Supporting Information

Stepwise Evolution of Photocatalytic Spinel-Structured (Co,Cr,Fe,Mn,Ni)$_3$O$_4$ High Entropy Oxides from First-Principles Calculations to Machine Learning
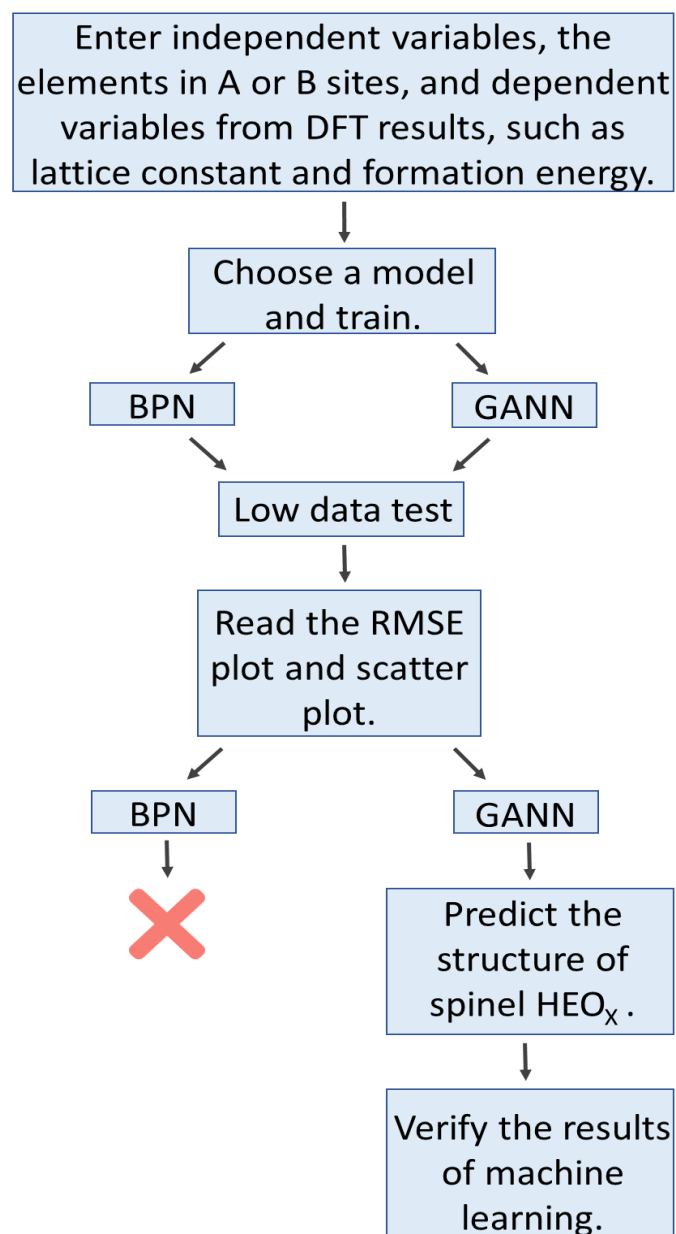
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┌─────────────────────────────────────────┐
│ Enter independent variables, the        │
│ elements in A or B sites, and dependent  │
│ variables from DFT results, such as      │
│ lattice constant and formation energy.   │
└─────────────────────────────────────────┘
                    │
                    ▼
        ┌───────────────────────┐
        │ Choose a model        │
        │ and train.            │
        └───────────────────────┘
          ╱                   ╲
    ┌──────────┐          ┌──────────┐
    │   BPN    │          │  GANN    │
    └──────────┘          └──────────┘
          ╲                   ╱
        ┌───────────────────┐
        │  Low data test    │
        └───────────────────┘
                    │
                    ▼
        ┌───────────────────┐
        │ Read the RMSE     │
        │ plot and scatter  │
        │ plot.             │
        └───────────────────┘
          ╱                   ╲
    ┌──────────┐          ┌──────────┐
    │   BPN    │          │  GANN    │
    └──────────┘          └──────────┘
         │                    │
         ✕                    ▼
                    ┌───────────────────┐
                    │ Predict the       │
                    │ structure of      │
                    │ spinel $HEO_X$.   │
                    └───────────────────┘
                              │
                              ▼
                    ┌───────────────────┐
                    │ Verify the results│
                    │ of machine        │
                    │ learning.         │
                    └───────────────────┘
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Supplementary Figure S1 Workflow of the HEOx investigation.
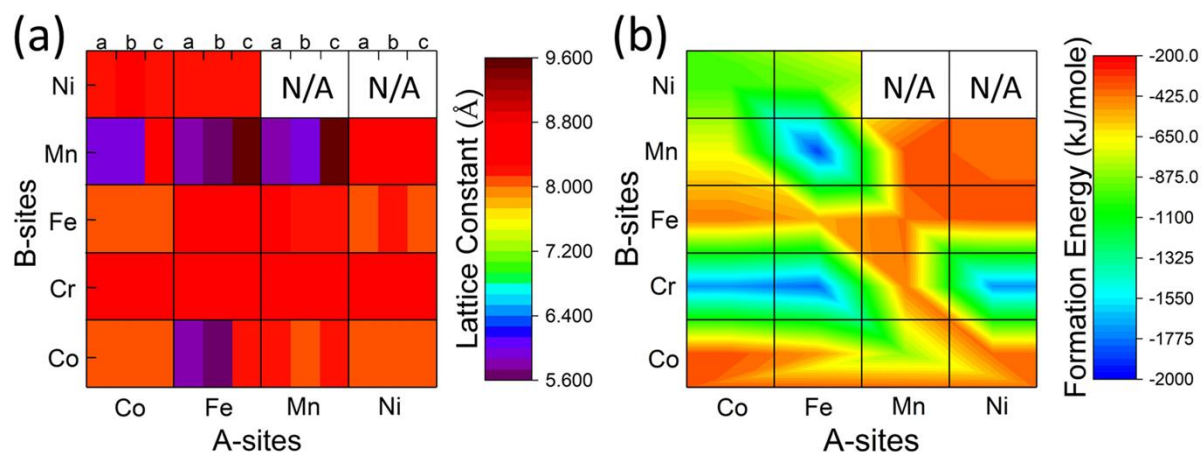
Supplementary Figure S2 Input data of the low data test: (a) lattice constants and (b) formation energies. The metal elements on A and B sites are represented in X-axis and Y-axis, respectively. The a, b, and c in Fig. (a) show the lattice constants of the structures. The color is related to the length and magnitude.
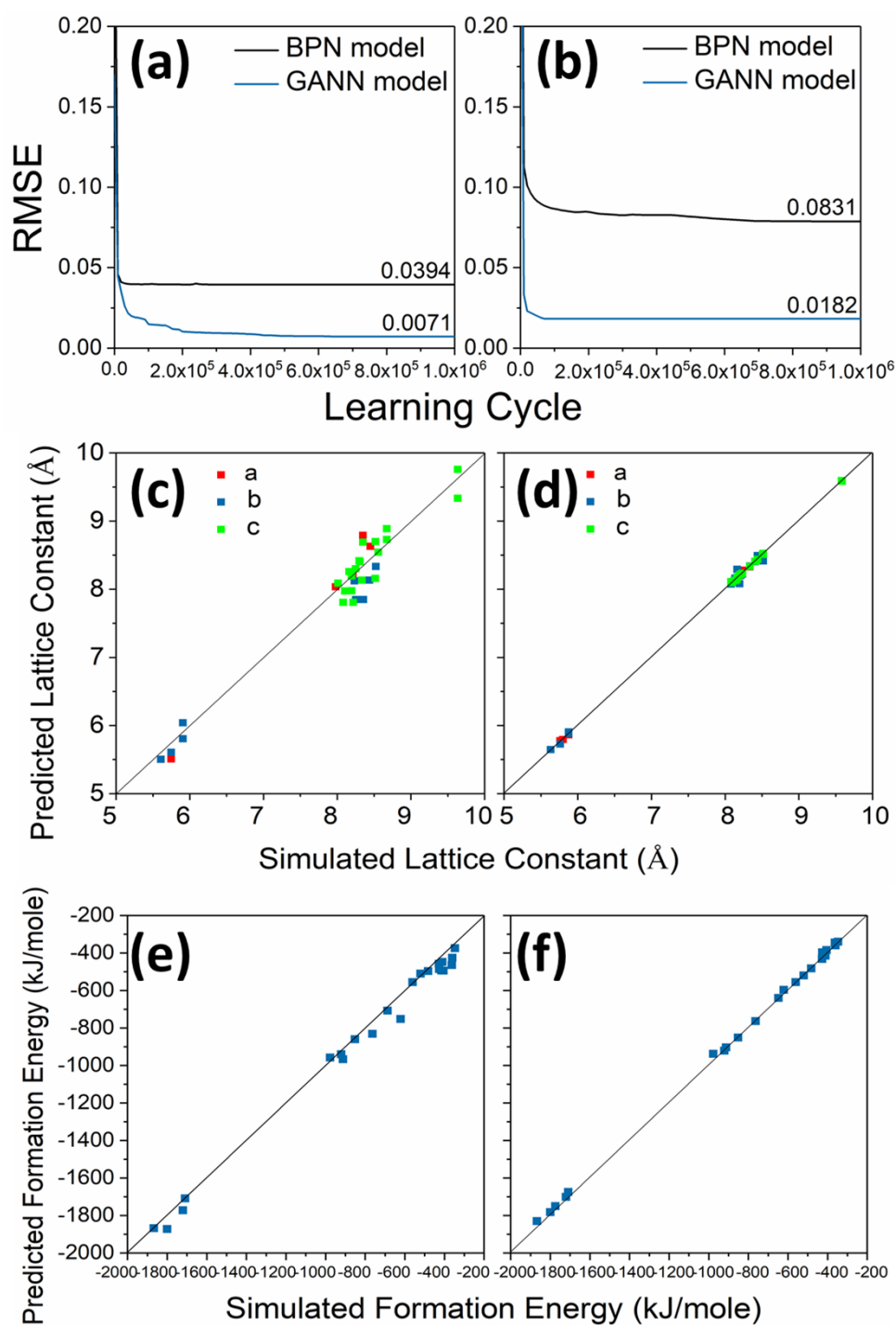
Supplementary Figure S3 Root Mean-Squared Errors of (a) the lattice constants and (b) formation energies. The DFT calculated versus ML predicted lattice constants from the (c) BPN and (d) GANN models, and formation energies from the (e) BPN and (f) GANN models.

Supplementary Table S1 Comparison of the computational results for the AB_2O_4 structures using DFT and ML

Computing method	Composition (Structure)	# of atoms in cell	Computing time (sec)	Results- lattice constant (Å) a/b/c	Results- formation energy (eV/Cell)
DFT	Co_3O_4 (Cubic)	56	1052.093	8.096/8.096/8.096	-1355.020
DFT	$CoCr_2O_4$ (Cubic)	56	751.268	8.408/8.408/8.408	-1751.270
DFT	$CoFe_2O_4$ (Cubic)	56	1163.274	8.121/8.121/8.121	-456.854
DFT	$CoMn_2O_4$ (Tetragonal)	28	851.38	5.876/ 5.876/8.515	-561.145
DFT	$CoNi_2O_4$ (Cubic)	56	994.785	8.163/8.163/8.163	-378.270
DFT	$FeCo_2O_4$ (Orthorhombic)	28	3097.944	5.799/ 5.632/8.160	-471.693
DFT	$FeCr_2O_4$ (Cubic)	56	695.639	8.439/8.439/8.439	-1799.830
DFT	Fe_3O_4 (Cubic)	56	1075.448	8.517/8.517/8.517	-520.681
DFT	$FeMn_2O_4$ (Tetragonal)	28	706.203	5.760/5.760/9.578	-632.056
DFT	$FeNi_2O_4$ (Cubic)	56	1150.191	8.212/8.212/8.212	-362.646
DFT	$MnCo_2O_4$ (Cubic)	56	792.678	8.195/8.195/8.195	-348.549
DFT	$MnCr_2O_4$ (Cubic)	56	935.966	8.507/8.507/8.507	-1867.26
DFT	$MnFe_2O_4$ (Cubic)	56	1031.612	8.234/8.234/8.234	-414.651
DFT	Mn_3O_4 (Tetragonal)	28	1331.249	5.875/5.875/9.580	-687.745
DFT	$NiCo_2O_4$ (Cubic)	56	1128.422	8.080/8.080/8.080	-405.259
DFT	$NiCr_2O_4$ (Cubic)	56	1282.038	8.336/8.336/8.336	-1708.99
DFT	$NiFe_2O_4$ (Cubic)	56	1165.679	8.136/8.136/8.136	-482.344
DFT	$NiMn_2O_4$ (Cubic)	56	755.241	8.335/8.335/8.335	-621.506
ML	Label I: $(Mn_3,Ni_5)(Co_7,Cr_3,Fe_2,Mn_4)O_{32}$ (Cubic)		> 0.1	8.161/8.184/8.136	-849.810
DFT	Label I: $(Mn_3,Ni_5)(Co_7,Cr_3,Fe_2,Mn_4)O_{32}$ (Cubic)	56	24695.295	8.342/8.313/8.317	-851.370
ML	Label II: $Co_8(Cr_4Fe_4Mn_4Ni_4)O_{32}$ (Cubic)		> 0.1	8.304/8.324/8.249	-763.000
DFT	Label II: $Co_8(Cr_4Fe_4Mn_4Ni_4)O_{32}$ (Cubic)	56	24572.371	8.309/8.325/8.249	-762.930
ML	Label III: $Fe_8(Co_4Cr_4Mn_4Ni_4)O_{32}$ (Cubic)		> 0.1	8.331/8.323/8.336	-921.860
DFT	Label III:	56	58048.316	8.363/8.242/8.301	-921.700

	Fe$_8$(Co$_4$Cr$_4$Mn$_4$Ni$_4$)O$_{32}$ (Cubic)				
ML	Label Ⅳ: Mn$_8$(Co$_4$Cr$_4$Fe$_4$Ni$_4$)O$_{32}$ (Cubic)		> 0.1	8.324/8.332/8.314	-978.910
DFT	Label Ⅳ: Mn$_8$(Co$_4$Cr$_4$Fe$_4$Ni$_4$)O$_{32}$ (Cubic)	56	21384.867	8.319/8.315/8.318	-977.020
ML	Co$_{1.0}$(Co$_{0.25}$Cr$_{0.25}$Fe$_{0.25}$Mn$_{0.25}$Ni$_1$)O$_4$ (Cubic Supercell)		> 0.1	8.188/8.166/8.169	-396.112
DFT	Co$_{16}$(Co$_4$Cr$_4$Fe$_4$Mn$_4$Ni$_{16}$)O$_{64}$ (Cubic Supercell)	112	110483.312	8.359/8.330/8.327	-400.279
ML	Ni$_{1.0}$(Co$_{0.25}$Cr$_{0.25}$Fe$_1$Mn$_{0.25}$Ni$_{0.25}$)O$_4$ (Cubic Supercell)		> 0.1	8.194/8.169/8.164	-522.275
DFT	Ni$_{32}$(Co$_8$Cr$_8$Fe$_{32}$Mn$_8$Ni$_8$)O$_{128}$ (Cubic Supercell)	224	253066.344	8.211/8.323/8.335	-527.184

Supplementary Table S2 Reported Major Spinels (AB$_2$O$_4$)[42]

A sites \ B sites	Co	Cr	Fe	Mn	Ni
Co	Co$_3$O$_4$	CoCr$_2$O$_4$	CoFe$_2$O$_4$	CoMn$_2$O$_4$	CoNi$_2$O$_4$
Cr	-	-	-	-	-
Fe	FeCo$_2$O$_4$	FeCr$_2$O$_4$	Fe$_3$O$_4$	FeMn$_2$O$_4$	FeNi$_2$O$_4$
Mn	MnCo$_2$O$_4$	MnCr$_2$O$_4$	MnFe$_2$O$_4$	Mn$_3$O$_4$	-
Ni	NiCo$_2$O$_4$	NiCr$_2$O$_4$	NiFe$_2$O$_4$	NiMn$_2$O$_4$	-

Supplementary Table S3 The HEOx compositions of each condition.

Symbol	Position	Composition
A$_1$	A sites	Co$_x$(Fe,Mn,Ni)$_{1-x}$
A$_2$	A sites	Fe$_x$(Co,Mn,Ni)$_{1-x}$

A₃	A sites	$Mn_x(Co,Fe,Ni)_{1-x}$
A₄	A sites	$Ni_x(Co,Fe,Mn)_{1-x}$
B₁	B sites	$Co_y(Cr,Fe,Mn,Ni)_{1-y}$
B₂	B sites	$Cr_y(Co,Fe,Mn,Ni)_{1-y}$
B₃	B sites	$Fe_y(Co,Cr,Mn,Ni)_{1-y}$
B₄	B sites	$Mn_y(Co,Cr,Fe,Ni)_{1-y}$
B₅	B sites	$Ni_y(Co,Cr,Fe,Mn)_{1-y}$

Supplementary Table S4 HEOx model for prediction and calculation.

Label	Co_A	Cr_A	Fe_A	Mn_A	Ni_A	Co_B	Cr_B	Fe_B	Mn_B	Ni_B
Ⅰ.	0	0	0	3	5	7	3	2	4	0
Ⅱ.	8	0	0	0	0	0	4	4	4	4
Ⅲ.	0	0	8	0	0	4	4	0	4	4
Ⅳ.	0	0	0	8	0	4	4	4	0	4

Supplementary information Structure card for VASP.

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# CRYSTAL DATA
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  _cell_angle_beta               90.000000
  _cell_angle_gamma              90.000000
  _cell_volume                   541.441554 'F d
  _space_group_name_H-M_alt      -3 m' 227
  _space_group_IT_number

  loop_
  _space_group_symop_operation_xyz
'x, y, z'
'-x, -y+1/2, z+1/2'
'-x+1/2, y+1/2, -z'
'x+1/2, -y, -z+1/2'
'z, x, y'
'z+1/2, -x, -y+1/2'
'-z, -x+1/2, y+1/2'
'-z+1/2, x+1/2, -y'
'y, z, x'
'-y+1/2, z+1/2, -x'
'y+1/2, -z, -x+1/2'
'-y, -z+1/2, x+1/2' 'y+3/4, x+1/4, -
z+3/4'
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'y, x, z'
'-y, x+1/2, -z+1/2'
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x, -z'
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9

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z'
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'y, -z+1/2, -x+1/2'

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'-z, -y+1/2, x+1/2'
'-z+1/2, y, -x+1/2'
'z, -y, -x' 'z+1/2, y+1/2, x'

loop_
_atom_site_label
_atom_site_occupancy
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
_atom_site_adp_type
_atom_site_B_iso_or_equiv
_atom_site_type_symbol

Co1	1.0	0.125000	0.125000	0.625000	Biso	1.000000	Co
Co2	1.0	0.375000	0.875000	0.125000	Biso	1.000000	Co
Co3	1.0	0.375000	0.125000	0.875000	Biso	1.000000	Co
Co4	1.0	0.125000	0.875000	0.375000	Biso	1.000000	Co
Co5	1.0	0.125000	0.375000	0.875000	Biso	1.000000	Co
Co6	1.0	0.375000	0.625000	0.375000	Biso	1.000000	Co
Co7	1.0	0.375000	0.375000	0.625000	Biso	1.000000	Co
Co8	1.0	0.125000	0.625000	0.125000	Biso	1.000000	Co
Co9	1.0	0.875000	0.625000	0.875000	Biso	1.000000	Co
Co10	1.0	0.625000	0.625000	0.625000	Biso	1.000000	Co
Co11	1.0	0.875000	0.875000	0.625000	Biso	1.000000	Co

Co12	1.0	0.625000	0.875000	0.875000	Biso	1.000000	Co
Co13	1.0	0.875000	0.125000	0.375000	Biso	1.000000	Co
Co14	1.0	0.625000	0.375000	0.375000	Biso	1.000000	Co
Co15	1.0	0.625000	0.125000	0.125000	Biso	1.000000	Co
Co16	1.0	0.875000	0.375000	0.125000	Biso	1.000000	Co
Co17	1.0	0.000000	0.000000	0.000000	Biso	1.000000	Co
Co18	1.0	0.750000	0.750000	0.250000	Biso	1.000000	Co
Co19	1.0	0.500000	0.000000	0.500000	Biso	1.000000	Co
Co20	1.0	0.000000	0.500000	0.500000	Biso	1.000000	Co
Co21	1.0	0.500000	0.500000	0.000000	Biso	1.000000	Co
Co22	1.0	0.250000	0.250000	0.250000	Biso	1.000000	Co
Co23	1.0	0.250000	0.750000	0.750000	Biso	1.000000	Co
Co24	1.0	0.750000	0.250000	0.750000	Biso	1.000000	Co
O1	1.0	0.111246	0.111246	0.388754	Biso	1.000000	O
O2	1.0	0.138754	0.861246	0.138754	Biso	1.000000	O
O3	1.0	0.388754	0.111246	0.111246	Biso	1.000000	O
O4	1.0	0.361246	0.861246	0.361246	Biso	1.000000	O
O5	1.0	0.111246	0.388754	0.111246	Biso	1.000000	O
O6	1.0	0.138754	0.638754	0.361246	Biso	1.000000	O
O7	1.0	0.388754	0.388754	0.388754	Biso	1.000000	O
O8	1.0	0.361246	0.638754	0.138754	Biso	1.000000	O
O9	1.0	0.888754	0.388754	0.888754	Biso	1.000000	O
O10	1.0	0.638754	0.638754	0.861246	Biso	1.000000	O
O11	1.0	0.888754	0.111246	0.611246	Biso	1.000000	O
O12	1.0	0.638754	0.861246	0.638754	Biso	1.000000	O
O13	1.0	0.611246	0.111246	0.888754	Biso	1.000000	O
O14	1.0	0.861246	0.861246	0.861246	Biso	1.000000	O
O15	1.0	0.611246	0.388754	0.611246	Biso	1.000000	O
O16	1.0	0.861246	0.638754	0.638754	Biso	1.000000	O
O17	1.0	0.611246	0.888754	0.111246	Biso	1.000000	O
O18	1.0	0.861246	0.361246	0.361246	Biso	1.000000	O
O19	1.0	0.888754	0.611246	0.111246	Biso	1.000000	O
O20	1.0	0.638754	0.138754	0.361246	Biso	1.000000	O
O21	1.0	0.888754	0.888754	0.388754	Biso	1.000000	O
O22	1.0	0.638754	0.361246	0.138754	Biso	1.000000	O
O23	1.0	0.611246	0.611246	0.388754	Biso	1.000000	O
O24	1.0	0.861246	0.138754	0.138754	Biso	1.000000	O
O25	1.0	0.388754	0.888754	0.888754	Biso	1.000000	O
O26	1.0	0.138754	0.138754	0.861246	Biso	1.000000	O
O27	1.0	0.388754	0.611246	0.611246	Biso	1.000000	O
O28	1.0	0.138754	0.361246	0.638754	Biso	1.000000	O
O29	1.0	0.111246	0.611246	0.888754	Biso	1.000000	O
O30	1.0	0.361246	0.361246	0.861246	Biso	1.000000	O
O31	1.0	0.111246	0.888754	0.611246	Biso	1.000000	O
O32	1.0	0.361246	0.138754	0.638754	Biso	1.000000	O

```
#========================================================================
# CRYSTAL DATA
#------------------------------------------------------------------------
data_VESTA_phase_1

 _chemical_name_common                'Mn8 Co4 O16                          '
 _cell_length_a                       5.903414
 _cell_length_b                       5.903414
 _cell_length_c                       8.348294
 _cell_angle_alpha                    90.000000
 _cell_angle_beta                     90.000000
 _cell_angle_gamma                    90.000000
 _cell_volume                         290.940558
 _space_group_name_H-M_alt            'I 41/a m d'
 _space_group_IT_number               141

 loop_
 _space_group_symop_operation_xyz
'x, y, z'
'-x+1/2, -y+1/2, z+1/2'
'-y, x+1/2, z+1/4'
'y+1/2, -x, z+3/4'
'-x+1/2, y, -z+3/4'
'x, -y+1/2, -z+1/4' 'y+1/2, x+1/2,
-z+1/2' '-y, -x, -z'
'-x, -y+1/2, -z+1/4'
'x+1/2, y, -z+3/4'
'y, -x, -z'
'-y+1/2, x+1/2, -z+1/2' 'x+1/2, -
y+1/2, z+1/2'
'-x, y, z'
'-y+1/2, -x, z+3/4'
'y, x+1/2, z+1/4' 'x+1/2, y+1/2,
z+1/2' '-x, -y, z'
'-y+1/2, x, z+3/4'
'y, -x+1/2, z+1/4'
'-x, y+1/2, -z+1/4'
'x+1/2, -y, -z+3/4'
'y, x, -z'
'-y+1/2, -x+1/2, -z+1/2'
'-x+1/2, -y, -z+3/4'
'x, y+1/2, -z+1/4' 'y+1/2, -x+1/2, -
z+1/2'
'-y, x, -z'
'x, -y, z'
'-x+1/2, y+1/2, z+1/2' '-y, -
x+1/2, z+1/4'
'y+1/2, x, z+3/4'

loop_
_atom_site_label
_atom_site_occupancy
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
```

_atom_site_adp_type
_atom_site_B_iso_or_equiv
_atom_site_type_symbol

Mn1	1.0	0.250000	0.500000	0.875000	Biso	1.000000	M
Mn2	1.0	0.750000	0.500000	0.875000	Biso	1.000000	M
Mn3	1.0	0.000000	0.250000	0.625000	Biso	1.000000	M
Mn4	1.0	0.000000	0.750000	0.625000	Biso	1.000000	M
Mn5	1.0	0.750000	0.000000	0.375000	Biso	1.000000	M
Mn6	1.0	0.250000	0.000000	0.375000	Biso	1.000000	M
Mn7	1.0	0.500000	0.750000	0.125000	Biso	1.000000	M
Mn8	1.0	0.500000	0.250000	0.125000	Biso	1.000000	M
Co1	1.0	0.500000	0.000000	0.750000	Biso	1.000000	Co
Co2	1.0	0.000000	0.000000	0.000000	Biso	1.000000	Co
Co3	1.0	0.000000	0.500000	0.250000	Biso	1.000000	Co
Co4	1.0	0.500000	0.500000	0.500000	Biso	1.000000	Co
O1	1.0	0.234984	0.500000	0.634084	Biso	1.000000	O
O2	1.0	0.765016	0.500000	0.634084	Biso	1.000000	O
O3	1.0	0.234984	0.000000	0.615916	Biso	1.000000	O
O4	1.0	0.765016	0.000000	0.615916	Biso	1.000000	O
O5	1.0	0.000000	0.265016	0.865916	Biso	1.000000	O
O6	1.0	0.000000	0.734984	0.865916	Biso	1.000000	O
O7	1.0	0.500000	0.265016	0.884084	Biso	1.000000	O
O8	1.0	0.500000	0.734984	0.884084	Biso	1.000000	O
O9	1.0	0.734984	0.000000	0.134084	Biso	1.000000	O
O10	1.0	0.265016	0.000000	0.134084	Biso	1.000000	O
O11	1.0	0.734984	0.500000	0.115916	Biso	1.000000	O
O12	1.0	0.265016	0.500000	0.115916	Biso	1.000000	O
O13	1.0	0.500000	0.765016	0.365916	Biso	1.000000	O
O14	1.0	0.500000	0.234984	0.365916	Biso	1.000000	O
O15	1.0	0.000000	0.765016	0.384084	Biso	1.000000	O
O16	1.0	0.000000	0.234984	0.384084	Biso	1.000000	O