Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Supplementary Information

Machine-learning prediction of thermal expansion coefficient for perovskite oxides with experimental validation

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Composition	TEC ($x10^{-6}$ K^{-1})	Initial Temperature (°C)	Final Temperature (°C)	Reference
La0.6Sr0.4Fe0.8Cu0.2O3	14.6	25	800	https://doi.org/10.1016/j.ijhydene.2012.05.114
La0.8Sr0.2Mn0.75Co0.25O3	13	30	1000	https://doi.org/10.1016/j.ssi.2005.12.017
La0.8Sr0.2Mn0.5Co0.5O3	15.6	30	1000	https://doi.org/10.1016/j.ssi.2005.12.017
La0.8Sr0.2Mn0.25Co0.75O3	17.5	30	1000	https://doi.org/10.1016/j.ssi.2005.12.017
La0.8Sr0.2Fe0.75Co0.25O3	15.6	30	1000	https://doi.org/10.1016/j.ssi.2005.12.017
La0.8Sr0.2Fe0.5Co0.5O3	18.3	30	1000	https://doi.org/10.1016/j.ssi.2005.12.017
La0.8Sr0.2Fe0.25Co0.75O3	19.1	30	1000	https://doi.org/10.1016/j.ssi.2005.12.017
La0.8Sr0.2Mn0.5Fe0.5O3	10.9	30	1000	https://doi.org/10.1016/j.ssi.2005.12.017
La0.7Sr0.3Fe0.8Ni0.2O3	13.7	30	1000	https://doi.org/10.1149/1.1483156
La0.6Sr0.4Co0.8Mn0.2O3	18.1	500	900	https://doi.org/10.1016/S0025-5408(03)00143-0
La0.6Sr0.4Co0.8Mn0.2O3	18.1	500	900	https://doi.org/10.1016/S0025-5408(03)00143-0
Gd0.6Sr0.4Co0.8Mn0.2O3	21.3	500	900	https://doi.org/10.1016/S0025-5408(03)00143-0
Sm0.6Sr0.4Co0.8Mn0.2O3	21.6	500	900	https://doi.org/10.1016/S0025-5408(03)00143-0
Nd0.6Sr0.4Co0.8Mn0.2O3	19.6	500	900	https://doi.org/10.1016/S0025-5408(03)00143-0
La0.6Sr0.4Co0.2Fe0.8O3	15.3	200	600	https://doi.org/10.1016/j.ssi.2012.01.001
La0.8Sr0.2Co0.2Fe0.8O3	14.8	30	1000	https://doi.org/10.1016/S0167-2738(00)00770-0
La0.8Sr0.2Co0.8Fe0.2O3	19.3	30	1000	https://doi.org/10.1016/S0167-2738(00)00770-0
La0.6Sr0.4Co0.9Cu0.1O3	19.2	30	900	https://doi.org/10.1016/S0167-2738(02)00115-7

Pr0.8Sr0.2Co0.2Fe0.8O3	12.8	30	1000	https://doi.org/10.1016/S0167-2738(00)00770-0
Pr0.7Sr0.3Co0.2Mn0.8O3	11.1	30	1000	https://doi.org/10.1007/BF02375916
Pr0.6Sr0.4Co0.8Fe0.2O3	19.69	30	850	https://doi.org/10.1016/j.jpowsour.2008.05.052
Pr0.4Sr0.6Co0.8Fe0.2O3	21.33	30	850	https://doi.org/10.1016/j.jpowsour.2008.05.052
Ba0.3Sr0.7Co0.8Fe0.2O3	20.44	50	1000	https://doi.org/10.1016/j.jeurceramsoc.2005.06.047
Ba0.4Sr0.6Co0.8Fe0.2O3	20.12	50	1000	https://doi.org/10.1016/j.jeurceramsoc.2005.06.047
Ba0.5Sr0.5Co0.8Fe0.2O3	19.95	50	1000	https://doi.org/10.1016/j.jeurceramsoc.2005.06.047
Ba0.6Sr0.4Co0.8Fe0.2O3	20.18	50	1000	https://doi.org/10.1016/j.jeurceramsoc.2005.06.047
Ba0.7Sr0.3Co0.8Fe0.2O3	20.27	50	1000	https://doi.org/10.1016/j.jeurceramsoc.2005.06.047
Sr0.9Ce0.1Fe0.8Ni0.2O3	18.9	30	1000	https://doi.org/10.1016/S0167-2738(00)00770-0
Sr0.7Ce0.3Mn0.9Al0.1O3	10.8	100	820	https://doi.org/10.1016/j.jeurceramsoc.2005.03.230
Sr0.7Ce0.3Mn0.8Al0.2O3	10.8	100	820	https://doi.org/10.1016/j.jeurceramsoc.2005.03.230
Sr0.85Ce0.15Fe0.8Co0.2O3	18.5	30	1000	https://doi.org/10.1016/S0167-2738(00)00770-0
La0.7Sr0.3Fe0.8Co0.2O3	14.9	30	1000	https://doi.org/10.1016/S0167-2738(00)00770-0
La0.6Sr0.4Fe0.8Co0.2O3	17.5	30	1000	https://doi.org/10.1016/S0167-2738(00)00770-0
La0.6Sr0.4Fe0.5Co0.5O3	20.3	30	1000	https://doi.org/10.1016/S0167-2738(00)00770-0
La0.6Sr0.4Fe0.2Co0.8O3	21.4	30	1000	https://doi.org/10.1016/S0167-2738(00)00770-0
La0.8Sr0.2Co0.1Fe0.9O3	13.9	30	1000	https://doi.org/10.1016/S0167-2738(00)00770-0
La0.8Sr0.2Co0.5Fe0.5O3	17.6	30	1000	https://doi.org/10.1016/S0167-2738(00)00770-0
Pr0.8Sr0.2Fe0.8Co0.2O3	12.8	30	1000	https://doi.org/10.1016/S0167-2738(00)00770-0
Pr0.8Sr0.2Mn0.8Co0.2O3	10.9	30	1000	https://doi.org/10.1016/S0167-2738(00)00770-0
La0.9Sr0.1Ga0.8Mg0.2O3	11.6	30	1000	https://doi.org/10.1016/S0167-2738(00)00770-0
La0.8Sr0.2Ga0.8Mg0.2O3	11.4	30	1000	https://doi.org/10.1016/S0167-2738(00)00770-0
La0.8Sr0.2Co0.9Fe0.1O3	20.1	100	900	https://doi.org/10.1016/0167-2738(94)00244-M
La0.8Sr0.2Co0.8Fe0.2O3	20.7	100	900	https://doi.org/10.1016/0167-2738(94)00244-M
La0.8Sr0.2Co0.7Fe0.3O3	20.3	100	900	https://doi.org/10.1016/0167-2738(94)00244-M
La0.8Sr0.2Co0.6Fe0.4O3	20	100	900	https://doi.org/10.1016/0167-2738(94)00244-M
La0.8Sr0.2Co0.5Fe0.5O3	18.7	100	900	https://doi.org/10.1016/0167-2738(94)00244-M
La0.8Sr0.2Co0.4Fe0.6O3	17.6	100	900	https://doi.org/10.1016/0167-2738(94)00244-M
La0.8Sr0.2Co0.3Fe0.7O3	16.5	100	900	https://doi.org/10.1016/0167-2738(94)00244-M
La0.8Sr0.2Co0.2Fe0.8O3	15.4	100	800	https://doi.org/10.1016/0167-2738(94)00244-M
La0.8Sr0.2Co0.1Fe0.9O3	14.5	200	900	https://doi.org/10.1016/0167-2738(94)00244-M
La0.9Sr0.1Co0.2Fe0.8O3	16	30	900	https://doi.org/10.1016/0167-2738(94)00245-N
La0.7Sr0.3Co0.2Fe0.8O3	14.6	30	700	https://doi.org/10.1016/0167-2738(94)00245-N
La0.6Sr0.4Co0.2Fe0.8O3	15.3	30	600	https://doi.org/10.1016/j.ssi.2012.01.001
La0.4Sr0.6Co0.2Fe0.8O3	16.8	30	400	https://doi.org/10.1016/0167-2738(94)00245-N
La0.3Sr0.7Co0.9Fe0.1O3	19.2	30	1000	https://doi.org/10.1016/S0167-2738(00)00394-5
La0.3Sr0.7Co0.8Fe0.2O3	21	30	1000	https://doi.org/10.1016/S0167-2738(00)00394-5
La0.3Sr0.7Co0.7Fe0.3O3	24.7	30	1000	https://doi.org/10.1016/S0167-2738(00)00394-5
La0.3Sr0.7Co0.6Fe0.4O3	24.1	30	1000	https://doi.org/10.1016/S0167-2738(00)00394-5
La0.3Sr0.7Co0.5Fe0.5O3	23.5	30	1000	https://doi.org/10.1016/S0167-2738(00)00394-5
La0.3Sr0.7Co0.4Fe0.6O3	23.9	30	1000	https://doi.org/10.1016/S0167-2738(00)00394-5
La0.3Sr0.7Co0.3Fe0.7O3	27.1	30	1000	https://doi.org/10.1016/S0167-2738(00)00394-5

La0.3Sr0.7Co0.2Fe0.8O3	27.1	30	1000	https://doi.org/10.1016/S0167-2738(00)00394-5
La0.3Sr0.7Co0.1Fe0.9O3	24.8	30	1000	https://doi.org/10.1016/S0167-2738(00)00394-5
La0.8Sr0.2Co0.2Fe0.8O3	14.8	30	1000	https://doi.org/10.1016/S0167-2738(00)00770-0
La0.7Sr0.3Co0.2Fe0.8O3	16	30	1000	https://doi.org/10.1016/S0167-2738(00)00394-5
La0.6Sr0.4Co0.2Fe0.8O3	17.5	30	1000	https://doi.org/10.1016/S0167-2738(00)00770-0
La0.4Sr0.6Ti0.4Mn0.6O3	11.6	30	800	https://doi.org/10.1002/fuce.200800018
La0.8Sr0.2Al0.5Mn0.5O3	10.9	30	800	https://doi.org/10.1002/fuce.200800018
La0.7Sr0.3Cr0.5Co0.5O3	19	30	600	https://doi.org/10.1007/s100080050161
La0.75Sr0.25Cr0.5Mn0.5O3	12	30	1000	https://doi.org/10.1016/j.ijhydene.2010.12.085
Bi0.5Sr0.5Fe0.85Ti0.15O3	13.4	30	800	https://doi.org/10.1021/acssuschemeng.9b05086
Bi0.5Sr0.5Fe0.95Ti0.05O3	13.7	30	800	https://doi.org/10.1021/acssuschemeng.9b05086
Bi0.5Sr0.5Fe0.9Ti0.1O3	13.5	30	800	https://doi.org/10.1021/acssuschemeng.9b05086
Bi0.5Sr0.5Fe0.8Ti0.2O3	13.3	30	800	https://doi.org/10.1021/acssuschemeng.9b05086
Bi0.5Sr0.5Fe0.9Sn0.1O3	12.9	30	800	https://doi.org/10.1016/j.jallcom.2020.155406
Bi0.5Sr0.5Fe0.8Cu0.2O3	13.1	30	800	https://doi.org/10.1016/j.jallcom.2017.01.026
Bi0.5Sr0.5Fe0.95Nb0.05O3	13.3	30	800	https://doi.org/10.1016/j.jpowsour.2017.10.036
Bi0.5Sr0.5Fe0.9Nb0.1O3	12.9	30	800	https://doi.org/10.1016/j.jpowsour.2017.10.036
Bi0.5Sr0.5Fe0.85Nb0.15O3	12.6	30	800	https://doi.org/10.1016/j.jpowsour.2017.10.036
Bi0.5Sr0.5Fe0.95Ta0.05O3	11.8	30	800	https://doi.org/10.1016/j.ceramint.2019.06.295
Bi0.5Sr0.5Fe0.9Ta0.1O3	11.4	30	800	https://doi.org/10.1016/j.ceramint.2019.06.295
La0.9Ca0.1Fe0.9Nb0.1O3	11.8	30	900	https://doi.org/10.1016/j.ijhydene.2017.04.291
Sm0.7Sr0.3Fe0.8Co0.2O3	13.7	25	600	https://doi.org/10.1016/10.1149/1.2818766
Nd0.7Sr0.3Fe0.8Co0.2O3	13.4	25	600	https://doi.org/10.1149/1.2818766
Ba0.7Sr0.3Fe0.8Co0.2O3	20.2	25	600	https://doi.org/10.1149/1.2818766
La0.7Sr0.3Fe0.8Co0.2O3	12.5	25	600	https://doi.org/10.1149/1.2818766
Pr0.7Sr0.3Fe0.8Co0.2O3	12.4	25	600	https://doi.org/10.1149/1.2818766
Gd0.7Sr0.3Fe0.8Co0.2O3	15.8	25	600	https://doi.org/10.1149/1.2818766
Dy0.7Sr0.3Fe0.8Co0.2O3	13.3	25	600	https://doi.org/10.1149/1.2818766
Er0.7Sr0.3Fe0.8Co0.2O3	13.3	25	600	https://doi.org/10.1149/1.2818766
La0.7Sr0.3Cr0.5Co0.5O3	19	30	600	https://doi.org/10.1007/s100080050161
La0.7Sr0.3Cr0.2Co0.8O3	19	30	600	https://doi.org/10.1007/s100080050161
La0.6Sr0.4Mn0.8Fe0.2O3	11.3	30	827	https://doi.org/10.1007/s100080050161
La0.6Sr0.4Mn0.6Fe0.4O3	12	30	827	https://doi.org/10.1007/s100080050161
La0.6Sr0.4Mn0.5Fe0.5O3	12.7	30	827	https://doi.org/10.1007/s100080050161
La0.6Sr0.4Mn0.8Ni0.2O3	12.7	30	827	https://doi.org/10.1007/s100080050161
La0.6Sr0.4Mn0.6Ni0.4O3	12.5	30	827	https://doi.org/10.1007/s100080050161
La0.5Sr0.5Co0.75Ni0.25O3	14.2	27	697	https://doi.org/10.1007/s100080050161
Sm0.5Sr0.5Cu0.2Fe0.8O3	15.9	30	900	https://doi.org/10.1016/j.ijhydene.2010.04.021
La0.9Sr0.1Cr0.9Ni0.1O3	9.11	30	800	http://203.158.7.72:8080/jspui/bitstream/123456789/3624/1/131555.pdf
La0.9Sr0.1Cr0.8Ni0.2O3	10.48	30	800	http://203.158.7.72:8080/jspui/bitstream/123456789/3624/1/131555.pdf
La0.9Sr0.1Cr0.7Ni0.3O3	10.52	30	800	http://203.158.7.72:8080/jspui/bitstream/123456789/3624/1/131555.pdf
La0.9Sr0.1Cr0.6Ni0.4O3	11.98	30	800	http://203.158.7.72:8080/jspui/bitstream/123456789/3624/1/131555.pdf
La0.9Sr0.1Cr0.5Ni0.5O3	12.51	30	800	http://203.158.7.72:8080/jspui/bitstream/123456789/3624/1/131555.pdf

La0.9Sr0.1Cr0.4Ni0.6O3	12.86	30	800	http://203.158.7.72:8080/jspui/bitstream/123456789/3624/1/131555.pdf
Ba0.5Sr0.5Fe0.9Sb0.1O3	17.2	700	1000	https://doi.org/10.1016/j.jallcom.2016.01.122
Ba0.5Sr0.5Fe0.95Sb0.05O3	29.1	700	1000	https://doi.org/10.1016/j.jallcom.2016.01.122
Ba0.5Sr0.5Fe0.8Cu0.2O3	25.8	30	800	https://doi.org/10.1007/s10832-014-9901-9
Ba0.5Sr0.5Fe0.9Nb0.1O3	19.2	30	1000	https://doi.org/10.1016/j.jallcom.2012.07.115
La0.5Sr0.5Fe0.8Cu0.2O3	15.8	30	850	https://doi.org/10.1016/j.jpowsour.2016.06.134
La0.6Ba0.4Fe0.8Ni0.2O3	17.5	30	900	https://doi.org/10.1007/s11581-015-1402-6
Nd0.5Sr0.5Fe0.8Cu0.2O3	14.7	30	800	https://doi.org/10.1021/jp500371w
Pr0.5Sr0.5Fe0.8Cu0.2O3	16.4	30	850	https://doi.org/10.1016/j.jpowsour.2016.06.134
Pr0.6Sr0.4Fe0.8Ni0.2O3	16.97	30	1000	https://doi.org/10.1016/j.electacta.2016.12.170
La0.5Sr0.5Co0.8Mn0.2O3	17.72	30	600	https://doi.org/10.1111/jace.14127
La0.5Sr0.5Co0.8Fe0.2O3	20.62	30	600	https://doi.org/10.1111/jace.14127
La0.5Sr0.5Co0.8Ni0.2O3	21.38	30	600	https://doi.org/10.1111/jace.14127
La0.5Sr0.5Co0.8Cu0.2O3	19.75	30	600	https://doi.org/10.1111/jace.14127
La0.95Sr0.05Ni0.5Mn0.5O3	11.29	30	850	https://doi.org/10.1016/j.ijhydene.2016.08.197
La0.9Sr0.1Ni0.5Mn0.5O3	11.33	30	850	https://doi.org/10.1016/j.ijhydene.2016.08.197
La0.85Sr0.15Ni0.5Mn0.5O3	11.83	30	850	https://doi.org/10.1016/j.ijhydene.2016.08.197
Bi0.7Sr0.3Fe0.5Mn0.5O3	13.4	30	800	https://doi.org/10.1016/j.ssi.2013.09.056
La0.6Ca0.4Fe0.8Ni0.2O3	11.2	30	1000	https://doi.org/10.1007/s40843-020-1567-2
La0.6Sr0.4Fe0.8Ni0.2O3	11.9	30	1000	https://doi.org/10.1021/acsaem.9b00115
Nd0.3Sr0.7Fe0.8Cu0.2O3	16.1	30	800	https://doi.org/10.1021/jp500371w
Nd0.4Sr0.6Fe0.8Cu0.2O3	15.6	30	800	https://doi.org/10.1021/jp500371w
Nd0.6Sr0.4Fe0.8Cu0.2O3	14.2	30	800	https://doi.org/10.1021/jp500371w
Nd0.7Sr0.3Fe0.8Cu0.2O3	14	30	800	https://doi.org/10.1021/jp500371w
La0.2Sr0.8Co0.9Sb0.1O3	22.99	30	900	https://doi.org/10.1016/j.ceramint.2017.02.070
La0.4Sr0.6Co0.9Sb0.1O3	22.49	30	900	https://doi.org/10.1016/j.ceramint.2017.02.070
La0.8Sr0.2Fe0.7Ni0.3O3	12.1	30	800	https://doi.org/10.1016/j.solidstatesciences.2020.106356
La0.6Sr0.4Fe0.7Ni0.3O3	13.8	30	800	https://doi.org/10.1016/j.solidstatesciences.2020.106356
La0.7Sr0.3Cu0.2Fe0.8O3	13.6	30	600	https://doi.org/10.1016/j.jallcom.2008.07.044
Sm0.5Sr0.5Fe0.7Cr0.3O3	12.8	30	1000	https://doi.org/10.1002/er.4377
Sm0.4Sr0.6Fe0.7Cr0.3O3	14	30	1000	https://doi.org/10.1002/er.4377
Sm0.3Sr0.7Fe0.7Cr0.3O3	14.1	30	1000	https://doi.org/10.1002/er.4377
Sm0.5Sr0.5Fe0.1Co0.9O3	20.4	30	900	https://doi.org/10.1016/j.materresbull.2007.02.007
Sm0.5Sr0.5Fe0.2Co0.8O3	20.8	30	900	https://doi.org/10.1016/j.materresbull.2007.02.007
Sm0.5Sr0.5Fe0.4Co0.6O3	19.5	30	900	https://doi.org/10.1016/j.materresbull.2007.02.007
Sm0.5Sr0.5Fe0.6Co0.4O3	18.2	30	900	https://doi.org/10.1016/j.materresbull.2007.02.007
Sm0.5Sr0.5Fe0.8Co0.2O3	15.8	30	900	https://doi.org/10.1016/j.materresbull.2007.02.007
Sm0.5Sr0.5Mn0.1Co0.9O3	16.7	30	900	https://doi.org/10.1016/j.materresbull.2007.02.007
Sm0.5Sr0.5Mn0.2Co0.8O3	15.6	30	900	https://doi.org/10.1016/j.materresbull.2007.02.007
Sm0.5Sr0.5Mn0.4Co0.6O3	14.8	30	900	https://doi.org/10.1016/j.materresbull.2007.02.007
Sm0.5Sr0.5Mn0.6Co0.4O3	13.8	30	900	https://doi.org/10.1016/j.materresbull.2007.02.007
Sm0.5Sr0.5Mn0.8Co0.2O3	11.7	30	900	https://doi.org/10.1016/j.materresbull.2007.02.007

Table S1. AA'BB'O_3 Dataset Used in this work

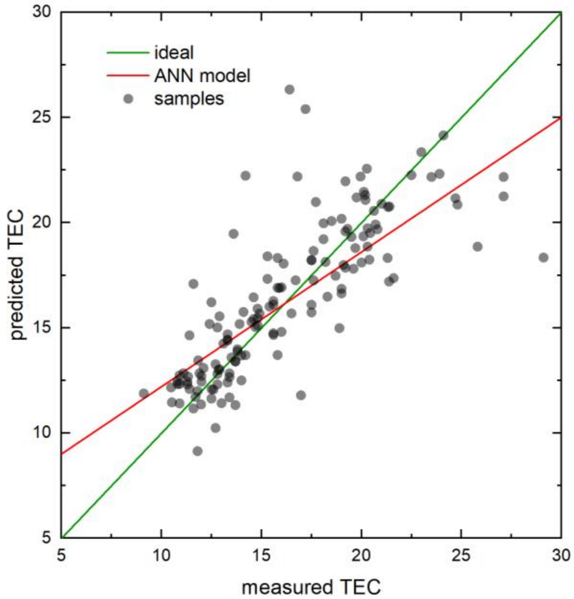


Figure S1. Plot of predicted TEC vs. measured TEC for the ANN model TEC predictions

Element	A occurrences	Element	B occurrences
Sr	143	Fe	103
La	84	Co	86
Sm	16	Mn	31
Bi	12	Ni	21
Ba	11	Cu	14
Pr	9	Cr	13
Nd	7	Ti	5
Ce	4	Nb	5
Gd	2	Sb	4
Ca	2	Al	3
Dy	1	Ga	2
Er	1	Mg	2
		Ta	2
		Sn	1

Table S2. Element occurrences in each site in the TEC dataset used for this work

Element	A occurrences	Element	B occurrences
Sr	204	Fe	116
La	171	Co	86
Ba	62	Ti	83
Ca	29	Mn	76
Pb	24	Mg	33

Bi	23	Cr	31
Nd	17	Al	26
Sm	16	Ni	23
Pr	13	Cu	22
Li	11	Nb	21
K	9	Zr	14
Na	7	Ga	12
Ce	6	Bi	10
Mn	4	Ta	8
Y	3	Zn	7
Gd	2	Sc	7
Eu	1	Ru	5
Dy	1	Ce	4
Er	1	Sb	4
		V	3
		Y	2
		Dy	2
		W	1
		Nd	1
		Sm	1
		Gd	1
		Er	1
		Yb	1
		Sn	1
		Cd	1

Table S3. Element occurrences in each site using AA'BB'O_3 compositions from the dataset used for this work, as well as compositions from the PCD and COD

A-site Combinations																			
	Ba	**Bi**	**Ca**	**Ce**	**Dy**	**Eu**	**Er**	**Gd**	**K**	**La**	**Li**	**Mn**	**Na**	**Nd**	**Pb**	**Pr**	**Sm**	**Sr**	**Y**
Ba	0	3	0	0	0	0	0	0	9	19	0	0	1	0	9	0	0	20	0
Bi	0	0	0	0	0	0	0	0	0	0	0	0	1	0	2	0	0	12	0
Ca	0	0	0	0	0	0	0	0	0	19	0	0	1	4	0	0	0	1	0
Ce	0	0	0	0	0	0	0	0	0	0	0	0	2	0	0	0	0	0	0
Dy	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1	0
Eu	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
Er	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1	0
Gd	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	2	0
K	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
La	1	0	2	0	0	0	0	0	0	0	6	0	2	0	6	0	0	116	0
Li	0	0	0	0	0	0	0	0	0	0	0	4	0	0	0	0	0	1	0
Mn	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0

Na	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
Nd	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1	0	0	12	0
Pb	0	4	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	2	0
Pr	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	10	0
Sm	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	16	0
Sr	0	1	0	4	0	0	0	0	0	0	0	0	0	0	0	2	0	0	3
Y	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0

Table S4. Occurrences of A and A' combinations using AA'BB'O_3 compositions from the dataset used for this work, as well as compositions from the PCD and COD

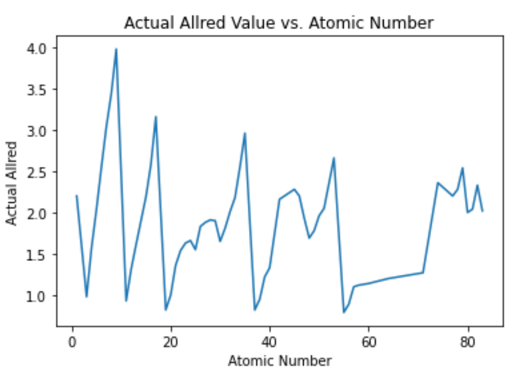
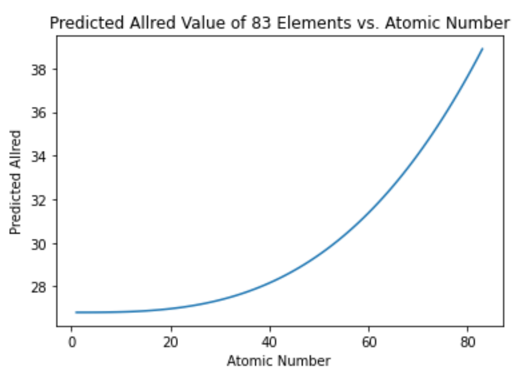
	B-site Combinations																													
	Al	**Bi**	**Ce**	**Cd**	**Co**	**Cr**	**Cu**	**Dy**	**Er**	**Fe**	**Ga**	**Gd**	**Mg**	**Mn**	**Nb**	**Nd**	**Ni**	**Ru**	**Sb**	**Sc**	**Sm**	**Sn**	**Ta**	**Ti**	**V**	**W**	**Y**	**Yb**	**Zn**	**Zr**
Al	0	0	0	0	0	0	0	0	0	1	0	0	0	3	1	0	0	0	0	0	0	0	3	13	1	0	0	0	0	0
Bi	0	0	0	1	0	0	1	2	1	0	0	1	0	0	0	1	0	0	0	0	1	0	0	0	0	0	0	1	0	0
Ce	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	2	0	0	0
Cd	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
Co	0	0	0	0	0	0	2	0	0	32	1	0	0	10	0	0	2	1	2	0	0	0	0	3	0	0	0	0	0	0
Cr	0	0	0	0	2	0	0	0	0	4	0	0	0	4	0	0	6	0	0	0	0	0	0	10	2	0	0	0	0	0
Cu	0	0	0	0	0	0	0	0	0	3	0	0	0	5	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0
Dy	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
Er	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
Fe	0	0	0	0	22	3	10	0	0	0	0	0	0	8	5	0	8	0	2	0	0	1	2	4	0	0	0	0	0	0
Ga	0	0	0	0	0	0	0	0	0	0	0	0	8	3	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
Gd	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
Mg	0	0	0	0	0	0	0	0	0	0	0	0	0	2	5	0	0	0	0	0	0	0	1	16	0	1	0	0	0	0
Mn	2	0	0	0	9	0	0	0	0	4	0	0	0	0	0	0	4	3	0	6	0	0	0	6	0	0	0	0	3	0
Nb	0	0	0	0	0	0	0	0	0	4	0	0	0	0	0	0	0	0	0	0	0	0	0	6	0	0	0	0	0	0
Nd	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
Ni	0	0	0	0	0	0	0	0	0	0	0	0	0	3	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
Ru	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
Sb	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
Sc	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0
Sm	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
Sn	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
Ta	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
Ti	1	0	2	0	0	0	0	0	0	3	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	4	14
V	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
W	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
Y	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
Yb	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
Zn	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
Zr	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0

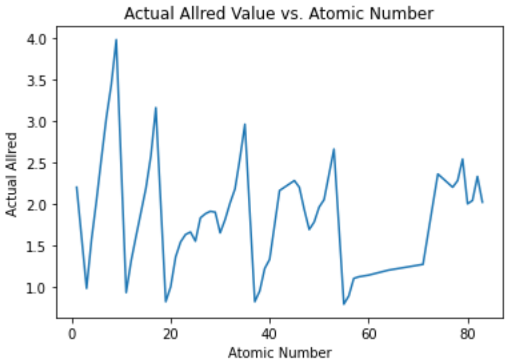
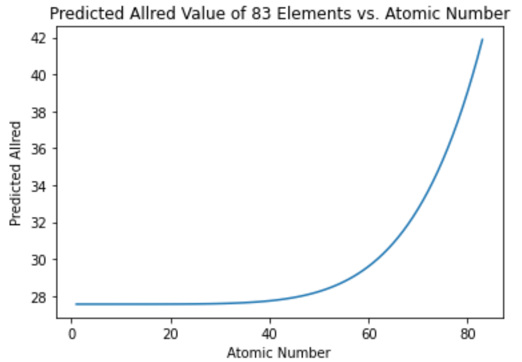
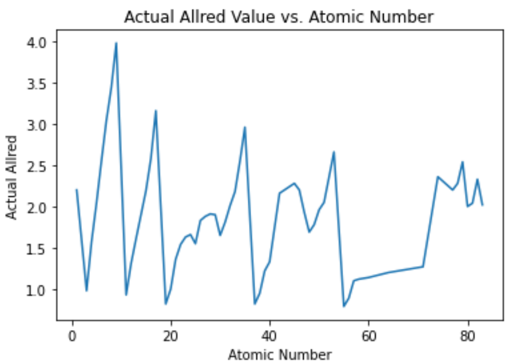
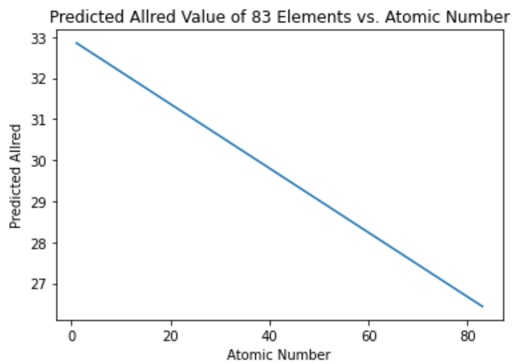
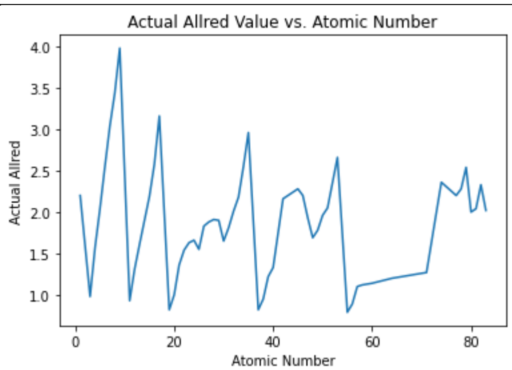
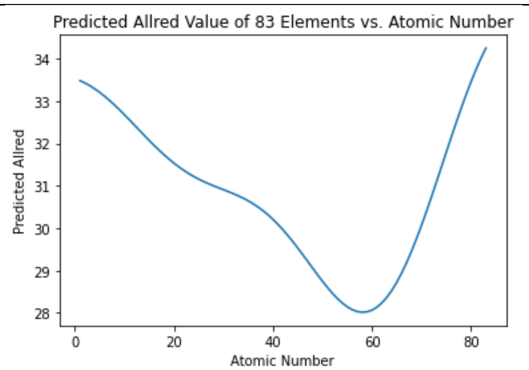
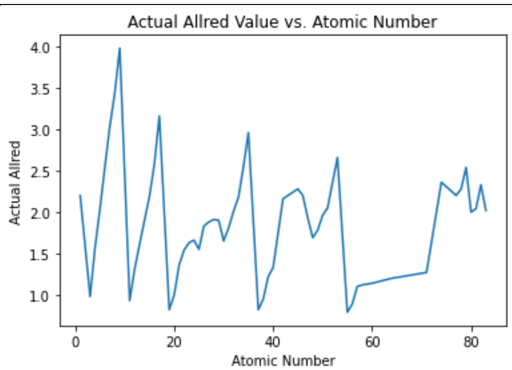
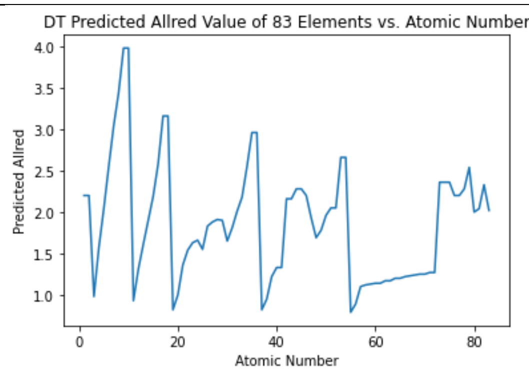
Table S5. Occurrences of B and B' combinations using AA'BB'O_3 compositions from the dataset used for this work, as well as compositions from the PCD and COD

		B-site Element																														
		Al	**Bi**	**Ce**	**Cd**	**Co**	**Cr**	**Cu**	**Dy**	**Er**	**Fe**	**Ga**	**Gd**	**La**	**Mg**	**Mn**	**Nb**	**Nd**	**Ni**	**Ru**	**Sb**	**Sc**	**Sm**	**Sn**	**Ta**	**Ti**	**V**	**W**	**Y**	**Yb**	**Zn**	**Zr**
A-site Element	**Ba**	0	9	4	1	9	0	4	2	1	12	0	1	1	10	10	7	1	1	1	2	4	1	0	1	26	0	0	2	1	1	12
	Bi	1	0	0	0	4	2	1	0	0	15	0	0	0	0	1	4	0	0	1	0	0	0	1	2	12	2	0	0	0	0	0

	Ca	2	1	0	0	0	11	1	0	0	3	0	0	0	6	3	2	0	1	2	0	0	0	0	0	22	0	0	0	0	4	0
	Ce	2	0	0	0	1	0	0	0	0	2	0	0	0	0	2	2	0	1	0	0	0	0	0	0	2	0	0	0	0	0	0
	Dy	0	0	0	0	1	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
	Eu	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	1	0
	Er	0	0	0	0	1	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
	Gd	0	0	0	0	2	0	0	0	0	1	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
	K	0	9	0	1	0	0	0	2	1	0	0	1	1	0	0	0	1	0	0	0	0	1	0	0	0	0	0	0	1	0	0
	La	15	0	2	0	47	25	11	0	0	56	11	0	0	28	59	3	0	21	2	2	6	0	0	3	44	0	1	2	0	4	0
	Li	7	0	0	0	0	0	0	0	0	4	0	0	0	0	0	4	0	0	0	0	0	0	0	1	6	0	0	0	0	0	0
	Mn	0	0	0	0	0	0	0	0	0	4	0	0	0	0	0	4	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
	Na	0	0	0	0	0	0	0	0	0	0	0	0	0	1	0	6	0	0	0	0	0	0	0	0	6	0	1	0	0	0	0
	Nd	4	0	0	0	2	1	6	0	0	7	0	0	0	1	5	1	0	0	2	0	0	0	0	1	3	0	0	0	0	1	0
	Pb	3	0	0	0	2	2	0	0	0	5	0	0	0	4	5	4	0	1	0	0	1	0	0	1	12	2	0	0	0	0	6
	Pr	2	0	0	0	8	0	1	0	0	8	0	0	0	0	2	0	0	1	0	0	0	0	0	0	3	0	0	0	0	1	0
	Sm	0	0	0	0	12	3	1	0	0	10	0	0	0	0	6	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
	Sr	15	1	2	0	81	18	19	0	0	102	12	0	0	16	58	5	0	20	2	4	3	0	1	7	29	1	0	0	0	2	10
	Y	1	0	0	0	2	0	0	0	0	1	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0

Table S6. Occurrences of A and B combinations using AA'BB'O_3 compositions from the dataset used for this work, as well as compositions from the PCD and COD

Actual	Predicted		RMSE
		svclassifier = SVR(kernel='poly', degree=3)	28.07

		svclassifier = SVR(kernel='poly', degree=6)	27.99
		svclassifier = SVR(kernel='linear')	28.07
		svclassifier = SVR(kernel='rbf')	29.15
		DTreg = tree.DecisionTreeRegressor() DTreg = DTreg.fit(X, y) *While the shape looks great, each missing value is identical to the value of its previous' element. It is not so useful. For example, H	0.0

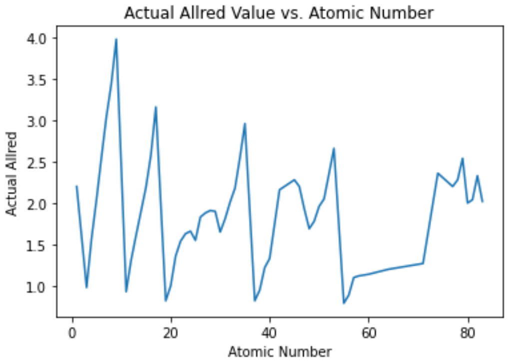
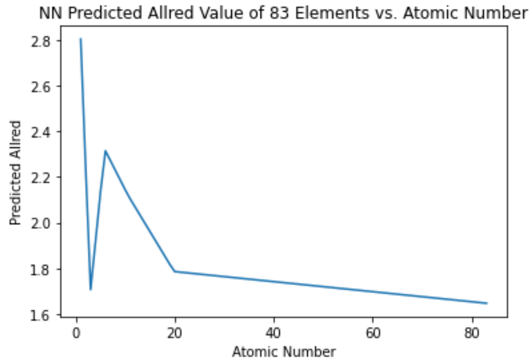
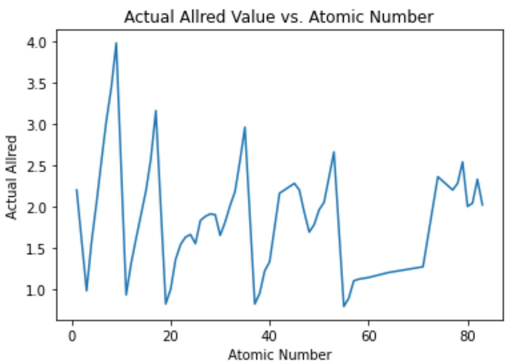
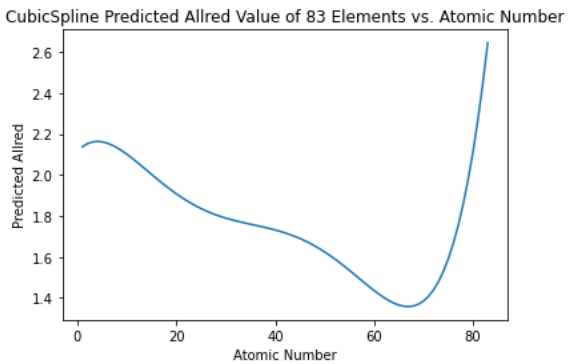
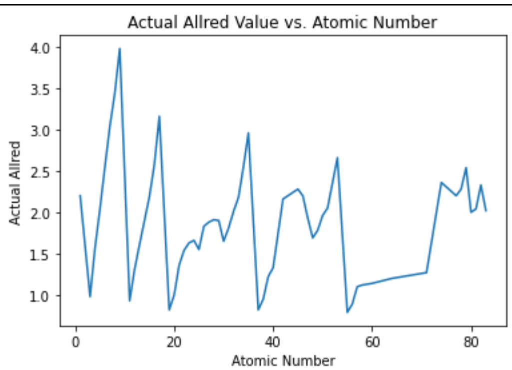
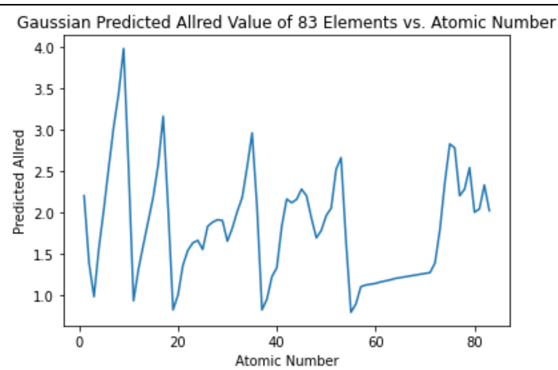
		has 2.2, and He (missing) also 2.2.	
		alpha_value = 0.001 max_iter = 10000 idden_layer_sizes=(100, 10) solver= 'lbfgs'	0.63
		degree = 5 clf = make_pipeline(PolynomialFeatures(degree), Ridge(alpha=1e-3))	0.61
		kernel = C(1.0, (1e-3, 1e3)) * RBF(10, (1e-2, 1e2)) clf = GaussianProcessRegressor(kernel=kernel, n_restarts_optimizer=9) clf.fit(X, y)	6.78e-10

Table S7. Comparison of the models used to predict the Allred electronegativity values for elements with a missing value