Online Supporting Information for

Pushing the Boundary of the Stability and Band Gap Pareto Front by Going Towards High-Entropy Perovskites

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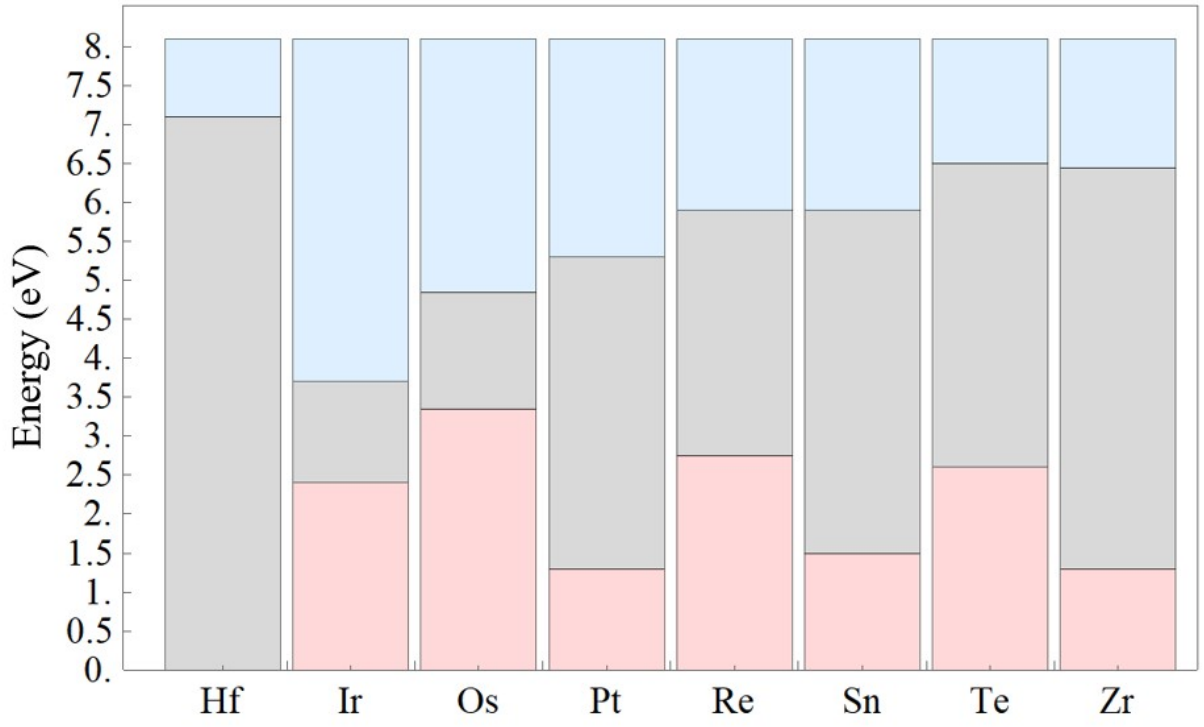

Figure S1. Conduction band minimum (CBM) and valence band maximum (VBM) of the eight constituent pure vacancy-ordered double perovskites: $CsHfCl_6$, $CsIrCl_6$, $CsOsCl_6$, $CsPtCl_6$, $CsReCl_6$, $CsSnCl_6$, $CsTeCl_6$. The VBM of $CsHfCl_6$ is used as the reference energy (zero).

Table S1. Calculated lattice constant, band gap, formation enthalpy, entropy and Gibbs free energy (at 298K) of the 546 medium-to-high-entropy vacancy-ordered double perovskites.

B-site Composition	X-site Composition	Lattice Constant (Å)	Band Gap (eV)	Enthalpy (eV)	Entropy (eV)	Gibbs Free Energy (eV)
Hf	Br	10.78276	4.329	-15.5867	0	-15.5867
Hf	Cl	10.32927	5.524	-18.2466	0	-18.2466
Hf	I	11.52272	2.903	-11.5279	0	-11.5279
Ir	Br	10.50874	0.337	-9.41883	0	-9.41883
Ir	Cl	10.14029	0.679	-11.1467	0	-11.1467
Ir	I	11.18599	0	-7.00829	0	-7.00829
Os	Br	10.53645	0.788	-8.9137	0	-8.9137
Os	Cl	10.152	0	-10.8986	0	-10.8986
Os	I	11.25247	0	-6.07162	0	-6.07162
Pt	Br	10.65152	2.313	-9.93094	0	-9.93094
Pt	Cl	10.20297	3.39	-11.4182	0	-11.4182
Pt	I	11.3011	1.131	-7.71749	0	-7.71749
Re	Br	10.60924	2.72	-9.67474	0	-9.67474
Re	Cl	10.2279	3.075	-11.9028	0	-11.9028
Re	I	11.35412	1.997	-6.46188	0	-6.46188
Sn	Br	10.86809	2.405	-11.8179	0	-11.8179
Sn	Cl	10.33736	3.934	-13.8553	0	-13.8553
Sn	I	11.5603	0.675	-8.57014	0	-8.57014
Te	Br	10.89327	2.851	-10.3454	0	-10.3454
Te	Cl	10.44218	3.438	-11.933	0	-11.933
Te	I	11.59152	2.013	-7.69636	0	-7.69636
Zr	Br	10.79601	3.862	-15.4306	0	-15.4306
Zr	Cl	10.36635	4.948	-17.9068	0	-17.9068
Zr	I	11.53911	2.575	-11.5571	0	-11.5571
Hf	Br2Cl	10.67823	4.218	-16.4575	0.016	-16.4735
Hf	Br2I	11.01062	3.5	-14.1796	0.016	-14.1956
Hf	Cl2Br	10.48398	4.821	-17.3388	0.016	-17.3548
Hf	I2Br	11.45331	3.029	-12.8373	0.016	-12.8533
Ir	Br2Cl	10.27007	1.007	-9.96994	0.016	-9.98594
Ir	Br2I	11.15218	0.661	-8.58201	0.016	-8.59801
Ir	Cl2Br	10.43199	1.326	-10.5537	0.016	-10.5697
Ir	I2Br	10.6234	0	-7.80595	0.016	-7.82195
Os	Br2Cl	10.39574	1.123	-9.55475	0.016	-9.57075
Os	Br2I	11.0197	1.219	-7.91477	0.016	-7.93077
Os	Cl2Br	10.41987	1.029	-10.2189	0.016	-10.2349
Os	I2Br	11.07288	0.885	-7.377895	0.016	-7.393895
Pt	Br2Cl	10.45061	2.323	-10.3997	0.016	-10.4157
Pt	Br2I	11.10865	1.488	-9.15253	0.016	-9.16853

Pt	Cl2Br	10.47238	2.682	-10.9029	0.016	-10.9189
Pt	I2Br	11.00435	1.022	-8.3902	0.016	-8.4062
Re	Br2Cl	10.51941	2.61	-10.4002	0.016	-10.4162
Re	Br2I	11.11154	2.364	-8.55219	0.016	-8.56819
Re	Cl2Br	10.46794	2.719	-11.1406	0.016	-11.1566
Re	I2Br	11.18084	1.778	-7.47273	0.016	-7.48873
Sn	Br2Cl	10.64349	2.525	-12.4651	0.016	-12.4811
Sn	Br2I	11.18396	1.818	-10.6745	0.016	-10.6905
Sn	Cl2Br	10.60375	3.228	-13.1461	0.016	-13.1621
Sn	I2Br	11.38255	0.905	-9.58634	0.016	-9.60234
Te	Br2Cl	10.64532	2.985	-11.8358	0.016	-11.8518
Te	Br2I	11.28351	2.144	-9.40581	0.016	-9.42181
Te	Cl2Br	10.64866	2.971	-11.3697	0.016	-11.3857
Te	I2Br	11.2181	2.145	-9.59221	0.016	-9.60821
Zr	Br2Cl	10.71592	3.864	-16.2353	0.016	-16.2513
Zr	Br2I	11.47428	2.565	-12.617	0.016	-12.633
Zr	Cl2Br	10.57373	4.339	-17.0599	0.016	-17.0759
Zr	I2Br	11.08726	3.042	-14.2796	0.016	-14.2956
HfOsIrPt	Br	10.64298	0.444	-10.9886	0.036	-11.0246
HfOsIrPt	Cl	10.23271	0.339	-12.957	0.036	-12.993
HfOsIrPt	I	11.25861	0.435	-8.09121	0.036	-8.12721
HfReIrPt	Br	10.63449	1.041	-11.1844	0.036	-11.2204
HfReIrPt	Cl	10.205	0.968	-13.2065	0.036	-13.2425
HfReIrPt	I	11.27124	0.438	-8.19637	0.036	-8.23237
HfReOsIr	Br	10.66705	1.453	-10.9302	0.036	-10.9662
HfReOsIr	Cl	10.25191	0	-13.0839	0.036	-13.1199
HfReOsIr	I	11.32008	1.583	-7.77808	0.036	-7.81408
HfReOsPt	Br	10.6603	1.518	-11.0335	0.036	-11.0695
HfReOsPt	Cl	10.22555	1.553	-13.1166	0.036	-13.1526
HfReOsPt	I	11.3263	0	-7.94816	0.036	-7.98416
ReOsIrPt	Br	10.57466	0.346	-9.51231	0.036	-9.54831
ReOsIrPt	Cl	10.12266	0	-11.3757	0.036	-11.4117
ReOsIrPt	I	11.22189	0	-6.82244	0.036	-6.85844
SnHfIrPt	Br	10.67393	1.242	-11.6928	0.036	-11.7288
SnHfIrPt	Cl	10.2456	1.494	-13.6683	0.036	-13.7043
SnHfIrPt	I	11.26376	0.545	-8.71363	0.036	-8.74963
SnHfOsIr	Br	10.67753	0.564	-11.4551	0.036	-11.4911
SnHfOsIr	Cl	10.26343	0.454	-13.5631	0.036	-13.5991
SnHfOsIr	I	11.32933	0.437	-8.2935	0.036	-8.3295
SnHfOsPt	Br	10.68132	1.579	-11.5675	0.036	-11.6035
SnHfOsPt	Cl	10.25073	1.702	-13.6043	0.036	-13.6403
SnHfOsPt	I	11.27671	1.216	-8.47472	0.036	-8.51072
SnHfReIr	Br	10.68882	1.012	-11.6472	0.036	-11.6832

SnHfReIr	Cl	10.27238	0.906	-13.8126	0.036	-13.8486
SnHfReIr	I	11.36882	0.438	-8.39787	0.036	-8.43387
SnHfReOs	Cl	10.2569	2.172	-13.7225	0.036	-13.7585
SnHfReOs	I	11.36904	1.323	-8.15082	0.036	-8.18682
SnHfRePt	Br	10.68314	2.586	-11.7722	0.036	-11.8082
SnHfRePt	Cl	10.25989	2.954	-13.8648	0.036	-13.9008
SnHfRePt	I	11.37609	1.43	-8.58714	0.036	-8.62314
SnOsIrPt	Br	10.63686	0.447	-10.0407	0.036	-10.0767
SnOsIrPt	Cl	10.22385	0.34	-11.8549	0.036	-11.8909
SnOsIrPt	I	11.26294	0.434	-7.34678	0.036	-7.38278
SnReIrPt	Br	10.63577	2.411	-10.237	0.036	-10.273
SnReIrPt	Cl	10.21796	2.865	-12.1037	0.036	-12.1397
SnReIrPt	I	11.28562	0.435	-7.45327	0.036	-7.48927
SnReOsIr	Br	10.66427	0	-9.98478	0.036	-10.0208
SnReOsIr	Cl	10.25372	1.682	-11.9832	0.036	-12.0192
SnReOsIr	I	11.32746	0	-7.03306	0.036	-7.06906
SnReOsPt	Br	10.65897	1.738	-10.0874	0.036	-10.1234
SnReOsPt	Cl	10.2333	3.217	-12.0154	0.036	-12.0514
SnReOsPt	I	11.33945	1.166	-7.2041	0.036	-7.2401
SnTeHfIr	Br	10.77811	1.132	-11.7875	0.036	-11.8235
SnTeHfIr	Cl	10.31478	1.35	-13.7923	0.036	-13.8283
SnTeHfIr	I	11.49078	0.656	-8.68923	0.036	-8.72523
SnTeHfOs	Br	10.77594	1.658	-11.6611	0.036	-11.6971
SnTeHfOs	Cl	10.32555	1.691	-13.7324	0.036	-13.7684
SnTeHfOs	I	11.49973	1.406	-8.45384	0.036	-8.48984
SnTeHfPt	Br	10.77635	2.515	-11.9357	0.036	-11.9717
SnTeHfPt	Cl	10.31355	2.992	-13.8711	0.036	-13.9071
SnTeHfPt	I	11.50355	1.673	-8.89263	0.036	-8.92863
SnTeHfRe	Br	10.78814	2.7	-11.8668	0.036	-11.9028
SnTeHfRe	Cl	10.33212	3.271	-13.9872	0.036	-14.0232
SnTeHfRe	I	11.51269	1.657	-8.56728	0.036	-8.60328
SnTeIrPt	Br	10.68809	1.235	-10.3788	0.036	-10.4148
SnTeIrPt	Cl	10.25085	1.362	-12.0851	0.036	-12.1211
SnTeIrPt	I	11.34914	0.543	-7.74845	0.036	-7.78445
SnTeOsIr	Br	10.69611	0.45	-10.1396	0.036	-10.1756
SnTeOsIr	Cl	10.28573	0.454	-11.9791	0.036	-12.0151
SnTeOsIr	I	11.3931	0.443	-7.32806	0.036	-7.36406
SnTeOsPt	Br	10.6928	1.587	-10.253	0.036	-10.289
SnTeOsPt	Cl	10.29639	1.589	-12.029	0.036	-12.065
SnTeOsPt	I	11.37998	1.334	-7.51147	0.036	-7.54747
SnTeReIr	Br	10.74697	0.899	-10.3349	0.036	-10.3709
SnTeReIr	Cl	10.29043	0.792	-12.2286	0.036	-12.2646
SnTeReIr	I	11.42143	1.738	-7.43425	0.036	-7.47025

SnTeReOs	Br	10.73492	1.58	-10.1857	0.036	-10.2217
SnTeReOs	Cl	10.27865	2.419	-12.1399	0.036	-12.1759
SnTeReOs	I	11.41426	1.315	-7.18874	0.036	-7.22474
SnTeRePt	Br	10.72687	2.395	-10.4581	0.036	-10.4941
SnTeRePt	Cl	10.29078	2.838	-12.2819	0.036	-12.3179
SnTeRePt	I	11.40311	1.441	-7.62495	0.036	-7.66095
TeHfIrPt	Br	10.67743	1.238	-11.3211	0.036	-11.3571
TeHfIrPt	Cl	10.24204	1.361	-13.1846	0.036	-13.2206
TeHfIrPt	I	11.29358	0.543	-8.48576	0.036	-8.52176
TeHfOsIr	Br	10.68474	0.447	-11.0814	0.036	-11.1174
TeHfOsIr	Cl	10.2729	0.454	-13.0773	0.036	-13.1133
TeHfOsIr	I	11.36924	0.544	-8.065	0.036	-8.101
TeHfOsPt	Br	10.68203	1.577	-11.1945	0.036	-11.2305
TeHfOsPt	Cl	10.2471	1.699	-13.1217	0.036	-13.1577
TeHfOsPt	I	11.33212	1.324	-8.24713	0.036	-8.28313
TeHfReIr	Br	10.71951	1.032	-11.2758	0.036	-11.3118
TeHfReIr	Cl	10.28229	0.643	-13.3271	0.036	-13.3631
TeHfReIr	I	11.39014	0.545	-8.17072	0.036	-8.20672
TeHfReOs	Br	10.6839	2.273	-11.1257	0.036	-11.1617
TeHfReOs	Cl	10.27886	2.257	-13.0336	0.036	-13.0696
TeHfReOs	I	11.38313	1.419	-7.92454	0.036	-7.96054
TeHfRePt	Br	10.68238	2.469	-11.3994	0.036	-11.4354
TeHfRePt	Cl	10.2647	2.836	-13.3809	0.036	-13.4169
TeHfRePt	I	11.36972	1.851	-8.36136	0.036	-8.39736
TeOsIrPt	Br	10.68615	0.453	-9.66876	0.036	-9.70476
TeOsIrPt	Cl	10.2588	0.344	-11.3712	0.036	-11.4072
TeOsIrPt	I	11.29555	0.447	-7.11687	0.036	-7.15287
TeReIrPt	Br	10.67344	1.022	-9.86462	0.036	-9.90062
TeReIrPt	Cl	10.25461	0.414	-11.622	0.036	-11.658
TeReIrPt	I	11.28984	0.447	-7.22396	0.036	-7.25996
TeReOsIr	Br	10.68632	0.508	-9.61171	0.036	-9.64771
TeReOsIr	Cl	10.27565	2.816	-11.4991	0.036	-11.5351
TeReOsIr	I	11.34964	0.53	-6.8035	0.036	-6.8395
TeReOsPt	Br	10.68493	1.568	-9.71558	0.036	-9.75158
TeReOsPt	Cl	10.21494	2.214	-11.3292	0.036	-11.3652
TeReOsPt	I	11.35887	1.303	-6.9766	0.036	-7.0126
ZrHfIrPt	Br	10.64348	1.239	-12.6005	0.036	-12.6365
ZrHfIrPt	Cl	10.22563	1.581	-14.6845	0.036	-14.7205
ZrHfIrPt	I	11.20794	0.544	-9.46714	0.036	-9.50314
ZrHfOsIr	Br	10.6721	0.466	-12.3606	0.036	-12.3966
ZrHfOsIr	Cl	10.25869	0.34	-14.5778	0.036	-14.6138
ZrHfOsIr	I	11.27947	0.439	-9.04587	0.036	-9.08187
ZrHfOsPt	Br	10.67311	1.584	-12.4743	0.036	-12.5103

ZrHfOsPt	Cl	10.2388	1.703	-14.6204	0.036	-14.6564
ZrHfOsPt	I	11.2927	1.323	-9.22674	0.036	-9.26274
ZrHfReIr	Br	10.68439	3.568	-12.554	0.036	-12.59
ZrHfReIr	Cl	10.25804	0	-14.8268	0.036	-14.8628
ZrHfReIr	I	11.35681	0.437	-9.14956	0.036	-9.18556
ZrHfReOs	Br	10.68278	3.388	-12.4037	0.036	-12.4397
ZrHfReOs	I	11.35106	2.811	-8.90145	0.036	-8.93745
ZrHfRePt	Br	10.67844	2.581	-12.6779	0.036	-12.7139
ZrHfRePt	Cl	10.25991	2.95	-14.8793	0.036	-14.9153
ZrHfRePt	I	11.33436	1.966	-9.33805	0.036	-9.37405
ZrOsIrPt	Br	10.63466	0.447	-10.9521	0.036	-10.9881
ZrOsIrPt	Cl	10.24271	0.341	-12.8738	0.036	-12.9098
ZrOsIrPt	I	11.25472	0.435	-8.10439	0.036	-8.14039
ZrReIrPt	Br	10.62643	2.416	-11.1478	0.036	-11.1838
ZrReIrPt	Cl	10.21015	0.408	-13.1255	0.036	-13.1615
ZrReIrPt	I	11.27481	0.332	-8.20901	0.036	-8.24501
ZrReOsIr	Br	10.66545	1.753	-10.8929	0.036	-10.9289
ZrReOsIr	Cl	10.24457	2.287	-13.0002	0.036	-13.0362
ZrReOsIr	I	11.3107	0	-7.78895	0.036	-7.82495
ZrReOsPt	Br	10.64496	1.694	-10.9964	0.036	-11.0324
ZrReOsPt	Cl	10.1988	1.513	-12.834	0.036	-12.87
ZrReOsPt	I	11.3007	1.306	-7.95931	0.036	-7.99531
ZrSnHfIr	Br	10.74368	1.336	-13.0611	0.036	-13.0971
ZrSnHfIr	Cl	10.31235	1.464	-15.2918	0.036	-15.3278
ZrSnHfIr	I	11.44466	0.549	-9.66036	0.036	-9.69636
ZrSnHfOs	Br	10.7431	1.543	-12.9349	0.036	-12.9709
ZrSnHfOs	Cl	10.31464	1.69	-15.2247	0.036	-15.2607
ZrSnHfOs	I	11.46794	1.303	-9.42321	0.036	-9.45921
ZrSnHfPt	Br	10.74762	2.853	-13.2098	0.036	-13.2458
ZrSnHfPt	Cl	10.31187	4.029	-15.3687	0.036	-15.4047
ZrSnHfPt	I	11.46761	1.558	-9.86162	0.036	-9.89762
ZrSnHfRe	Br	10.76903	2.931	-13.1393	0.036	-13.1753
ZrSnHfRe	Cl	10.32274	3.249	-15.4868	0.036	-15.5228
ZrSnHfRe	I	11.49151	1.656	-9.53571	0.036	-9.57171
ZrSnIrPt	Br	10.65081	1.243	-11.657	0.036	-11.693
ZrSnIrPt	Cl	10.24864	1.483	-13.5847	0.036	-13.6207
ZrSnIrPt	I	11.26765	0.546	-8.72591	0.036	-8.76191
ZrSnOsIr	Br	10.67696	0.449	-11.4173	0.036	-11.4533
ZrSnOsIr	Cl	10.273	0.34	-13.4835	0.036	-13.5195
ZrSnOsIr	I	11.33682	0.436	-8.30539	0.036	-8.34139
ZrSnOsPt	Br	10.68117	1.582	-11.5315	0.036	-11.5675
ZrSnOsPt	Cl	10.24972	1.712	-13.5222	0.036	-13.5582
ZrSnOsPt	I	11.282	1.211	-8.4862	0.036	-8.5222

ZrSnReIr	Br	10.72165	0.504	-11.6121	0.036	-11.6481
ZrSnReIr	Cl	10.27797	3.393	-13.7287	0.036	-13.7647
ZrSnReIr	I	11.37112	1.916	-8.41012	0.036	-8.44612
ZrSnReOs	Br	10.70291	1.554	-11.4624	0.036	-11.4984
ZrSnReOs	Cl	10.25584	1.7	-13.6387	0.036	-13.6747
ZrSnReOs	I	11.3689	1.248	-8.16287	0.036	-8.19887
ZrSnRePt	Br	10.69294	2.498	-11.7361	0.036	-11.7721
ZrSnRePt	Cl	10.26378	2.961	-13.7812	0.036	-13.8172
ZrSnRePt	I	11.36494	1.331	-8.59819	0.036	-8.63419
ZrSnTeHf	Br	10.80072	2.85	-13.3012	0.036	-13.3372
ZrSnTeHf	Cl	10.36219	3.57	-15.4871	0.036	-15.5231
ZrSnTeHf	I	11.55374	1.789	-9.84013	0.036	-9.87613
ZrSnTeIr	Br	10.76406	1.113	-11.75	0.036	-11.786
ZrSnTeIr	Cl	10.33329	1.35	-13.7079	0.036	-13.7439
ZrSnTeIr	I	11.45721	0.541	-8.69974	0.036	-8.73574
ZrSnTeOs	Br	10.76207	1.587	-11.6235	0.036	-11.6595
ZrSnTeOs	Cl	10.33063	1.692	-13.6441	0.036	-13.6801
ZrSnTeOs	I	11.48524	1.333	-8.46438	0.036	-8.50038
ZrSnTePt	Br	10.77316	2.507	-11.8984	0.036	-11.9344
ZrSnTePt	Cl	10.33573	2.996	-13.7881	0.036	-13.8241
ZrSnTePt	I	11.4745	1.567	-8.90331	0.036	-8.93931
ZrSnTeRe	Br	10.78644	2.678	-11.8291	0.036	-11.8651
ZrSnTeRe	Cl	10.34178	3.288	-13.9029	0.036	-13.9389
ZrSnTeRe	I	11.49909	1.755	-8.57755	0.036	-8.61355
ZrTeHfIr	Br	10.77017	1.122	-12.6887	0.036	-12.7247
ZrTeHfIr	Cl	10.31349	1.339	-14.805	0.036	-14.841
ZrTeHfIr	I	11.45995	0.543	-9.43415	0.036	-9.47015
ZrTeHfOs	Br	10.76731	1.561	-12.5617	0.036	-12.5977
ZrTeHfOs	Cl	10.32061	1.686	-14.7411	0.036	-14.7771
ZrTeHfOs	I	11.4777	1.407	-9.19793	0.036	-9.23393
ZrTeHfPt	Br	10.77212	2.608	-12.8372	0.036	-12.8732
ZrTeHfPt	Cl	10.31537	2.994	-14.8857	0.036	-14.9217
ZrTeHfPt	I	11.4762	2.006	-9.63734	0.036	-9.67334
ZrTeHfRe	Br	10.78946	2.923	-12.767	0.036	-12.803
ZrTeHfRe	Cl	10.32783	3.244	-14.9995	0.036	-15.0355
ZrTeHfRe	I	11.49989	2.299	-9.31124	0.036	-9.34724
ZrTeIrPt	Br	10.67125	1.129	-11.2843	0.036	-11.3203
ZrTeIrPt	Cl	10.25844	1.368	-13.103	0.036	-13.139
ZrTeIrPt	I	11.2548	0.543	-8.49773	0.036	-8.53373
ZrTeOsIr	Br	10.68097	0.447	-11.0434	0.036	-11.0794
ZrTeOsIr	Cl	10.26977	0.341	-12.9943	0.036	-13.0303
ZrTeOsIr	I	11.35748	0.543	-8.07636	0.036	-8.11236
ZrTeOsPt	Br	10.6836	1.577	-11.1577	0.036	-11.1937

ZrTeOsPt	Cl	10.26457	1.718	-13.0399	0.036	-13.0759
ZrTeOsPt	I	11.34142	1.317	-8.25932	0.036	-8.29532
ZrTeReIr	Br	10.72418	2.777	-11.2381	0.036	-11.2741
ZrTeReIr	Cl	10.28341	0.903	-13.2431	0.036	-13.2791
ZrTeReIr	I	11.38593	2.179	-8.1816	0.036	-8.2176
ZrTeReOs	Br	10.71654	2.178	-11.0888	0.036	-11.1248
ZrTeReOs	Cl	10.28265	1.573	-13.1011	0.036	-13.1371
ZrTeReOs	I	11.37046	1.416	-7.93536	0.036	-7.97136
ZrTeRePt	Br	10.71831	2.473	-11.3622	0.036	-11.3982
ZrTeRePt	Cl	10.30449	2.829	-13.2963	0.036	-13.3323
ZrTeRePt	I	11.3723	1.766	-8.37243	0.036	-8.40843
HfOsIrPt	Br2Cl	10.46435	0.447	-11.6189	0.052	-11.6709
HfOsIrPt	Br2I	11.07929	0.438	-9.97795	0.052	-10.0299
HfOsIrPt	Cl2Br	10.46065	0.447	-12.2809	0.052	-12.3329
HfOsIrPt	I2Br	11.03605	0	-8.99691	0.052	-9.04891
HfReIrPt	Br2Cl	10.46573	0.999	-11.83	0.052	-11.882
HfReIrPt	Br2I	11.06321	0.657	-10.1402	0.052	-10.1922
HfReIrPt	Cl2Br	10.47132	1.005	-12.5129	0.052	-12.5649
HfReIrPt	I2Br	11.04496	0.22	-9.13844	0.052	-9.19044
HfReOsIr	Br2Cl	10.46237	0	-11.6241	0.052	-11.6761
HfReOsIr	Br2I	11.08132	0.359	-9.82503	0.052	-9.87703
HfReOsIr	Cl2Br	10.48399	0.461	-12.3456	0.052	-12.3976
HfReOsIr	I2Br	11.09094	1.317	-8.77326	0.052	-8.82526
HfReOsPt	Br2Cl	10.46557	1.922	-11.7028	0.052	-11.7548
HfReOsPt	Br2I	11.07417	2.099	-9.95383	0.052	-10.0058
HfReOsPt	Cl2Br	10.47201	1.777	-12.4011	0.052	-12.4531
HfReOsPt	I2Br	11.14645	1.039	-8.91833	0.052	-8.97033
ReOsIrPt	Br2Cl	10.39408	0	-10.1102	0.052	-10.1622
ReOsIrPt	Br2I	11.05278	0	-8.5658	0.052	-8.6178
ReOsIrPt	Cl2Br	10.44864	0	-10.7315	0.052	-10.7835
ReOsIrPt	I2Br	10.93038	0	-7.66418	0.052	-7.71618
SnHfIrPt	Br2Cl	10.45689	1.245	-12.3295	0.052	-12.3815
SnHfIrPt	Br2I	11.07707	0.885	-10.6443	0.052	-10.6963
SnHfIrPt	Cl2Br	10.48389	1.453	-12.9842	0.052	-13.0362
SnHfIrPt	I2Br	11.06259	0.441	-9.66306	0.052	-9.71506
SnHfOsIr	Br2Cl	10.47689	0.448	-12.1316	0.052	-12.1836
SnHfOsIr	Br2I	11.14621	0.441	-10.3472	0.052	-10.3992
SnHfOsIr	Cl2Br	10.49097	0.449	-12.8358	0.052	-12.8878
SnHfOsIr	I2Br	11.14897	0.22	-9.2919	0.052	-9.3439
SnHfOsPt	Br2Cl	10.484	1.58	-12.2247	0.052	-12.2767
SnHfOsPt	Br2I	11.07577	1.44	-10.4821	0.052	-10.5341
SnHfOsPt	Cl2Br	10.48179	1.598	-12.9013	0.052	-12.9533
SnHfOsPt	I2Br	11.175	1.335	-9.45398	0.052	-9.50598

SnHfReIr	Br2Cl	10.514	3.007	-12.3428	0.052	-12.3948
SnHfReIr	Br2I	11.1617	0.774	-10.5108	0.052	-10.5628
SnHfReIr	Cl2Br	10.5023	0.226	-13.0664	0.052	-13.1184
SnHfReIr	I2Br	11.167	1.737	-9.42735	0.052	-9.47935
SnHfReOs	Br2Cl	10.52428	2.053	-12.2147	0.052	-12.2667
SnHfReOs	Br2I	11.07711	3.423	-10.3265	0.052	-10.3785
SnHfReOs	Cl2Br	10.49924	1.601	-12.9572	0.052	-13.0092
SnHfReOs	I2Br	11.22737	1.451	-9.21162	0.052	-9.26362
SnHfRePt	Br2Cl	10.52047	2.774	-12.4463	0.052	-12.4983
SnHfRePt	Br2I	11.09574	2.004	-10.6557	0.052	-10.7077
SnHfRePt	Cl2Br	10.48798	2.706	-13.1424	0.052	-13.1944
SnHfRePt	I2Br	11.21071	1.544	-9.59563	0.052	-9.64763
SnOsIrPt	Br2Cl	10.46679	0.447	-10.6167	0.052	-10.6687
SnOsIrPt	Br2I	11.10973	0.44	-9.0977	0.052	-9.1497
SnOsIrPt	Cl2Br	10.49327	0.336	-11.2299	0.052	-11.2819
SnOsIrPt	I2Br	11.03399	0	-8.18509	0.052	-8.23709
SnReIrPt	Br2Cl	10.46866	1.067	-10.8281	0.052	-10.8801
SnReIrPt	Br2I	11.09654	0.665	-9.26007	0.052	-9.31207
SnReIrPt	Cl2Br	10.50399	2.844	-11.4626	0.052	-11.5146
SnReIrPt	I2Br	11.02781	0	-8.32399	0.052	-8.37599
SnReOsIr	Br2Cl	10.46614	0.538	-10.6247	0.052	-10.6767
SnReOsIr	Br2I	11.11639	0.677	-8.94699	0.052	-8.99899
SnReOsIr	Cl2Br	10.51196	0.369	-11.2905	0.052	-11.3425
SnReOsIr	I2Br	11.07546	0	-7.95647	0.052	-8.00847
SnReOsPt	Br2Cl	10.47101	1.53	-10.7034	0.052	-10.7554
SnReOsPt	Br2I	11.10015	1.383	-9.07422	0.052	-9.12622
SnReOsPt	Cl2Br	10.48472	1.631	-11.3487	0.052	-11.4007
SnReOsPt	I2Br	11.13245	1.235	-8.10409	0.052	-8.15609
SnTeHfIr	Br2Cl	10.57826	1.122	-12.428	0.052	-12.48
SnTeHfIr	Br2I	11.24711	0.888	-10.7017	0.052	-10.7537
SnTeHfIr	Cl2Br	10.58411	1.229	-13.0987	0.052	-13.1507
SnTeHfIr	I2Br	11.26802	0.442	-9.66564	0.052	-9.71764
SnTeHfOs	Br2Cl	10.60501	1.669	-12.3224	0.052	-12.3744
SnTeHfOs	Br2I	11.20259	1.446	-10.54	0.052	-10.592
SnTeHfOs	Cl2Br	10.57367	1.686	-13.0146	0.052	-13.0666
SnTeHfOs	I2Br	11.34546	1.421	-9.46505	0.052	-9.51705
SnTeHfPt	Br2Cl	10.5744	2.634	-12.5538	0.052	-12.6058
SnTeHfPt	Br2I	11.18272	2.151	-10.8732	0.052	-10.9252
SnTeHfPt	Cl2Br	10.58567	2.753	-13.2018	0.052	-13.2538
SnTeHfPt	I2Br	11.31846	1.684	-9.84959	0.052	-9.90159
SnTeHfRe	Br2Cl	10.62781	2.931	-12.5444	0.052	-12.5964
SnTeHfRe	Br2I	11.17066	2.236	-10.715	0.052	-10.767
SnTeHfRe	Cl2Br	10.59444	3.168	-13.2551	0.052	-13.3071

SnTeHfRe	I2Br	11.36965	1.881	-9.60942	0.052	-9.66142
SnTeIrPt	Br2Cl	10.48093	1.233	-10.9212	0.052	-10.9732
SnTeIrPt	Br2I	11.18155	0.886	-9.44741	0.052	-9.49941
SnTeIrPt	Cl2Br	10.51308	1.261	-11.4906	0.052	-11.5426
SnTeIrPt	I2Br	11.09244	0.332	-8.57541	0.052	-8.62741
SnTeOsIr	Br2Cl	10.50118	0.335	-10.7224	0.052	-10.7744
SnTeOsIr	Br2I	11.18573	0.443	-9.15037	0.052	-9.20237
SnTeOsIr	Cl2Br	10.52023	0.45	-11.3422	0.052	-11.3942
SnTeOsIr	I2Br	11.1822	0.438	-8.20435	0.052	-8.25635
SnTeOsPt	Br2Cl	10.53238	1.483	-10.8165	0.052	-10.8685
SnTeOsPt	Br2I	11.13576	1.44	-9.2855	0.052	-9.3375
SnTeOsPt	Cl2Br	10.51326	1.699	-11.4071	0.052	-11.4591
SnTeOsPt	I2Br	11.20243	1.335	-8.3667	0.052	-8.4187
SnTeReIr	Br2Cl	10.54855	0.898	-10.9355	0.052	-10.9875
SnTeReIr	Br2I	11.20594	0.778	-9.31402	0.052	-9.36602
SnTeReIr	Cl2Br	10.5429	0.995	-11.5713	0.052	-11.6233
SnTeReIr	I2Br	11.20643	0.446	-8.33991	0.052	-8.39191
SnTeReOs	Br2Cl	10.56166	2.224	-10.8084	0.052	-10.8604
SnTeReOs	Br2I	11.16327	1.686	-9.13053	0.052	-9.18253
SnTeReOs	Cl2Br	10.52783	1.603	-11.4623	0.052	-11.5143
SnTeReOs	I2Br	11.25975	1.437	-8.12551	0.052	-8.17751
SnTeRePt	Br2Cl	10.54501	2.492	-11.0381	0.052	-11.0901
SnTeRePt	Br2I	11.18243	2.036	-9.46016	0.052	-9.51216
SnTeRePt	Cl2Br	10.53484	2.652	-11.6519	0.052	-11.7039
SnTeRePt	I2Br	11.23953	1.677	-8.51025	0.052	-8.56225
TeHfIrPt	Br2Cl	10.48119	1.233	-11.9216	0.052	-11.9736
TeHfIrPt	Br2I	11.07137	0.895	-10.3187	0.052	-10.3707
TeHfIrPt	Cl2Br	10.47821	1.166	-12.5378	0.052	-12.5898
TeHfIrPt	I2Br	11.09816	0.439	-9.38645	0.052	-9.43845
TeHfOsIr	Br2Cl	10.49889	0.447	-11.7217	0.052	-11.7737
TeHfOsIr	Br2I	11.11054	0.551	-10.0198	0.052	-10.0718
TeHfOsIr	Cl2Br	10.49151	0	-12.39	0.052	-12.442
TeHfOsIr	I2Br	11.17991	0.219	-9.01483	0.052	-9.06683
TeHfOsPt	Br2Cl	10.49807	1.589	-11.8154	0.052	-11.8674
TeHfOsPt	Br2I	11.06061	1.786	-10.1571	0.052	-10.2091
TeHfOsPt	Cl2Br	10.48185	1.582	-12.4565	0.052	-12.5085
TeHfOsPt	I2Br	11.19635	1.441	-9.17668	0.052	-9.22868
TeHfReIr	Br2Cl	10.53199	0.912	-11.9342	0.052	-11.9862
TeHfReIr	Br2I	11.16757	0.666	-10.1845	0.052	-10.2365
TeHfReIr	Cl2Br	10.50567	0.422	-12.6185	0.052	-12.6705
TeHfReIr	I2Br	11.20442	0.331	-9.15106	0.052	-9.20306
TeHfReOs	Br2Cl	10.5467	1.649	-11.8056	0.052	-11.8576
TeHfReOs	Br2I	11.11567	0	-10.0012	0.052	-10.0532

TeHfReOs	Cl2Br	10.4991	1.466	-12.5113	0.052	-12.5633
TeHfReOs	I2Br	11.25175	1.282	-8.93656	0.052	-8.98856
TeHfRePt	Br2Cl	10.5316	2.613	-12.0372	0.052	-12.0892
TeHfRePt	Br2I	11.11778	2.106	-10.3314	0.052	-10.3834
TeHfRePt	Cl2Br	10.51378	2.59	-12.6976	0.052	-12.7496
TeHfRePt	I2Br	11.2338	1.865	-9.32086	0.052	-9.37286
TeOsIrPt	Br2Cl	10.47643	0.456	-10.2064	0.052	-10.2584
TeOsIrPt	Br2I	11.11429	0.451	-8.77302	0.052	-8.82502
TeOsIrPt	Cl2Br	10.50368	0	-10.7831	0.052	-10.8351
TeOsIrPt	I2Br	11.06513	0.336	-7.90412	0.052	-7.95612
TeReIrPt	Br2Cl	10.4863	2.652	-10.4197	0.052	-10.4717
TeReIrPt	Br2I	11.10563	0	-8.93442	0.052	-8.98642
TeReIrPt	Cl2Br	10.49482	0.915	-11.0133	0.052	-11.0653
TeReIrPt	I2Br	11.05864	0.337	-8.04282	0.052	-8.09482
TeReOsIr	Br2Cl	10.48484	0	-10.2138	0.052	-10.2658
TeReOsIr	Br2I	11.15376	0.515	-8.61761	0.052	-8.66961
TeReOsIr	Cl2Br	10.52041	1.222	-10.8447	0.052	-10.8967
TeReOsIr	I2Br	11.11739	0	-7.67771	0.052	-7.72971
TeReOsPt	Br2Cl	10.48367	2.706	-10.2924	0.052	-10.3444
TeReOsPt	Br2I	11.11872	0	-8.75111	0.052	-8.80311
TeReOsPt	Cl2Br	10.50021	1.595	-10.9058	0.052	-10.9578
TeReOsPt	I2Br	11.14948	1.41	-7.82513	0.052	-7.87713
ZrHfIrPt	Br2Cl	10.44977	1.351	-13.2769	0.052	-13.3289
ZrHfIrPt	Br2I	11.04243	0.773	-11.4975	0.052	-11.5495
ZrHfIrPt	Cl2Br	10.47431	1.565	-13.9642	0.052	-14.0162
ZrHfIrPt	I2Br	11.07385	0.219	-10.4734	0.052	-10.5254
ZrHfOsIr	Br2Cl	10.48017	0.337	-13.0763	0.052	-13.1283
ZrHfOsIr	Br2I	11.05328	0.44	-11.1991	0.052	-11.2511
ZrHfOsIr	Cl2Br	10.48105	0.451	-13.8168	0.052	-13.8688
ZrHfOsIr	I2Br	11.13641	0	-10.101	0.052	-10.153
ZrHfOsPt	Br2Cl	10.47371	1.484	-13.1709	0.052	-13.2229
ZrHfOsPt	Br2I	11.02081	1.54	-11.3358	0.052	-11.3878
ZrHfOsPt	Cl2Br	10.46881	1.601	-13.8829	0.052	-13.9349
ZrHfOsPt	I2Br	11.17325	1.316	-10.262	0.052	-10.314
ZrHfReIr	Br2Cl	10.50828	0.468	-13.2871	0.052	-13.3391
ZrHfReIr	Br2I	11.08749	3.14	-11.3628	0.052	-11.4148
ZrHfReIr	Cl2Br	10.49298	0.901	-14.0473	0.052	-14.0993
ZrHfReIr	I2Br	11.16102	2.246	-10.2355	0.052	-10.2875
ZrHfReOs	Br2Cl	10.52453	1.521	-13.158	0.052	-13.21
ZrHfReOs	Br2I	11.02494	1.4	-11.179	0.052	-11.231
ZrHfReOs	Cl2Br	10.47981	2.133	-13.8877	0.052	-13.9397
ZrHfReOs	I2Br	11.22663	1.179	-10.018	0.052	-10.07
ZrHfRePt	Br2Cl	10.52251	2.582	-13.3914	0.052	-13.4434

ZrHfRePt	Br2I	11.05014	2.218	-11.5095	0.052	-11.5615
ZrHfRePt	Cl2Br	10.49933	2.811	-14.1238	0.052	-14.1758
ZrHfRePt	I2Br	11.21174	1.87	-10.4032	0.052	-10.4552
ZrOsIrPt	Br2Cl	10.46909	0.557	-11.5656	0.052	-11.6176
ZrOsIrPt	Br2I	11.10283	0.468	-9.95762	0.052	-10.0096
ZrOsIrPt	Cl2Br	10.48907	0.449	-12.2153	0.052	-12.2673
ZrOsIrPt	I2Br	11.03288	0	-8.99517	0.052	-9.04717
ZrReIrPt	Br2Cl	10.46515	1.103	-11.7805	0.052	-11.8325
ZrReIrPt	Br2I	11.06606	0.661	-10.1184	0.052	-10.1704
ZrReIrPt	Cl2Br	10.47282	1.158	-12.442	0.052	-12.494
ZrReIrPt	I2Br	11.03655	0	-9.1323	0.052	-9.1843
ZrReOsIr	Br2Cl	10.46094	0.931	-11.5707	0.052	-11.6227
ZrReOsIr	Br2I	11.10807	0.873	-9.8024	0.052	-9.8544
ZrReOsIr	Cl2Br	10.49187	0	-12.274	0.052	-12.326
ZrReOsIr	I2Br	11.08457	0	-8.76832	0.052	-8.82032
ZrReOsPt	Br2Cl	10.47052	2.52	-11.6513	0.052	-11.7033
ZrReOsPt	Br2I	11.09247	1.584	-9.93435	0.052	-9.98635
ZrReOsPt	Cl2Br	10.47322	0	-12.3326	0.052	-12.3846
ZrReOsPt	I2Br	11.14265	1.435	-8.91299	0.052	-8.96499
ZrSnHfIr	Br2Cl	10.57413	1.35	-13.7747	0.052	-13.8267
ZrSnHfIr	Br2I	11.16301	0.889	-11.877	0.052	-11.929
ZrSnHfIr	Cl2Br	10.52587	1.345	-14.5239	0.052	-14.5759
ZrSnHfIr	I2Br	11.23425	0.331	-10.7387	0.052	-10.7907
ZrSnHfOs	Br2Cl	10.59189	1.664	-13.671	0.052	-13.723
ZrSnHfOs	Br2I	11.14073	1.426	-11.7147	0.052	-11.7667
ZrSnHfOs	Cl2Br	10.53424	1.556	-14.4393	0.052	-14.4913
ZrSnHfOs	I2Br	11.35714	1.56	-10.5376	0.052	-10.5896
ZrSnHfPt	Br2Cl	10.57212	2.964	-13.9015	0.052	-13.9535
ZrSnHfPt	Br2I	11.15092	2.257	-12.0476	0.052	-12.0996
ZrSnHfPt	Cl2Br	10.53999	3.446	-14.6276	0.052	-14.6796
ZrSnHfPt	I2Br	11.30213	1.571	-10.9203	0.052	-10.9723
ZrSnHfRe	Br2Cl	10.59934	3.039	-13.8927	0.052	-13.9447
ZrSnHfRe	Br2I	11.1381	2.342	-11.887	0.052	-11.939
ZrSnHfRe	Cl2Br	10.55589	3.276	-14.6792	0.052	-14.7312
ZrSnHfRe	I2Br	11.36874	1.77	-10.681	0.052	-10.733
ZrSnIrPt	Br2Cl	10.45677	1.461	-12.2759	0.052	-12.3279
ZrSnIrPt	Br2I	11.09803	0.877	-10.6235	0.052	-10.6755
ZrSnIrPt	Cl2Br	10.51312	1.363	-12.9168	0.052	-12.9688
ZrSnIrPt	I2Br	11.0664	0.33	-9.65855	0.052	-9.71055
ZrSnOsIr	Br2Cl	10.47744	0.449	-12.0782	0.052	-12.1302
ZrSnOsIr	Br2I	11.11708	0.444	-10.3256	0.052	-10.3776
ZrSnOsIr	Cl2Br	10.5267	0.451	-12.7681	0.052	-12.8201
ZrSnOsIr	I2Br	11.12904	0	-9.28796	0.052	-9.33996

ZrSnOsPt	Br2Cl	10.47667	1.696	-12.1703	0.052	-12.2223
ZrSnOsPt	Br2I	11.10258	1.455	-10.4618	0.052	-10.5138
ZrSnOsPt	Cl2Br	10.50868	1.588	-35.8492	0.052	-35.9012
ZrSnOsPt	I2Br	11.16786	1.331	-9.4476	0.052	-9.4996
ZrSnReIr	Br2Cl	10.49976	1.068	-12.2889	0.052	-12.3409
ZrSnReIr	Br2I	11.16327	0.668	-10.4902	0.052	-10.5422
ZrSnReIr	Cl2Br	10.53235	0.891	-13.001	0.052	-13.053
ZrSnReIr	I2Br	11.15074	1.951	-9.42145	0.052	-9.47345
ZrSnReOs	Br2Cl	10.53174	1.674	-12.1604	0.052	-12.2124
ZrSnReOs	Br2I	11.10221	1.955	-10.306	0.052	-10.358
ZrSnReOs	Cl2Br	10.50812	4.138	-12.8888	0.052	-12.9408
ZrSnReOs	I2Br	11.24003	1.427	-9.20468	0.052	-9.25668
ZrSnRePt	Br2Cl	10.5234	2.59	-12.3912	0.052	-12.4432
ZrSnRePt	Br2I	11.11293	2.113	-10.6362	0.052	-10.6882
ZrSnRePt	Cl2Br	10.53365	2.594	-13.0752	0.052	-13.1272
ZrSnRePt	I2Br	11.20581	1.545	-9.58858	0.052	-9.64058
ZrSnTeHf	Br2Cl	10.68029	3.018	-14.0027	0.052	-14.0547
ZrSnTeHf	Br2I	11.18709	2.37	-12.0956	0.052	-12.1476
ZrSnTeHf	Cl2Br	10.59165	3.313	-14.7334	0.052	-14.7854
ZrSnTeHf	I2Br	11.43536	1.909	-10.9412	0.052	-10.9932
ZrSnTeIr	Br2Cl	10.59485	1.136	-12.3721	0.052	-12.4241
ZrSnTeIr	Br2I	11.16597	1.002	-10.6826	0.052	-10.7346
ZrSnTeIr	Cl2Br	10.57408	1.231	-13.032	0.052	-13.084
ZrSnTeIr	I2Br	11.25196	0.442	-9.65695	0.052	-9.70895
ZrSnTeOs	Br2Cl	10.59937	1.674	-12.2677	0.052	-12.3197
ZrSnTeOs	Br2I	11.14431	1.446	-10.5194	0.052	-10.5714
ZrSnTeOs	Cl2Br	10.5716	1.582	-12.9468	0.052	-12.9988
ZrSnTeOs	I2Br	11.36269	1.525	-9.45715	0.052	-9.50915
ZrSnTePt	Br2Cl	10.5868	2.638	-12.4978	0.052	-12.5498
ZrSnTePt	Br2I	11.17001	2.262	-10.8535	0.052	-10.9055
ZrSnTePt	Cl2Br	10.57087	2.747	-13.1351	0.052	-13.1871
ZrSnTePt	I2Br	11.30051	1.64	-9.84012	0.052	-9.89212
ZrSnTeRe	Br2Cl	10.61045	2.931	-12.4895	0.052	-12.5415
ZrSnTeRe	Br2I	11.1522	2.339	-10.6922	0.052	-10.7442
ZrSnTeRe	Cl2Br	10.58093	3.051	-13.1871	0.052	-13.2391
ZrSnTeRe	I2Br	11.34715	1.768	-9.60126	0.052	-9.65326
ZrTeHfIr	Br2Cl	10.59856	1.232	-13.3679	0.052	-13.4199
ZrTeHfIr	Br2I	11.16359	0.884	-11.5505	0.052	-11.6025
ZrTeHfIr	Cl2Br	10.57091	1.127	-14.0762	0.052	-14.1282
ZrTeHfIr	I2Br	11.26914	0.439	-10.4642	0.052	-10.5162
ZrTeHfOs	Br2Cl	10.62084	1.66	-13.2626	0.052	-13.3146
ZrTeHfOs	Br2I	11.15685	1.427	-11.3889	0.052	-11.4409
ZrTeHfOs	Cl2Br	10.56774	1.558	-13.992	0.052	-14.044

ZrTeHfOs	I2Br	11.38489	1.447	-10.2635	0.052	-10.3155
ZrTeHfPt	Br2Cl	10.6015	2.557	-13.4943	0.052	-13.5463
ZrTeHfPt	Br2I	11.15828	2.361	-11.7216	0.052	-11.7736
ZrTeHfPt	Cl2Br	10.56878	2.739	-14.1811	0.052	-14.2331
ZrTeHfPt	I2Br	11.31942	1.793	-10.6481	0.052	-10.7001
ZrTeHfRe	Br2Cl	10.62845	2.024	-13.4847	0.052	-13.5367
ZrTeHfRe	Br2I	11.15851	2.661	-11.5617	0.052	-11.6137
ZrTeHfRe	Cl2Br	10.56789	3.162	-14.232	0.052	-14.284
ZrTeHfRe	I2Br	11.39153	2.319	-10.408	0.052	-10.46
ZrTeIrPt	Br2Cl	10.46731	1.126	-11.8677	0.052	-11.9197
ZrTeIrPt	Br2I	11.11031	0.884	-10.2973	0.052	-10.3493
ZrTeIrPt	Cl2Br	10.49536	1.249	-12.4712	0.052	-12.5232
ZrTeIrPt	I2Br	11.0868	0.439	-9.38231	0.052	-9.43431
ZrTeOsIr	Br2Cl	10.51594	0.448	-11.6685	0.052	-11.7205
ZrTeOsIr	Br2I	11.08984	0.442	-9.99891	0.052	-10.0509
ZrTeOsIr	Cl2Br	10.50511	0.449	-12.3217	0.052	-12.3737
ZrTeOsIr	I2Br	11.16617	0.437	-9.01016	0.052	-9.06216
ZrTeOsPt	Br2Cl	10.48494	1.58	-11.7622	0.052	-11.8142
ZrTeOsPt	Br2I	11.11062	1.45	-10.1352	0.052	-10.1872
ZrTeOsPt	Cl2Br	10.49832	1.585	-12.3875	0.052	-12.4395
ZrTeOsPt	I2Br	11.18585	1.332	-9.17291	0.052	-9.22491
ZrTeReIr	Br2Cl	10.53807	0.97	-11.8798	0.052	-11.9318
ZrTeReIr	Br2I	11.15794	0.775	-10.1626	0.052	-10.2146
ZrTeReIr	Cl2Br	10.5244	3.371	-12.5523	0.052	-12.6043
ZrTeReIr	I2Br	11.18263	0.416	-9.14427	0.052	-9.19627
ZrTeReOs	Br2Cl	10.55963	1.821	-11.7513	0.052	-11.8033
ZrTeReOs	Br2I	11.10133	1.669	-9.97921	0.052	-10.0312
ZrTeReOs	Cl2Br	10.52987	1.541	-12.4407	0.052	-12.4927
ZrTeReOs	I2Br	11.25731	1.487	-8.92858	0.052	-8.98058
ZrTeRePt	Br2Cl	10.54186	2.594	-11.9833	0.052	-12.0353
ZrTeRePt	Br2I	11.12674	2.103	-10.3095	0.052	-10.3615
ZrTeRePt	Cl2Br	10.52928	2.592	-12.6288	0.052	-12.6808
ZrTeRePt	I2Br	11.22524	1.757	-9.31444	0.052	-9.36644

Table S2. Calculated lattice constant, band gap, formation enthalpy, entropy and Gibbs free energy (at 298K) of the 99 promising vacancy-ordered double perovskites that exhibit a band gap between 1.1 and 1.5 eV.

B-site Composition	X-site Composition	Lattice Constant (Å)	Band Gap (eV)	Enthalpy (eV)	Entropy (eV)	Gibbs Free Energy (eV)
Pt	I	11.3011	1.131	-7.71749	0	-7.71749
Ir	Cl2Br	10.43199	1.326	-10.5537	0.016	-10.5697
Os	Br2Cl	10.39574	1.123	-9.55475	0.016	-9.57075
Os	Br2I	11.0197	1.219	-7.91477	0.016	-7.93077
Pt	Br2I	11.10865	1.488	-9.15253	0.016	-9.16853
HfReOsIr	Br	10.66705	1.453	-10.9302	0.036	-10.9662
SnHfIrPt	Br	10.67393	1.242	-11.6928	0.036	-11.7288
SnHfIrPt	Cl	10.2456	1.494	-13.6683	0.036	-13.7043
SnHfOsPt	I	11.27671	1.216	-8.47472	0.036	-8.51072
SnHfReOs	I	11.36904	1.323	-8.15082	0.036	-8.18682
SnHfRePt	I	11.37609	1.43	-8.58714	0.036	-8.62314
SnReOsPt	I	11.33945	1.166	-7.2041	0.036	-7.2401
SnTeHfIr	Br	10.77811	1.132	-11.7875	0.036	-11.8235
SnTeHfIr	Cl	10.31478	1.35	-13.7923	0.036	-13.8283
SnTeHfOs	I	11.49973	1.406	-8.45384	0.036	-8.48984
SnTeIrPt	Br	10.68809	1.235	-10.3788	0.036	-10.4148
SnTeIrPt	Cl	10.25085	1.362	-12.0851	0.036	-12.1211
SnTeOsPt	I	11.37998	1.334	-7.51147	0.036	-7.54747
SnTeReOs	I	11.41426	1.315	-7.18874	0.036	-7.22474
SnTeRePt	I	11.40311	1.441	-7.62495	0.036	-7.66095
TeHfIrPt	Br	10.67743	1.238	-11.3211	0.036	-11.3571
TeHfIrPt	Cl	10.24204	1.361	-13.1846	0.036	-13.2206
TeHfOsPt	I	11.33212	1.324	-8.24713	0.036	-8.28313
TeHfReOs	I	11.38313	1.419	-7.92454	0.036	-7.96054
TeReOsPt	I	11.35887	1.303	-6.9766	0.036	-7.0126
ZrHfIrPt	Br	10.64348	1.239	-12.6005	0.036	-12.6365
ZrHfOsPt	I	11.2927	1.323	-9.22674	0.036	-9.26274
ZrReOsPt	I	11.3007	1.306	-7.95931	0.036	-7.99531
ZrSnHfIr	Br	10.74368	1.336	-13.0611	0.036	-13.0971
ZrSnHfIr	Cl	10.31235	1.464	-15.2918	0.036	-15.3278
ZrSnHfOs	I	11.46794	1.303	-9.42321	0.036	-9.45921
ZrSnIrPt	Br	10.65081	1.243	-11.657	0.036	-11.693
ZrSnIrPt	Cl	10.24864	1.483	-13.5847	0.036	-13.6207
ZrSnOsPt	I	11.282	1.211	-8.4862	0.036	-8.5222
ZrSnReOs	I	11.3689	1.248	-8.16287	0.036	-8.19887
ZrSnRePt	I	11.36494	1.331	-8.59819	0.036	-8.63419
ZrSnTeIr	Br	10.76406	1.113	-11.75	0.036	-11.786

ZrSnTeIr	Cl	10.33329	1.35	-13.7079	0.036	-13.7439
ZrSnTeOs	I	11.48524	1.333	-8.46438	0.036	-8.50038
ZrTeHfIr	Br	10.77017	1.122	-12.6887	0.036	-12.7247
ZrTeHfIr	Cl	10.31349	1.339	-14.805	0.036	-14.841
ZrTeHfOs	I	11.4777	1.407	-9.19793	0.036	-9.23393
ZrTeIrPt	Br	10.67125	1.129	-11.2843	0.036	-11.3203
ZrTeIrPt	Cl	10.25844	1.368	-13.103	0.036	-13.139
ZrTeOsPt	I	11.34142	1.317	-8.25932	0.036	-8.29532
ZrTeReOs	I	11.37046	1.416	-7.93536	0.036	-7.97136
HfReOsIr	I2Br	11.09094	1.317	-8.77326	0.052	-8.82526
SnHfIrPt	Br2Cl	10.45689	1.245	-12.3295	0.052	-12.3815
SnHfIrPt	Cl2Br	10.48389	1.453	-12.9842	0.052	-13.0362
SnHfOsPt	Br2I	11.07577	1.44	-10.4821	0.052	-10.5341
SnHfOsPt	I2Br	11.175	1.335	-9.45398	0.052	-9.50598
SnHfReOs	I2Br	11.22737	1.451	-9.21162	0.052	-9.26362
SnReOsPt	Br2I	11.10015	1.383	-9.07422	0.052	-9.12622
SnReOsPt	I2Br	11.13245	1.235	-8.10409	0.052	-8.15609
SnTeHfIr	Br2Cl	10.57826	1.122	-12.428	0.052	-12.48
SnTeHfIr	Cl2Br	10.58411	1.229	-13.0987	0.052	-13.1507
SnTeHfOs	Br2I	11.20259	1.446	-10.54	0.052	-10.592
SnTeHfOs	I2Br	11.34546	1.421	-9.46505	0.052	-9.51705
SnTeIrPt	Br2Cl	10.48093	1.233	-10.9212	0.052	-10.9732
SnTeIrPt	Cl2Br	10.51308	1.261	-11.4906	0.052	-11.5426
SnTeOsPt	Br2Cl	10.53238	1.483	-10.8165	0.052	-10.8685
SnTeOsPt	Br2I	11.13576	1.44	-9.2855	0.052	-9.3375
SnTeOsPt	I2Br	11.20243	1.335	-8.3667	0.052	-8.4187
SnTeReOs	I2Br	11.25975	1.437	-8.12551	0.052	-8.17751
TeHfIrPt	Br2Cl	10.48119	1.233	-11.9216	0.052	-11.9736
TeHfIrPt	Cl2Br	10.47821	1.166	-12.5378	0.052	-12.5898
TeHfOsPt	I2Br	11.19635	1.441	-9.17668	0.052	-9.22868
TeHfReOs	Cl2Br	10.4991	1.466	-12.5113	0.052	-12.5633
TeHfReOs	I2Br	11.25175	1.282	-8.93656	0.052	-8.98856
TeReOsIr	Cl2Br	10.52041	1.222	-10.8447	0.052	-10.8967
TeReOsPt	I2Br	11.14948	1.41	-7.82513	0.052	-7.87713
ZrHfIrPt	Br2Cl	10.44977	1.351	-13.2769	0.052	-13.3289
ZrHfOsPt	Br2Cl	10.47371	1.484	-13.1709	0.052	-13.2229
ZrHfOsPt	I2Br	11.17325	1.316	-10.262	0.052	-10.314
ZrHfReOs	Br2I	11.02494	1.4	-11.179	0.052	-11.231
ZrHfReOs	I2Br	11.22663	1.179	-10.018	0.052	-10.07
ZrReIrPt	Br2Cl	10.46515	1.103	-11.7805	0.052	-11.8325
ZrReIrPt	Cl2Br	10.47282	1.158	-12.442	0.052	-12.494
ZrReOsPt	I2Br	11.14265	1.435	-8.91299	0.052	-8.96499
ZrSnHfIr	Br2Cl	10.57413	1.35	-13.7747	0.052	-13.8267

ZrSnHfIr	Cl2Br	10.52587	1.345	-14.5239	0.052	-14.5759
ZrSnHfOs	Br2I	11.14073	1.426	-11.7147	0.052	-11.7667
ZrSnIrPt	Br2Cl	10.45677	1.461	-12.2759	0.052	-12.3279
ZrSnIrPt	Cl2Br	10.51312	1.363	-12.9168	0.052	-12.9688
ZrSnOsPt	Br2I	11.10258	1.455	-10.4618	0.052	-10.5138
ZrSnOsPt	I2Br	11.16786	1.331	-9.4476	0.052	-9.4996
ZrSnReOs	I2Br	11.24003	1.427	-9.20468	0.052	-9.25668
ZrSnTeIr	Br2Cl	10.59485	1.136	-12.3721	0.052	-12.4241
ZrSnTeIr	Cl2Br	10.57408	1.231	-13.032	0.052	-13.084
ZrSnTeOs	Br2I	11.14431	1.446	-10.5194	0.052	-10.5714
ZrTeHfIr	Br2Cl	10.59856	1.232	-13.3679	0.052	-13.4199
ZrTeHfIr	Cl2Br	10.57091	1.127	-14.0762	0.052	-14.1282
ZrTeHfOs	Br2I	11.15685	1.427	-11.3889	0.052	-11.4409
ZrTeHfOs	I2Br	11.38489	1.447	-10.2635	0.052	-10.3155
ZrTeIrPt	Br2Cl	10.46731	1.126	-11.8677	0.052	-11.9197
ZrTeIrPt	Cl2Br	10.49536	1.249	-12.4712	0.052	-12.5232
ZrTeOsPt	Br2I	11.11062	1.45	-10.1352	0.052	-10.1872
ZrTeOsPt	I2Br	11.18585	1.332	-9.17291	0.052	-9.22491
ZrTeReOs	I2Br	11.25731	1.487	-8.92858	0.052	-8.98058

Table S3. Comparison of calculated fundamental band gaps (VBM-CBM) from this work with previous work and the experimentally measured optical band gaps.

Compound	Calculated band gap (this work)/ eV	Calculated band gap (previous work)/ eV	Measured optical band gap / eV
Cs_2SnCl_6	3.9	3.9[1]	3.9[2]
Cs_2SnBr_6	2.4	2.4[1]	2.7[2]
Cs_2SnIBr_2	1.6	N/A	1.8[3]
Cs_2SnI_2Br	0.9	N/A	1.4[3]
Cs_2SnI_6	0.7	0.7[1]	1.3[4]
Cs_2PtI_6	1.1	1.1[5]	1.4[6]

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