Supplementary Materials

A. Brief review of the structure types

The compounds with the perovskite, spinel, garnet, hexagonal perovskite, layered perovskite, -o-tp- perovskite, ilmenite, halite, and fluorite structures (Figure 1) were used to create different collections to develop the ANNs. Fluorite and halite are typical structures in AX_2 and AX binary compounds, respectively. The characteristic polyhedron formed around cations in normal fluorite is the cube, whereas a tetrahedron is formed around anions. In antifluorite structure (formula XA_2) the first coordination polyhedral are reversed, i.e., a cube of cations surrounds the anion, and a tetrahedron of anions surrounds the cation. In this article, we did not distinguish between fluorite or antifluorite compounds. In halite structure, counterions surround each other forming octahedral geometry.

In this article, we refer as perovskite structures to those compounds characterized only by a vertex-shared octahedral framework. This octahedral framework of the perovskite structure can be distorted, which is mainly due to rotations among octahedra. We refer to Ruddlesden-Popper and Dion-Jacobson structures as layered perovskites. In the layered perovskite, alternate phases between perovskite with halite or cesium chloride structure occur. Hexagonal perovskite compounds possess column-like structure. The columns consist of face-share octahedra. Additionally, there are polytypes in the hexagonal perovskite structure, wherein the columns are connected by octahedral vertices. These polytypes are consequence of alternate stacking of spheres layer in close packing fashion. -o-tp-perovskite compounds are similar to hexagonal perovskite: the column is formed by an alternate stacking of trigonal prisms and octahedra via face sharing. In all before mentioned structures, there is always an interstitial cation left in within the characteristic framework. Ilmenite, spinel, and garnet structures lack of interstitial cation.

Ilmenite structure is the structure of corundum, $\alpha - Al_2O_3$. In corundum, oxygen atoms adopt the hexagonal closest packing, wherein 2/3 of the octahedral sites are occupied by cations and the remaining 1/3 are vacant. These arrangement leads to face, vertex and edge sharing of the octahedra. Additionally, the anion (vertex) is four coordinated in the ilmenite stucture. Spinel structure is characterized by vertex sharing of one tetrahedron a three octahedra; i.e., anion is four coordinated. The three octahedra are connected by edge-

sharing. Garnet structure also has four coordinated anions, which connect one tetrahedral cation, one octahedral cation and two eight-coordinated cations.

B. Definitions of the structure types

In this part, each structure type is defined in terms of the occupied Wyckoff sites in each space group. The Wyckoff sites are pointed out with the labels corresponding to each space group. The different crystal descriptions for the same space groups are pointed out as option. These different descriptions in a space group may correspond to instances such as double or simple unit cell in perovskite compounds, polytypes in the hexagonal perovskites, or single – or double Ruddlesden-Popper or Dion Jacobson structures of layered perovskite compounds. The capital letter in each row refers to an atom type in the compound formula.

1. Fluorite structure

Space group: $Fm\bar{3}m$

option: 0

A: a

X: c

2. Garnet structure

Space group: $Ia\bar{3}d$

option: 0

D: c

O: a

T: d

X: h

3. Halite structure

Space group: $Fm\bar{3}m$

option: 0

A: a

X: b

4. Hexagonal perovskite structure

Space group: $P6_3/mmc$

option: 0

A: d

B: a

X: h

option: 1

A: a,d

B: f

X: g,h

option: 2

A: b, f

B: a, f

X: h, k

option: 3

A: b,f,f

B: a,f,f

X: h,k,k

Space group: $P6_3mc$

option: 0

A: b

B: a

X: c

option: 1

A: a, b, b

B: a, b, b

X: c, c, c

Space group: $P6_3cm$

option:0

A: a, b

B: c

X: d, c

Space group: $R\bar{3}m$

option: 0

A: a,c

B: b,c

X: e,h

5. Ilmenite structure

Space group: $R\bar{3}$

option: 0

A: c

B: c

X: f

6. Layered perovskite structure

Space group: $I4/mmm$

option: 0

A: e

B: a

X: e, c

option: 1

A: b, e

B: e

X: a, e, g

option: 2

A1: d

A2: a

B: e

X: b, e, g

option: 3

A1: d

A2: e

B: a, e

X: c, e, e, g

Space group: $P4/nmm$

option: 0

A: c, c

B: c

X: a, c, f

Space group: $P4/mmm$

option: 0

A1: d

A2: c

B: g

X: a, g, i

option: 1

A1: d

A2: h

B: a, g

X: f, g, g, i

Space group: $Cmce$

option: 0

A: f

B: a

X: e, f

7. -o-tp- perovskite structure

Space group: $R\bar{3}c$

option: 0

A1: e

A2: a

B: b

X: f

8. Perovskite structure

Space group: $Pm\bar{3}m$

option: 0

A: b

B: a

X: d

Space group: $P4/mbm$

option: 0

A: c

B: a

X: b, g

Space group: $I4/mmm$

option: 0

A: a, b, c

B: f

X: h, n

Space group: $Im\bar{3}$

option: 0

A: a, b

B: c

X: g

Space group: $Immm$

option: 0

A: a,b,c,d

B: k

X: l, m, n

Space group: $I4/mcm$

option: 0

A: b

B: c

X: a, h

X: e, f

Space group: $Imma$

option: 0

A: e

B: b

X: e, g

Space group: $R\bar{3}c$

option: 0

A: a

B: b

X: e

Space group: $C2/m$

option: 0

A: i

B: e

X: i, g, h

option: 1

A: i

B1: a

B2: d

X: i, j

Space group: $C2/c$

option: 0

A: e

B: b

option: 1

A: e, e

B1: c

B2: d

X: f, f, f

Space group: $P\bar{1}$

option: 0

A: i

B: a, b

X: i, i, i

option: 1

A: i, i, i, i

B1: a, e, f, g

B2: b, c, d, h

X: i, i, i, i, i, i

Space group: $Cmcm$

option: 0

A: c, c

B: d

X: e, f, g

Space group: $Pnma$

option: 0

A: c

B: b

X: c, d

Space group: $P2_1/m$

option: 0

A: e, e

B: b, c

X: e, e, f, f

Space group: $P4_2/nmc$

option: 0

A: a, b, d

B: e

X: g, g, f

Space group: $Pmmn$

option: 0

A: a, a, b, b

B: c, d

X: e, e, f, f, g

Space group: $Pnnn$

option: 0

A: a, b, c, d

B1: e

B2: f

X: m, m, m

Space group: $Pn\bar{3}$

option: 0

A: a, d

B1: b

B2: c

X: h

Space group: $P2/c$

option: 0

A: e, e, f, f

B1: a, b

B2: c, d

X: g, g, g, g

Space group: $P4_2/n$

option: 0

A : a, b, e

B1: c

B2: d

X: g, g, g

Space group: $P2_1/c$

option: 0

A : e

B1: c

B2: d

X: e, e, e

Space group: $R\bar{3}$

option: 0

A: c

B1: a

B2: b

X: f

Space group: $P4_2/nnm$

option: 0

A: a, b, c

B1: e

B2: f

X: m, n

Space group: $P4/mnc$

option: 0

A: c

B1: a

B2: b

X: e, h

Space group: $I4/m$

option: 0

A: b

B1: a

B2: b

X: e, h

Space group: $Fm\bar{3}m$

option: 0

A: c

B1: a

B2: b

X: e

9. Spinel structure

(In the 4S – ANNs, the space group $Fd\bar{3}m$ was the only used).

Space group: $Fd\bar{3}m$

option: 0

A: a

B: d

X: e

Space group: $F\bar{4}3m$

option: 0

A1: a

A2: d

B: e

X: e, e

Space group: $P4_332$

option: 0

A: c

B1: b

B2: d

X: c, e

Space group: $P2_13$

option: 0

A: a, a

B1: a

B2: b

X: a, a, b, b

Space group: $I4_1/amd$

option: 0

A: a

B: d

X: h

Space group: $P4_122$

option: 0

A: c

B1: a

B2: b

X: d, d

Space group: $P4_322$

option: 0

A: c

B: a, b

X: d, d

Space group: $Imma$

option: 0

A: h

B: a, e, g

X: e, e, h, j

C. Precisions with the compounds of the TRAining – VALidation set | Recall in the 2nd test

1. 4 sites, 4 outputs: garnet, perovskite, spinel and others.

	Traval	
	No density	With density
Garnet	100.00	100.00
Perovskite	95.93	97.39
Spinel	97.80	98.34
Other phases	97.83	98.56
Number of samples	4197	

In case that the scores of the NEF – and WEF – ANN were different, the scores of the WEF – ANNs are shown in bold.

	2nd test: 12,264 not used compounds			
	1	2	3	4
	(1189)	(4306)	(3757)	(3012)
Garnet	0.00	0.14 **(0.00)**	0.00	0.27 **(0.20)**
Perovskite	0.00 **(0.17)**	1.42 **(3.37)**	2.45 **(1.89)**	3.19 **(2.95)**
Spinel	0.00	0.02 **(2.42)**	1.14	0.00
Other phases	100.00 **(99.83)**	98.42 **(94.22)**	96.41 **(96.97)**	96.55 **(96.85)**

2. 6 sites, 4 outputs: garnet, perovskite, spinel, and other phases.

	Traval	
	No density	With density
Garnet	99.40	100.00
Perovskite	95.28	96.21
Spinel	96.53	97.67
Other phases	95.48	95.81
Number of samples	4322	

	2nd test					
	1	2	3	4	5	6
	(1189)	(4306)	(3711)	(3012)	(3557)	(3454)
Garnet	0.00	0.00	0.00	0.37 **(0.27)**	0.00	0.00
Perovskite	0.00 **(0.08)**	0.81 **(1.11)**	4.23 **(3.96)**	3.45 **(3.49)**	6.16 **(7.59)**	7.47 **(6.98)**
Spinel	0.00	1.86 **(8.10)**	3.05 **(2.32)**	0.03	11.13 **(8.52)**	0.00
Other phases	100.00 **(99.92)**	97.33 **(90.78)**	92.72 **(93.72)**	96.15 **(96.22)**	82.71 **(83.89)**	92.53 **(93.02)**

3. 6 sites, 8 output: garnet, hexagonal perovskite, ilmenite, layered perovskite, -o-tp-perovskite, perovskite, spinel, and others

	Traval	
	No density	With density
Garnet	98.80	98.20
Hexagonal perovskite	93.20	89.62
Ilmenite	76.19	74.47
Layered perovskite	94.94	95.28
-o-tp perovskite	94.03	98.31
Perovskite	95.75	95.12
Spinel	98.69	97.93
Other phases	95.39	94.61
Number of samples	*5519*	

	2nd test					
	1	2	3	4	5	6
	(1189)	(4306)	(3537)	(2504)	(3523)	(3120)
Garnet	0.00	0.00	0.00	0.28 **(0.32)**	0.09 **(0.00)**	0.00
Hexagonal perovskite	0.00	0.00	0.20 **(0.23)**	0.00	3.46 **(5.59)**	4.17 **(4.26)**
Ilmenite	0.00	0.00	0.57 **(0.71)**	0.00	0.00	0.00
Layered perovskite	0.00	0.00	0.00	0.56 **(0.44)**	0.14 **(0.00)**	1.51 **(2.02)**
-o-tp perovskite	0.00	0.00	0.00	0.52 **(0.40)**	0.00	0.00
Perovskite	0.00 **(0.17)**	0.37 **(0.49)**	3.28 **(4.04)**	2.64 **(2.24)**	4.54 **(3.75)**	3.24 **(2.44)**
Spinel	0.00	2.02 **(0.44)**	1.84 **(2.01)**	0.00 **(0.04)**	6.02 **(5.31)**	0.03 **(0.00)**
Other phases	100.00 **(99.83)**	97.61 **(99.07)**	94.12 **(93.02)**	96.01 **(96.57)**	85.75 **(85.35)**	91.06 **(91.28)**

4. 6 sites, 10 outputs: fluorite, garnet, halite, hexagonal perovskite, ilmenite, layered perovskite, -o-tp- perovskite, perovskite, spinel, and others.

	% Precision (traval)
Fluorite	92.43 (191)
Garnet	97.63 (165)
Halite	89.98 (454)
Hexagonal perovskite	96.00 (104)
Ilmenite	86.67 (44)
Layered perovskite	95.47 (237)
-o-tp- perovskite	96.92 (63)
Perovskite	96.63 (1383)
Spinel	97.94 (764)
Others	96.45 (3398)
Number of samples	*6803*

	1 (1189)	2 (2793)	3 (3537)	4 (2504)	5 (3524)	6 (3120)
Fluorite	2.78 (33)	4.19 (117)	0.00	0.00	0.00	0.00
Garnet	0.00	0.00	0.00	0.36 (9)	0.00	0.00
Halite	0.00	10.67 (298)	0.00	0.00	0.00	0.00
Hexagonal perovskite	0.00	0.00	0.25 (9)	0.00	3.69 (130)	2.37 (74)
Ilmenite	0.00	0.00	0.42 (15)	0.00	0.00	0.00
Layered perovskite	0.00	0.00	0.00	0.96 (24)	0.26 (9)	1.67 (52)
-o-tp- perovskite	0.00	0.00	0.00	0.84 (21)	0.00	0.00
Perovskite	0.00	0.00	2.97 (105)	3.31 (83)	5.51 (194)	2.53 (79)
Spinel	0.00	0.00	2.23 (79)	0.00	5.99 (211)	0.00
Others	97.22	85.14	94.12	94.53	84.56	93.43

D. Retrieved compounds of the second test

Hexagonal perovskites			
Space group	Sites	Atoms	Compounds
$P6_3/mmc$	6	30	Ba3NaRu2O9, Ba3YRu2O9, Ba3GdRu2O9, Ba6Fe3.98Te2.02O18
	5	28	Cs3W2Cl9, Cs3Tm2I9, Cs3Y2I9, Cs3Zr2I9, Rb3Nb2Br9, Cs3Er2I9
	5	20	SrMnO3
$P\bar{6}m2$	6	30	BaCoO3
	5	10	BaCoO3
$P6_322$	6	30	Ba3Fe2WO9
$P6_3/m$	6	30	Ba6Sr0.4Ca1.6Ru4O18, Ba3SrNb2O9, Ba3SrTa2O9, Ba4Ta2O9
$R\bar{3}m$	6	57	Sr4Re2NiO12, Ba3LaZnReWO12, Sr3LaTa3O12, Ba4ScReWO12
	5	42	RbBa2Fe2F9, CsBa2Co2F9, KBa2Ni2F9, RbBa2Ni2F9, CsBa2Ni2F9, CsBa2Zn2F9

Ilmenite			
$R3c$	3	30	Ta4.002Mn7.998O18, Li5.64Nb5.88Zn0.48O18, Li6Nb6O12.006F5.994, Mn8.1Nb3.9O18, ScFeO3, AlBiO3, Li3.6Ta6Cu2.4O18, TiMnO3, Li5.25Nb5.25Te0.75O18

Layered perovskites			
$I4/mmm$	6	32	CsBa2Cr2F11
		24	Li3.92Y4Ti4S4O10, Li0.92Y4Ti4S4O10, Li0.6Y4Ti4S4O10, Ba3.964Tl4.016Cu1.988O12
		14	Na0.2La7.8Ni4O16
$P4/nmm$	6	14	Sr0.82Ce0.54Nd2.64Cu2O7.8608, Sr0.5La2Ho1.5Cu2O7.78
$Immm$	4	12	Ba2PdO3, Ce2MnN3
		11	Li4WO6
$Fmmm$	4	28	K4Br2O
$Ccce$	6	48	K3Ag2F7
$Cccm$	6	44	Sr2MnBiPbO6
$Cmce$	5	36	Ba2CuF6
$Pbam$	4	14	Sr2PrO4, Sr2PbO4, Ca2SnO4, Ca3.8Eu0.4Sn1.8O8, Ca3.4Eu1.2Sn1.4O8, Ca2PbO4

-o-tp perovskites			
$R\bar{3}m$	4	33	K4MnCl6

Perovskite			
$Im\bar{3}m$	5	40	K1.92Ba6.08Na1.262Bi6.738O24, K4CaU3O12, K4SrU3O12, K4BaU3O12, Ba4Na(SbO4)3, Ba8Li1.98Sb6.02O24, Ba8Ca1.84Cu6O17.4, K6Ba2CaU6O24
	4	40	CaTi4(CuO4)3
	4	28	Ca9.016B6N12
$Fd\bar{3}m$	4	84	Na2Sr2Nb4O13, Eu10.72Ti16Fe5.28O50.72, Nd13.44Ti16O52.16, Na16Ta16.0O47.984, Ca10.4Re16O52.8, Na14.72Ta16O39.9984F8.0016, Na2.88Y6.88Sb16O51.76, Na2.88Gd6.4Sb16O51.04, K3.36Gd5.6Sb16O50.08
	3	80	SnPbO3, Nb2CdO7, Ta2CdO7, Nb2PbO7, KTaWO7, MnRe(PbO3)2, Ta12.8Ti3.2Pb9.6O48, Ta2PbO7, NaSbO3, AgSbO3, K2.576Ag13.424Sb16O48, Nb8Cr8Bi10.72O48, SbWNO6, TaWNO6, W2O7, NbWNO6, Nb2O7, Ta2O7, Ta11.2W4.8O56, TaWO7, Al8(O5F4)3, Ta8W8O50.16 Nb8W8O48.56
$Fm\bar{3}m$	5	64	K2FeCu(CN)6, K2FeNi(CN)6, K2FeCo(CN)6, KFe(CN)3, Rb2FeCu(CN)6
	3	36	Cs2SiF6, Cs2GeF6, Sr2H6Ru, Cs2PdF6, Rb2PdF6, NaPF6, HfVF6, ZrTiF6, NaMoF6, CaPbF6, NaSbF6
$Pm\bar{3}m$	4	8	CaTiO3
$F\bar{4}3m$	5	40	KBaLiZnF6
$Pa\bar{3}$	4	40	Ba2UCrO6, Ba8Mg2U3.332Fe2.668O24, K2NaAlF6, Ba8U2.668In0.532Fe4.8O24, Ba8U2.668In0.268Fe5.064O24, Ba8U2.668In1.064Fe4.268O24, Ba8U2.668In1.332Fe4O24 Sr8Sc2Al6O19.9992
$R\bar{3}c$	3	30	Sr0.32La1.68Mn2O6

$R\bar{3}m$	4	30	Ba2SrIrO6, Ba2Ca0.7333Nb1.2667O5.8998, Ba2Ca0.7867Nb1.2133O5.823, Ba2Ca0.8333Nb1.1667O5.7498 Ba2Ca0.9Nb1.1O5.6502
	3	24	BaGeF6, KAuF6, BaCrF6, SrCrF6, CaTiF6, BaPbF6 SrNiF6
$P\bar{3}m1$	3	9	K2PdF6
$P\bar{3}1m$	3	9	Li2HfF6, Li2ZrF6
$R3c$	3	30	K0.6Na2.4Ti6Bi3O18, K1.2Na1.8Ti6Bi3O18, Sr0.3La5.7Mg0.6Ga5.4O17.46
$R3m$	3	15	Ta1.5Fe1.5Pb3O9, Ba3Ta1.5Fe1.5O9, Ba2TaFeO6, Nb0.5Fe0.5Pb1O3, Zr0.58Ti0.42Pb1O3, BaTiO3
$R\bar{3}$	3	24	NaFeF6, MgCrF6, LiBiF6, RbBiF6, CsBiF6, TiCdF6, CsSbF6, CsReF6, LiIrF6, CaPtF6, MnPtF6, CaPdF6, CsBrF6, CsUF6, ZnPdF6, CdPdF6
$I4/mcm$	4	20	KCuF3
$I4/mmm$	5	20	CsAuCl3, Cs2AgAuCl6, CsAgCl3, Ba2FeReO6, Cs2KMnF6, Sr2FeMoO6, Cs3TlF6, Sr4Fe2.2Mo1.8O12, Sr4Fe1.6Mo2.4O12, Rb2NaMnF6, Sr2MgReO6, Cs2HgPdCl6, CoTe(PbO3)2, CsAuI3, CsAuBr3, Ba2SmMoO6
$P4/mmm$	6	10	Ba2Sc1Cu1O4.5, Ba2Cu1Hg1O4.34, Ba2Cu1Hg0.98O4.34, Ba2Cu1Hg1O4.31, Ba2Cu1Hg0.96O4.34, Ba2Cu1Hg1O4.27, Ba2Cu1Hg1O4.24, Ba2Cu1Hg1O4.172, Ba2Ce0.15Cu1Hg0.85O4.15, Ba2Cu1Hg1O4.12, Ba2Cu1Hg1O4.1, Ba2Cu1Hg1O4.069, Ba2Cu1Hg1O4.054
	5	9	Li0.5La0.5Nb2O6, Li0.32La0.56Nb2O6, Li0.08La0.64Nb2O6, La0.667Nb2O6, La0.66Ta2O6, Y1.32Ta4O12, Y0.6Ta1.8W0.2O6, U0.5Nb2O6
	4	10	Sr1Ca1Cu1.5Bi0.5O4
$P4bm$	4	10	NaTi2BiO6
$P4mm$	6	20	Nd3Ta4O12
	5	5	Hf0.42Ti0.58Pb1O3, Ba0.3Fe1Bi0.7O2.7F0.3, Ba0.2Fe1Bi0.8O2.799F0.201, Sr0.06Zr0.5Ti0.5Pb0.91O3, Ba0.2Fe1Bi0.8O2.9001, Ba0.3Fe1Bi0.7O2.85
	4	5	Mg0.213Ti0.36Nb0.427Pb1O3, Mg0.227Ti0.32Nb0.453Pb1O3, Mg0.237Ti0.29Nb0.473Pb1O3, Mg0.203Ti0.39Nb0.407Pb1O3, Zr0.1Ti0.9Pb1O3, Zr0.52Ti0.48Pb1O3, TiPbO3, Hf0.2Ti0.8Pb1O3, Zr0.44Ti0.44Mn0.04Nb0.04Ni0.04Pb1O3, Zr0.525Ti0.475Pb1O3, Zr0.45Ti0.55Pb1O3, Zr0.945Ti0.029Nb0.026Pb0.987O3, Ca0.42Ti1Pb0.58O3, Ca0.388Ti1Pb0.612O3, Zr0.45Ti0.55Pb1O3, ZrPbO3, Zr0.945Ti0.029Nb0.026Pb0.987O3, Ti1Pb0.9926O2.9342, Ti1Pb0.9633O2.6098, Ti0.962Pb0.9909O2.9794, Ti0.984Pb0.9923O2.9426, Ti0.96Pb0.9844O2.96, Ti0.964Pb0.9981O2.8972
$I4/m$	5	20	BaLaMgRuO6, BaLaZnRuO6, Ba2CuWO6, Sr2CuWO6, Sr2CuTeO6, Ba2CuTeO6, BaLaCuRuO6, Sr2NiWO6, Sr2FeMoO6, Sr3.8Nd0.2Fe2Mo2O12, Sr2MnSbO6, Ba2GdNbO6, Ba2TbNbO6, Ba2CaWO6, Ba2CaReO6, Sr4V0.5Fe1.5Mo2.0O12, KRb2InF6, Ba2FeWO6, Sr2TaInO6, Sr2TaGaO6, Sr2ReNiO6, Sr2CoReO6, Sr2ZnReO6, Sr2NiMoO6, Ba2YTaO6, Sr4Fe2.94Te1.06O12, Sr4Fe1.98Mo1.98O12, Sr4Ti0.5Fe1.48Mo1.96O12, Sr4Cr0.5Fe1.5Mo2O11.796, Sr4Fe1.94Mo1.88O11.616, Sr3.82Fe1.5Co0.5Mo2O11.364
$Imma$	4	20	SrNdMn2O6, Ba1.0912Sr2.9088Zr2.624Ti1.376O12, Sr2Nd0.25Sm1.75Mn4O12, Ba4Bi(PbO4)3, BaLaMnInO6, Na1.32La2.66Ti2.68Mn1.32O12, Sr0.2La3.8Mg0.428Ga3.572O11.1612
$Pnma$	5	20	Mg3.9Al0.2Si3.9O12
$Pbam$	6	20	Sr3.6La0.4Mn4O10.2
$Pmmm$	5	5	TiPbO3
$Amm2$	5	10	K1.7156Na0.2844Nb2O5.612, K1.6786Na0.3214Nb2O5.612
	4	10	KNbO3, K1.4032Na0.5968Nb1O6, K1.5238Na0.4762Nb1O6, K1.5098Na0.49Nb1O6, K1.45Na0.55Nb1O6
$C2/m$	6	20	KCrF3

Cm	5	10	Zr1.08Ti0.92Pb2O6, Zr1.04Ti0.96Pb2O6
	4	10	NbFe(PbO3)2
Pm	5	5	Mg0.213Ti0.36Nb0.427Pb1O3, Mg0.227Ti0.32Nb0.453Pb1O3, KNbO3
Spinel			
I4₁/amd	*3*	*28*	*Mn3O4, Cu2GeO4, MgMn2O4, Mn8.196Co0.76Cu0.36Ni2.684O16, Mn2CuO4, Cr2NiO4, Cr2CuO4, Cu(RhO2)2, Li3.628Mn8.372O16, Fe2SnS4, Mn8.344Co3.656O16, Mn11.752Fe0.248O16, Mn10.812Fe1.188O16, Fe2CuO4, Mn8.0004Ni3.9996O16, Li3.56Mn8O15.36*
Imma	5	28	LiVCuO4, Li2.196V4.02Co4.956O16
Fddd	3	56	Na2SO4, Na2SeO4, Hg2GeO4, AgHgAsO4, Ag2SeO4, Cr2SiO4
C2/c	5	28	Li2CrCl4

E. List of features

In this part of the supplementary information, we enlist the features $[x_1, x_2, \ldots, x_n]$ in the input data used to characterize the compounds in the WEF - ANNs. In the NEF - ANNs, atomic radii and electronegativities per site, as well as the density of the compound, were not part of the input data. The subscripts appearing with average atomic radius r_i, electronegativity χ_i, and local function f_{ij} refer to a site in the crystal compound. The average atomic radius per site, r_i is calculated as follows:

$$r_i = \sum r_{elem} s_{elem} \text{ (eq. 1)}$$

where r_{elem} refers to the atomic radius of the chemical element in the i - Wyckoff site, and s_{elem} to its occupation fraction. If the occupation fraction of all elements occupying the i - Wyckoff site does not sum one, this means that there are vacancies in the compound.

The number of features corresponding to geometric factors, as well as to packing factors, is calculated with the number of combinations formula:

$$_k^n C = \frac{n!}{k!(n-k)!} \text{ (eq. 2)}$$

where n is the number of sites in the crystal compound and k is the number of elements in the set to form. From this formula, there are six different pairs of atomic radii when the crystal compounds are characterized with four sites (4S - ANNs). Similarly, there are fifteen different pairs of atomic radii when the crystal compounds are characterized with six sites (6S - ANNs). These different pairs corresponded to the different quotients in the geometric factors. To generate the 15 packing factors in the 4S - ANNs, the six different combinations previously calculated were first expressed in terms of a sum; i.e., there were six different sums. These different sums were used again with the number of combinations formula to calculate different pairs to generate the quotients corresponding to packing factors. This procedure was the same to generate the 105 packing factors in the 6S - ANNs. The local environment functions were calculated as follows:

$$f_{ij} = (\chi_i - \chi_j) \sum_{n=1}^{d_{ij[n]} \leq R_c} \left[\frac{1}{2} \left(\cos \frac{\pi d_{ij[n]}}{R_c} + 1 \right) \right] \exp \left[-\left(\frac{d_{ij[n]}}{r_i^{norm} + r_i^{norm}} \right)^2 \right] \text{ (eq. 3)}$$

The sum in the equation 2 is performed over all neighbor atoms located in the same j - Wyckoff site within a cutoff radius, R_c, equal to 25 Å. $d_{ij[n]}$ stands for the distance between a neighbor atom and the central one, which is located in the i - Wyckoff site. The atomic radii of the species are normalized, which implies that the occupation fraction of each element in the i - Wyckoff site, s_{elem}, was considered:

$$r_i^{norm} = \frac{r_i}{\sum s_{elem}}$$

E.1 Features in the 4S - WEF ANNs

E.1.1 Average atomic radii and electronegativities per site

(This set of features was not used in the NEF - ANNs)

$x_1: r_1$ $x_3: r_2$ $x_5: r_3$ $x_7: r_4$

$x_2: \chi_1$ $x_4: \chi_2$ $x_6: \chi_3$ $x_8: \chi_4$

E.1.2 Geometric factors

$$x_9: \frac{r_1}{r_2} \qquad\qquad x_{11}: \frac{r_1}{r_4} \qquad\qquad x_{13}: \frac{r_2}{r_4}$$

$$x_{10}: \frac{r_1}{r_3} \qquad\qquad x_{12}: \frac{r_2}{r_3} \qquad\qquad x_{14}: \frac{r_3}{r_4}$$

E.1.3 Packing factors

$$x_{15}: \frac{r_1 + r_2}{r_1 + r_3} \qquad\qquad x_{20}: \frac{r_1 + r_3}{r_1 + r_4} \qquad\qquad x_{25}: \frac{r_1 + r_4}{r_2 + r_4}$$

$$x_{16}: \frac{r_1 + r_2}{r_1 + r_4} \qquad\qquad x_{21}: \frac{r_1 + r_3}{r_2 + r_3} \qquad\qquad x_{26}: \frac{r_1 + r_4}{r_3 + r_4}$$

$$x_{17}: \frac{r_1 + r_2}{r_2 + r_3} \qquad\qquad x_{22}: \frac{r_1 + r_3}{r_2 + r_4} \qquad\qquad x_{27}: \frac{r_2 + r_3}{r_2 + r_4}$$

$$x_{18}: \frac{r_1 + r_2}{r_2 + r_4} \qquad\qquad x_{23}: \frac{r_1 + r_3}{r_3 + r_4} \qquad\qquad x_{28}: \frac{r_2 + r_3}{r_3 + r_4}$$

$$x_{19}: \frac{r_1 + r_2}{r_3 + r_4} \qquad\qquad x_{24}: \frac{r_1 + r_4}{r_2 + r_3} \qquad\qquad x_{29}: \frac{r_2 + r_4}{r_3 + r_4}$$

E.1.4 Local environment functions

$x_{30}: f_{12}$ $x_{33}: f_{21}$ $x_{36}: f_{31}$ $x_{39}: f_{41}$

$x_{31}: f_{13}$ $x_{34}: f_{23}$ $x_{37}: f_{32}$ $x_{40}: f_{42}$

$x_{32}: f_{14}$ $x_{35}: f_{24}$ $x_{38}: f_{34}$ $x_{41}: f_{43}$

E.1.5 Density of the crystal 2 compound

(This feature was not used in the NEF - ANNs)

$x_{42}: \rho_{compound}$

E.2 Features in the 6S - WEF ANNs

E.2.1 Average atomic radii and electronegativities per site

(This set of features was not used in the NEF - ANNs)

$x_1 : r_1$ $x_3 : r_2$ $x_5 : r_3$ $x_7 : r_4$ $x_9 : r_5$ $x_{11} : r_6$

$x_2 : \chi_1$ $x_4 : \chi_2$ $x_6 : \chi_3$ $x_8 : \chi_4$ $x_{10} : \chi_5$ $x_{12} : \chi_6$

E.2.2 Geometric factors

$x_{13} : \dfrac{r_1}{r_2}$ $x_{18} : \dfrac{r_2}{r_3}$ $x_{23} : \dfrac{r_3}{r_5}$

$x_{14} : \dfrac{r_1}{r_3}$ $x_{19} : \dfrac{r_2}{r_4}$ $x_{24} : \dfrac{r_3}{r_6}$

$x_{15} : \dfrac{r_1}{r_4}$ $x_{20} : \dfrac{r_2}{r_5}$ $x_{25} : \dfrac{r_4}{r_5}$

$x_{16} : \dfrac{r_1}{r_5}$ $x_{21} : \dfrac{r_2}{r_6}$ $x_{26} : \dfrac{r_4}{r_6}$

$x_{17} : \dfrac{r_1}{r_6}$ $x_{22} : \dfrac{r_3}{r_4}$ $x_{27} : \dfrac{r_5}{r_6}$

E.2.3 Packing factors

$x_{28} : \dfrac{r_1 + r_2}{r_1 + r_3}$ $x_{37} : \dfrac{r_1 + r_2}{r_3 + r_5}$ $x_{46} : \dfrac{r_1 + r_3}{r_2 + r_4}$ $x_{55} : \dfrac{r_1 + r_4}{r_1 + r_5}$

$x_{29} : \dfrac{r_1 + r_2}{r_1 + r_4}$ $x_{38} : \dfrac{r_1 + r_2}{r_3 + r_6}$ $x_{47} : \dfrac{r_1 + r_3}{r_2 + r_5}$ $x_{56} : \dfrac{r_1 + r_4}{r_1 + r_6}$

$x_{30} : \dfrac{r_1 + r_2}{r_1 + r_5}$ $x_{39} : \dfrac{r_1 + r_2}{r_4 + r_5}$ $x_{48} : \dfrac{r_1 + r_3}{r_2 + r_6}$ $x_{57} : \dfrac{r_1 + r_4}{r_2 + r_3}$

$x_{31} : \dfrac{r_1 + r_2}{r_1 + r_6}$ $x_{40} : \dfrac{r_1 + r_2}{r_4 + r_6}$ $x_{49} : \dfrac{r_1 + r_3}{r_3 + r_4}$ $x_{58} : \dfrac{r_1 + r_4}{r_2 + r_4}$

$x_{32} : \dfrac{r_1 + r_2}{r_2 + r_3}$ $x_{41} : \dfrac{r_1 + r_2}{r_5 + r_6}$ $x_{50} : \dfrac{r_1 + r_3}{r_3 + r_5}$ $x_{59} : \dfrac{r_1 + r_4}{r_2 + r_5}$

$x_{33} : \dfrac{r_1 + r_2}{r_2 + r_4}$ $x_{42} : \dfrac{r_1 + r_3}{r_1 + r_4}$ $x_{51} : \dfrac{r_1 + r_3}{r_3 + r_6}$ $x_{60} : \dfrac{r_1 + r_4}{r_2 + r_6}$

$x_{34} : \dfrac{r_1 + r_2}{r_2 + r_5}$ $x_{43} : \dfrac{r_1 + r_3}{r_1 + r_5}$ $x_{52} : \dfrac{r_1 + r_3}{r_4 + r_5}$ $x_{61} : \dfrac{r_1 + r_4}{r_3 + r_4}$

$x_{35} : \dfrac{r_1 + r_2}{r_2 + r_6}$ $x_{44} : \dfrac{r_1 + r_3}{r_1 + r_6}$ $x_{53} : \dfrac{r_1 + r_3}{r_4 + r_6}$ $x_{62} : \dfrac{r_1 + r_4}{r_3 + r_5}$

$x_{36} : \dfrac{r_1 + r_2}{r_3 + r_4}$ $x_{45} : \dfrac{r_1 + r_3}{r_2 + r_3}$ $x_{54} : \dfrac{r_1 + r_3}{r_5 + r_6}$ $x_{63} : \dfrac{r_1 + r_4}{r_3 + r_6}$

$x_{64}: \dfrac{r_1 + r_4}{r_4 + r_5}$

$x_{65}: \dfrac{r_1 + r_4}{r_4 + r_6}$

$x_{66}: \dfrac{r_1 + r_4}{r_5 + r_6}$

$x_{67}: \dfrac{r_1 + r_5}{r_1 + r_6}$

$x_{68}: \dfrac{r_1 + r_5}{r_2 + r_3}$

$x_{69}: \dfrac{r_1 + r_5}{r_2 + r_4}$

$x_{70}: \dfrac{r_1 + r_5}{r_2 + r_5}$

$x_{71}: \dfrac{r_1 + r_5}{r_2 + r_6}$

$x_{72}: \dfrac{r_1 + r_5}{r_3 + r_4}$

$x_{73}: \dfrac{r_1 + r_5}{r_3 + r_5}$

$x_{74}: \dfrac{r_1 + r_5}{r_3 + r_6}$

$x_{75}: \dfrac{r_1 + r_5}{r_4 + r_5}$

$x_{76}: \dfrac{r_1 + r_5}{r_4 + r_6}$

$x_{77}: \dfrac{r_1 + r_5}{r_5 + r_6}$

$x_{78}: \dfrac{r_1 + r_6}{r_2 + r_3}$

$x_{79}: \dfrac{r_1 + r_6}{r_2 + r_4}$

$x_{80}: \dfrac{r_1 + r_6}{r_2 + r_5}$

$x_{81}: \dfrac{r_1 + r_6}{r_2 + r_6}$

$x_{82}: \dfrac{r_1 + r_6}{r_3 + r_4}$

$x_{83}: \dfrac{r_1 + r_6}{r_3 + r_5}$

$x_{84}: \dfrac{r_1 + r_6}{r_3 + r_6}$

$x_{85}: \dfrac{r_1 + r_6}{r_4 + r_5}$

$x_{86}: \dfrac{r_1 + r_6}{r_4 + r_6}$

$x_{87}: \dfrac{r_1 + r_6}{r_5 + r_6}$

$x_{88}: \dfrac{r_2 + r_3}{r_2 + r_4}$

$x_{89}: \dfrac{r_2 + r_3}{r_2 + r_5}$

$x_{90}: \dfrac{r_2 + r_3}{r_2 + r_6}$

$x_{91}: \dfrac{r_2 + r_3}{r_3 + r_4}$

$x_{92}: \dfrac{r_2 + r_3}{r_3 + r_5}$

$x_{93}: \dfrac{r_2 + r_3}{r_3 + r_6}$

$x_{94}: \dfrac{r_2 + r_3}{r_4 + r_5}$

$x_{95}: \dfrac{r_2 + r_3}{r_4 + r_6}$

$x_{96}: \dfrac{r_2 + r_3}{r_5 + r_6}$

$x_{97}: \dfrac{r_2 + r_4}{r_2 + r_5}$

$x_{98}: \dfrac{r_2 + r_4}{r_2 + r_6}$

$x_{99}: \dfrac{r_2 + r_4}{r_3 + r_4}$

$x_{100}: \dfrac{r_2 + r_4}{r_3 + r_5}$

$x_{101}: \dfrac{r_2 + r_4}{r_3 + r_6}$

$x_{102}: \dfrac{r_2 + r_4}{r_4 + r_5}$

$x_{103}: \dfrac{r_2 + r_4}{r_4 + r_6}$

$x_{104}: \dfrac{r_2 + r_4}{r_5 + r_6}$

$x_{105}: \dfrac{r_2 + r_5}{r_2 + r_6}$

$x_{106}: \dfrac{r_2 + r_5}{r_3 + r_4}$

$x_{107}: \dfrac{r_2 + r_5}{r_3 + r_5}$

$x_{108}: \dfrac{r_2 + r_5}{r_3 + r_6}$

$x_{109}: \dfrac{r_2 + r_5}{r_4 + r_5}$

$x_{110}: \dfrac{r_2 + r_5}{r_4 + r_6}$

$x_{111}: \dfrac{r_2 + r_5}{r_5 + r_6}$

$x_{112}: \dfrac{r_2 + r_6}{r_3 + r_4}$

$x_{113}: \dfrac{r_2 + r_6}{r_3 + r_5}$

$x_{114}: \dfrac{r_2 + r_6}{r_3 + r_6}$

$x_{115}: \dfrac{r_2 + r_6}{r_4 + r_5}$

$x_{116}: \dfrac{r_2 + r_6}{r_4 + r_6}$

$x_{117}: \dfrac{r_2 + r_6}{r_5 + r_6}$

$x_{118}: \dfrac{r_3 + r_4}{r_3 + r_5}$

$x_{119}: \dfrac{r_3 + r_4}{r_3 + r_6}$

$x_{120}: \dfrac{r_3 + r_4}{r_4 + r_5}$

$x_{121}: \dfrac{r_3 + r_4}{r_4 + r_6}$

$x_{122}: \dfrac{r_3 + r_4}{r_5 + r_6}$

$x_{123}: \dfrac{r_3 + r_5}{r_3 + r_6}$

$x_{124}: \dfrac{r_3 + r_5}{r_4 + r_5}$

$x_{125}: \dfrac{r_3 + r_5}{r_4 + r_6}$

$x_{126}: \dfrac{r_3 + r_5}{r_5 + r_6}$

$x_{127}: \dfrac{r_3 + r_6}{r_4 + r_5}$

$x_{128}: \dfrac{r_3 + r_6}{r_4 + r_6}$

$x_{129}: \dfrac{r_3 + r_6}{r_5 + r_6}$

$x_{130}: \dfrac{r_4 + r_5}{r_4 + r_6}$

$x_{131}: \dfrac{r_4 + r_5}{r_5 + r_6}$

$x_{132}: \dfrac{r_4 + r_6}{r_5 + r_6}$

E.2.4 Local environment functions

$x_{133}: f_{12}$ $x_{138}: f_{21}$ $x_{143}: f_{31}$ $x_{148}: f_{41}$ $x_{153}: f_{51}$ $x_{158}: f_{61}$

$x_{134}: f_{13}$ $x_{139}: f_{23}$ $x_{144}: f_{32}$ $x_{149}: f_{42}$ $x_{154}: f_{52}$ $x_{159}: f_{62}$

$x_{135}: f_{14}$ $x_{140}: f_{24}$ $x_{145}: f_{34}$ $x_{150}: f_{43}$ $x_{155}: f_{53}$ $x_{160}: f_{63}$

$x_{136}: f_{15}$ $x_{141}: f_{25}$ $x_{146}: f_{35}$ $x_{151}: f_{45}$ $x_{156}: f_{54}$ $x_{161}: f_{64}$

$x_{137}: f_{16}$ $x_{142}: f_{26}$ $x_{147}: f_{36}$ $x_{152}: f_{46}$ $x_{157}: f_{56}$ $x_{162}: f_{65}$

E.2.5 Density of the crystal compound

(This feature was not used in the NEF - ANNs)

$x_{42}: \rho_{compound}$