	2.356	1.540	1.082	–	0.638
$MgGeO_3$	40333	2.356	1.898	0.878	–	0.607
$MgTiO_3$	65794	2.356	1.965	0.848	–	0.704
$MgVO_3$	15927	2.356	1.934	0.861	–	0.662
$MnCO_3$	80867	2.453	1.540	1.126	–	1.139
$MnGeO_3$	69591	2.453	1.898	0.914	–	0.480
$MnSiO_3$	87277	2.453	1.790	0.969	–	0.196
$MnSnO_3$	29203	2.453	2.055	0.844	–	0.729

$MnSO_3$	15554	2.453	1.794	0.967	–	0.210
$MnTiO_3$	60006	2.453	1.965	0.883	–	0.605
$NiMnO_3$	31853	2.317	1.903	0.861	–	0.657
$NiTiO_3$	79284	2.317	1.965	0.834	–	0.737
$PbCO_3$	36164	2.775	1.540	1.274	1.310	4.153
$PbSeO_3$	94763	2.775	1.961	1.001	1.076	0.005
$PbSiO_3$	26812	2.775	1.790	1.096	1.135	0.962
$PbSO_3$	30993	2.775	1.794	1.094	1.155	0.932
$PbTeO_3$	61343	2.775	2.127	0.923	0.862	0.483
$SrCO_3$	56099	2.781	1.540	1.277	1.287	4.237
$SrSiO_3$	59308	2.781	1.790	1.099	1.116	0.994
$SrTeO_3$	74396	2.781	2.127	0.924	0.847	0.474
$ZnGeO_3$	33722	2.367	1.898	0.882	–	0.595
$ZnSiO_3$	1861	2.367	1.790	0.935	–	0.371
$ZnSnO_3$	50404	2.367	2.055	0.814	–	0.792
$ZnTeO_3$	16937	2.367	2.127	0.787	–	0.850
$ZnTiO_3$	22382	2.367	1.965	0.852	–	0.694
$ZnSeO_3$	61341	2.367	1.961	0.853	–	0.688
$NiSeO_3$	497	2.317	1.961	0.835	–	0.732
$BaTeO_3$	10107	2.948	2.127	0.980	0.898	0.155
$MgSeO_3$	494	2.356	1.961	0.850	–	0.698
$CoSeO_3$	496	2.355	1.961	0.849	–	0.699
$CoTeO_3$	500	2.355	2.127	0.783	–	0.856
$CuSeO_3$	498	2.342	1.961	0.844	–	0.711
$HgSeO_3$	79694	2.635	1.961	0.950	–	0.322
$CdSeO_3$	75273	2.567	1.961	0.926	1.009	0.442
$MnSeO_3$	495	2.453	1.961	0.884	–	0.598

† Notation of the column: Muller refers to (Muller, O. & Roy, R. 1974), the codes indicate the collection codes in ICSD and P refers to (Mizoguchi *et al.*, 2004; Ito *et al.*, 2001; Belik *et al.*, 2006), respectively.

(b) Perovskites in $A^{2+}B^{4+}O_3$-type compounds

Compound	Citation†	d_{A-O} (Å)	d_{B-O} (Å)	t_{BV}	t_{IR}	GII (v.u.)
$BaAmO_3$	61317	2.948	2.230	0.935	0.946	0.441
$BaNpO_3$	61316	2.948	2.330	0.895	0.938	0.629
$BaPaO_3$	61315	2.948	2.292	0.910	0.925	0.565
$BaPuO_3$	65033	2.948	2.232	0.934	0.942	0.445
$CaNbO_3$	51202	2.630	2.030	0.916	0.931	0.494
$CdTiO_3$	62150	2.567	1.965	0.924	0.956	0.450
$SrCoO_3$	77142	2.781	1.870	1.052	1.041	0.460
$SrIrO_3$	16295	2.781	2.020	0.973	0.992	0.191

$SrMnO_3$	Muller	2.781	1.903	1.033	1.041	0.283
$SrNbO_3$	42004	2.781	2.030	0.969	0.965	0.223
$BaCeO_3$	2751	2.948	2.178	0.957	0.938	0.310
$BaMoO_3$	43799	2.948	2.006	1.039	1.038	0.362
$BaNbO_3$	50257	2.948	2.030	1.027	1.023	0.239
$BaPbO_3$	72269	2.948	2.192	0.951	0.979	0.348
$BaSnO_3$	43138	2.948	2.055	1.014	1.018	0.123
$BaThO_3$	29110	2.948	2.317	0.900	0.910	0.608
$BaTiO_3$	95437	2.948	1.965	1.061	1.062	0.598
$BaUO_3$	77627	2.948	2.262	0.922	0.929	0.509
$BaZrO_3$	63136	2.948	2.078	1.003	1.004	0.026
$CaMnO_3$	50997	2.630	1.903	0.977	1.004	0.158
$CaRuO_3$	82970	2.630	1.984	0.937	0.954	0.391
$CaSnO_3$	59160	2.630	2.055	0.905	0.927	0.543
$CaTiO_3$	74212	2.630	1.965	0.946	0.966	0.342
$CaVO_3$	88978	2.630	1.934	0.962	0.979	0.256
$CaZrO_3$	37264	2.630	2.078	0.895	0.914	0.585
$PbTiO_3$	93553	2.775	1.965	0.999	1.019	0.010
$PbZrO_3$	280469	2.775	2.078	0.944	0.964	0.370
$SrCeO_3$	78536	2.781	2.178	0.903	0.885	0.573
$SrHfO_3$	89383	2.781	2.073	0.949	0.952	0.346
$SrMoO_3$	71994	2.781	2.006	0.980	0.980	0.108
$SrRuO_3$	78628	2.781	1.984	0.991	0.994	0.067
$SrSnO_3$	90846	2.781	2.055	0.957	0.961	0.297
$SrTiO_3$	80873	2.781	1.965	1.001	1.002	0.006
$SrVO_3$	88982	2.781	1.934	1.017	1.014	0.136
$SrZrO_3$	650	2.781	2.078	0.946	0.947	0.359
$CaPbO_3$	87825	2.630	2.192	0.848	0.891	0.743
$CaUO_3$	Muller	2.630	2.262	0.822	0.846	0.811
$CaMoO_3$	Muller	2.630	2.006	0.927	0.945	0.443
$CaHfO_3$	Muller	2.630	2.073	0.897	0.918	0.576
$BaHfO_3$	Muller	2.948	2.073	1.006	1.009	0.046
$SrPuO_3$	Muller	2.781	2.232	0.881	0.889	0.658
$SrAmO_3$	Muller	2.781	2.230	0.882	0.893	0.656
$CaCrO_3$	Muller	2.630	1.960	0.949	0.994	0.329
$CdSnO_3$	Muller	2.567	2.055	0.883	0.917	0.620
$CaGeO_3$	31338	2.630	1.898	0.980	1.004	0.141
$CdGeO_3$	Muller	2.567	1.898	0.956	0.993	0.281
$PbHfO_3$	Muller	2.775	2.073	0.947	0.969	0.357
$SrPbO_3$	78682	2.781	2.192	0.897	0.923	0.597
$BaIrO_3$	65466	2.948	2.020	1.032	1.051	0.289
$CaSiO_3$	40658	2.630	1.790	1.039	1.076	0.315
$CaIrO_3$	25524	2.630	2.020	0.921	0.957	0.473

$MgSiO_3$	64964	2.356	1.790	0.931	–	0.390
$HgTiO_3$	19005	2.635	1.965	0.948	–	0.333
$SrGeO_3$	28603	2.781	1.898	1.036	1.041	0.309
$PbGeO_3$	200595	2.775	1.898	1.034	1.059	0.287

† Notation of the column: Muller refers to (Muller, O. & Roy, R. 1974), the codes indicate the collection codes in ICSD and P refers to (Mizoguchi *et al.*, 2004; Ito *et al.*, 2001; Belik *et al.*, 2006), respectively.

Table S3
(a) Non-perovskites in $A^{3+}B^{3+}O_3$-type compounds

Compound	Citation†	$d_{A–O}$ (Å)	$d_{B–O}$ (Å)	t_{BV}	t_{IR}	GII (v.u.)
$AlBO_3$	30538	2.133	1.627	0.927	–	0.567
$AlFeO_3$	203202	2.133	2.015	0.748	–	1.326
$AsSbO_3$	37187	2.302	2.229	0.730	–	1.394
$CoMnO_3$	31854	2.213	2.016	0.776	–	1.274
$CrBO_3$	43311	2.237	1.627	0.972	–	0.248
$CrMoO_3$	27551	2.237	2.090	0.757	–	1.328
$CuNbO_3$	201899	2.248	2.153	0.738	–	1.369
$CuVO_3$	9414	2.248	1.999	0.795	–	1.226
$DyBO_3$	27935	2.514	1.627	1.092	–	1.201
$ErBO_3$	27937	2.501	1.627	1.087	–	1.106
$EuBO_3$	27933	2.587	1.627	1.124	–	1.801
$FeBO_3$	34474	2.272	1.627	0.987	–	0.119
$FeMnO_3$	30237	2.272	2.016	0.797	–	1.226
$FeTiO_3$	30669	2.272	2.047	0.785	–	1.262
$GaFeO_3$	35079	2.243	2.015	0.787	–	1.249
$GaInO_3$	30339	2.243	2.158	0.735	–	1.375
$GdBO_3$	87778	2.578	1.627	1.120	–	1.720
$HoBO_3$	27936	2.538	1.627	1.103	–	1.385
$InBO_3$	75254	2.415	1.627	1.049	–	0.555
$InFeO_3$	80469	2.415	2.015	0.847	–	1.072
$InMnO_3$	67671	2.415	2.016	0.847	–	1.073
$LaBO_3$	23608	2.685	1.627	1.167	1.169	2.817
$LuBO_3$	16525	2.484	1.627	1.079	–	0.987
$MnTiO_3$	44407	2.273	2.047	0.785	–	1.261
$NiMnO_3$	31853	2.263	2.016	0.794	–	1.234
$ScBO_3$	65010	2.362	1.627	1.026	–	0.274
$SmBO_3$	20650	2.601	1.627	1.130	1.118	1.930
$SmYO_3$	85359	2.601	2.275	0.808	0.812	1.257
$TiBO_3$	402039	2.304	1.627	1.001	–	0.010
$TlLaO_3$	200088	2.516	2.428	0.733	–	1.420

$TmBO_3$	27942	2.513	1.627	1.092	–	1.194
$TmYO_3$	90666	2.513	2.275	0.781	–	1.319
VBO_3	45060	2.256	1.627	0.980	–	0.180
$VCrO_3$	9420	2.256	1.980	0.805	–	1.194
YBO_3	44162	2.532	1.627	1.100	–	1.338
$YbYO_3$	84135	2.478	2.275	0.770	–	1.340
$YInO_3$	251	2.532	2.158	0.829	–	1.170

† Notation of the column: Muller refers to (Muller, O. & Roy, R. 1974), the codes indicate the collection codes in ICSD and P refers to (Mizoguchi *et al.*, 2004; Ito *et al.*, 2001; Belik *et al.*, 2006), respectively.

(b) Perovskites in $A^{3+}B^{3+}O_3$-type compounds

Compound	Citation†	$d_{A–O}$ (Å)	$d_{B–O}$ (Å)	t_{BV}	t_{IR}	GII (v.u.)
$BiFeO_3$	28622	2.607	2.015	0.915	–	0.747
$CeAlO_3$	72559	2.664	1.876	1.004	1.001	0.043
$CeCrO_3$	28931	2.664	1.980	0.951	0.962	0.479
$CeVO_3$	63521	2.664	1.999	0.942	0.950	0.554
$DyCrO_3$	16505	2.514	1.980	0.898	–	0.836
$DyFeO_3$	27280	2.514	2.015	0.882	–	0.925
$DyMnO_3$	91711	2.514	2.016	0.882	–	0.927
$DyNiO_3$	88041	2.514	2.006	0.886	–	0.903
$DyVO_3$	40392	2.514	1.999	0.889	–	0.886
$ErCrO_3$	28487	2.501	1.980	0.893	–	0.860
$ErFeO_3$	27282	2.501	2.015	0.877	–	0.947
$ErVO_3$	40393	2.501	1.999	0.884	–	0.909
$EuFeO_3$	27277	2.587	2.015	0.908	–	0.789
$EuMnO_3$	95492	2.587	2.016	0.907	–	0.792
$EuNiO_3$	88039	2.587	2.006	0.912	–	0.762
$EuScO_3$	4128	2.587	2.105	0.869	–	1.010
$EuTiO_3$	24669	2.587	2.047	0.893	–	0.876
$GdCoO_3$	45153	2.578	1.956	0.932	–	0.619
$GdCrO_3$	38023	2.578	1.980	0.920	–	0.701
$GdFeO_3$	27278	2.578	2.015	0.904	–	0.807
$GdMnO_3$	95493	2.578	2.016	0.904	–	0.810
$GdNiO_3$	88040	2.578	2.006	0.908	–	0.781
$GdScO_3$	65513	2.578	2.105	0.866	–	1.023
$GdTiO_3$	8149	2.578	2.047	0.890	–	0.893
$GdVO_3$	40391	2.578	1.999	0.912	–	0.760
$HoFeO_3$	27281	2.538	2.015	0.890	–	0.883
$HoMnO_3$	92838	2.538	2.016	0.890	–	0.886
$HoNiO_3$	88042	2.538	2.006	0.894	–	0.860

$LaAlO_3$	90535	2.685	1.876	1.012	1.009	0.136
$LaCoO_3$	201763	2.685	1.956	0.970	0.971	0.308
$LaCrO_3$	81984	2.685	1.980	0.959	0.969	0.417
$LaErO_3$	16237	2.685	2.244	0.846	0.852	1.136
$LaFeO_3$	93611	2.685	2.015	0.942	0.954	0.558
$LaLuO_3$	51449	2.685	2.227	0.852	0.863	1.109
$LaMnO_3$	83761	2.685	2.016	0.942	0.954	0.562
$LaNiO_3$	93919	2.685	2.006	0.946	0.976	0.524
$LaTiO_3$	63575	2.685	2.047	0.927	0.943	0.672
$LaVO_3$	86554	2.685	1.999	0.950	0.957	0.496
$LaYbO_3$	30399	2.685	2.221	0.855	0.861	1.098
$LaYO_3$	89455	2.685	2.275	0.834	0.849	1.182
$LuFeO_3$	27285	2.484	2.015	0.871	–	0.974
$NdAlO_3$	90572	2.618	1.876	0.987	0.976	0.143
$NdCoO_3$	82078	2.618	1.956	0.946	0.939	0.513
$NdCrO_3$	38022	2.618	1.980	0.935	0.937	0.604
$NdFeO_3$	78587	2.618	2.015	0.918	0.923	0.722
$NdMnO_3$	15719	2.618	2.016	0.918	0.923	0.726
$NdTiO_3$	82008	2.618	2.047	0.904	0.912	0.818
$NdVO_3$	63522	2.618	1.999	0.926	0.925	0.670
$PrAlO_3$	90558	2.651	1.876	0.999	–	0.012
$PrCoO_3$	88738	2.651	1.956	0.958	–	0.417
$PrCrO_3$	28932	2.651	1.980	0.946	–	0.516
$PrFeO_3$	63645	2.651	2.015	0.930	–	0.645
$PrLuO_3$	50758	2.651	2.227	0.842	–	1.147
$PrMnO_3$	84922	2.651	2.016	0.930	–	0.649
$PrVO_3$	28927	2.651	1.999	0.937	–	0.588
$SmCoO_3$	90969	2.601	1.956	0.940	0.929	0.560
$SmCrO_3$	28934	2.601	1.980	0.929	0.926	0.647
$SmFeO_3$	27276	2.601	2.015	0.913	0.913	0.760
$SmMnO_3$	95491	2.601	2.016	0.912	0.913	0.763
$SmTiO_3$	51180	2.601	2.047	0.898	0.902	0.851
$SmVO_3$	28929	2.601	1.999	0.920	0.915	0.710
$TbFeO_3$	84412	2.545	2.015	0.893	–	0.870
$TbMnO_3$	15720	2.545	2.016	0.892	–	0.873
$TmFeO_3$	27283	2.513	2.015	0.882	–	0.927
$YbFeO_3$	27284	2.478	2.015	0.869	–	0.983
$YCrO_3$	28909	2.532	1.980	0.904	–	0.800
$YFeO_3$	80865	2.532	2.015	0.888	–	0.894
$YMnO_3$	56617	2.532	2.016	0.888	–	0.896
$YNiO_3$	92047	2.532	2.006	0.892	–	0.871
$YTiO_3$	84610	2.532	2.047	0.874	–	0.969
YVO_3	95579	2.532	1.999	0.895	–	0.853

$YbNiO_3$	92050	2.478	2.006	0.873	–	0.963
$ErNiO_3$	92048	2.501	2.006	0.881	–	0.926
$SmNiO_3$	90959	2.601	2.006	0.917	0.933	0.732
$NdNiO_3$	78319	2.618	2.006	0.923	0.944	0.694
$PrNiO_3$	67721	2.651	2.006	0.934	–	0.614
$LaCuO_3$	73554	2.685	1.991	0.953	1.006	0.463
$TlNiO_3$	93507	2.516	2.006	0.887	–	0.900
$PrRuO_3$	75570	2.651	2.026	0.925	–	0.683
$DyCoO_3$	23658	2.514	1.956	0.909	–	0.767
$LaRuO_3$	75569	2.685	2.026	0.937	0.938	0.599
$HoCoO_3$	23659	2.538	1.956	0.917	–	0.715
$PrRhO_3$	Muller	2.651	2.049	0.915	–	0.755
$PrScO_3$	Muller	2.651	2.105	0.890	–	0.908
$PrTiO_3$	Muller	2.651	2.047	0.916	–	0.749
$PuCrO_3$	Muller	2.623	1.980	0.936	–	0.591
$PuVO_3$	Muller	2.623	1.999	0.928	–	0.658
$SmInO_3$	Muller	2.601	2.158	0.852	0.849	1.092
$SmRhO_3$	Muller	2.601	2.049	0.897	0.904	0.856
$SmScO_3$	Muller	2.601	2.105	0.874	0.870	0.989
$TbCrO_3$	Muller	2.545	1.980	0.909	–	0.773
$TbRhO_3$	Muller	2.545	2.049	0.878	–	0.953
$TbTiO_3$	Muller	2.545	2.047	0.879	–	0.949
$TmTiO_3$	Muller	2.513	2.047	0.868	–	0.998
$YbTiO_3$	Muller	2.478	2.047	0.856	–	1.048
$YCoO_3$	Muller	2.532	1.956	0.915	–	0.728
$YScO_3$	Muller	2.532	2.105	0.850	–	1.085
$DyAlO_3$	Muller	2.514	1.876	0.947	–	0.487
$ErAlO_3$	Muller	2.501	1.876	0.942	–	0.524
$EuAlO_3$	Muller	2.587	1.876	0.975	–	0.256
$EuCrO_3$	Muller	2.587	1.980	0.924	–	0.680
$EuGaO_3$	Muller	2.587	1.986	0.921	–	0.700
$GdAlO_3$	Muller	2.578	1.876	0.971	–	0.287
$HoCrO_3$	Muller	2.538	1.980	0.906	–	0.788
$LuCrO_3$	Muller	2.484	1.980	0.887	–	0.891
$TmAlO_3$	Muller	2.513	1.876	0.947	–	0.490
$TmCrO_3$	Muller	2.513	1.980	0.897	–	0.838
$YbAlO_3$	Muller	2.478	1.876	0.934	–	0.586
$YbCrO_3$	Muller	2.478	1.980	0.885	–	0.902
$AmVO_3$	Muller	2.623	1.999	0.928	–	0.658
$CeFeO_3$	Muller	2.664	2.015	0.935	0.947	0.613
$CeTiO_3$	Muller	2.664	2.047	0.920	0.936	0.721
$DyRhO_3$	Muller	2.514	2.049	0.867	–	1.001
$DyScO_3$	Muller	2.514	2.105	0.844	–	1.107

$DyTiO_3$	Muller	2.514	2.047	0.868	–	0.997
$ErRhO_3$	Muller	2.501	2.049	0.863	–	1.020
$ErTiO_3$	Muller	2.501	2.047	0.864	–	1.016
$EuRhO_3$	Muller	2.587	2.049	0.893	–	0.882
$GdRhO_3$	Muller	2.578	2.049	0.889	–	0.898
$HoRhO_3$	Muller	2.538	2.049	0.876	–	0.964
$HoScO_3$	Muller	2.538	2.105	0.852	–	1.077
$HoTiO_3$	Muller	2.538	2.047	0.876	–	0.960
$LaHoO_3$	Muller	2.685	2.281	0.832	0.848	1.191
$LaInO_3$	Muller	2.685	2.158	0.880	0.887	0.976
$LaRhO_3$	Muller	2.685	2.049	0.926	0.945	0.679
$LaScO_3$	Muller	2.685	2.105	0.902	0.910	0.847
$LaTmO_3$	Muller	2.685	2.256	0.841	0.856	1.155
$LuTiO_3$	Muller	2.484	2.047	0.858	–	1.040
$NdInO_3$	Muller	2.618	2.158	0.858	0.858	1.071
$NdRhO_3$	Muller	2.618	2.049	0.903	0.914	0.823
$NdScO_3$	Muller	2.618	2.105	0.879	0.880	0.963
$TbAlO_3$	84422	2.545	1.876	0.959	–	0.395
$TbCoO_3$	23657	2.545	1.956	0.920	–	0.699
$ErMnO_3$	280583	2.501	2.016	0.877	–	0.949
$NdGaO_3$	83348	2.618	1.986	0.932	0.935	0.626
$SmAlO_3$	10334	2.601	1.876	0.980	0.965	0.206
$GdGaO_3$	492	2.578	1.986	0.918	–	0.720
$HoAlO_3$	39606	2.538	1.876	0.956	–	0.416
$LaGaO_3$	51285	2.685	1.986	0.956	0.966	0.442
$YAlO_3$	83027	2.532	1.876	0.954	–	0.435
$BiMnO_3$	56842	2.607	2.016	0.914	–	0.750
$PrGaO_3$	73766	2.651	1.986	0.944	–	0.539
$YGaO_3$	Muller	2.532	1.986	0.901	–	0.817
$YbMnO_3$	Muller	2.478	2.016	0.869	–	0.985
$LuMnO_3$	Muller	2.484	2.016	0.871	–	0.976
$CeGaO_3$	76048	2.664	1.986	0.948	0.959	0.503
$TmNiO_3$	92049	2.513	2.006	0.886	–	0.905
$ScAlO_3$	66883	2.362	1.876	0.890	–	0.845
$ScCrO_3$	85141	2.362	1.980	0.843	–	1.076
$PrYbO_3$	P	2.651	2.221	0.844	–	1.138
$CeTmO_3$	P	2.664	2.256	0.835	0.850	1.177
$CeYbO_3$	P	2.664	2.221	0.848	0.854	1.123
$CeLuO_3$	P	2.664	2.227	0.846	0.857	1.133
$BiInO_3$	P	2.607	2.158	0.854	–	1.085
$BiAlO_3$	P	2.607	1.876	0.982	–	0.184
$BiScO_3$	P	2.607	2.105	0.876	–	0.98

† Notation of the column: Muller refers to (Muller, O. & Roy, R. 1974), the codes indicate the collection codes

in ICSD and P refers to (Mizoguchi *et al.*, 2004; Ito *et al.*, 2001; Belik *et al.*, 2006), respectively.