Supplementary Information 2 for

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Impact of alkaline-earth doping on electronic properties of the photovoltaic perovskite $CsSnI_3$: Insights from a DFT perspective

CsSnI3 - Orthorhombic				6X4X6; 0.02 eV		
	Ry	Energy total	Free energy	% ET	% FE	ΔE_{Total}
1	40	-14912.3005	-14912.3013			
2	80	-14895.8328	-14895.8336	-0.1104	-0.1104	-16.4677
3	120	-14894.0615	-14894.0623	-0.0119	-0.0119	-1.7713
4	160	-14893.7075	-14893.7083	-0.0024	-0.0024	-0.3540
5	200	-14893.5787	-14893.5795	-0.0009	-0.0009	-0.1288
6	240	-14893.5116	-14893.5124	-0.0005	-0.0005	-0.0671
7	280	-14893.5024	-14893.5032	-0.0001	-0.0001	-0.0092
8	320	-14893.4788	-14893.4796	-0.0002	-0.0002	-0.0236
9	360	-14893.4740	-14893.4749	0.0000	0.0000	-0.0048
10	400	-14893.4637	-14893.4645	-0.0001	-0.0001	-0.0104
11	440	-14893.4547	-14893.4555	-0.0001	-0.0001	-0.0090
12	480	-14893.4538	-14893.4546	0.0000	0.0000	-0.0009
13	520	-14893.4519	-14893.4528	0.0000	0.0000	-0.0018
14	560	-14893.4495	-14893.4503	0.0000	0.0000	-0.0024
15	600	-14893.4475	-14893.4484	0.0000	0.0000	-0.0020
16	640	-14893.4463	-14893.4471	0.0000	0.0000	-0.0013
17	680	-14893.4459	-14893.4468	0.0000	0.0000	-0.0003

MgI2				6X6X4; 0.02 eV		
	Ry	Energy total	Free energy	% ET	% FE	ΔE_{Total}
1	40	-2444.5588	-2444.5588			
2	80	-2441.8979	-2441.8979	-0.1089	-0.1089	-2.6609
3	120	-2441.3140	-2441.3140	-0.0239	-0.0239	-0.5839
4	160	-2441.1136	-2441.1136	-0.0082	-0.0082	-0.2004
5	200	-2441.0857	-2441.0857	-0.0011	-0.0011	-0.0279
6	240	-2441.0612	-2441.0612	-0.0010	-0.0010	-0.0245
7	280	-2441.0481	-2441.0481	-0.0005	-0.0005	-0.0130
8	320	-2441.0465	-2441.0465	-0.0001	-0.0001	-0.0016
9	360	-2441.0392	-2441.0392	-0.0003	-0.0003	-0.0073
10	400	-2441.0383	-2441.0383	0.0000	0.0000	-0.0009
11	440	-2441.0383	-2441.0383	0.0000	0.0000	0.0000
12	480	-2441.0383	-2441.0383	0.0000	0.0000	0.0000
13	520					
14	560					
15	600					
16	640					
17	680					

CaI2				6X6X3; 0.02 eV		
	Ry	Energy total	Free energy	% ET	% FE	
1	40	-2481.0065	-2481.0065			
2	80	-2476.5986	-2476.5986	-0.1777	-0.1777	-4.4080
3	120	-2476.2352	-2476.2352	-0.0147	-0.0147	-0.3633
4	160	-2476.2153	-2476.2153	-0.0008	-0.0008	-0.0200
5	200	-2476.1417	-2476.1417	-0.0030	-0.0030	-0.0736
6	240	-2476.1200	-2476.1200	-0.0009	-0.0009	-0.0217
7	280	-2476.1200	-2476.1200	0.0000	0.0000	0.0000
8	320	-2476.1072	-2476.1072	-0.0005	-0.0005	-0.0128
9	360	-2476.1072	-2476.1072	0.0000	0.0000	0.0000
10	400	-2476.1062	-2476.1062	0.0000	0.0000	-0.0010
11	440	-2476.1050	-2476.1050	0.0000	0.0000	-0.0012
12	480	-2476.1030	-2476.1030	-0.0001	-0.0001	-0.0020
13	520	-2476.1030	-2476.1030	0.0000	0.0000	0.0000
14	560	-2476.1016	-2476.1016	-0.0001	-0.0001	-0.0014
15	600	-2476.1014	-2476.1014	0.0000	0.0000	-0.0002
16	640	-2476.1014	-2476.1014	0.0000	0.0000	0.0000

		CsSnI3 - Orthorhombic		480 Ry; 0.02 eV		
		Energy total	Free energy	% ET	% FE	ΔE_{Total}
1	1X1X1	-14888.0832	-14888.1851			
2	2X2X2	-14893.0954	-14893.1057	0.0337	0.0331	5.0122
3	3X2X3	-14893.2993	-14893.3038	0.0014	0.0013	0.2039
4	4X3X4	-14893.4265	-14893.4283	0.0009	0.0008	0.1272
5	5X3X5	-14893.4355	-14893.4368	0.0001	0.0001	0.0090
6	5X4X5	-14893.4499	-14893.4509	0.0001	0.0001	0.0144
7	6X4X6	-14893.4519	-14893.4528	0.0000	0.0000	0.0020
8	7X5X7	-14893.4570	-14893.4576	0.0000	0.0000	0.0051
9	8X5X8	-14893.4567	-14893.4571	0.0000	0.0000	-0.0004
10	8X6X8	-14893.4578	-14893.4582	0.0000	0.0000	0.0012
11	9X6X9	-14893.4582	-14893.4586	0.0000	0.0000	0.0004
12	9X7X9	-14893.4587	-14893.4590	0.0000	0.0000	0.0005

		MgI2		440 Ry; 0.02 eV		
		Energy total	Free energy	% ET	% FE	ΔE_{Total}
1	1X1X1	-2431.8427	-2431.8427			
2	2X2X1	-2440.2514	-2440.2514	0.3458	0.3458	8.4087
3	3X3X2	-2440.9112	-2440.9112	0.0270	0.0270	0.6598
4	4X4X2	-2441.0183	-2441.0183	0.0044	0.0044	0.1070
5	5X5X3	-2441.0350	-2441.0350	0.0007	0.0007	0.0168
6	6X6X3	-2441.0383	-2441.0383	0.0001	0.0001	0.0033
7	7X7X4	-2441.0396	-2441.0396	0.0001	0.0001	0.0012
8	8X8X4	-2441.0397	-2441.0397	0.0000	0.0000	0.0002
9	9X9X5	-2441.0397	-2441.0397	0.0000	0.0000	0.0000
10						
11						
12						

		CaI2		520 Ry; 0.02 eV		
		Energy total	Free energy	% ET	% FE	ΔE_{Total}
1	1X1X1	-2470.5289	-2470.5289			
2	2X2X1	-2475.7840	-2475.7840	0.2127	0.2127	5.2551
3	3X3X2	-2476.0637	-2476.0637	0.0113	0.0113	0.2797
4	4X4X2	-2476.0986	-2476.0986	0.0014	0.0014	0.0349
5	5X5X3	-2476.1023	-2476.1023	0.0001	0.0001	0.0037
6	6X6X3	-2476.1030	-2476.1030	0.0000	0.0000	0.0007
7	7X7X4	-2476.1032	-2476.1032	0.0000	0.0000	0.0002
8	8X8X4	-2476.1032	-2476.1032	0.0000	0.0000	0.0000
9	9X9X5	-2476.1032	-2476.1032	0.0000	0.0000	0.0000
10						
11						
12						

CsSnI3 - Orthorhombic

480 Ry; 6X4X6

	PAOEnergyShift (eV)	Energy total	Free energy		Calls	SCF Time/call	Total
1	0.02	-14894.3327	-14894.3327	0.00000	148.00000	1785.779	264295.29
2	0.04	-14893.3981	-14893.3981	0.00000	292.00000	876.995	256082.54
3	0.06	-14892.6192	-14892.6192	0.00000	425.00000	835.366	355030.55
4	0.08	-14892.0178	-14892.0178	0.00000	296.00000	824.704	244112.38
5	0.10	-14891.2376	-14891.2376	0.00000	243.00000	685.148	166490.96
6	0.12	-14890.2364	-14890.2364	0.00000	183.00000	772.669	141398.43
7	0.14	-14889.2821	-14889.2821	0.00000	181.00000	778.028	140823.07
8	0.16	-14888.7364	-14888.7364	0.00000	210.00000	977.943	205368.03
9	0.18	-14887.0928	-14887.0928	0.00000	221.00000	543.150	120036.15
10	0.20	-14886.9464	-14886.9464	0.00000	212.00000	478.328	101405.54
11	0.22	-14885.6766	-14885.6766	0.00000	167.00000	689.105	115080.54
12	0.24	-14884.9857	-14884.9857	0.00000	170.00000	730.001	124100.17
13	0.26	-14882.9194	-14882.9194	0.00001	226.00000	636.812	143919.51
14	0.28	-14882.9194	-14882.9194	0.00001	226.00000	797.343	180199.52
15	0.30	-14880.2714	-14880.2715	0.00005	205.00000	958.055	196401.28
16	0.32	-14880.0493	-14880.0494	0.00008	184.00000	805.996	148303.26
17	0.34	-14879.7906	-14879.7907	0.00010	220.00000	1405.342	309175.24

480 Ry; 6X4X6

PAOEnergyShift (eV)	a	a - exp	error	b	b - exp	error	c	c - exp	error	Prom error	Standard deviation	a/c	a/c exp	error	Volume/Z	Volume/Z exp	Error
0.02	9.149313	8.6885	5.304	12.936738	12.3775	4.518	8.952640	8.6384	3.638	**4.487**	**0.833**	1.022	1.006	1.608	264.9137	232.25	**14.064**
0.04	9.185956	8.6885	5.725	12.836905	12.3775	3.712	8.984334	8.6384	4.005	**4.481**	**1.088**	1.022	1.006	1.655	264.8565	232.25	**14.039**
0.06	9.136131	8.6885	5.152	12.870595	12.3775	3.984	8.962641	8.6384	3.753	**4.296**	**0.750**	1.019	1.006	1.348	263.4735	232.25	**13.444**
0.08	9.123395	8.6885	5.005	12.844817	12.3775	3.776	8.942903	8.6384	3.525	**4.102**	**0.792**	1.020	1.006	1.430	262.0010	232.25	**12.810**
0.10	9.128167	8.6885	5.060	12.785703	12.3775	3.298	8.896432	8.6384	2.987	**3.782**	**1.118**	1.026	1.006	2.013	259.5757	232.25	**11.766**
0.12	9.094133	8.6885	4.669	12.748477	12.3775	2.997	8.883348	8.6384	2.836	**3.500**	**1.015**	1.024	1.006	1.783	257.4757	232.25	**10.861**
0.14	9.039386	8.6885	4.039	12.688971	12.3775	2.516	8.880783	8.6384	2.806	**3.120**	**0.808**	1.018	1.006	1.199	254.6576	232.25	**9.648**
0.16	9.039031	8.6885	4.034	12.674873	12.3775	2.403	8.844907	8.6384	2.391	**2.943**	**0.946**	1.022	1.006	1.605	253.3871	232.25	**9.101**
0.18	8.995057	8.6885	3.528	12.599158	12.3775	1.791	8.793982	8.6384	1.801	**2.373**	**1.000**	1.023	1.006	1.697	249.1558	232.25	**7.279**
0.20	8.965805	8.6885	3.192	12.595241	12.3775	1.759	8.818495	8.6384	2.085	**2.345**	**0.751**	1.017	1.006	1.084	248.9604	232.25	**7.195**
0.22	8.906245	8.6885	2.506	12.545244	12.3775	1.355	8.803181	8.6384	1.908	**1.923**	**0.576**	1.012	1.006	0.587	245.8971	232.25	**5.876**
0.24	8.899775	8.6885	2.432	12.531255	12.3775	1.242	8.757213	8.6384	1.375	**1.683**	**0.652**	1.016	1.006	1.042	244.1628	232.25	**5.129**
0.26	8.876071	8.6885	2.159	12.462047	12.3775	0.683	8.697178	8.6384	0.680	**1.174**	**0.853**	1.021	1.006	1.468	240.5075	232.25	**3.555**
0.28	8.876071	8.6885	2.159	12.462047	12.3775	0.683	8.697178	8.6384	0.680	**1.174**	**0.853**	1.021	1.006	1.468	240.5075	232.25	**3.555**
0.30	8.822579	8.6885	1.543	12.416764	12.3775	0.317	8.629116	8.6384	-0.107	**0.656**	**0.857**	1.022	1.006	1.652	236.3254	232.25	**1.755**
0.32	8.791082	8.6885	1.181	12.392219	12.3775	0.119	8.649468	8.6384	0.128	**0.476**	**0.610**	1.016	1.006	1.051	235.5705	232.25	**1.430**
0.34	8.784599	8.6885	1.106	12.409503	12.3775	0.259	8.635470	8.6384	-0.034	**0.466**	**0.592**	1.017	1.006	1.140	235.3436	232.25	**1.332**

520 Ry; 7X5X7

PAOEnergyShift (eV)	Energy total	Free energy		Calls	SCF Time/call	Total time	E_Fermi
0.20	-14886.945719	-14886.945719	0.000000	231	2012.833	464964.423	-3.3784
0.22	-14885.676861	-14885.676861	0.000000	207	2022.959	418752.513	-3.2660

PAOEnergyShift (eV)	a	a - exp	error	b	b - exp	error	c	c - exp	error	Prom error	Standard deviation	a/c	a/c exp	error	Volume/Z	Volume/Z exp	Error
0.20	8.983605	8.6885	3.397	12.5912	12.3775	1.727	8.799056	8.6384	1.860	**2.328**	**0.928**	1.021	1.006	1.509	248.8249	232.25	**7.137**
0.22	8.909978	8.6885	2.549	12.552947	12.3775	1.417	8.793455	8.6384	1.795	**1.921**	**0.576**	1.013	1.006	0.741	245.8792	232.25	**5.868**

600 Ry; 7X5X7

PAOEnergyShift (eV)	Energy total	Free energy		Calls	SCF Time/call	Total time	E_Fermi
0.20	-14886.942326	-14886.942326		261	1967.263	513455.643	-3.3864
0.22	-14885.673173	-14885.673173		219	1191.795	261003.105	-3.2725

PAOEnergyShift (eV)	a	a - exp	error	b	b - exp	error	c	c - exp	error	Prom error	Standard deviation	a/c	a/c exp	error	Volume/Z	Volume/Z exp	Error
0.20	8.99663	8.6885	3.546	12.598181	12.3775	1.783	8.784417	8.6384	1.690	**2.340**	**1.046**	1.024	1.006	1.825	248.9090	232.25	**7.173**
0.22	8.924318	8.6885	2.714	12.546561	12.3775	1.366	8.791186	8.6384	1.769	**1.950**	**0.692**	1.015	1.006	0.929	246.0862	232.25	**5.957**

Voronoi				Hirshfeld			
520Ry - 0.20 eV	520Ry - 0.22 eV	600Ry - 0.20 eV	600Ry - 0.22 eV	520Ry - 0.20 eV	520Ry - 0.22 eV	600Ry - 0.20 eV	600Ry - 0.22 eV
0.275	0.260	0.276	0.261	0.229	0.216	0.230	0.216
-0.150	-0.141	-0.150	-0.141	-0.121	-0.112	-0.121	-0.113
-0.149	-0.141	-0.150	-0.141	-0.123	-0.115	-0.123	-0.115
0.175	0.162	0.174	0.162	0.137	0.124	0.136	0.124
0.004	**-0.004**	**0.000**	**0.000**	**0.004**	**0.004**	**0.004**	**-0.004**

	600 Ry; 7X5X7; 0.22 eV					
Functional	Energy total	Free energy	Calls	SCF Time/call	Total time	**E_Fermi**
PBE	-14871.859633	-14871.859633	327	1278.214	417975.978	-3.3065
RPBE	-14890.993393	-14890.993393	226	1199.153	271008.578	-3.2435
PBEsol	-14774.402013	-14774.402013	1009	1133.341	1143541.069	-3.4438
WC	-14833.153620	-14833.153620	465	1541.793	716933.745	-3.4435

Functional	**a**	**a - exp**	**error**	**b**	**b - exp**	**error**	**c**	**c - exp**	**error**	**Prom error**	**Standard deviation**	**a/c**	**a/c exp**	**error**	**Volume/Z**	**Volume/Z exp**	**Error**
PBE	8.985193	8.6885	3.415	12.415199	12.3775	0.305	8.421892	8.6384	-2.506	**2.075**	**2.962**	1.067	1.006	6.073	234.8718	232.25	**1.129**
RPBE	8.921279	8.6885	2.679	12.596974	12.3775	1.773	8.843677	8.6384	2.376	**2.276**	**0.461**	1.009	1.006	0.296	248.4656	232.25	**6.982**
PBEsol	9.066314	8.6885	4.348	12.314073	12.3775	-0.512	7.842087	8.6384	-9.218	**4.693**	**6.874**	1.156	1.006	14.944	248.9090	232.25	**7.173**
WC	9.058197	8.6885	4.255	12.313587	12.3775	-0.516	7.898122	8.6384	-8.570	**4.447**	**6.482**	1.147	1.006	14.027	220.2370	232.25	**-5.172**

Voronoi				Hirshfeld			
PBE	RPBE	PBEsol	WC	PBE	RPBE	PBEsol	WC
0.244	0.265	0.226	0.229	0.200	0.220	0.182	0.185
-0.126	-0.145	-0.107	-0.109	-0.095	-0.117	-0.077	-0.078
-0.124	-0.146	-0.098	-0.100	-0.098	-0.119	-0.071	-0.073
0.131	0.171	0.086	0.088	0.088	0.133	0.042	0.043
-0.004	**0.000**	**0.000**	**-0.004**	**0.000**	**0.000**	**-0.004**	**-0.004**

MgI2					440 Ry; 6X6X3		
	PAOEnergyShift (eV)	Energy total	Free energy		Calls	SCF Time/call	Total
1	0.02	-2441.1884	-2441.1884	0.00000	93.00	48.508	4511.24
2	0.04	-2441.1244	-2441.1244	0.00000	151.00	41.146	6213.05
3	0.06	-2441.0779	-2441.0779	0.00000	127.00	40.084	5090.67
4	0.08	-2440.9977	-2440.9977	0.00000	126.00	37.550	4731.30
5	0.10	-2440.9025	-2440.9025	0.00000	122.00	25.203	3074.77
6	0.12	-2440.7708	-2440.7708	0.00000	119.00	35.76	4255.44
7	0.14	-2440.6390	-2440.6390	0.00000	78.00	38.643	3014.15
8	0.16	-2440.5721	-2440.5721	0.00000	78.00	51.172	3991.42
9	0.18	-2440.3392	-2440.3392	0.00000	106.00	40.424	4284.94
10	0.20	-2440.3149	-2440.3149	0.00000	131.00	31.753	4159.64
11	0.22	-2440.0972	-2440.0972	0.00000	97.00	25.387	2462.54
12	0.24	-2440.0056	-2440.0056	0.00000	85.00	35.842	3046.57
13	0.26			0.00000			0.00
14	0.28			0.00000			0.00
15	0.30			0.00000			0.00
16	0.32			0.00000			0.00
17	0.34			0.00000			0.00

	440 Ry; 6X6X3																
PAOEnergyShift (eV)	a	a - exp		b	b - exp		c	c - exp		Prom error	Standard deviation	c/a	c/a exp	error	Volume/Z	Volume/Z exp	Error
0.02	4.397158	4.1537	5.861	4.397155	4.1537	5.861	7.176313	6.862	4.580	**5.434**	**0.739**	1.632	1.652	**-1.210**	120.1378	102.53	**17.173**
0.04	4.394197	4.1537	5.790	4.394195	4.1537	5.790	7.172169	6.862	4.520	**5.367**	**0.733**	1.632	1.652	**-1.200**	119.9068	102.53	**16.948**
0.06	4.345005	4.1537	4.606	4.344970	4.1537	4.605	7.290905	6.862	6.250	**5.154**	**0.950**	1.678	1.652	**1.572**	119.1669	102.53	**16.226**
0.08	4.346962	4.1537	4.653	4.346961	4.1537	4.653	7.132049	6.862	3.935	**4.414**	**0.414**	1.641	1.652	**-0.685**	116.6897	102.53	**13.810**
0.10	4.324385	4.1537	4.109	4.324385	4.1537	4.109	7.103570	6.862	3.520	**3.913**	**0.340**	1.643	1.652	**-0.566**	115.0198	102.53	**12.182**
0.12	4.297333	4.1537	3.458	4.297331	4.1537	3.458	7.067815	6.862	2.999	**3.305**	**0.265**	1.645	1.652	**-0.443**	113.0158	102.53	**10.227**
0.14	4.268503	4.1537	2.764	4.268502	4.1537	2.764	7.030603	6.862	2.457	**2.662**	**0.177**	1.647	1.652	**-0.299**	110.9152	102.53	**8.178**
0.16	4.260140	4.1537	2.563	4.260139	4.1537	2.563	7.020315	6.862	2.307	**2.477**	**0.147**	1.648	1.652	**-0.249**	110.3210	102.53	**7.599**
0.18	4.207751	4.1537	1.301	4.207746	4.1537	1.301	7.053679	6.862	2.793	**1.799**	**0.861**	1.676	1.652	**1.473**	108.1175	102.53	**5.450**
0.20	4.203072	4.1537	1.189	4.203084	4.1537	1.189	7.086787	6.862	3.276	**1.884**	**1.205**	1.686	1.652	**2.063**	108.3860	102.53	**5.711**
0.22	4.187689	4.1537	0.818	4.187688	4.1537	0.818	6.902964	6.862	0.597	**0.745**	**0.128**	1.648	1.652	**-0.220**	104.8203	102.53	**2.234**
0.24	4.182426	4.1537	0.692	4.182426	4.1537	0.692	6.886624	6.862	0.359	**0.581**	**0.192**	1.647	1.652	**-0.330**	104.3115	102.53	**1.738**
0.26		4.1537	-100.000		4.1537	-100.000		6.862	-100.000	**100.000**	**0.000**	#¡DIV/0!				102.53	**-100.000**
0.28		4.1537	-100.000		4.1537	-100.000		6.862	-100.000	**100.000**	**0.000**	#¡DIV/0!				102.53	**-100.000**
0.30		4.1537	-100.000		4.1537	-100.000		6.862	-100.000	**100.000**	**0.000**	#¡DIV/0!				102.53	**-100.000**
0.32		4.1537	-100.000		4.1537	-100.000		6.862	-100.000	**100.000**	**0.000**	#¡DIV/0!				102.53	**-100.000**
0.34		4.1537	-100.000		4.1537	-100.000		6.862	-100.000	**100.000**	**0.000**	#¡DIV/0!				102.53	**-100.000**

	600 Ry; 7X7X4; 0.22 eV						
PAOEnergyShift (eV)	Energy total	Free energy		Calls	SCF Time/call	Total	**E_Fermi**
revPBE	-2440.095087	-2440.095087		93	127.209	11830.437	-4.5565
RPBE	-2441.054552	-2441.054552		100	26.392	2639.2	-4.6915

PAOEnergyShift (eV)	a	a - exp	error	b	b - exp	error	c	c - exp	error	Prom error	Standard deviation	c/a	c/a exp	error	Volume/Z	Volume/Z exp	Error
revPBE	4.187449	4.1537	0.813	4.187449	4.1537	0.813	6.902502	6.862	0.590	**0.738**	**0.128**	**1.648**	**1.652**	**-0.220**	104.8105	102.53	**2.224**
RPBE	4.208537	4.1537	1.320	4.208538	4.1537	1.320	6.923057	6.862	0.890	**1.177**	**0.249**	**1.645**	**1.652**	**-0.425**	106.1834	102.53	**3.563**

Atom	Voronoi		Hirshfeld	
	revPBE	RPBE	revPBE	RPBE
Mg	0.227	0.220	0.171	0.166
I_1	-0.113	-0.110	-0.086	-0.083
I_2	-0.113	-0.110	-0.086	-0.083
SUMA	**0.001**	**0.000**	**-0.001**	**0.000**

	CaI2				440 Ry; 6X6X3		
	PAOEnergyShift (eV)	Energy total	Free energy		Calls	SCF Time/call	Total
1	0.02	-2476.6381	-2476.6381	0.00000	449.00	54.067	24276.08
2	0.04	-2476.5154	-2476.5154	0.00000	293.00	48.793	14296.35
3	0.06	-2476.4243	-2476.4243	0.00000	165.00	38.809	6403.49
4	0.08	-2476.3286	-2476.3286	0.00000	168.00	36.066	6059.09
5	0.10	-2476.1984	-2476.1984	0.00000	207.00	80.865	16739.06
6	0.12	-2476.0121	-2476.0121	0.00000	149.00	81.417	12131.13
7	0.14	-2475.8397	-2475.8397	0.00000	145.00	36.350	5270.75
8	0.16	-2475.7671	-2475.7671	0.00000	111.00	32.102	3563.32
9	0.18	-2475.4354	-2475.4354	0.00000	113.00	83.151	9396.06
10	0.20	-2475.4354	-2475.4354	0.00000	112.00	32.947	3690.06
11	0.22	-2475.1597	-2475.1597	0.00000	103.00	40.085	4128.76
12	0.24			0.00000	98.00	28.764	2818.87
13	0.26			0.00000			0.00
14	0.28			0.00000			0.00
15	0.30			0.00000			0.00
16	0.32			0.00000			0.00
17	0.34			0.00000			0.00

	440 Ry; 6X6X3																
PAOEnergyShift (eV)	a	a - exp		b	b - exp		c	c - exp		Prom error	Standard deviation	c/a	c/a exp	error	Volume/Z	Volume/Z exp	Error
0.02	4.912886	4.4900	9.418	4.912849	4.4900	9.418	8.797170	6.975	26.124	**14.987**	**9.645**	1.791	1.553	**15.268**	183.7357	121.78	**50.875**
0.04	4.966268	4.4900	10.607	4.966269	4.4900	10.607	7.355761	6.975	5.459	**8.891**	**2.972**	1.481	1.553	**-4.655**	157.0977	121.78	**29.001**
0.06	4.916090	4.4900	9.490	4.916090	4.4900	9.490	7.335510	6.975	5.169	**8.049**	**2.495**	1.492	1.553	**-3.947**	153.5147	121.78	**26.059**
0.08	4.885560	4.4900	8.810	4.885560	4.4900	8.810	7.320618	6.975	4.955	**7.525**	**2.226**	1.498	1.553	**-3.543**	151.3069	121.78	**24.246**
0.10	4.827945	4.4900	7.527	4.827951	4.4900	7.527	7.495836	6.975	7.467	**7.507**	**0.034**	1.553	1.553	**-0.055**	151.2724	121.78	**24.218**
0.12	4.787502	4.4900	6.626	4.787501	4.4900	6.626	7.375006	6.975	5.735	**6.329**	**0.514**	1.540	1.553	**-0.836**	146.3617	121.78	**20.185**
0.14	4.753093	4.4900	5.860	4.753078	4.4900	5.859	7.314208	6.975	4.863	**5.527**	**0.575**	1.539	1.553	**-0.941**	143.0689	121.78	**17.481**
0.16	4.748092	4.4900	5.748	4.748088	4.4900	5.748	7.201238	6.975	3.244	**4.913**	**1.446**	1.517	1.553	**-2.368**	140.5848	121.78	**15.442**
0.18	4.697930	4.4900	4.631	4.697929	4.4900	4.631	7.136331	6.975	2.313	**3.858**	**1.338**	1.519	1.553	**-2.215**	136.3897	121.78	**11.997**
0.20	4.697927	4.4900	4.631	4.697927	4.4900	4.631	7.136336	6.975	2.313	**3.858**	**1.338**	1.519	1.553	**-2.215**	136.3896	121.78	**11.997**
0.22	4.659164	4.4900	3.768	4.659162	4.4900	3.768	7.074175	6.975	1.422	**2.986**	**1.354**	1.518	1.553	**-2.261**	132.9790	121.78	**9.196**
0.24	4.654416	4.4900	3.662	4.654418	4.4900	3.662	7.055921	6.975	1.160	**2.828**	**1.444**	1.516	1.553	**-2.413**	132.3681	121.78	**8.694**
0.26		4.4900	-100.000		4.4900	-100.000		6.975	-100.000	**100.000**	**0.000**	#¡DIV/0!	1.553	**#¡DIV/0!**		121.78	**-100.000**
0.28		4.4900	-100.000		4.4900	-100.000		6.975	-100.000	**100.000**	**0.000**	#¡DIV/0!	1.553	**#¡DIV/0!**		121.78	**-100.000**
0.30		4.4900	-100.000		4.4900	-100.000		6.975	-100.000	**100.000**	**0.000**	#¡DIV/0!				121.78	**-100.000**
0.32		4.4900	-100.000		4.4900	-100.000		6.975	-100.000	**100.000**	**0.000**	#¡DIV/0!				121.78	**-100.000**
0.34		4.4900	-100.000		4.4900	-100.000		6.975	-100.000	**100.000**	**0.000**	#¡DIV/0!				121.78	**-100.000**

	600 Ry; 7X7X4; 0.22 eV					
PAOEnergyShift (eV)	Energy total	Free energy		Calls	SCF Time/call	Total	**E_Fermi**
revPBE	-2475.159982	-2475.159982		79	154.5140	12206.606	
RPBE	-2476.104605	-2476.104605		72	155.7450	11213.64	

											Standard						
PAOEnergyShift (eV)	a	a - exp	error	b	b - exp	error	c	c - exp	error	Prom error	deviation	c/a	c/a exp	error	Volume/Z	Volume/Z exp	Error
revPBE	4.657130	4.4900	3.722	4.657132	4.4900	3.722	7.073561	6.975	1.413	**2.953**	**1.333**	**1.519**	**1.553**	**-2.226**	132.8538	121.78	**9.093**
RPBE	4.666776	4.4900	3.937	4.666775	4.4900	3.937	7.091708	6.975	1.673	**3.182**	**1.307**	**1.520**	**1.553**	**-2.178**	133.7476	121.78	**9.827**

Atom	Voronoi		Hirshfeld	
	revPBE	RPBE	revPBE	RPBE
Ca	0.321	0.329	0.232	0.238
l_1	-0.160	-0.164	-0.116	-0.119
l_2	-0.160	-0.164	-0.116	-0.119
SUMA	**0.001**	**0.001**	**0.000**	**0.000**

Structural data

CsSnI3 - Bonds - Optimized structure

	revPBE (Å)	RPBE (Å)	Exp. (Å)	revPBE - Relative error (%)	RPBE - Relative error (%)
Bond lenght					
Sn-I apical	3.192	3.201		2.340	2.629
	3.191	3.200		2.308	2.597
	3.192	3.201		2.340	2.629
	3.191	3.200	3.119	2.308	2.597
	3.192	3.201		2.340	2.629
	3.191	3.200		2.308	2.597
	3.192	3.201		2.340	2.629
	3.191	3.200		2.308	2.597
Mean value	**3.192**	3.201		**2.324**	**2.613**
Sn-I equatorial	3.203	3.209		2.529	2.721
	3.205	3.210		2.593	2.753
	3.202	3.209		2.497	2.721
	3.205	3.209		2.593	2.721
	3.203	3.209		2.529	2.721
	3.205	3.209		2.593	2.721
	3.203	3.209		2.529	2.721
	3.205	3.210	3.124	2.593	2.753
	3.203	3.209		2.529	2.721
	3.205	3.210		2.593	2.753
	3.203	3.209		2.529	2.721
	3.205	3.209		2.593	2.721
	3.205	3.210		2.593	2.753
	3.203	3.209		2.529	2.721
	3.205	3.209		2.593	2.721
	3.203	3.209		2.529	2.721
Mean value	**3.204**	3.209		**2.559**	**2.729**
Angles					
Sn-I apical	158.719	159.478		-4.386	-3.929
	158.715	159.480	166.000	-4.389	-3.928
	158.719	159.486		-4.386	-3.924
	158.716	159.481		-4.388	-3.927
Mean value	**158.717**	159.481		**-4.387**	**-3.927**
Sn-I equatorial	155.614	156.236		-1.260	-0.865
	155.616	156.233		-1.259	-0.867
	155.616	156.232		-1.259	-0.868
	155.617	156.237	157.600	-1.258	-0.865
	155.630	156.249		-1.250	-0.857
	155.631	156.250		-1.249	-0.857
	155.631	156.249		-1.249	-0.857
	155.632	156.250		-1.249	-0.857
Mean value	**155.623**	156.242		**-1.254**	**-0.862**

CsSnI3 - Cell dimensions - FINE Optimization

	revPBE (Å)	RPBE (Å)	Exp. (Å)	revPBE - Relative error (%)	RPBE - Relative error (%)
Lattice constants					
a	8.92	8.921	8.689	2.71	2.679
b	12.55	12.597	12.378	1.37	1.773
c	8.79	8.844	8.638	1.77	2.376
Mean error				**1.950**	**2.276**
α	90.000	90.000	90.000	0.000	0.000
β	90.000	90.002	90.000	0.000	0.002
γ	90.000	90.000	90.000	0.000	0.000
Mean error				**0.000**	**0.001**
Volume	984.34	993.862	928.990	**5.96**	**6.983**

Structural data

CsSnI3 - w/Grimme corrections - Bonds - Optimized structure

	Grimme1 (Å)	Grimme2 (Å)	Grimme3 (Å)	Exp. (Å)	Grimme1 - Relative error (%)	Grimme2 - Relative error (%)	Grimme3 - Relative error (%)
Bond lenght							
Sn-I apical	3.170	3.171	3.169		1.635	1.667	1.603
	3.170	3.171	3.168		1.635	1.667	1.571
	3.170	3.171	3.169		1.635	1.667	1.603
	3.170	3.171	3.169	3.119	1.635	1.667	1.603
	3.170	3.171	3.169		1.635	1.667	1.603
	3.170	3.171	3.169		1.635	1.667	1.603
	3.170	3.172	3.169		1.635	1.699	1.603
	3.170	3.172	3.169		1.635	1.699	1.603
Mean value	3.170	3.171	3.169		**1.635**	**1.675**	**1.599**
Sn-I equatorial	3.178	3.179	3.180		1.729	1.761	1.793
	3.199	3.199	3.195		2.401	2.401	2.273
	3.178	3.180	3.180		1.729	1.793	1.793
	3.199	3.200	3.196		2.401	2.433	2.305
	3.178	3.179	3.178		1.729	1.761	1.729
	3.200	3.199	3.198		2.433	2.401	2.369
	3.178	3.181	3.178		1.729	1.825	1.729
	3.200	3.199	3.198	3.124	2.433	2.401	2.369
	3.178	3.178	3.177		1.729	1.729	1.697
	3.199	3.200	3.198		2.401	2.433	2.369
	3.178	3.178	3.177		1.729	1.729	1.697
	3.199	3.201	3.199		2.401	2.465	2.401
	3.200	3.200	3.201		2.433	2.433	2.465
	3.178	3.179	3.174		1.729	1.761	1.601
	3.200	3.201	3.201		2.433	2.465	2.465
	3.178	3.178	3.175		1.729	1.729	1.633
Mean value	3.189	3.189	3.188		**2.073**	**2.095**	**2.043**
Angles							
Sn-I apical	160.803	160.896	160.996		-3.131	-3.075	-3.014
	160.805	160.867	161.005	166.000	-3.130	-3.092	-3.009
	160.806	160.846	160.953		-3.129	-3.105	-3.040
	160.804	160.833	160.944		-3.130	-3.113	-3.046
Mean value	160.805	160.861	160.975		**-3.130**	**-3.096**	**-3.027**
Sn-I equatorial	146.097	145.876	146.308		-7.299	-7.439	-7.165
	146.095	145.907	146.303		-7.300	-7.419	-7.168
	146.072	145.848	146.220		-7.315	-7.457	-7.221
	146.070	145.848	146.240	157.600	-7.316	-7.457	-7.208
	146.095	145.903	146.213		-7.300	-7.422	-7.225
	146.095	145.895	146.231		-7.300	-7.427	-7.214
	146.072	145.847	146.151		-7.315	-7.457	-7.265
	146.071	145.866	146.143		-7.315	-7.445	-7.270
Mean value	146.083	145.874	146.226		**-7.308**	**-7.441**	**-7.217**

CsSnI3 - Cell dimensions - FINE Optimization - revPBE

	Grimme1	Grimme2	Grimme3	Exp. (Å)	Grimme1 - Relative error (%)	Grimme2 - Relative error (%)	Grimme3 - Relative error (%)
Lattice constants							
a	9.20	9.21	9.20	8.69	5.92	6.00	5.91
b	12.50	12.51	12.50	12.38	1.01	1.06	1.00
c	8.01	8.00	8.01	8.64	-7.28	-7.44	-7.26
Mean error					**4.74**	**4.83**	**4.72**
α	90.00	90.00	90.00	90.00	0.00	0.00	0.00
β	90.00	89.99	90.00	90.00	0.00	-0.01	0.00
γ	90.00	90.00	90.00	90.00	0.00	0.00	0.00
Mean error					**0.00**	**0.01**	**0.00**
Volume	921.60	921.13	921.66	928.99	**-0.80**	**-0.85**	**-0.79**

Structural data

Mg-doped perovskite - Bonds - Optimized structure

		Mg1	Mg2	Mg3	Mg4
Bond lenght					
	Sn-I apical	3.19	3.16	3.12	3.15
		3.12	3.15	3.19	3.16
		3.15	3.15	3.16	3.16
		3.16	3.16	3.15	3.15
		3.29	3.32	3.02	2.98
		3.01	2.98	3.28	3.32
		3.02	3.02	3.29	3.29
		3.29	3.29	3.02	3.02
	Mean value	**3.15**	**3.15**	**3.15**	**3.15**
	Sn-I equatorial	3.20	3.19	3.24	3.00
		3.14	3.14	3.06	3.30
		3.19	3.20	3.00	3.24
		3.14	3.14	3.30	3.06
		3.27	3.27	3.17	3.17
		3.03	3.03	3.17	3.17
		3.02	3.02	3.17	3.17
		3.26	3.27	3.18	3.18
		3.28	3.27	3.17	3.16
		3.02	3.02	3.17	3.18
		3.02	3.02	3.17	3.17
		3.27	3.27	3.17	3.17
		3.17	3.17	3.27	3.03
		3.17	3.17	3.02	3.27
		3.17	3.18	3.03	3.27
		3.17	3.16	3.27	3.02
	Mean value	**3.16**	**3.16**	**3.16**	**3.16**
Angles					
	Sn-I apical	159.93	160.02	159.89	160.01
		160.02	160.04	160.01	160.03
		160.63	160.73	160.67	160.64
		160.63	160.63	160.65	160.62
	Mean value	**160.30**	**160.35**	**160.31**	**160.33**
	Sn-I equatorial	155.25	155.36	157.91	158.06
		155.00	154.94	158.28	158.27
		158.90	158.70	154.34	154.51
		158.35	158.90	154.14	154.07
		158.72	159.15	154.45	154.33
		159.22	158.50	154.64	154.81
		154.54	154.33	158.88	158.71
		154.69	154.81	158.35	158.51
	Mean value	**156.83**	**156.84**	**156.37**	**156.41**

CsSnMgI3 - revPBE - Cell dimensions - FINE Optimization

	Mg1	Mg2	Mg3	Mg4
Lattice constants				
a	8.78	8.78	8.78	8.78
b	12.43	12.43	12.42	12.43
c	8.71	8.71	8.71	8.71
α	90.01	89.99	90.02	90.01
β	90.04	89.97	90.01	89.97
γ	89.59	89.59	90.40	90.41
Volume	950.60	950.52	950.35	950.54

Apical

Bond	Times	Length
Sn-I	2	3.19
	6	3.16
	6	3.15
	2	3.12
Total/Average	**16**	**3.15**
Sn-I	2	3.32
	5	3.29
	1	3.28
Total/Average	**8**	**3.29**
Mg-I	5	3.02
	1	3.01
	2	2.98
Total	**8**	**3.01**

Angle	Average
Sn-I-Sn	159.99
Mg-I-Sn	160.65

Lattice constants average

a	8.78
b	12.43
c	8.71
Volume	950.50
α	90.01
β	90.00
γ	90.00

Equatorial

Equatorial	Times	Length
Sn-I	2	3.20
	2	3.19
	4	3.18
	18	3.17
	2	3.16
	4	3.14
Total/Average	**32**	**3.17**
Sn-I	2	3.30
	1	3.28
	10	3.27
	1	3.26
	2	3.24
Total/Average	**16**	**3.27**
Mg-I	2	3.06
	4	3.03
	8	3.02
	2	3.00
Total/Average	**16**	**3.03**

Angle	Average
Sn-I-Sn	154.64
Mg-I-Sn	158.59

Structural data

Ca-doped perovskite - Bonds - Optimized structure

		Ca1	Ca2	Ca3	Ca4
Bond lenght					
	Sn-I apical	3.18	3.21	3.22	3.19
		3.22	3.19	3.18	3.21
		3.20	3.21	3.20	3.20
		3.20	3.20	3.20	3.21
		3.21	3.21	3.24	3.24
		3.25	3.25	3.21	3.21
		3.23	3.23	3.22	3.22
		3.22	3.22	3.23	3.23
Mean value		**3.21**	**3.21**	**3.21**	**3.21**
	Sn-I equatorial	3.22	3.19	3.23	3.28
		3.23	3.25	3.25	3.21
		3.19	3.22	3.28	3.23
		3.25	3.22	3.22	3.25
		3.24	3.24	3.22	3.22
		3.25	3.25	3.22	3.22
		3.25	3.25	3.21	3.22
		3.24	3.24	3.22	3.22
		3.23	3.24	3.21	3.22
		3.25	3.25	3.22	3.22
		3.25	3.19	3.22	3.22
		3.24	3.31	3.22	3.22
		3.22	3.22	3.24	3.25
		3.22	3.22	3.25	3.24
		3.22	3.22	3.25	3.24
		3.22	3.22	3.23	3.25
Mean value		**3.23**	**3.23**	**3.23**	**3.23**
Angles					
	Sn-I apical	158.80	158.75	158.08	157.97
		158.37	158.38	158.30	158.36
		153.98	153.96	154.57	154.54
		154.29	154.29	154.32	154.29
Mean value		**156.36**	**156.34**	**156.32**	**156.29**
	Sn-I equatorial	154.02	155.16	151.58	150.78
		155.38	154.17	150.62	151.45
		150.88	150.74	154.75	155.18
		150.59	150.22	155.37	154.97
		150.92	150.77	154.97	154.99
		151.22	150.70	154.49	155.18
		155.02	155.00	150.88	150.74
		154.49	155.19	151.17	150.77
Mean value		**152.82**	**152.74**	**152.98**	**153.01**

CsSnCaI3 - revPBE - Cell dimensions - FINE Optimization

	Ca1	Ca2	Ca3	Ca4
Lattice constants				
a	9.02	9.02	9.02	9.02
b	12.58	12.58	12.58	12.58
c	8.74	8.74	8.74	8.74
α	89.82	90.18	90.18	89.82
β	89.99	90.01	89.96	90.02
γ	90.20	90.20	89.82	89.81
Volume	992.25	992.26	992.23	992.25

Apical

Bond	Times	Length
Sn-I	2	3.22
	4	3.21
	6	3.20
	2	3.19
	2	3.18
Total/Average	**16**	**3.20**
Sn-I	4	3.22
	4	3.21
Total/Average	**8**	**3.21**
Ca-I	2	3.25
	2	3.24
	4	3.23
Total	**8**	**3.24**

Angle	Average
Sn-I-Sn	158.38
Ca-I-Sn	154.28

Lattice constants average

a	9.02
b	12.58
c	8.74
Volume	992.25
α	90.00
β	89.99
γ	90.01

Equatorial

Equatorial	Times	Length
Sn-I	2	3.25
	1	3.23
	25	3.22
	2	3.21
	2	3.19
Total/Average	**32**	**3.22**
Sn-I	1	3.31
	9	3.24
	4	3.23
	1	3.22
	1	3.21
Total/Average	**16**	**3.24**
Ca-I	2	3.28
	13	3.25
	1	3.19
Total/Average	**16**	**3.25**

Angle	Average
Sn-I-Sn	154.89
Ca-I-Sn	150.88

Mg-doped perovskite					
Atom	**1 - Voronoi charges**	**2 - Voronoi charges**	**3 - Voronoi charges**	**4 - Voronoi charges**	**Average**
Sn - HP	0.305	0.304	0.305	0.303	0.304
Sn - VP	0.281	0.279	0.281	0.278	0.280
Sn - DP	0.248	0.250	0.247	0.249	0.249
Mg	0.334	0.335	0.333	0.335	0.334
I - eq - HP	-0.164	-0.164	-0.165	-0.165	-0.163
I - eq - HP	-0.164	-0.164	-0.165	-0.165	
I - eq - HP	-0.163	-0.163	-0.163	-0.163	
I - eq - HP	-0.162	-0.162	-0.162	-0.161	
I - eq - DHP	-0.133	-0.133	-0.132	-0.133	-0.132
I - eq - DHP	-0.132	-0.133	-0.132	-0.132	
I - eq - DHP	-0.132	-0.132	-0.131	-0.132	
I - eq - DHP	-0.131	-0.131	-0.131	-0.131	
I - ap - VP	-0.175	-0.176	-0.175	-0.176	-0.175
I - ap - VP	-0.175	-0.173	-0.175	-0.174	
I - ap - DVP	-0.123	-0.123	-0.123	-0.123	-0.123
I - ap - DVP	-0.123	-0.123	-0.123	-0.123	
Cs	0.152	0.152	0.153	0.153	0.153
Suma	-0.001	-0.001	0.001	-0.001	-0.001

CsSnI - orthorhombic	
Atom	**Averaged Voronoi charges**
Sn	0.261
I - equatoria	-0.141
I - apical	-0.141
Cs	0.162
Suma	0.000

Ca-doped perovskite					
Atom	**Voronoi charges**	**2 - Voronoi charges**	**3 - Voronoi charges**	**4 - Voronoi charges**	**Average**
Sn - HP	0.305	0.306	0.307	0.309	0.307
Sn - VP	0.290	0.290	0.289	0.289	0.290
Sn - DP	0.270	0.269	0.272	0.271	0.271
Ca	0.394	0.393	0.392	0.392	0.393
I - eq - HP	-0.174	-0.173	-0.176	-0.176	-0.173
I - eq - HP	-0.173	-0.173	-0.173	-0.172	
I - eq - HP	-0.172	-0.171	-0.172	-0.171	
I - eq - HP	-0.172	-0.171	-0.172	-0.170	
I - eq - DHP	-0.139	-0.140	-0.139	-0.140	-0.139
I - eq - DHP	-0.139	-0.139	-0.139	-0.139	
I - eq - DHP	-0.138	-0.139	-0.137	-0.139	
I - eq - DHP	-0.137	-0.138	-0.137	-0.138	
I - ap - VP	-0.170	-0.172	-0.173	-0.173	-0.171
I - ap - VP	-0.171	-0.170	-0.170	-0.170	
I - ap - DVP	-0.141	-0.141	-0.140	-0.140	-0.140
I - ap - DVP	-0.141	-0.141	-0.140	-0.139	
Cs	0.153	0.153	0.152	0.152	0.152
Suma	0.002	0.000	0.000	0.002	0.001

CsSnI3								
	a	b	c	Volume	Energy (eV)	Birch-Murnaghan	Residual	Residual^2
11	9.427612	13.254135	9.286972	1160.4521	-14884.2381	-14884.2298	-0.008328	0.00007
10	9.380709	13.188194	9.240768	1143.2180	-14884.4704	-14884.4682	-0.002241	0.00001
9	9.334039	13.122581	9.194794	1126.2398	-14884.6849	-14884.6872	0.002293	0.00001
8	9.287601	13.057294	9.149049	1109.5137	-14884.8804	-14884.8862	0.005856	0.00003
7	9.241394	12.992333	9.103532	1093.0362	-14885.0565	-14885.0645	0.008023	0.00006
6	9.195417	12.927694	9.058240	1076.8031	-14885.2121	-14885.2214	0.009269	0.00009
5	9.149668	12.863377	9.013174	1060.8112	-14885.3468	-14885.3562	0.009459	0.00009
4	9.104147	12.799380	8.968333	1045.0569	-14885.4592	-14885.4683	0.009010	0.00008
3	9.058853	12.735702	8.923714	1029.5365	-14885.5489	-14885.5567	0.007864	0.00006
2	9.013784	12.672340	8.879318	1014.2466	-14885.6141	-14885.6209	0.006821	0.00005
1	8.968940	12.609294	8.835142	999.1839	-14885.6554	-14885.6600	0.004537	0.00002
0	8.924318	12.546561	8.791186	984.3447	-14885.6732	-14885.6732	0.000000	0.00000
-1	8.879696	12.483828	8.747230	969.6532	-14885.6604	-14885.6596	-0.000870	0.00000
-2	8.835298	12.421409	8.703494	955.1811	-14885.6212	-14885.6181	-0.003118	0.00001
-3	8.791121	12.359302	8.659976	940.9247	-14885.5539	-14885.5480	-0.005862	0.00003
-4	8.747166	12.297505	8.616677	926.8814	-14885.4553	-14885.4484	-0.006936	0.00005
-5	8.703430	12.236018	8.573593	913.0476	-14885.3252	-14885.3182	-0.006971	0.00005
-6	8.659913	12.174838	8.530725	899.4203	-14885.1643	-14885.1567	-0.007602	0.00006
-7	8.616613	12.113964	8.488072	885.9963	-14884.9680	-14884.9628	-0.005273	0.00003
-8	8.573530	12.053394	8.445631	872.7726	-14884.7383	-14884.7355	-0.002752	0.00001
-9	8.530663	11.993127	8.403403	859.7465	-14884.4732	-14884.4739	0.000668	0.00000
-10	8.488009	11.933161	8.361386	846.9146	-14884.1722	-14884.1769	0.004683	0.00002

B_{0}	B'_{0}	B0 (GPa)	SSR
0.1211	4.0649	19.402746	8.21E-04

Birch – Murnaghan EOS

$$E(V) = E_0 + \frac{9V_0B_0}{16}\left\{\left[\left(\frac{V_0}{V}\right)^{\frac{2}{3}} - 1\right]^3 B'_0 + \left[\left(\frac{V_0}{V}\right)^{\frac{2}{3}} - 1\right]^2 \left[6 - 4\left(\frac{V_0}{V}\right)^{\frac{2}{3}}\right]\right\}$$

Mg-doped perovskite

	a	b	c	Volume	Energy (eV)	Birch-Murnaghan	Residual	Residual^2
11	9.278046	13.127258	9.201496	1120.6707	-14866.8875	-14866.8825	-0.00501	0.00003
10	9.231886	13.061949	9.155718	1104.0275	-14867.1172	-14867.1150	-0.00217	0.00000
9	9.185956	12.996964	9.110167	1087.6312	-14867.3293	-14867.3291	-0.00019	0.00000
8	9.140255	12.932302	9.064842	1071.4784	-14867.5216	-14867.5239	0.00225	0.00001
7	9.094781	12.867963	9.019744	1055.5658	-14867.6946	-14867.6987	0.00410	0.00002
6	9.049534	12.803943	8.974869	1039.8893	-14867.8474	-14867.8528	0.00545	0.00003
5	9.004511	12.740242	8.930218	1024.4456	-14867.9786	-14867.9855	0.00688	0.00005
4	8.959713	12.676857	8.885789	1009.2314	-14868.0884	-14868.0959	0.00753	0.00006
3	8.915137	12.613788	8.841581	994.2430	-14868.1754	-14868.1833	0.00782	0.00006
2	8.870783	12.551033	8.797593	979.4772	-14868.2388	-14868.2467	0.00796	0.00006
1	8.826650	12.488590	8.753824	964.9308	-14868.2781	-14868.2855	0.00741	0.00005
0	8.782736	12.426458	8.710273	950.6005	-14868.2986	-14868.2986	0.00000	0.00000
1	8.738822	12.364326	8.666722	936.4126	-14868.2801	-14868.2850	0.00489	0.00002
2	8.695128	12.302504	8.623388	922.4365	-14868.2393	-14868.2437	0.00445	0.00002
3	8.651653	12.240992	8.580271	908.6691	-14868.1707	-14868.1737	0.00302	0.00001
4	8.608394	12.179787	8.537370	895.1071	-14868.0720	-14868.0740	0.00200	0.00000
5	8.565352	12.118888	8.494683	881.7475	-14867.9416	-14867.9436	0.00200	0.00000
6	8.522526	12.058293	8.452209	868.5872	-14867.7796	-14867.7814	0.00183	0.00000
7	8.479913	11.998002	8.409948	855.6235	-14867.5852	-14867.5863	0.00113	0.00000
8	8.437513	11.938012	8.367899	842.8532	-14867.3572	-14867.3572	0.00001	0.00000
9	8.395326	11.878322	8.326059	830.2735	-14867.0942	-14867.0929	-0.00121	0.00000
10	8.353349	11.818930	8.284429	817.8816	-14866.7950	-14866.7924	-0.00267	0.00001

B_{0}	B'_{0}	B0 (GPa)	SSR
0.1246	4.3104	**19.966983**	4.39E-04

Ca-doped perovskite

	a	b	c	Volume	Energy (eV)	irch-Murnagha	Residual	Residual^2
11	9.532628	13.289869	9.233616	1169.7692	-14902.2387	-14902.2349	-0.00372	0.00001
10	9.485202	13.223751	9.187677	1152.3966	-14902.4670	-14902.4656	-0.00141	0.00000
9	9.438012	13.157961	9.141968	1135.2822	-14902.6773	-14902.6778	0.00048	0.00000
8	9.391056	13.092498	9.096485	1118.4217	-14902.8684	-14902.8708	0.00237	0.00001
7	9.344335	13.027362	9.051229	1101.8119	-14903.0409	-14903.0440	0.00302	0.00001
6	9.297845	12.962549	9.006198	1085.4485	-14903.1925	-14903.1966	0.00404	0.00002
5	9.251587	12.898059	8.961391	1069.3282	-14903.3233	-14903.3279	0.00460	0.00002
4	9.205560	12.833889	8.916807	1053.4474	-14903.4325	-14903.4371	0.00462	0.00002
3	9.159761	12.770039	8.872445	1037.8025	-14903.5189	-14903.5235	0.00465	0.00002
2	9.114190	12.706506	8.828303	1022.3897	-14903.5821	-14903.5863	0.00413	0.00002
1	9.068846	12.643290	8.784381	1007.2060	-14903.6210	-14903.6245	0.00356	0.00001
0	9.023727	12.580388	8.740678	992.2477	-14903.6375	-14903.6375	0.00000	0.00000
1	8.978608	12.517486	8.696975	977.4383	-14903.6215	-14903.6241	0.00262	0.00001
2	8.933715	12.454899	8.653490	962.8500	-14903.5827	-14903.5834	0.00070	0.00000
3	8.889047	12.392624	8.610222	948.4793	-14903.5139	-14903.5143	0.00041	0.00000
4	8.844602	12.330661	8.567171	934.3231	-14903.4158	-14903.4160	0.00023	0.00000
5	8.800379	12.269008	8.524335	920.3783	-14903.2875	-14903.2874	-0.00011	0.00000
6	8.756377	12.207663	8.481714	906.6416	-14903.1285	-14903.1276	-0.00087	0.00000
7	8.712595	12.146624	8.439305	893.1097	-14902.9359	-14902.9355	-0.00046	0.00000
8	8.669032	12.085891	8.397109	879.7800	-14902.7110	-14902.7099	-0.00111	0.00000
9	8.625687	12.025462	8.355123	866.6492	-14902.4504	-14902.4499	-0.00046	0.00000
10	8.582558	11.965334	8.313347	853.7142	-14902.1542	-14902.1543	0.00007	0.00000

B_{0}	B'_{0}	B0 (GPa)	SSR
0.1179	4.2554	**18.891085**	1.51E-04

n=2		k	T	Energy kT
2		8.6173E-05	298.15	2.5693E-02

Mg-doped perovskite

	1.317	n=2					n=2			
n_ext	**qVoc**	qVoc_theo	residual	residual^2	**qV_mp (n_2)**	**J_MP / J_SC (n_2)**	**V_oc'**	**ff_1**	**ff_2**	**FF**
1.00E-03	8.808E-01	8.808E-01	0.000E+00	0.000E+00	7.40E-01	9.344E+01	1.714E+01	8.411E-01	9.344E-01	0.786
2.00E-03	8.986E-01	8.986E-01	0.000E+00	0.000E+00	7.57E-01	9.358E+01	1.749E+01	8.430E-01	9.358E-01	0.789
3.00E-03	9.090E-01	9.090E-01	0.000E+00	0.000E+00	7.67E-01	9.366E+01	1.769E+01	8.441E-01	9.366E-01	0.791
4.00E-03	9.164E-01	9.164E-01	0.000E+00	0.000E+00	7.74E-01	9.371E+01	1.783E+01	8.449E-01	9.371E-01	0.792
5.00E-03	9.221E-01	9.221E-01	0.000E+00	0.000E+00	7.79E-01	9.375E+01	1.795E+01	8.455E-01	9.375E-01	0.793
6.00E-03	9.268E-01	9.268E-01	0.000E+00	0.000E+00	7.84E-01	9.379E+01	1.804E+01	8.460E-01	9.379E-01	0.793
7.00E-03	9.308E-01	9.308E-01	0.000E+00	0.000E+00	7.87E-01	9.381E+01	1.811E+01	8.464E-01	9.381E-01	0.794
8.00E-03	9.342E-01	9.342E-01	0.000E+00	0.000E+00	7.91E-01	9.384E+01	1.818E+01	8.467E-01	9.384E-01	0.795
9.00E-03	9.372E-01	9.372E-01	0.000E+00	0.000E+00	7.93E-01	9.386E+01	1.824E+01	8.470E-01	9.386E-01	0.795
1.00E-02	9.399E-01	9.399E-01	0.000E+00	0.000E+00	7.96E-01	9.388E+01	1.829E+01	8.473E-01	9.388E-01	0.795

Ca-doped perovskite

	1.546	n=2					n=2			
n_ext	**qVoc**	qVoc_theo	residual	residual^2	**qV_mp (n_2)**	**J_MP / J_SC (n_2)**	**V_oc'**	**ff_1**	**ff_2**	**FF**
1.00E-03	1.096E+00	1.096E+00	0.000E+00	0.000E+00	9.44E-01	9.480E+01	2.133E+01	8.614E-01	9.480E-01	0.817
2.00E-03	1.114E+00	1.114E+00	0.000E+00	0.000E+00	9.61E-01	9.489E+01	2.168E+01	8.629E-01	9.489E-01	0.819
3.00E-03	1.124E+00	1.124E+00	0.000E+00	0.000E+00	9.71E-01	9.494E+01	2.188E+01	8.637E-01	9.494E-01	0.820
4.00E-03	1.132E+00	1.132E+00	0.000E+00	0.000E+00	9.78E-01	9.497E+01	2.203E+01	8.642E-01	9.497E-01	0.821
5.00E-03	1.138E+00	1.138E+00	0.000E+00	0.000E+00	9.83E-01	9.500E+01	2.214E+01	8.647E-01	9.500E-01	0.821
6.00E-03	1.142E+00	1.142E+00	0.000E+00	0.000E+00	9.88E-01	9.502E+01	2.223E+01	8.651E-01	9.502E-01	0.822
7.00E-03	1.146E+00	1.146E+00	0.000E+00	0.000E+00	9.92E-01	9.504E+01	2.231E+01	8.654E-01	9.504E-01	0.822
8.00E-03	1.150E+00	1.150E+00	0.000E+00	0.000E+00	9.95E-01	9.506E+01	2.237E+01	8.656E-01	9.506E-01	0.823
9.00E-03	1.153E+00	1.153E+00	0.000E+00	0.000E+00	9.98E-01	9.507E+01	2.243E+01	8.658E-01	9.507E-01	0.823
1.00E-02	1.155E+00	1.155E+00	0.000E+00	0.000E+00	1.00E+00	9.508E+01	2.249E+01	8.660E-01	9.508E-01	0.823

n=2		k	T	Energy kT
2		8.6173E-05	298.15	2.5693E-02

Sr-doped perovskite

	1.868	n=2						n=2		
n_ext	**qVoc**	qVoc_theo	residual	residual^2	**qV_mp (n_2)**	**J_MP / J_SC (n_2)**	**V_oc'**	**ff_1**	**ff_2**	**FF**
1.00E-03	1.399E+00	1.399E+00	0.000E+00	0.000E+00	1.23E+00	9.598E+01	2.723E+01	8.820E-01	9.598E-01	0.847
2.00E-03	1.417E+00	1.417E+00	0.000E+00	0.000E+00	1.25E+00	9.604E+01	2.758E+01	8.830E-01	9.604E-01	0.848
3.00E-03	1.427E+00	1.427E+00	0.000E+00	0.000E+00	1.26E+00	9.607E+01	2.778E+01	8.835E-01	9.607E-01	0.849
4.00E-03	1.435E+00	1.435E+00	0.000E+00	0.000E+00	1.27E+00	9.609E+01	2.792E+01	8.839E-01	9.609E-01	0.849
5.00E-03	1.441E+00	1.441E+00	0.000E+00	0.000E+00	1.27E+00	9.610E+01	2.804E+01	8.842E-01	9.610E-01	0.850
6.00E-03	1.445E+00	1.445E+00	0.000E+00	0.000E+00	1.28E+00	9.612E+01	2.813E+01	8.845E-01	9.612E-01	0.850
7.00E-03	1.449E+00	1.449E+00	0.000E+00	0.000E+00	1.28E+00	9.613E+01	2.820E+01	8.847E-01	9.613E-01	0.850
8.00E-03	1.453E+00	1.453E+00	0.000E+00	0.000E+00	1.29E+00	9.614E+01	2.827E+01	8.849E-01	9.614E-01	0.851
9.00E-03	1.456E+00	1.456E+00	0.000E+00	0.000E+00	1.29E+00	9.615E+01	2.833E+01	8.851E-01	9.615E-01	0.851
1.00E-02	1.458E+00	1.458E+00	0.000E+00	0.000E+00	1.29E+00	9.615E+01	2.838E+01	8.852E-01	9.615E-01	0.851

Ba-doped perovskite

	2.118	n=2						n=2		
n_ext	**qVoc**	qVoc_theo	residual	residual^2	**qV_mp (n_2)**	**J_MP / J_SC (n_2)**	**V_oc'**	**ff_1**	**ff_2**	**FF**
1.00E-03	1.635E+00	1.635E+00	0.000E+00	0.000E+00	1.46E+00	9.659E+01	3.181E+01	8.938E-01	9.659E-01	0.863
2.00E-03	1.652E+00	1.652E+00	0.000E+00	0.000E+00	1.48E+00	9.663E+01	3.216E+01	8.946E-01	9.663E-01	0.864
3.00E-03	1.663E+00	1.663E+00	0.000E+00	0.000E+00	1.49E+00	9.665E+01	3.236E+01	8.950E-01	9.665E-01	0.865
4.00E-03	1.670E+00	1.670E+00	0.000E+00	0.000E+00	1.50E+00	9.667E+01	3.250E+01	8.954E-01	9.667E-01	0.866
5.00E-03	1.676E+00	1.676E+00	0.000E+00	0.000E+00	1.50E+00	9.668E+01	3.261E+01	8.956E-01	9.668E-01	0.866
6.00E-03	1.681E+00	1.681E+00	0.000E+00	0.000E+00	1.51E+00	9.669E+01	3.271E+01	8.958E-01	9.669E-01	0.866
7.00E-03	1.685E+00	1.685E+00	0.000E+00	0.000E+00	1.51E+00	9.670E+01	3.278E+01	8.960E-01	9.670E-01	0.866
8.00E-03	1.688E+00	1.688E+00	0.000E+00	0.000E+00	1.51E+00	9.670E+01	3.285E+01	8.961E-01	9.670E-01	0.867
9.00E-03	1.691E+00	1.691E+00	0.000E+00	0.000E+00	1.52E+00	9.671E+01	3.291E+01	8.963E-01	9.671E-01	0.867
1.00E-02	1.694E+00	1.694E+00	0.000E+00	0.000E+00	1.52E+00	9.671E+01	3.296E+01	8.964E-01	9.671E-01	0.867

CsSnI3

	1.3	n=2						n=2		
n_ext	**qVoc**	qVoc_theo	residual	residual^2	**qV_mp (n_2)**	**J_MP / J_SC (n_2)**	**V_oc'**	**ff_1**	**ff_2**	**FF**
1.00E-03	8.648E-01	8.648E-01	0.000E+00	0.000E+00	7.25E-01	9.331E+01	1.683E+01	8.393E-01	9.331E-01	0.783
2.00E-03	8.826E-01	8.826E-01	0.000E+00	0.000E+00	7.42E-01	9.345E+01	1.718E+01	8.413E-01	9.345E-01	0.786
3.00E-03	8.930E-01	8.930E-01	0.000E+00	0.000E+00	7.52E-01	9.353E+01	1.738E+01	8.424E-01	9.353E-01	0.788
4.00E-03	9.004E-01	9.004E-01	0.000E+00	0.000E+00	7.59E-01	9.359E+01	1.752E+01	8.432E-01	9.359E-01	0.789
5.00E-03	9.061E-01	9.061E-01	0.000E+00	0.000E+00	7.64E-01	9.363E+01	1.763E+01	8.438E-01	9.363E-01	0.790
6.00E-03	9.108E-01	9.108E-01	0.000E+00	0.000E+00	7.68E-01	9.367E+01	1.773E+01	8.443E-01	9.367E-01	0.791
7.00E-03	9.148E-01	9.148E-01	0.000E+00	0.000E+00	7.72E-01	9.370E+01	1.780E+01	8.447E-01	9.370E-01	0.791
8.00E-03	9.182E-01	9.182E-01	0.000E+00	0.000E+00	7.75E-01	9.372E+01	1.787E+01	8.451E-01	9.372E-01	0.792
9.00E-03	9.212E-01	9.212E-01	0.000E+00	0.000E+00	7.78E-01	9.375E+01	1.793E+01	8.454E-01	9.375E-01	0.793
1.00E-02	9.239E-01	9.239E-01	0.000E+00	0.000E+00	7.81E-01	9.376E+01	1.798E+01	8.457E-01	9.376E-01	0.793

	J_MP (mA)	J_SC (mA)	V_oc	V_MP	FF	FF -Calculated
Champion	18.81	20.32	0.84	0.71	0.78	0.78

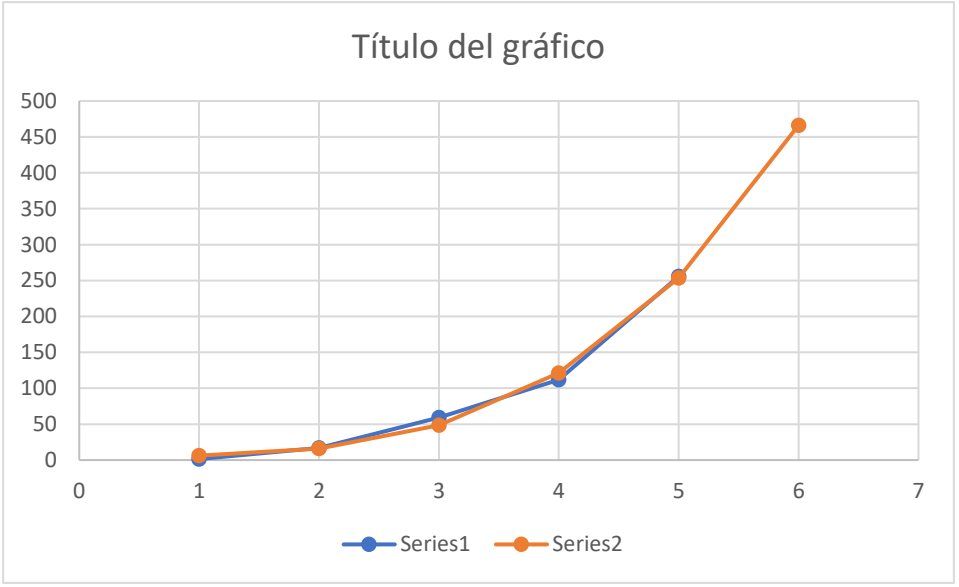
E_g	h (eV*s)	c (m/s)	h^3	c^2	h^3*c^2	2pi/h^3*c^2	Integral	1/m^2*s
1.30	4.1357E-15	2.9979E+08	7.0735E-44	8.9876E+16	6.3574E-27	9.8833E+26	4.7897E-24	4.7338E+03
1.32	4.1357E-15	2.9979E+08	7.0735E-44	8.9876E+16	6.3574E-27	9.8833E+26	2.2659E-24	2.2395E+03
1.55	4.1357E-15	2.9979E+08	7.0735E-44	8.9876E+16	6.3574E-27	9.8833E+26	4.0220E-28	3.9751E-01
1.87	4.1357E-15	2.9979E+08	7.0735E-44	8.9876E+16	6.3574E-27	9.8833E+26	2.2693E-33	2.2428E-06
2.12	4.1357E-15	2.9979E+08	7.0735E-44	8.9876E+16	6.3574E-27	9.8833E+26	1.7282E-37	1.7080E-10

	Q_c	Q_s	J_sc	q*Q_c	V_oc	V_max	qV/kT	EXP(qV/kT)	J_rr	J_max	P_max	FF	n
E_g	1/cm^2*s	1/cm^2*s	mA/cm^2	mA/cm^2	V	V	adimensional	adimensional	mA/cm^2	mA/cm^2	mA/cm^2	adimensional	%
1.30	**4.734E-01**	**2.236E+17**	**35.83**	7.58E-17	**1.07**	**0.95**	3.71E+01	1.24E+16	0.94	**34.88**	**33.21**	**0.865**	**33.20**
1.32	2.239E-01	2.211E+17	35.43	3.59E-17	1.09	0.97	3.78E+01	2.55E+16	0.91	34.52	33.50	0.867	33.49
1.55	**3.975E-05**	**1.702E+17**	**27.27**	6.37E-21	**1.31**	**1.18**	4.60E+01	9.12E+19	0.58	**26.69**	**31.52**	**0.885**	**31.50**
1.87	2.243E-10	1.106E+17	17.72	3.59E-26	1.60	1.47	5.74E+01	8.44E+24	0.30	17.42	25.68	0.903	25.67
2.12	1.708E-14	7.558E+16	12.11	2.74E-30	1.84	1.70	6.64E+01	6.57E+28	0.18	11.93	20.34	0.913	20.33

	x	C_{6}	C_{6} - Exponential	residual	residual^2
H	1	1.451	6.15	-4.7003	22.0930
Li	2	16.6865	15.95	0.7332	0.5376
Na	3	59.18	48.48	10.7047	114.5916
K	4	111.9341	121.05	-9.1200	83.1747
Rb	5	255.6865	253.30	2.3824	5.6757
Cs	6		**466.12**		**SSR**
					226.072751

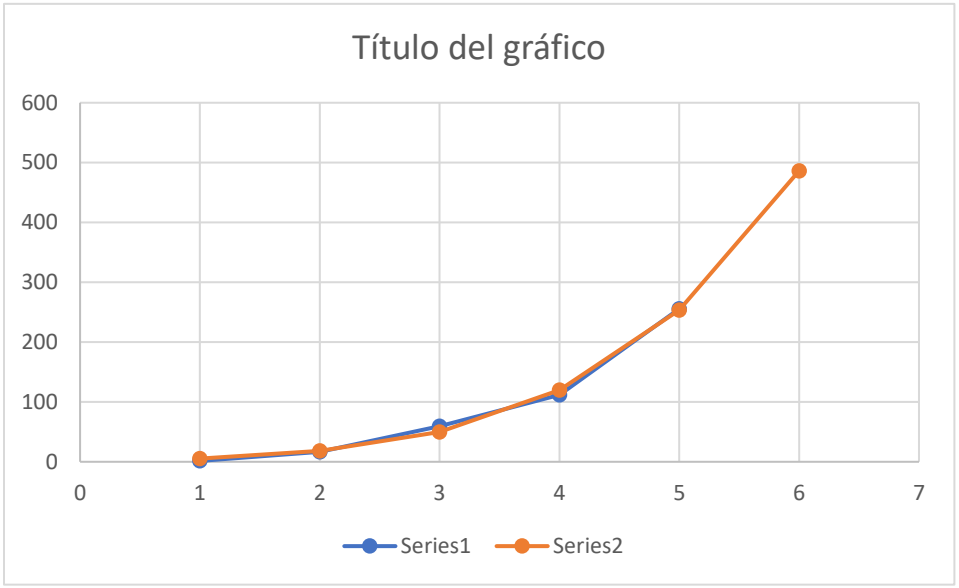
A	k	n	B	D
19602.3636	0.00431062	3.42680136	1.011967368	1.00026253

Ba	**466.12**	Exponential fit
Ba	**476.20**	Promedio
Ba	**486.28**	Polynomial fit



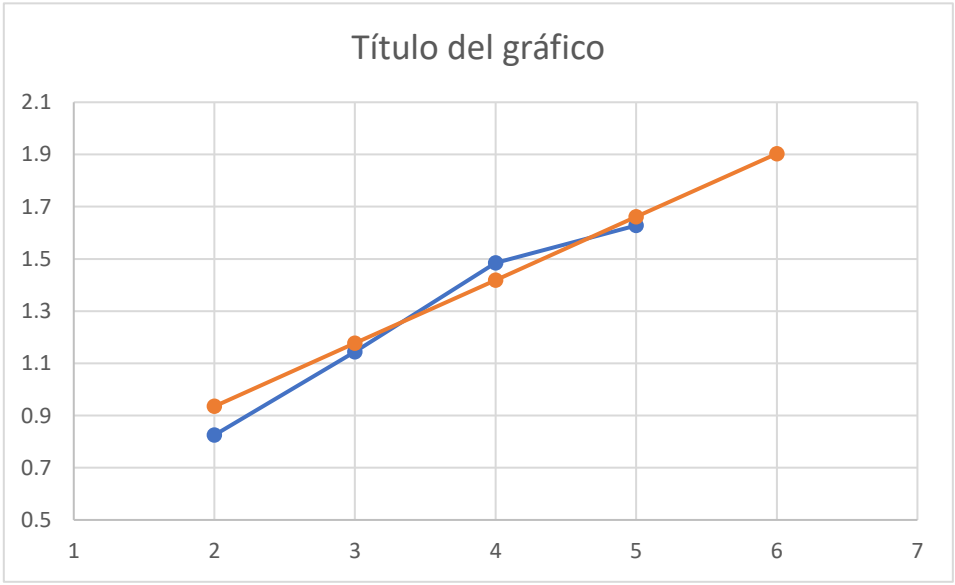
	x	C_{6}	C_{6} - PolyFourth	residual	residual^2
H	1	1.451	5.32	-3.8723415	14.995028
Li	2	16.6865	18.19	-1.5022748	2.2568296
Na	3	59.18	49.97	9.21006834	84.8253588
K	4	111.9341	119.62	-7.6887648	59.1171034
Rb	5	255.6865	253.69	2.00045209	4.00180857
Cs	6		**486.28**		**SSR**
					165.196129

A	B	C	D	E
0	3.4479008	1.55950645	0	0.31593421



	x	$R\_\{0\}$	$R\_\{0\}$ - Lineal	residual	residual^2
H	1	1.001			
Li	2	0.825	0.935	-0.1100	0.0121
Na	3	1.144	1.177	-0.0330	0.0011
K	4	1.485	1.419	0.0660	0.0044
Rb	5	1.628	1.661	-0.0330	0.0011
Cs	6		**1.903**		**SSR**
					0.006534

A	**B**
0.45099998	0.24199997



	Octahedron 1	Octahedron 2	Octahedron 3	Octahedron 4
l_1	3.122	3.122	3.122	3.122
l_2	3.123	3.123	3.123	3.123
l_3	3.122	3.122	3.122	3.122
l_4	3.123	3.123	3.123	3.123
l_5	3.118	3.118	3.118	3.118
l_6	3.118	3.118	3.118	3.118
Average	**3.121**	**3.121**	**3.121**	**3.121**
Standard deviation	**0.002**	**0.002**	**0.002**	**0.002**
Φ*_1*	91.427	88.573	91.427	88.573
Φ*_2*	91.101	88.899	88.899	91.101
Φ*_3*	88.573	91.427	88.573	91.427
Φ*_4*	88.899	91.101	91.101	88.899
Φ*_5*	88.573	91.427	88.573	91.427
Φ*_6*	88.899	91.101	91.101	88.899
Φ*_7*	91.427	88.573	91.427	88.573
Φ*_8*	91.101	88.899	88.899	91.101
Φ*_9*	90.050	90.050	89.950	89.950
Φ*_10*	89.950	89.950	90.050	90.050
Φ*_11*	90.050	90.050	89.950	89.950
Φ*_12*	89.950	89.950	90.050	90.050
Average	**90.000**	**90.000**	**90.000**	**90.000**
Standard deviation	**1.087**	**1.087**	**1.087**	**1.087**
Θ_1	55.19	55.19	55.19	55.19
Θ_2	55.52	55.52	55.52	55.52
Θ_3	7.02	7.02	7.02	7.02
Average	**39.246**	**39.246**	**39.246**	**39.246**
Standard deviation	**27.905**	**27.905**	**27.905**	**27.905**

	Octahedron 1		
	x	*y*	*z*
v_1	3.56402	0.50500	5.10184
v_2	5.12448	-0.50500	-3.53656
v_3	-0.06082	6.18875	-0.76018
a_1	8.68850	0.00000	0.00000
a_2	0.00000	0.00000	8.63840
a_3	0.00000	12.37750	0.00000
*v_1 * a_1 / |v_1||a_1|*		0.57080	
*v_2 * a_2 / |v_2||a_2|*		0.56614	
*v_3 * a_3 / |v_3||a_3|*		0.99249	

	Octahedron 2		
	x	*y*	*z*
v_1	3.56402	-0.50500	5.10184
v_2	5.12448	0.50500	-3.53656
v_3	0.06082	6.18875	0.76018
a_1	8.68850	0.00000	0.00000
a_2	0.00000	0.00000	8.63840
a_3	0.00000	12.37750	0.00000
*v_1 * a_1 / |v_1||a_1|*		0.57080	
*v_2 * a_2 / |v_2||a_2|*		0.56614	
*v_3 * a_3 / |v_3||a_3|*		0.99249	

	Octahedron 3		
	x	*y*	*z*
v_1	3.56402	0.50500	-5.10184
v_2	5.12448	-0.50500	3.53656
v_3	-0.06082	6.18875	0.76018
a_1	8.68850	0.00000	0.00000
a_2	0.00000	0.00000	8.63840
a_3	0.00000	12.37750	0.00000
*v_1 * a_1 / |v_1||a_1|*		0.57080	
*v_2 * a_2 / |v_2||a_2|*		0.56614	
*v_3 * a_3 / |v_3||a_3|*		0.99249	

	Octahedron 4		
	x	*y*	*z*
v_1	3.56402	-0.50500	-5.10184
v_2	5.12448	0.50500	3.53656
v_3	0.06082	6.18875	-0.76018
a_1	8.68850	0.00000	0.00000
a_2	0.00000	0.00000	8.63840
a_3	0.00000	12.37750	0.00000
*v_1 * a_1 / |v_1||a_1|*		0.57080	
*v_2 * a_2 / |v_2||a_2|*		0.56614	
*v_3 * a_3 / |v_3||a_3|*		0.99249	

	Octahedron 1	Octahedron 2	Octahedron 3	Octahedron 4
l_1	3.203	3.202	3.203	3.203
l_2	3.205	3.205	3.205	3.205
l_3	3.203	3.203	3.203	3.203
l_4	3.205	3.205	3.205	3.205
l_5	3.191	3.191	3.191	3.191
l_6	3.192	3.192	3.192	3.192
Average	**3.200**	**3.200**	**3.200**	**3.200**
Standard deviation	**0.007**	**0.006**	**0.007**	**0.007**
Φ*_1*	90.609	89.403	90.611	89.402
Φ*_2*	91.375	88.634	88.636	91.375
Φ*_3*	89.400	90.607	89.402	90.610
Φ*_4*	88.635	91.374	91.377	88.637
Φ*_5*	89.391	90.602	89.388	90.598
Φ*_6*	88.623	91.367	91.365	88.620
Φ*_7*	90.599	89.388	90.599	89.390
Φ*_8*	91.367	88.624	88.622	91.367
Φ*_9*	90.227	90.229	89.773	89.771
Φ*_10*	89.772	89.772	90.227	90.226
Φ*_11*	90.227	90.224	89.773	89.774
Φ*_12*	89.774	89.775	90.227	90.229
Average	**90.000**	**90.000**	**90.000**	**90.000**
Standard deviation	**0.914**	**0.914**	**0.914**	**0.914**
Θ_1	54.33	54.33	54.33	54.33
Θ_2	55.17	55.17	55.17	55.17
Θ_3	10.64	10.64	10.64	10.64
Average	**40.047**	**40.047**	**40.047**	**40.047**
Standard deviation	**25.469**	**25.469**	**25.470**	**25.470**

	Octahedron 1				Octahedron 2		
	x	*y*	*z*		*x*	*y*	*z*
v_1	3.73510	0.87332	5.12974	*v_1*	3.73508	-0.87334	5.12971
v_2	5.18921	-0.87331	-3.66143	*v_2*	5.18926	0.87332	-3.66139
v_3	0.03582	6.27331	-1.17813	*v_3*	-0.03582	6.27325	1.17819
a_1	8.92432	0.00000	0.00000	*a_1*	8.92432	0.00000	0.00000
a_2	-0.00005	0.00005	8.79119	*a_2*	-0.00005	0.00005	8.79119
a_3	-0.00002	12.54656	0.00000	*a_3*	-0.00002	12.54656	0.00000
*v_1 * a_1 / |v_1||a_1|*		0.58313		*v_1 * a_1 / |v_1||a_1|*		0.58313	
*v_2 * a_2 / |v_2||a_2|*		0.57115		*v_2 * a_2 / |v_2||a_2|*		0.57114	
*v_3 * a_3 / |v_3||a_3|*		0.98280		*v_3 * a_3 / |v_3||a_3|*		0.98280	

	Octahedron 3				Octahedron 4		
	x	*y*	*z*		*x*	*y*	*z*
v_1	3.73511	0.87330	-5.12980	*v_1*	3.73506	-0.87334	-5.12984
v_2	5.18922	-0.87334	3.66140	*v_2*	5.18924	0.87333	3.66143
v_3	0.03582	6.27327	1.17817	*v_3*	-0.03582	6.27329	-1.17810
a_1	8.92432	0.00000	0.00000	*a_1*	8.92432	0.00000	0.00000
a_2	-0.00005	0.00005	8.79119	*a_2*	-0.00005	0.00005	8.79119
a_3	-0.00002	12.54656	0.00000	*a_3*	-0.00002	12.54656	0.00000
*v_1 * a_1 / |v_1||a_1|*		0.58312		*v_1 * a_1 / |v_1||a_1|*		0.58311	
*v_2 * a_2 / |v_2||a_2|*		0.57114		*v_2 * a_2 / |v_2||a_2|*		0.57114	
*v_3 * a_3 / |v_3||a_3|*		0.98280		*v_3 * a_3 / |v_3||a_3|*		0.98280	

	Mg	Apical w/Mg	Equatorial w/Mg	Alone
	Octahedron 1	Octahedron 2	Octahedron 3	Octahedron 4
l_1	3.022	3.192	3.269	3.198
l_2	3.024	3.169	3.262	3.139
l_3	3.024	3.168	3.275	3.172
l_4	3.026	3.135	3.267	3.173
l_5	3.014	3.288	3.118	3.160
l_6	3.015	3.289	3.149	3.191
Average	**3.021**	**3.207**	**3.223**	**3.172**
Standard deviation	**0.005**	**0.066**	**0.070**	**0.021**
Φ*_1*	90.603	89.388	91.182	88.948
Φ*_2*	91.162	87.268	89.939	92.826
Φ*_3*	89.409	90.619	89.351	91.619
Φ*_4*	88.850	92.762	90.593	87.764
Φ*_5*	89.432	90.182	88.926	90.558
Φ*_6*	88.867	92.146	90.151	87.806
Φ*_7*	90.556	89.805	90.541	88.868
Φ*_8*	91.121	87.820	89.316	91.599
Φ*_9*	90.408	89.982	89.655	89.772
Φ*_10*	89.621	89.411	90.430	90.838
Φ*_11*	90.343	91.039	89.472	89.644
Φ*_12*	89.628	89.568	90.438	89.739
Average	**90.000**	**89.999**	**90.000**	**89.998**
Standard deviation	**0.805**	**1.564**	**0.666**	**1.556**
Θ_1	53.28	55.19	52.77	55.10
Θ_2	53.79	55.67	53.10	55.88
Θ_3	10.12	9.26	10.09	9.95
Average	**39.064**	**40.043**	**38.651**	**40.312**
Standard deviation	**25.065**	**26.658**	**24.738**	**26.293**

	Octahedron 1				Octahedron 2			
	x	*y*	*z*		*x*	*y*	*z*	
v_1	3.61468	0.78935	4.78116	*v_1*	3.63047	-0.79413	5.16120	
v_2	-4.82324	0.76163	3.57089	*v_2*	-5.13812	-0.85425	3.55166	
v_3	0.00261	5.93534	-1.05897	*v_3*	-0.00261	6.49111	1.05747	
a_1	8.78274	0.00000	0.00000	*a_1*	8.78274	0.00000	0.00000	
a_2	-0.00538	-0.00101	8.71027	*a_2*	-0.00538	-0.00101	8.71027	
a_3	0.08790	12.42615	0.00000	*a_3*	0.08790	12.42615	0.00000	
*v_1 * a_1 / |v_1||a_1|*		0.59791		*v_1 * a_1 / |v_1||a_1|*		0.57083		
*v_2 * a_2 / |v_2||a_2|*		0.59077		*v_2 * a_2 / |v_2||a_2|*		0.56389		
*v_3 * a_3 / |v_3||a_3|*		0.98443		*v_3 * a_3 / |v_3||a_3|*		0.98696		

	Octahedron 3				Octahedron 4			
	x	*y*	*z*		*x*	*y*	*z*	
v_1	3.95927	0.82376	-5.14481	*v_1*	3.64440	-0.79212	-5.16404	
v_2	5.16783	-0.72722	3.92368	*v_2*	5.15205	0.85626	3.54365	
v_3	-0.01531	6.17066	1.09602	*v_3*	0.01531	6.25580	-1.09752	
a_1	8.78274	0.00000	0.00000	*a_1*	8.78274	0.00000	0.00000	
a_2	-0.00538	-0.00101	8.71027	*a_2*	-0.00538	-0.00101	8.71027	
a_3	0.08790	12.42615	0.00000	*a_3*	0.08790	12.42615	0.00000	
*v_1 * a_1 / |v_1||a_1|*		0.60503		*v_1 * a_1 / |v_1||a_1|*		0.57212		
*v_2 * a_2 / |v_2||a_2|*		0.60047		*v_2 * a_2 / |v_2||a_2|*		0.56094		
*v_3 * a_3 / |v_3||a_3|*		0.98454		*v_3 * a_3 / |v_3||a_3|*		0.98495		

	Ca	Apical w/Ca	Equatorial w/Ca	Alone
	Octahedron 1	Octahedron 2	Octahedron 3	Octahedron 4
l_1	3.252	3.185	3.237	3.220
l_2	3.250	3.223	3.244	3.246
l_3	3.249	3.216	3.234	3.217
l_4	3.252	3.226	3.241	3.217
l_5	3.246	3.219	3.222	3.200
l_6	3.233	3.210	3.204	3.178
Average	**3.247**	**3.213**	**3.230**	**3.213**
Standard deviation	**0.007**	**0.015**	**0.015**	**0.023**
Φ*_1*	89.924	88.376	89.294	89.734
Φ*_2*	91.000	90.767	86.612	90.518
Φ*_3*	89.830	91.426	90.409	89.882
Φ*_4*	88.754	89.054	93.095	89.095
Φ*_5*	90.029	92.173	90.647	90.219
Φ*_6*	89.024	89.299	93.342	88.972
Φ*_7*	90.216	88.026	89.649	90.160
Φ*_8*	91.121	90.875	86.951	91.415
Φ*_9*	89.585	89.248	90.020	89.990
Φ*_10*	90.441	90.815	89.925	89.514
Φ*_11*	89.608	88.644	90.132	90.532
Φ*_12*	90.365	91.293	89.922	89.962
Average	**89.991**	**90.000**	**90.000**	**89.999**
Standard deviation	**0.707**	**1.374**	**1.972**	**0.662**
Θ_1	55.67	54.26	55.82	54.64
Θ_2	57.58	56.43	57.55	55.88
Θ_3	12.72	13.14	10.86	10.55
Average	**41.992**	**41.280**	**41.412**	**40.356**
Standard deviation	**25.365**	**24.392**	**26.469**	**25.819**

	Octahedron 1				Octahedron 2			
	x	*y*	*z*		*x*	*y*	*z*	
v_1	3.66575	1.06999	5.26063	*v_1*	3.73880	-0.88169	5.12058	
v_2	-5.38816	1.05356	3.48378	*v_2*	-5.29859	-0.87815	3.56926	
v_3	0.17013	6.32043	-1.41390	*v_3*	-0.17013	6.25989	1.45428	
a_1	9.02373	0.00000	0.00000	*a_1*	9.02373	0.00000	0.00000	
a_2	0.00159	0.02806	8.74063	*a_2*	0.00159	0.02806	8.74063	
a_3	-0.04470	12.58031	0.00000	*a_3*	-0.04470	12.58031	0.00000	
*v_1 * a_1 / |v_1||a_1|*		0.56392		*v_1 * a_1 / |v_1||a_1|*		0.58407		
*v_2 * a_2 / |v_2||a_2|*		0.53615		*v_2 * a_2 / |v_2||a_2|*		0.55290		
*v_3 * a_3 / |v_3||a_3|*		0.97544		*v_3 * a_3 / |v_3||a_3|*		0.97381		

	Octahedron 3				Octahedron 4			
	x	*y*	*z*		*x*	*y*	*z*	
v_1	3.63551	1.02149	-5.25526	*v_1*	3.72508	-0.91022	-5.16978	
v_2	5.35792	-1.10206	3.48169	*v_2*	5.28487	0.84961	3.62174	
v_3	0.07710	6.31065	1.20701	*v_3*	-0.07710	6.26967	-1.16663	
a_1	9.02373	0.00000	0.00000	*a_1*	9.02373	0.00000	0.00000	
a_2	0.00159	0.02806	8.74063	*a_2*	0.00159	0.02806	8.74063	
a_3	-0.04470	12.58031	0.00000	*a_3*	-0.04470	12.58031	0.00000	
*v_1 * a_1 / |v_1||a_1|*		0.56179		*v_1 * a_1 / |v_1||a_1|*		0.57872		
*v_2 * a_2 / |v_2||a_2|*		0.53656		*v_2 * a_2 / |v_2||a_2|*		0.56096		
*v_3 * a_3 / |v_3||a_3|*		0.98208		*v_3 * a_3 / |v_3||a_3|*		0.98309		

	Equatorial w/Mg	Alone	Mg	Apical w/Mg
	Octahedron 1	Octahedron 2	Octahedron 3	Octahedron 4
l_1	3.269	3.198	3.022	3.193
l_2	3.267	3.175	3.023	3.142
l_3	3.267	3.172	3.024	3.160
l_4	3.269	3.136	3.026	3.171
l_5	3.149	3.160	2.983	3.288
l_6	3.149	3.159	3.015	3.318
Average	**3.228**	**3.167**	**3.016**	**3.212**
Standard deviation	**1.495**	**1.466**	**0.016**	**0.073**
Φ*_1*	90.635	88.950	90.612	89.389
Φ*_2*	88.956	87.757	89.520	93.312
Φ*_3*	89.353	91.043	89.983	91.162
Φ*_4*	91.031	92.256	91.074	87.263
Φ*_5*	89.325	90.588	89.421	90.043
Φ*_6*	91.079	91.537	90.521	87.222
Φ*_7*	90.687	89.410	89.984	89.401
Φ*_8*	88.934	88.447	88.884	92.197
Φ*_9*	89.554	89.715	89.655	89.444
Φ*_10*	90.483	89.583	90.392	91.090
Φ*_11*	89.558	90.881	89.575	89.498
Φ*_12*	90.406	89.821	90.372	89.963
Average	**90.000**	**89.999**	**89.999**	**89.999**
Standard deviation	**0.797**	**1.309**	**0.618**	**1.780**
Θ_1	52.74	55.13	53.31	55.18
Θ_2	53.11	55.85	53.75	55.70
Θ_3	10.00	9.98	10.15	9.19
Average	**38.616**	**40.323**	**39.072**	**40.023**
Standard deviation	**24.783**	**26.278**	**25.050**	**26.706**

	Octahedron 1			Octahedron 2		
	x	*y*	*z*	*x*	*y*	*z*
v_1	3.95703	0.79146	5.14173	3.64122	-0.82331	5.16098
v_2	-5.17008	0.75721	3.92671	-5.15500	-0.82520	3.54550
v_3	-0.01298	6.20247	-1.09219	0.01298	6.22337	1.09494
a_1	8.78242	0.00000	0.00000	8.78242	0.00000	0.00000
a_2	0.00497	0.00190	8.71025	0.00497	0.00190	8.71025
a_3	0.08811	12.42553	0.00000	0.08811	12.42553	0.00000
*v_1 * a_1 / |v_1||a_1|*		0.60540		*v_1 * a_1 / |v_1||a_1|*		0.57165
*v_2 * a_2 / |v_2||a_2|*		0.60034		*v_2 * a_2 / |v_2||a_2|*		0.56133
*v_3 * a_3 / |v_3||a_3|*		0.98481		*v_3 * a_3 / |v_3||a_3|*		0.98486

	Octahedron 3			Octahedron 4		
	x	*y*	*z*	*x*	*y*	*z*
v_1	3.61211	0.81948	-4.77853	3.62720	-0.76292	-5.15974
v_2	4.82516	-0.72919	3.57354	5.14097	0.88559	3.55429
v_3	0.00543	5.90455	1.05613	-0.00543	6.52129	-1.05338
a_1	8.78242	0.00000	0.00000	8.78242	0.00000	0.00000
a_2	0.00497	0.00190	8.71025	0.00497	0.00190	8.71025
a_3	0.08811	12.42553	0.00000	0.08811	12.42553	0.00000
*v_1 * a_1 / |v_1||a_1|*		0.59744		*v_1 * a_1 / |v_1||a_1|*		0.57094
*v_2 * a_2 / |v_2||a_2|*		0.59125		*v_2 * a_2 / |v_2||a_2|*		0.56356
*v_3 * a_3 / |v_3||a_3|*		0.98436		*v_3 * a_3 / |v_3||a_3|*		0.98717

	Equatorial w/Ca	Alone	Ca	Apical w/Ca
	Octahedron 1	Octahedron 2	Octahedron 3	Octahedron 4
l_1	3.242	3.219	3.252	3.186
l_2	3.240	3.215	3.254	3.224
l_3	3.241	3.215	3.250	3.217
l_4	3.237	3.247	3.252	3.219
l_5	3.190	3.198	3.248	3.219
l_6	3.206	3.210	3.232	3.208
Average	**3.226**	**3.217**	**3.248**	**3.212**
Standard deviation	**1.493**	**1.489**	**0.008**	**0.014**
Φ*_1*	93.288	89.760	89.936	88.385
Φ*_2*	90.844	89.361	88.478	88.777
Φ*_3*	86.969	90.430	89.789	91.396
Φ*_4*	89.414	90.820	91.247	91.022
Φ*_5*	86.693	90.155	90.029	92.188
Φ*_6*	89.108	91.206	91.493	91.141
Φ*_7*	93.050	89.649	90.246	88.030
Φ*_8*	90.634	88.612	88.782	89.053
Φ*_9*	90.001	89.943	90.329	91.335
Φ*_10*	89.951	90.627	89.632	88.591
Φ*_11*	90.077	89.454	90.403	90.845
Φ*_12*	89.970	89.975	89.635	89.229
Average	**90.000**	**89.999**	**90.000**	**89.999**
Standard deviation	**1.966**	**0.710**	**0.865**	**1.447**
Θ_1	55.85	54.61	55.67	54.27
Θ_2	57.55	55.88	57.61	56.41
Θ_3	10.93	10.52	12.73	13.15
Average	**41.441**	**40.336**	**42.001**	**41.276**
Standard deviation	**26.440**	**25.834**	**25.371**	**24.381**

	Octahedron 1				Octahedron 2			
	x	*y*	*z*		*x*	*y*	*z*	
v_1	3.63660	1.05199	5.25614	*v_1*	3.72600	-0.87994	5.17060	
v_2	-5.35710	1.09992	3.48083	*v_2*	-5.28439	-0.85194	3.62078	
v_3	0.07656	6.28024	-1.20824	*v_3*	-0.07656	6.29985	1.16814	
a_1	9.02391	0.00000	0.00000	*a_1*	9.02391	0.00000	0.00000	
a_2	-0.00168	-0.02786	8.74072	*a_2*	-0.00168	-0.02786	8.74072	
a_3	-0.04409	12.58007	0.00000	*a_3*	-0.04409	12.58007	0.00000	
*v_1 * a_1 / |v_1||a_1|*		0.56142		*v_1 * a_1 / |v_1||a_1|*		0.57914		
*v_2 * a_2 / |v_2||a_2|*		0.53656		*v_2 * a_2 / |v_2||a_2|*		0.56087		
*v_3 * a_3 / |v_3||a_3|*		0.98187		*v_3 * a_3 / |v_3||a_3|*		0.98321		

	Octahedron 3				Octahedron 4			
	x	*y*	*z*		*x*	*y*	*z*	
v_1	3.66675	1.06829	-5.26167	*v_1*	3.73946	-0.88357	-5.12171	
v_2	5.38725	-1.08362	3.48290	*v_2*	5.29785	0.84831	3.56844	
v_3	0.16993	6.32216	1.41473	*v_3*	-0.16993	6.25792	-1.45482	
a_1	9.02391	0.00000	0.00000	*a_1*	9.02391	0.00000	0.00000	
a_2	-0.00168	-0.02786	8.74072	*a_2*	-0.00168	-0.02786	8.74072	
a_3	-0.04409	12.58007	0.00000	*a_3*	-0.04409	12.58007	0.00000	
*v_1 * a_1 / |v_1||a_1|*		0.56397		*v_1 * a_1 / |v_1||a_1|*		0.58403		
*v_2 * a_2 / |v_2||a_2|*		0.53571		*v_2 * a_2 / |v_2||a_2|*		0.55321		
*v_3 * a_3 / |v_3||a_3|*		0.97543		*v_3 * a_3 / |v_3||a_3|*		0.97377		

	Apical w/Mg	Mg	Alone	Equatorial w/Mg
	Octahedron 1	Octahedron 2	Octahedron 3	Octahedron 4
l_1	3.167	2.999	3.172	3.240
l_2	3.171	3.025	3.177	3.297
l_3	3.168	3.023	3.169	3.273
l_4	3.172	3.062	3.174	3.268
l_5	3.284	3.015	3.189	3.148
l_6	3.286	3.016	3.159	3.119
Average	**3.208**	**3.023**	**3.173**	**3.224**
Standard deviation	**1.486**	**1.400**	**0.010**	**0.073**
Φ*_1*	90.609	89.435	90.939	88.891
Φ*_2*	92.770	88.896	87.152	90.131
Φ*_3*	89.422	90.588	88.512	90.582
Φ*_4*	87.263	91.117	92.303	89.352
Φ*_5*	89.404	91.018	88.988	91.711
Φ*_6*	87.238	91.806	92.809	89.330
Φ*_7*	90.565	88.951	91.561	88.810
Φ*_8*	92.729	88.177	87.736	91.181
Φ*_9*	90.623	91.073	89.534	89.548
Φ*_10*	89.384	89.637	90.400	89.932
Φ*_11*	90.604	89.902	89.656	89.493
Φ*_12*	89.389	89.387	90.404	91.022
Average	**90.000**	**89.999**	**90.000**	**89.999**
Standard deviation	**1.735**	**1.109**	**1.749**	**0.939**
Θ_1	55.54	53.67	55.43	53.08
Θ_2	55.95	54.08	56.06	53.34
Θ_3	9.27	10.09	9.92	10.14
Average	**40.251**	**39.277**	**40.473**	**38.855**
Standard deviation	**26.834**	**25.282**	**26.462**	**24.869**

	Octahedron 1			Octahedron 2		
	x	*y*	*z*	*x*	*y*	*z*
v_1	3.58444	0.79808	5.16227	3.56784	-0.78648	4.78789
v_2	-5.18559	0.85670	3.55155	-4.87115	-0.75894	3.57002
v_3	-0.03893	6.48488	-1.05814	0.03893	5.93806	1.05300
a_1	8.78299	0.00000	0.00000	8.78299	0.00000	0.00000
a_2	-0.00166	-0.00362	8.71016	-0.00166	-0.00362	8.71016
a_3	-0.08666	12.42264	0.00000	-0.08666	12.42264	0.00000
*v_1 * a_1 / |v_1||a_1|*		0.56580		*v_1 * a_1 / |v_1||a_1|*		0.59241
*v_2 * a_2 / |v_2||a_2|*		0.55999		*v_2 * a_2 / |v_2||a_2|*		0.58672
*v_3 * a_3 / |v_3||a_3|*		0.98695		*v_3 * a_3 / |v_3||a_3|*		0.98455

	Octahedron 3			Octahedron 4		
	x	*y*	*z*	*x*	*y*	*z*
v_1	3.59719	0.79543	-5.16028	3.91163	-0.82021	-5.14182
v_2	5.19834	-0.85935	3.54622	5.21494	0.72521	3.92060
v_3	-0.05816	6.25318	1.09349	0.05816	6.16977	-1.09862
a_1	8.78299	0.00000	0.00000	8.78299	0.00000	0.00000
a_2	-0.00166	-0.00362	8.71016	-0.00166	-0.00362	8.71016
a_3	-0.08666	12.42264	0.00000	-0.08666	12.42264	0.00000
*v_1 * a_1 / |v_1||a_1|*		0.56734		*v_1 * a_1 / |v_1||a_1|*		0.60064
*v_2 * a_2 / |v_2||a_2|*		0.55826		*v_2 * a_2 / |v_2||a_2|*		0.59705
*v_3 * a_3 / |v_3||a_3|*		0.98505		*v_3 * a_3 / |v_3||a_3|*		0.98438

	Apical w/Ca	Ca	Alone	Equatorial w/Ca
	Octahedron 1	Octahedron 2	Octahedron 3	Octahedron 4
l_1	3.213	3.281	3.215	3.232
l_2	3.224	3.251	3.221	3.218
l_3	3.216	3.249	3.214	3.232
l_4	3.219	3.245	3.218	3.241
l_5	3.206	3.232	3.184	3.204
l_6	3.219	3.242	3.201	3.223
Average	**3.216**	**3.250**	**3.209**	**3.225**
Standard deviation	**1.489**	**1.505**	**0.014**	**0.013**
Φ*_1*	91.697	89.962	90.190	90.713
Φ*_2*	89.184	89.025	89.357	93.350
Φ*_3*	88.535	90.212	90.086	89.613
Φ*_4*	91.057	91.151	90.915	86.998
Φ*_5*	88.336	89.483	89.796	89.282
Φ*_6*	90.727	90.858	90.598	87.070
Φ*_7*	91.431	90.343	89.928	90.388
Φ*_8*	89.033	88.960	89.130	92.582
Φ*_9*	89.122	89.445	90.510	90.551
Φ*_10*	90.798	90.446	89.453	89.855
Φ*_11*	89.172	90.105	90.564	90.145
Φ*_12*	90.907	90.004	89.471	89.447
Average	**90.000**	**90.000**	**90.000**	**90.000**
Standard deviation	**1.206**	**0.677**	**0.573**	**1.845**
Θ_1	54.24	55.65	54.39	55.59
Θ_2	56.25	57.41	55.89	57.56
Θ_3	12.98	12.57	10.75	11.06
Average	**41.158**	**41.877**	**40.340**	**41.403**
Standard deviation	**24.423**	**25.392**	**25.638**	**26.294**

	Octahedron 1				Octahedron 2			
	x	*y*	*z*		*x*	*y*	*z*	
v_1	3.75714	0.88142	5.14292	*v_1*	3.68450	-1.07077	5.28375	
v_2	-5.28010	0.88022	3.58658	*v_2*	-5.37027	-1.05208	3.50004	
v_3	0.19242	6.26059	-1.43283	*v_3*	-0.19242	6.31930	1.39339	
a_1	9.02390	0.00000	0.00000	*a_1*	9.02390	0.00000	0.00000	
a_2	0.00665	-0.02742	8.74061	*a_2*	0.00665	-0.02742	8.74061	
a_3	0.03930	12.57989	0.00000	*a_3*	0.03930	12.57989	0.00000	
*v_1 * a_1 / |v_1||a_1|*		0.58433		*v_1 * a_1 / |v_1||a_1|*		0.56425		
*v_2 * a_2 / |v_2||a_2|*		0.55557		*v_2 * a_2 / |v_2||a_2|*		0.53868		
*v_3 * a_3 / |v_3||a_3|*		0.97445		*v_3 * a_3 / |v_3||a_3|*		0.97601		

	Octahedron 3				Octahedron 4			
	x	*y*	*z*		*x*	*y*	*z*	
v_1	3.74375	0.90844	-5.14721	*v_1*	3.65358	-1.02387	-5.23375	
v_2	5.26671	-0.85321	3.60460	*v_2*	5.33935	1.09898	3.46378	
v_3	0.09998	6.27216	1.18794	*v_3*	-0.09998	6.30773	-1.22738	
a_1	9.02390	0.00000	0.00000	*a_1*	9.02390	0.00000	0.00000	
a_2	0.00665	-0.02742	8.74061	*a_2*	0.00665	-0.02742	8.74061	
a_3	0.03930	12.57989	0.00000	*a_3*	0.03930	12.57989	0.00000	
*v_1 * a_1 / |v_1||a_1|*		0.58230		*v_1 * a_1 / |v_1||a_1|*		0.56518		
*v_2 * a_2 / |v_2||a_2|*		0.56085		*v_2 * a_2 / |v_2||a_2|*		0.53639		
*v_3 * a_3 / |v_3||a_3|*		0.98246		*v_3 * a_3 / |v_3||a_3|*		0.98142		

	Alone	Equatorial w/Mg	Apical w/Mg	Mg
	Octahedron 1	Octahedron 2	Octahedron 3	Octahedron 4
l_1	3.173	3.243	3.166	2.995
l_2	3.175	3.269	3.177	3.058
l_3	3.172	3.267	3.161	3.024
l_4	3.173	3.303	3.171	3.025
l_5	3.159	3.149	3.318	3.015
l_6	3.160	3.150	3.288	2.984
Average	**3.169**	**3.230**	**3.214**	**3.017**
Standard deviation	**1.467**	**1.496**	**0.070**	**0.026**
Φ*_1*	91.042	88.929	90.501	89.426
Φ*_2*	92.207	89.329	86.647	90.518
Φ*_3*	88.974	91.078	88.944	89.984
Φ*_4*	87.808	90.678	92.806	88.893
Φ*_5*	88.938	91.504	89.390	91.137
Φ*_6*	87.754	91.288	93.283	88.851
Φ*_7*	91.046	88.483	91.164	89.446
Φ*_8*	92.231	88.702	87.264	91.733
Φ*_9*	90.378	91.049	89.293	89.516
Φ*_10*	89.583	89.553	90.604	89.864
Φ*_11*	90.438	90.024	89.498	89.575
Φ*_12*	89.601	89.374	90.600	91.039
Average	**90.000**	**89.999**	**90.000**	**89.999**
Standard deviation	**1.499**	**1.080**	**1.953**	**0.917**
Θ_1	55.46	53.06	55.50	53.64
Θ_2	56.06	53.32	55.93	54.01
Θ_3	9.97	10.02	9.19	10.19
Average	**40.498**	**38.800**	**40.208**	**39.281**
Standard deviation	**26.439**	**24.925**	**26.861**	**25.194**

	Octahedron 1				Octahedron 2			
	x	*y*	*z*		*x*	*y*	*z*	
v_1	3.59752	0.82324	5.16209	*v_1*	3.91305	-0.79170	5.14301	
v_2	-5.19909	0.82533	3.54725	*v_2*	-5.21443	-0.75752	3.92835	
v_3	-0.05726	6.22320	-1.09406	*v_3*	0.05726	6.20263	1.09113	
a_1	8.78266	0.00000	0.00000	*a_1*	8.78266	0.00000	0.00000	
a_2	0.00476	-0.00202	8.71019	*a_2*	0.00476	-0.00202	8.71019	
a_3	-0.08824	12.42551	0.00000	*a_3*	-0.08824	12.42551	0.00000	
*v_1 * a_1 / |v_1||a_1|*		0.56693		*v_1 * a_1 / |v_1||a_1|*		0.60102		
*v_2 * a_2 / |v_2||a_2|*		0.55834		*v_2 * a_2 / |v_2||a_2|*		0.59730		
*v_3 * a_3 / |v_3||a_3|*		0.98489		*v_3 * a_3 / |v_3||a_3|*		0.98475		

	Octahedron 3				Octahedron 4			
	x	*y*	*z*		*x*	*y*	*z*	
v_1	3.58335	0.76296	-5.15815	*v_1*	3.56801	-0.81990	-4.77705	
v_2	5.18492	-0.88561	3.55290	*v_2*	4.86939	0.72933	3.57198	
v_3	-0.03883	6.52121	1.05530	*v_3*	0.03883	5.90462	-1.05823	
a_1	8.78266	0.00000	0.00000	*a_1*	8.78266	0.00000	0.00000	
a_2	0.00476	-0.00202	8.71019	*a_2*	0.00476	-0.00202	8.71019	
a_3	-0.08824	12.42551	0.00000	*a_3*	-0.08824	12.42551	0.00000	
*v_1 * a_1 / |v_1||a_1|*		0.56637		*v_1 * a_1 / |v_1||a_1|*		0.59283		
*v_2 * a_2 / |v_2||a_2|*		0.56021		*v_2 * a_2 / |v_2||a_2|*		0.58762		
*v_3 * a_3 / |v_3||a_3|*		0.98716		*v_3 * a_3 / |v_3||a_3|*		0.98423		

	Alone	Equatorial w/Ca	Apical w/Ca	Ca
	Octahedron 1	Octahedron 2	Octahedron 3	Octahedron 4
l_1	3.216	3.233	3.215	3.281
l_2	3.216	3.242	3.217	3.246
l_3	3.215	3.240	3.218	3.251
l_4	3.218	3.212	3.219	3.252
l_5	3.214	3.206	3.205	3.232
l_6	3.198	3.194	3.219	3.244
Average	**3.213**	**3.221**	**3.216**	**3.251**
Standard deviation	**1.487**	**1.491**	**0.005**	**0.016**
Φ*_1*	90.155	90.701	91.735	89.968
Φ*_2*	90.677	86.706	91.320	91.418
Φ*_3*	89.577	89.108	88.525	90.233
Φ*_4*	89.058	93.131	88.936	88.784
Φ*_5*	89.827	89.423	88.320	89.512
Φ*_6*	89.359	92.772	88.733	88.679
Φ*_7*	90.442	90.763	91.420	90.287
Φ*_8*	90.906	87.390	91.012	91.115
Φ*_9*	89.418	89.472	90.946	89.969
Φ*_10*	90.623	90.008	89.104	90.121
Φ*_11*	89.392	89.864	90.846	90.397
Φ*_12*	90.565	90.655	89.103	89.512
Average	**90.000**	**89.999**	**90.000**	**90.000**
Standard deviation	**0.634**	**1.861**	**1.305**	**0.813**
Θ_1	54.35	55.59	54.22	55.62
Θ_2	55.92	57.59	56.18	57.38
Θ_3	10.71	11.13	13.00	12.59
Average	**40.326**	**41.437**	**41.132**	**41.861**
Standard deviation	**25.658**	**26.267**	**24.381**	**25.367**

	Octahedron 1				Octahedron 2			
	x	*y*	*z*		*x*	*y*	*z*	
v_1	3.74801	0.87982	5.15065	*v_1*	3.65839	-1.05223	5.23625	
v_2	-5.26254	0.85237	3.60049	*v_2*	-5.33539	-1.09980	3.46051	
v_3	0.09836	6.30000	-1.18940	*v_3*	-0.09836	6.27991	1.22936	
a_1	9.02410	0.00000	0.00000	*a_1*	9.02410	0.00000	0.00000	
a_2	-0.00302	0.02778	8.74062	*a_2*	-0.00302	0.02778	8.74062	
a_3	0.04227	12.57989	0.00000	*a_3*	0.04227	12.57989	0.00000	
*v_1 * a_1 / |v_1||a_1|*		0.58285		*v_1 * a_1 / |v_1||a_1|*		0.56511		
*v_2 * a_2 / |v_2||a_2|*		0.56039		*v_2 * a_2 / |v_2||a_2|*		0.53594		
*v_3 * a_3 / |v_3||a_3|*		0.98257		*v_3 * a_3 / |v_3||a_3|*		0.98120		

	Octahedron 3				Octahedron 4			
	x	*y*	*z*		*x*	*y*	*z*	
v_1	3.76151	0.88270	-5.14329	*v_1*	3.68866	-1.06947	-5.28327	
v_2	5.27604	-0.84949	3.58689	*v_2*	5.36566	1.08256	3.50130	
v_3	0.19140	6.25866	1.43524	*v_3*	-0.19140	6.32124	-1.39528	
a_1	9.02410	0.00000	0.00000	*a_1*	9.02410	0.00000	0.00000	
a_2	-0.00302	0.02778	8.74062	*a_2*	-0.00302	0.02778	8.74062	
a_3	0.04227	12.57989	0.00000	*a_3*	0.04227	12.57989	0.00000	
*v_1 * a_1 / |v_1||a_1|*		0.58473		*v_1 * a_1 / |v_1||a_1|*		0.56473		
*v_2 * a_2 / |v_2||a_2|*		0.55660		*v_2 * a_2 / |v_2||a_2|*		0.53909		
*v_3 * a_3 / |v_3||a_3|*		0.97436		*v_3 * a_3 / |v_3||a_3|*		0.97596		

	l	Φ	Θ_a	Θ_b	Θ_c
CsSnI3 Exp	3.12	90.00	55.19	7.02	55.52
CsSnI3 Theo	3.20	90.00	54.33	10.64	55.17
CsSnMgI3	3.16	90.00	54.26	9.85	54.73
Mg	3.02	90.00	53.33	10.10	53.75
Sn	3.20	90.00	54.52	9.75	55.00
CsSnCaI3	3.23	90.00	55.03	11.84	56.82
Ca	3.25	90.00	55.65	12.65	57.50
Sn	3.22	90.00	54.82	11.57	56.59

CsSnI3

	Octahedrons in the unit cell	l - mean value	$l\_standdev$	Φ - mean value	$\Phi\_standdev$	Θ_a - mean value	$\Theta\_a\_standdev$	Θ_b - mean value	$\Theta\_b\_standdev$	Θ_c - mean value	$\Theta\_c\_standdev$
CsSnI3 Exp	4	3.121	0.002	90.000	1.052	55.19	0.000	7.02	0.000	55.52	0.000
CsSnI3 Theo	4	3.200	0.006	90.000	0.884	54.33	0.000	10.64	0.000	55.17	0.000

Structure 1: All values were averaged over the octahedrons indicated below.

	Octahedrons in the unit cell	l - mean value	$l\_standdev$	Φ - mean value	$\Phi\_standdev$	Θ_a - mean value	$\Theta\_a\_standdev$	Θ_b - mean value	$\Theta\_b\_standdev$	Θ_c - mean value	$\Theta\_c\_standdev$
CsSnMgI3	4	3.156	0.094	89.999	1.181	54.09	1.243	9.86	0.403	54.61	1.379
Mg	1	3.021	0.005	90.000	0.805	53.28		10.12		53.79	
Sn	3	3.201	0.058	89.999	1.292	54.35	1.373	9.77	0.442	54.88	1.551
CsSnCaI3	4	3.226	0.021	89.998	1.254	55.10	0.766	11.82	1.302	56.86	0.844
Ca	1	3.247	0.007	89.991	0.707	55.67		12.72		57.58	
Sn	3	3.219	0.019	90.000	1.398	54.91	0.813	11.52	1.414	56.62	0.852

Structure 2: All values were averaged over the octahedrons indicated below.

	Octahedrons in the unit cell	l - mean value	$l\_standdev$	Φ - mean value	$\Phi\_standdev$	Θ_a - mean value	$\Theta\_a\_standdev$	Θ_b - mean value	$\Theta\_b\_standdev$	Θ_c - mean value	$\Theta\_c\_standdev$
CsSnMgI3	4	3.156	0.097	89.999	1.175	54.09	1.253	9.83	0.435	54.60	1.381
Mg	1	3.016	0.016	90.000	0.797	52.74		10.00		53.11	
Sn	3	3.202	0.059	89.999	1.317	54.35	1.396	9.72	0.465	54.89	1.543
CsSnCaI3	4	3.226	0.020	90.000	1.299	55.10	0.778	11.83	1.303	56.86	0.854
Ca	1	3.248	0.008	90.000	0.865	55.67		12.73		57.61	
Sn	3	3.219	0.018	90.000	1.425	54.91	0.831	11.53	1.418	56.62	0.851

Structure 3: All values were averaged over the octahedrons indicated below.											
	Octahedrons in the unit cell	*l - mean value*	*l_standdev*	*Φ - mean value*	*Φ_standdev*	*Θ_a - mean value*	*Θ_a_standdev*	*Θ_b - mean value*	*Θ_b_standdev*	*Θ_c - mean value*	*Θ_c_standdev*
CsSnMgI3	4	3.157	0.093	89.999	1.384	54.43	1.243	9.85	0.401	54.86	1.360
Mg	1	3.023	1.400	89.999	1.109	53.67		10.09		54.08	
Sn	3	3.202	0.056	89.999	1.478	54.69	1.389	9.78	0.454	55.12	1.539
CsSnCaI3	4	3.225	0.020	90.000	1.150	54.97	0.754	11.84	1.101	56.78	0.834
Ca	1	3.250	1.505	90.000	0.677	55.65		12.57		57.41	
Sn	3	3.217	0.013	90.000	1.277	54.74	0.736	11.60	1.208	56.57	0.882

Structure 4: All values were averaged over the octahedrons indicated below.											
	Octahedrons in the unit cell	*l - mean value*	*l_standdev*	*Φ - mean value*	*Φ_standdev*	*Θ_a - mean value*	*Θ_a_standdev*	*Θ_b - mean value*	*Θ_b_standdev*	*Θ_c - mean value*	*Θ_c_standdev*
CsSnMgI3	4	3.157	0.098	89.999	1.374	54.42	1.255	9.84	0.444	54.83	1.374
Mg	1	3.017	0.026	89.999	0.917	53.64		10.19		54.01	
Sn	3	3.204	0.059	90.000	1.507	54.67	1.401	9.73	0.464	55.10	1.544
CsSnCaI3	4	3.225	0.020	90.000	1.207	54.94	0.765	11.86	1.109	56.77	0.841
Ca	1	3.251	0.016	90.000	0.813	55.62		12.59		57.38	
Sn	3	3.217	0.012	90.000	1.323	54.72	0.758	11.61	1.220	56.56	0.901