Electronic Supplementary Material (ESI) for Dalton Transactions.

Supporting Information for "Investigation on the predictive power of tolerance factor τ for A-site double perovskite oxides"

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I. DATABASE OF INVESTIGATED DOUBLE PEROVSKITE OXIDE COMPOSITIONS

Database of investigated double perovskite oxide compositions is provided as a separate file in Excel format. On the first worksheet in the file, only Shannon ionic radii have been used to obtain the τ values. On the second worksheet, BVS parameters have been additionally used to obtain ionic radii for ions which lack Shannon ionic radii for 12-coordination. In the database, the final four columns tell whether a composition is currently found in the Inorganic Crystal Structure Database (ICSD). **tau Per ICSD Per**: is predicted to be a perovskite and found in ICSD as a perovskite; **tau Per ICSD NonPer**: is predicted to be a perovskite but found with a different structure in ICSD; **tau Nonper ICSD NonPer**: is predicted to not be a perovskite and found in ICSD with a non-perovskite structure type; **tau Nonper ICSD Per**: is predicted to not be a perovskite but found in ICSD as a perovskite.

II. CRYSTAL STRUCTURES OF THE STUDIED SYSTEMS

The optimized crystal structures of the studied systems are provided as separate files in CIF format.

III. ABSOLUTE ELECTRONIC ENERGIES PER FORMULA UNIT (Z)

Absolute energies are given in atomic units (Hartree). Relative energies in kJ/mol per Z are given relative to the lowest-energy structure of each chemical composition.

Table I. Columnar A-Site Ordering of $CsScTi_2O_6$

Tilt System	**Energy/Z [a.u.]**	**Relative Energy [kJ/mol]**
$a^+a^+a^+$	-2930.970416	220
$a^+a^+c^-$	-2930.983304	186
$a^-b^+a^-$	-2930.970689	219
$a^-b^-b^-$	-2930.962572	240
$a^-a^-a^-$	-2930.958352	251
$a^0b^+b^+$	-2930.970211	220
$a^+b^0c^-$	-2930.970494	219
$a^0b^-b^-$	-2930.962532	240
$a^0a^0c^+$	-2930.942609	293
$a^0a^0c^-$	-2930.938555	303
$a^0a^0a^0$	-2930.937672	306

Table II. Planar A-Site Ordering of $CsScTi_2O_6$

Tilt System	**Energy/Z [a.u.]**	**Relative Energy [kJ/mol]**
$a^+a^+a^+$	-2930.979370	172
$a^+a^+c^-$	-2930.982923	162
$a^-b^+a^-$	-2931.044726	0
$a^-b^-b^-$	-2931.031960	34
$a^-a^-a^-$	-2931.020189	64
$a^0b^+b^+$	-2930.974386	185
$a^+b^0c^-$	-2931.019126	67
$a^0b^-b^-$	-2931.001419	114
$a^0a^0c^+$	-2930.972935	188
$a^0a^0c^-$	-2930.976981	178
$a^0a^0a^0$	-2930.967520	203

Table III. Rock Salt A-Site Ordering of $CsScTi_2O_6$

Tilt System	**Energy/Z [a.u.]**	**Relative Energy [kJ/mol]**
$a^+a^+a^+$	-2930.933176	317
$a^+a^+c^-$	-2930.953032	265
$a^-b^+a^-$	-2931.023285	81
$a^-b^-b^-$	-	-
$a^-a^-a^-$	-	-
$a^0b^+b^+$	-2930.941958	294
$a^+b^0c^-$	-2931.013493	106
$a^0b^-b^-$	-	-
$a^0a^0c^+$	-2930.935727	311
$a^0a^0c^-$	-2930.949965	273
$a^0a^0a^0$	-2930.873833	473

Table IV. Columnar A-Site Ordering of $YRbTi_2O_6$

Tilt System	**Energy/Z [a.u.]**	**Relative Energy [kJ/mol]**
$a^+a^+a^+$	-2212.815026	74
$a^+a^+c^-$	-2212.814905	74
$a^-b^+a^-$	-2212.810291	86
$a^-b^-b^-$	-2212.807763	93
$a^-a^-a^-$	-2212.805262	100
$a^0b^+b^+$	-2212.814899	74
$a^+b^0c^-$	-2212.843203	0
$a^0b^-b^-$	-2212.807772	93
$a^0a^0c^+$	-2212.802939	106
$a^0a^0c^-$	-2212.803378	105
$a^0a^0a^0$	-2212.797404	120

Table V. Planar A-Site Ordering of $YRbTi_2O_6$

Tilt System	**Energy/Z [a.u.]**	**Relative Energy [kJ/mol]**
$a^+a^+a^+$	-2212.823192	53
$a^+a^+c^-$	-2212.823046	53
$a^-b^+a^-$	-2212.830042	35
$a^-b^-b^-$	-2212.823397	52
$a^-a^-a^-$	-2212.822985	53
$a^0b^+b^+$	-2212.821915	56
$a^+b^0c^-$	-2212.826897	43
$a^0b^-b^-$	-2212.823317	52
$a^0a^0c^+$	-2212.815461	73
$a^0a^0c^-$	-2212.821135	58
$a^0a^0a^0$	-2212.820837	59

Table VI. Rock Salt A-Site Ordering of $YRbTi_2O_6$

Tilt System	**Energy/Z [a.u.]**	**Relative Energy [kJ/mol]**
$a^+a^+a^+$	-2212.783521	157
$a^+a^+c^-$	-2212.795828	124
$a^-b^+a^-$	-2212.802313	107
$a^-b^-b^-$	-2212.798448	118
$a^-a^-a^-$	-2212.801118	110
$a^0b^+b^+$	-2212.786199	150
$a^+b^0c^-$	-2212.803817	103
$a^0b^-b^-$	-2212.798429	118
$a^0a^0c^+$	-2212.785915	150
$a^0a^0c^-$	-2212.795261	126
$a^0a^0a^0$	-2212.766282	202