

Supplementary Information

High-Throughput Screening of High-Activity Oxygen Carriers for Chemical Looping Argon purification via Machine Learning - Density Functional Theory Method

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Table S1. The U-values for different transition state metal elements in this paper.

Element	Zn	Cd	Fe	Cu	Co	Ni	Mn	Cr	Ti	V
U value	4.7	4.2	3.5	5	3	5.5	5	3.2	3.8	2.1

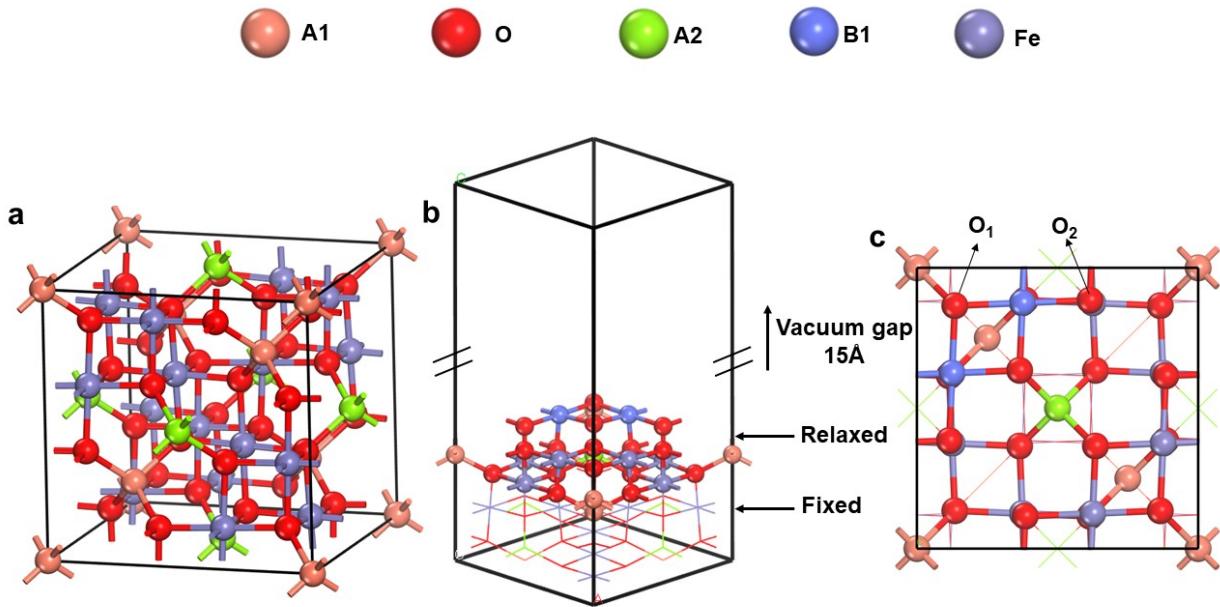


Fig. S1. Crystal structure of $\text{Al}_{1-x}\text{A2}_{1-x}\text{B1}_y\text{Fe}_{2-y}\text{O}_4$ oxygen carrier. (a) perfect bulk structure. (b) the optimized configuration of $\text{Al}_{1-x}\text{A2}_{1-x}\text{B1}_y\text{Fe}_{2-y}\text{O}_4(100)$. (c) top view.

DFT Calculation details

The calculated expression for the formation energy of a crystalline material is shown below:

$$E_f = \frac{E_{\text{Al}_x\text{A2}_{1-x}\text{B1}_y\text{Fe}_{2-y}\text{O}_4} - x * E_{\text{A1}} - (1-x) * E_{\text{A2}} - y * E_{\text{B1}} - (2-y) * E_{\text{B2}} - 4 * E_{\text{O}}}{7} \quad (\text{S1})$$

where $E_{\text{Al}_x\text{A2}_{1-x}\text{B1}_y\text{Fe}_{2-y}\text{O}_4}$ denotes the total energy of the oxygen carrier structure, x, y denotes the mass fractions of the elements A1 and B1, respectively, and $E_{\text{A1}}, E_{\text{A2}}, E_{\text{B1}}, E_{\text{B2}}$, and E_{O} denote the energies of the elemental monomers in the steady state, respectively.

The derivation of Gibbs formation energy(ΔG_f) and its formula are shown below:

$$\Delta G_f(T) = \Delta H_f(298K) + G^\delta(T) - \sum_{i=1}^N a_i G_i(T) \quad (\text{S2})$$

In the above equation S2, $\Delta G_f(T)$ represents the variation of Gibbs formation energy with temperature. $\Delta H_f(298K)$ represents the enthalpy of formation of the oxygen carriers at 298 K,

which can be obtained by simple DFT calculations. N is the number of elements in the oxygen carriers, a_i is the stoichiometric weight of element i, and G_i is the absolute Gibbs energy of element i. $G^\delta(T)$ is the enthalpic contribution to the Gibbs energy.

The derivation of oxygen vacancy formation energy (E_{vac}) and its formula are shown below:

$$E_{vac} = E_{A1_x A2_{1-x} B1_y B2_{2-y} O_4} - E_{defect} - \frac{1}{2} E_{O_2} \quad (S3)$$

In equation S3, $E_{A1_x A2_{1-x} B1_y B2_{2-y} O_4}$ is the surface energy of the intact oxygen-containing oxygen carriers. E_{defect} is the total surface energy of the oxygen carriers containing surface oxygen vacancy. E_{O_2} is the energy of the oxygen molecule.

The adsorption energy (E_{ads}) of $A1_x A2_{1-x} B1_y B2_{2-y} O_4$ with the CO surface can be expressed as:

$$E_{ads} = E_{A1_x A2_{1-x} B1_y B2_{2-y} O_4 + CO} - (E_{A1_x A2_{1-x} B1_y B2_{2-y} O_4} + E_{CO}) \quad (S4)$$

Where $E_{A1_x A2_{1-x} B1_y B2_{2-y} O_4 + CO}$ denotes the total energy of CO adsorbed on the surface of the oxygen carriers, $E_{A1_x A2_{1-x} B1_y B2_{2-y} O_4}$ denotes the surface energy of the oxygen carriers and E_{CO} denotes the energy of the CO molecule.

The reaction pathway for CO oxidation by oxygen carriers includes the initial, transition, and end states. The activation energy of the reaction (E_a) is shown below:

$$E_a = E_{TS} - E_{IS} \quad (S5)$$

Where E_{TS} denotes the energy at the transition state and E_{IS} denotes the initial state energy.

Table S2. Oxygen carrier energy from 756 sets of DFT calculations.

	Oxygen carrier	ΔG	ΔG	ΔG	Ef	Evac
		600K	900K	1200K		
1	Cu0.5Ca0.5Al0.25Fe1.75O4	-2.01	-1.67	-1.33	-1.11	2.57
2	Cu0.5Ca0.5Al0.375Fe1.625O4	-2.03	-1.66	-1.33	-1.16	2.52
3	Cu0.5Ca0.5Al0.5Fe1.5O4	-2.03	-1.65	-1.35	-1.17	2.23
4	Cu0.5Ca0.5Co0.25Fe1.75O4	-2.03	-1.22	-0.93	-0.40	2.50
5	Cu0.5Ca0.5Co0.375Fe1.625O4	-2.03	-1.16	-0.95	-0.40	2.42
6	Cu0.5Ca0.5Co0.5Fe1.5O4	-2.01	-1.17	-0.95	-0.40	2.38
7	Cu0.5Ca0.5V0.25Fe1.75O4	-2.04	-1.51	-1.22	-1.04	2.67
8	Cu0.5Ca0.5V0.375Fe1.625O4	-2.05	-1.51	-1.22	-1.04	2.82

9	Cu0.5Ca0.5V0.5Fe1.5O4	-2.02	-1.51	-1.22	-1.13	2.57
10	Cu0.5Mg0.5Al0.25Fe1.75O4	-1.12	-0.96	-0.74	-0.34	1.68
11	Cu0.5Mg0.5Al0.375Fe1.625O4	-1.18	-1.05	-0.78	-0.34	1.45
12	Cu0.5Mg0.5Al0.5Fe1.5O4	-1.36	-1.17	-1.05	-0.52	1.61
13	Cu0.5Mg0.5Co0.25Fe1.75O4	-1.08	-0.91	-0.67	-0.23	2.77
14	Cu0.5Mg0.5Co0.375Fe1.625O4	-1.11	-0.92	-0.67	-0.26	2.66
15	Cu0.5Mg0.5Co0.5Fe1.5O4	-1.13	-0.93	-0.68	-0.27	2.39
16	Cu0.5Mg0.5V0.25Fe1.75O4	-1.07	-0.92	-0.72	-0.36	2.78
17	Cu0.5Mg0.5V0.375Fe1.625O4	-1.08	-0.93	-0.75	-0.36	2.71
18	Cu0.5Mg0.5V0.5Fe1.5O4	-1.11	-0.91	-0.73	-0.41	2.64
19	Cu0.5Zn0.5Al0.25Fe1.75O4	-1.30	-1.06	-0.91	-0.45	2.55
20	Cu0.5Zn0.5Al0.375Fe1.625O4	-1.32	-1.10	-0.90	-0.43	2.36
21	Cu0.5Zn0.5Al0.5Fe1.5O4	-1.35	-1.13	-1.06	-0.52	2.34
22	Cu0.5Zn0.5Co0.25Fe1.75O4	-1.20	-0.99	-0.78	-0.25	2.66
23	Cu0.5Zn0.5Co0.375Fe1.625O4	-1.21	-0.99	-0.80	-0.25	2.59
24	Cu0.5Zn0.5Co0.5Fe1.5O4	-1.24	-1.01	-0.81	-0.26	2.46
25	Cu0.5Zn0.5V0.25Fe1.75O4	-1.22	-1.06	-0.77	-0.40	2.73
26	Cu0.5Zn0.5V0.375Fe1.625O4	-1.25	-1.01	-0.82	-0.43	2.65
27	Cu0.5Zn0.5V0.5Fe1.5O4	-1.27	-1.00	-0.85	-0.48	2.58
28	Cu0.625Ca0.375Al0.25Fe1.75O4	-2.01	-1.41	-1.09	-0.62	2.47
29	Cu0.625Ca0.375Al0.375Fe1.625O4	-2.03	-1.67	-1.34	-1.12	2.36
30	Cu0.625Ca0.375Al0.5Fe1.5O4	-2.02	-1.67	-1.34	-1.12	2.23
31	Cu0.625Ca0.375Co0.25Fe1.75O4	-2.03	-1.20	-0.96	-0.39	2.47
32	Cu0.625Ca0.375Co0.375Fe1.625O4	-2.04	-1.22	-0.96	-0.40	2.49
33	Cu0.625Ca0.375Co0.5Fe1.5O4	-2.02	-1.20	-0.96	-0.40	2.48
34	Cu0.625Ca0.375V0.25Fe1.75O4	-2.01	-1.25	-1.05	-0.54	2.50
35	Cu0.625Ca0.375V0.375Fe1.625O4	-2.03	-1.51	-1.32	-0.99	2.69
36	Cu0.625Ca0.375V0.5Fe1.5O4	-2.03	-1.55	-1.31	-1.06	2.72
37	Cu0.625Mg0.375Al0.25Fe1.75O4	-1.16	-0.98	-0.76	-0.37	1.39
38	Cu0.625Mg0.375Al0.375Fe1.625O4	-1.36	-1.08	-0.93	-0.44	1.43
39	Cu0.625Mg0.375Al0.5Fe1.5O4	-1.40	-1.20	-1.00	-0.60	2.64

40	Cu0.625Mg0.375Co0.25Fe1.75O4	-1.09	-0.93	-0.69	-0.21	2.43
41	Cu0.625Mg0.375Co0.375Fe1.625O4	-1.07	-0.90	-0.69	-0.21	2.47
42	Cu0.625Mg0.375Co0.5Fe1.5O4	-1.06	-0.89	-0.68	-0.20	2.47
43	Cu0.625Mg0.375V0.25Fe1.75O4	-1.11	-0.93	-0.73	-0.23	2.46
44	Cu0.625Mg0.375V0.375Fe1.625O4	-1.11	-0.91	-0.70	-0.23	2.50
45	Cu0.625Mg0.375V0.5Fe1.5O4	-1.07	-0.90	-0.74	-0.28	2.48
46	Cu0.625Zn0.375Al0.25Fe1.75O4	-1.29	-1.08	-0.92	-0.49	2.39
47	Cu0.625Zn0.375Al0.375Fe1.625O4	-1.48	-1.20	-1.14	-0.63	2.28
48	Cu0.625Zn0.375Al0.5Fe1.5O4	-1.51	-1.32	-1.11	-0.65	2.11
49	Cu0.625Zn0.375Co0.25Fe1.75O4	-1.19	-0.99	-0.73	-0.25	2.42
50	Cu0.625Zn0.375Co0.375Fe1.625O4	-1.23	-0.97	-0.74	-0.25	2.42
51	Cu0.625Zn0.375Co0.5Fe1.5O4	-1.25	-0.99	-0.76	-0.25	2.40
52	Cu0.625Zn0.375V0.25Fe1.75O4	-1.20	-1.02	-0.82	-0.35	2.44
53	Cu0.625Zn0.375V0.375Fe1.625O4	-1.31	-1.06	-0.88	-0.34	2.44
54	Cu0.625Zn0.375V0.5Fe1.5O4	-1.30	-1.05	-0.87	-0.34	2.46
55	Cu0.75Ca0.25Al0.25Fe1.75O4	-2.01	-1.38	-1.10	-0.60	2.57
56	Cu0.75Ca0.25Al0.375Fe1.625O4	-1.86	-1.43	-1.10	-0.63	2.41
57	Cu0.75Ca0.25Al0.5Fe1.5O4	-1.73	-1.36	-1.08	-0.66	2.24
58	Cu0.75Ca0.25Co0.25Fe1.75O4	-2.00	-1.28	-1.08	-0.55	2.46
59	Cu0.75Ca0.25Co0.375Fe1.625O4	-2.00	-1.27	-1.08	-0.42	2.46
60	Cu0.75Ca0.25Co0.5Fe1.5O4	-2.00	-1.21	-1.00	-0.42	2.44
61	Cu0.75Ca0.25V0.25Fe1.75O4	-1.99	-1.22	-1.06	-0.54	2.69
62	Cu0.75Ca0.25V0.375Fe1.625O4	-2.01	-1.35	-1.07	-0.60	2.66
63	Cu0.75Ca0.25V0.5Fe1.5O4	-2.02	-1.39	-1.07	-0.61	2.57
64	Cu0.75Mg0.25Al0.25Fe1.75O4	-1.26	-1.09	-0.94	-0.51	1.53
65	Cu0.75Mg0.25Al0.375Fe1.625O4	-1.33	-1.17	-1.01	-0.66	1.56
66	Cu0.75Mg0.25Al0.5Fe1.5O4	-1.45	-1.27	-1.09	-0.65	1.56
67	Cu0.75Mg0.25Co0.25Fe1.75O4	-1.13	-0.94	-0.75	-0.24	2.45
68	Cu0.75Mg0.25Co0.375Fe1.625O4	-1.12	-0.94	-0.72	-0.23	2.37
69	Cu0.75Mg0.25Co0.5Fe1.5O4	-1.12	-0.94	-0.71	-0.23	2.34
70	Cu0.75Mg0.25V0.25Fe1.75O4	-1.18	-0.95	-0.77	-0.30	2.64

71	Cu0.75Mg0.25V0.375Fe1.625O4	-1.17	-1.01	-0.82	-0.34	2.61
72	Cu0.75Mg0.25V0.5Fe1.5O4	-1.24	-1.07	-0.87	-0.32	2.56
73	Cu0.75Zn0.25Al0.25Fe1.75O4	-1.42	-1.17	-1.09	-0.50	2.37
74	Cu0.75Zn0.25Al0.375Fe1.625O4	-1.52	-1.33	-1.11	-0.67	2.41
75	Cu0.75Zn0.25Al0.5Fe1.5O4	-1.55	-1.32	-1.13	-0.66	1.99
76	Cu0.75Zn0.25Co0.25Fe1.75O4	-1.22	-1.00	-0.82	-0.33	2.41
77	Cu0.75Zn0.25Co0.375Fe1.625O4	-1.20	-1.00	-0.81	-0.33	2.33
78	Cu0.75Zn0.25Co0.5Fe1.5O4	-1.25	-1.01	-0.83	-0.32	2.34
79	Cu0.75Zn0.25V0.25Fe1.75O4	-1.30	-1.12	-0.89	-0.36	2.46
80	Cu0.75Zn0.25V0.375Fe1.625O4	-1.32	-1.10	-0.89	-0.36	2.42
81	Cu0.75Zn0.25V0.5Fe1.5O4	-1.32	-1.09	-0.89	-0.35	2.39
82	Cu0.875Ca0.125Al0.25Fe1.75O4	-1.45	-1.31	-1.05	-0.56	2.32
83	Cu0.875Ca0.125Al0.375Fe1.625O4	-1.52	-1.29	-1.07	-0.54	2.34
84	Cu0.875Ca0.125Al0.5Fe1.5O4	-1.50	-1.29	-1.10	-0.69	1.98
85	Cu0.875Ca0.125Co0.25Fe1.75O4	-1.23	-1.06	-0.92	-0.33	2.57
86	Cu0.875Ca0.125Co0.375Fe1.625O4	-1.19	-1.00	-0.83	-0.33	2.51
87	Cu0.875Ca0.125Co0.5Fe1.5O4	-1.19	-0.99	-0.79	-0.32	2.56
88	Cu0.875Ca0.125V0.25Fe1.75O4	-1.33	-1.11	-1.02	-0.49	2.56
89	Cu0.875Ca0.125V0.375Fe1.625O4	-1.45	-1.18	-1.04	-0.55	2.23
90	Cu0.875Ca0.125V0.5Fe1.5O4	-1.41	-1.21	-1.02	-0.50	2.49
91	Cu0.875Mg0.125Al0.25Fe1.75O4	-1.75	-1.36	-1.10	-0.60	1.57
92	Cu0.875Mg0.125Al0.375Fe1.625O4	-1.45	-1.32	-1.05	-0.58	1.54
93	Cu0.875Mg0.125Al0.5Fe1.5O4	-1.48	-1.34	-1.04	-0.60	1.62
94	Cu0.875Mg0.125Co0.25Fe1.75O4	-1.82	-1.28	-1.12	-0.55	2.46
95	Cu0.875Mg0.125Co0.375Fe1.625O4	-1.83	-1.26	-1.14	-0.57	2.45
96	Cu0.875Mg0.125Co0.5Fe1.5O4	-1.83	-1.26	-1.13	-0.56	2.51
97	Cu0.875Mg0.125V0.25Fe1.75O4	-1.87	-1.36	-1.09	-0.59	2.55
98	Cu0.875Mg0.125V0.375Fe1.625O4	-1.87	-1.32	-1.08	-0.58	2.56
99	Cu0.875Mg0.125V0.5Fe1.5O4	-1.84	-1.31	-1.07	-0.58	2.55
100	Cu0.875Zn0.125Al0.25Fe1.75O4	-1.48	-1.31	-1.07	-0.55	2.36
101	Cu0.875Zn0.125Al0.375Fe1.625O4	-1.51	-1.33	-1.10	-0.55	2.37

102	Cu0.875Zn0.125Al0.5Fe1.5O4	-1.52	-1.26	-1.09	-0.69	1.96
103	Cu0.875Zn0.125Co0.25Fe1.75O4	-1.25	-1.07	-0.88	-0.38	2.42
104	Cu0.875Zn0.125Co0.375Fe1.625O4	-1.27	-1.07	-0.89	-0.38	2.43
105	Cu0.875Zn0.125Co0.5Fe1.5O4	-1.24	-1.08	-0.86	-0.37	2.38
106	Cu0.875Zn0.125V0.25Fe1.75O4	-1.40	-1.14	-1.04	-0.51	2.37
107	Cu0.875Zn0.125V0.375Fe1.625O4	-1.37	-1.14	-1.06	-0.51	2.50
108	Cu0.875Zn0.125V0.5Fe1.5O4	-1.39	-1.30	-1.02	-0.51	2.44
109	Co0.625Zn0.375Al0.375Fe1.625O4	-1.00	-0.85	-0.60	-0.18	2.70
110	Co0.625Zn0.375Al0.5Fe1.5O4	-1.05	-0.87	-0.69	-0.25	2.47
111	Co0.75Zn0.25Al0.25Fe1.75O4	-1.09	-0.88	-0.65	-0.10	3.24
112	Co0.75Zn0.25Al0.375Fe1.625O4	-0.93	-0.79	-0.60	-0.18	2.84
113	Co0.625Cd0.375Al0.375Fe1.625O4	-0.99	-0.88	-0.60	-0.15	2.73
114	Co0.625Cd0.375Al0.5Fe1.5O4	-0.89	-0.78	-0.53	-0.13	2.71
115	Co0.75Cd0.25Al0.25Fe1.75O4	-0.97	-0.78	-0.59	-0.16	3.43
116	Co0.75Cd0.25Al0.375Fe1.625O4	-0.99	-0.84	-0.59	-0.07	3.07
117	Co0.5Cd0.5Cr0.25Fe1.75O4	-1.07	-1.00	-0.68	0.10	3.25
118	Co0.5Cd0.5Cr0.375Fe1.625O4	-1.20	-1.09	-0.71	0.06	3.35
119	Co0.5Cd0.5Cr0.5Fe1.5O4	-1.52	-1.30	-0.94	0.08	3.40
120	Co0.75Cd0.25Cr0.25Fe1.75O4	-1.33	-1.11	-0.93	-0.48	3.44
121	Co0.75Cu0.25Al0.5Fe1.5O4	-1.06	-0.88	-0.68	-0.15	2.06
122	Co0.625Cu0.375Al0.5Fe1.5O4	-1.08	-0.90	-0.70	-0.04	2.07
123	Co0.5Cu0.5Al0.5Fe1.5O4	-1.07	-0.87	-0.68	-0.10	2.08
124	Co0.875Cu0.125Al0.5Fe1.5O4	-0.98	-0.79	-0.59	-0.10	2.13
125	Co0.5Cu0.5Cr0.375Fe1.625O4	-0.91	-0.74	-0.51	0.06	2.35
126	Co0.5Cu0.5In0.375Fe1.625O4	-1.48	-1.33	-0.85	-0.01	2.39
127	Co0.625Cu0.375Al0.25Fe1.75O4	-0.86	-0.59	-0.49	-0.01	2.40
128	Co0.5Cu0.5In0.5Fe1.5O4	-0.84	-0.79	-0.51	0.16	2.44
129	Co0.625Cu0.375Al0.375Fe1.625O4	-0.96	-0.82	-0.58	-0.13	2.44
130	Co0.625Cu0.375Cr0.25Fe1.75O4	-0.89	-0.73	-0.52	0.16	2.44
131	Co0.5Cu0.5Al0.25Fe1.75O4	-1.02	-0.86	-0.61	-0.14	2.45
132	Co0.5Cd0.5In0.5Fe1.5O4	-0.95	-0.98	-0.63	0.05	2.45

133	Co0.75Zn0.25Al0.5Fe1.5O4	-1.02	-0.88	-0.67	-0.15	2.48
134	Co0.5Cu0.5Cr0.25Fe1.75O4	-1.02	-0.78	-0.62	-0.03	2.49
135	Co0.5Zn0.5Al0.5Fe1.5O4	-1.18	-0.99	-0.78	-0.29	2.49
136	Co0.5Cu0.5Al0.375Fe1.625O4	-1.02	-0.82	-0.60	-0.10	2.51
137	Co0.625Cu0.375Cr0.5Fe1.5O4	-0.88	-0.71	-0.49	0.05	2.51
138	Co0.5Zn0.5In0.5Fe1.5O4	-0.86	-0.90	-0.59	0.08	2.53
139	Co0.5Cu0.5Cr0.5Fe1.5O4	-0.89	-0.72	-0.48	-0.02	2.54
140	Co0.625Cd0.375In0.5Fe1.5O4	-0.79	-0.87	-0.52	0.18	2.54
141	Co0.5Cd0.5In0.375Fe1.625O4	-0.82	-0.97	-0.52	0.21	2.55
142	Co0.5Cu0.5In0.25Fe1.75O4	-1.62	-1.42	-1.05	-0.56	2.55
143	Co0.5Zn0.5Al0.25Fe1.75O4	-0.90	-0.77	-0.51	-0.12	2.56
144	Co0.75Cu0.25Al0.375Fe1.625O4	-1.14	-0.97	-0.77	-0.13	2.57
145	Co0.875Zn0.125Al0.5Fe1.5O4	-1.02	-0.87	-0.66	-0.18	2.59
146	Co0.625Zn0.375In0.5Fe1.5O4	-0.80	-0.81	-0.48	0.24	2.59
147	Co0.5Cd0.5In0.25Fe1.75O4	-0.83	-0.90	-0.50	0.17	2.59
148	Co0.75Cu0.25Al0.25Fe1.75O4	-0.81	-0.60	-0.52	-0.05	2.59
149	Co0.5Zn0.5In0.375Fe1.625O4	-0.89	-0.88	-0.58	0.08	2.60
150	Co0.625Cu0.375Cr0.375Fe1.625O4	-0.88	-0.69	-0.46	0.08	2.60
151	Co0.625Cu0.375In0.5Fe1.5O4	-0.96	-0.88	-0.54	0.18	2.61
152	Co0.625Cd0.375In0.375Fe1.625O4	-0.81	-0.83	-0.52	0.16	2.62
153	Co0.625Zn0.375In0.375Fe1.625O4	-1.11	-0.96	-0.66	0.13	2.64
154	Co0.5Zn0.5In0.25Fe1.75O4	-1.25	-1.10	-0.90	-0.38	2.64
155	Co0.5Cd0.5Al0.25Fe1.75O4	-1.18	-1.11	-0.83	-0.34	2.64
156	Co0.75Cd0.25In0.5Fe1.5O4	-0.83	-0.77	-0.48	0.16	2.64
157	Co0.5Zn0.5Al0.375Fe1.625O4	-1.02	-0.83	-0.62	-0.21	2.65
158	Co0.5Cd0.5Al0.5Fe1.5O4	-1.31	-1.07	-0.81	-0.33	2.66
159	Co0.75Cu0.25Cr0.375Fe1.625O4	-0.87	-0.69	-0.48	0.07	2.67
160	Co0.875Cu0.125Cr0.375Fe1.625O4	-0.85	-0.67	-0.48	0.03	2.67
161	Co0.75Cd0.25Al0.5Fe1.5O4	-0.96	-0.81	-0.59	-0.14	2.67
162	Co0.75Zn0.25In0.5Fe1.5O4	-0.90	-0.75	-0.47	0.22	2.69
163	Co0.75Cu0.25Cr0.5Fe1.5O4	-0.87	-0.67	-0.48	0.08	2.70

164	Co0.875Cu0.125Cr0.5Fe1.5O4	-0.85	-0.67	-0.47	0.09	2.71
165	Co0.5Cd0.5Al0.375Fe1.625O4	-1.18	-1.01	-0.74	-0.32	2.72
166	Co0.75Cu0.25Cr0.25Fe1.75O4	-0.89	-0.72	-0.51	0.02	2.73
167	Co0.625Zn0.375In0.25Fe1.75O4	-1.47	-1.27	-1.01	-0.46	2.82
168	Co0.625Cd0.375In0.25Fe1.75O4	-1.11	-1.09	-0.73	0.11	2.83
169	Co0.875Cd0.125In0.5Fe1.5O4	-1.11	-1.11	-0.71	0.13	2.85
170	Co0.75Cd0.25In0.375Fe1.625O4	-1.10	-1.09	-0.73	0.12	2.85
171	Co0.625Cu0.375In0.375Fe1.625O4	-1.55	-1.40	-0.96	0.00	2.86
172	Co0.625Zn0.375Al0.25Fe1.75O4	-0.95	-0.79	-0.54	-0.13	2.86
173	Co0.875Zn0.125In0.5Fe1.5O4	-1.16	-1.09	-0.71	0.14	2.89
174	Co0.75Zn0.25In0.375Fe1.625O4	-1.47	-1.27	-0.91	0.05	2.89
175	Co0.875Cd0.125Al0.5Fe1.5O4	-1.00	-0.80	-0.62	-0.24	2.91
176	Co0.875Cu0.125Cr0.25Fe1.75O4	-0.90	-0.73	-0.53	0.02	2.92
177	Co0.75Cu0.25In0.5Fe1.5O4	-1.15	-1.20	-0.79	0.12	2.95
178	Co0.625Cu0.375In0.25Fe1.75O4	-1.57	-1.42	-1.06	-0.55	2.96
179	Co0.75Cd0.25In0.25Fe1.75O4	-1.09	-1.10	-0.69	0.15	2.99
180	Co0.875Cd0.125Cr0.375Fe1.625O4	-0.95	-0.80	-0.61	-0.03	3.01
181	Co0.875Cu0.125Al0.375Fe1.625O4	-0.82	-0.66	-0.53	0.03	2.62
182	Co0.875Zn0.125Al0.375Fe1.625O4	-0.90	-0.76	-0.55	-0.01	3.03
183	Co0.875Cd0.125Cr0.5Fe1.5O4	-0.91	-0.75	-0.56	-0.02	3.03
184	Co0.875Cu0.125In0.5Fe1.5O4	-1.16	-1.22	-0.77	0.11	3.04
185	Co0.75Zn0.25Cr0.25Fe1.75O4	-0.86	-0.67	-0.48	0.02	3.07
186	Co0.75Cu0.25In0.375Fe1.625O4	-1.56	-1.43	-0.97	0.04	3.08
187	Co0.625Cd0.375Al0.25Fe1.75O4	-1.46	-1.21	-0.98	-0.46	3.09
188	Co0.875Zn0.125Cr0.5Fe1.5O4	-0.84	-0.66	-0.44	0.07	3.14
189	Co0.875Cd0.125Al0.375Fe1.625O4	-1.10	-0.99	-0.67	-0.07	3.14
190	Co0.625Zn0.375Cr0.375Fe1.625O4	-0.84	-0.67	-0.47	-0.02	3.16
191	Co0.875Zn0.125Cr0.375Fe1.625O4	-0.85	-0.67	-0.47	0.06	3.18
192	Co0.875Cu0.125Al0.25Fe1.75O4	-0.82	-0.62	-0.51	-0.01	2.20
193	Co0.875Cd0.125In0.375Fe1.625O4	-1.10	-1.14	-0.70	0.14	3.22
194	Co0.75Zn0.25In0.25Fe1.75O4	-1.41	-1.21	-0.99	-0.48	3.25

195	Co0.5Zn0.5Cr0.5Fe1.5O4	-1.03	-0.80	-0.51	-0.08	3.27
196	Co0.875Cd0.125Cr0.25Fe1.75O4	-0.95	-0.80	-0.61	-0.04	3.28
197	Co0.875Zn0.125In0.375Fe1.625O4	-1.42	-1.25	-0.88	0.05	3.30
198	Co0.75Cd0.25Cr0.375Fe1.625O4	-1.32	-1.10	-0.90	-0.46	3.30
199	Co0.875Zn0.125Al0.25Fe1.75O4	-0.82	-0.67	-0.50	-0.03	3.31
200	Co0.875Zn0.125Cr0.25Fe1.75O4	-0.86	-0.70	-0.49	0.04	3.32
201	Co0.625Cd0.375Cr0.25Fe1.75O4	-1.32	-1.10	-0.84	0.10	3.33
202	Co0.75Cd0.25Cr0.5Fe1.5O4	-1.34	-1.11	-0.97	-0.35	3.34
203	Co0.625Cd0.375Cr0.5Fe1.5O4	-1.33	-1.13	-0.91	-0.36	3.34
204	Co0.875Cd0.125In0.25Fe1.75O4	-1.42	-1.19	-0.91	0.04	3.34
205	Co0.75Cu0.25In0.25Fe1.75O4	-1.54	-1.32	-1.09	-0.49	3.36
206	Co0.875Zn0.125In0.25Fe1.75O4	-1.41	-1.15	-0.97	-0.50	3.37
207	Co0.5Zn0.5Cr0.375Fe1.625O4	-1.06	-0.96	-0.64	-0.12	3.41
208	Co0.625Zn0.375Cr0.5Fe1.5O4	-0.82	-0.68	-0.42	0.01	3.41
209	Co0.875Cu0.125In0.25Fe1.75O4	-1.53	-1.31	-1.06	-0.49	3.43
210	Co0.75Zn0.25Cr0.5Fe1.5O4	-0.83	-0.67	-0.45	0.07	3.45
211	Co0.75Zn0.25Cr0.375Fe1.625O4	-0.84	-0.67	-0.46	0.02	3.45
212	Co0.875Cu0.125In0.375Fe1.625O4	-1.71	-1.53	-1.11	0.06	3.46
213	Co0.5Zn0.5Cr0.25Fe1.75O4	-1.08	-0.92	-0.64	-0.12	3.52
214	Co0.875Cd0.125Al0.25Fe1.75O4	-0.84	-0.67	-0.47	-0.05	3.92
215	Co0.625Zn0.375Cr0.25Fe1.75O4	-0.90	-0.69	-0.51	-0.10	4.04
216	Co0.625Cd0.375Cr0.375Fe1.625O4	-1.34	-1.12	-0.92	-0.37	4.10
217	Ca0.5Ni0.5Cr0.375Fe1.625O4	-1.34	-1.08	-0.72	-0.32	3.13
218	Ca0.5Ni0.5Cr0.5Fe1.5O4	-1.46	-1.07	-0.76	-0.36	2.96
219	Ca0.5Ni0.5Ga0.25Fe1.75O4	-1.13	-1.01	-0.68	-0.24	2.49
220	Ca0.5Ni0.5Ga0.375Fe1.625O4	-1.15	-1.02	-0.72	-0.26	2.53
221	Ca0.5Ni0.5Ga0.5Fe1.5O4	-1.16	-1.05	-0.73	-0.25	2.46
222	Ca0.625Ni0.375Ga0.375Fe1.625O4	-1.24	-1.06	-0.69	-0.27	2.31
223	Ca0.625Ni0.375Ga0.5Fe1.5O4	-1.27	-1.09	-0.75	-0.28	2.31
224	Ca0.625Cd0.375Mn0.25Fe1.75O4	-1.62	-1.37	-0.78	-0.32	3.09
225	Ca0.75Ni0.25Ga0.5Fe1.5O4	-1.69	-1.31	-0.94	-0.42	2.02

226	Ca0.875Ni0.125Ga0.5Fe1.5O4	-1.79	-1.67	-1.13	-0.57	2.04
227	Ca0.875Ni0.125Ga0.375Fe1.625O4	-1.82	-1.66	-1.13	-0.58	2.10
228	Ca0.75Ni0.25Ga0.375Fe1.625O4	-1.68	-1.32	-0.94	-0.41	2.12
229	Ca0.875Ni0.125Ga0.25Fe1.75O4	-1.92	-1.87	-1.36	-0.57	2.12
230	Ca0.875Mg0.125Cr0.375Fe1.625O4	-2.08	-1.91	-1.73	-1.27	2.14
231	Ca0.5Mg0.5Cr0.5Fe1.5O4	-2.03	-1.57	-1.22	-1.12	2.15
232	Ca0.625Mg0.375Cr0.5Fe1.5O4	-2.05	-1.89	-1.69	-1.23	2.15
233	Ca0.5Mg0.5Cr0.375Fe1.625O4	-2.04	-1.60	-1.23	-1.08	2.16
234	Ca0.625Mg0.375Cr0.375Fe1.625O4	-2.04	-1.86	-1.69	-1.25	2.16
235	Ca0.75Mg0.25Cr0.375Fe1.625O4	-2.07	-1.91	-1.69	-1.27	2.17
236	Ca0.75Mg0.25Cr0.5Fe1.5O4	-2.04	-1.89	-1.69	-1.23	2.17
237	Ca0.875Cd0.125Cr0.5Fe1.5O4	-1.96	-1.92	-1.41	-0.62	2.17
238	Ca0.875Mg0.125Cr0.5Fe1.5O4	-2.04	-1.89	-1.71	-1.24	2.18
239	Ca0.625Cd0.375Cr0.375Fe1.625O4	-1.67	-1.41	-0.83	-0.34	2.19
240	Ca0.625Cd0.375Cr0.5Fe1.5O4	-1.66	-1.40	-0.82	-0.33	2.19
241	Ca0.75Ni0.25Ga0.25Fe1.75O4	-1.67	-1.30	-0.93	-0.40	2.19
242	Ca0.75Cd0.25Cr0.375Fe1.625O4	-1.61	-1.62	-0.89	-0.44	2.19
243	Ca0.75Cd0.25Cr0.5Fe1.5O4	-1.59	-1.63	-0.87	-0.42	2.20
244	Ca0.875Cd0.125Cr0.375Fe1.625O4	-1.98	-1.96	-1.39	-0.62	2.20
245	Ca0.75Mg0.25Ga0.5Fe1.5O4	-1.95	-1.87	-1.37	-1.27	2.25
246	Ca0.875Mg0.125Ga0.5Fe1.5O4	-1.95	-1.88	-1.36	-0.54	2.26
247	Ca0.625Mg0.375Ga0.5Fe1.5O4	-2.12	-1.83	-1.68	-1.22	2.28
248	Ca0.5Mg0.5Ga0.5Fe1.5O4	-2.05	-1.22	-0.96	-0.44	2.30
249	Ca0.5Cd0.5Cr0.5Fe1.5O4	-1.67	-1.39	-0.85	-0.47	2.32
250	Ca0.875Mg0.125Ga0.375Fe1.625O4	-1.95	-1.88	-1.36	-0.59	2.33
251	Ca0.5Cd0.5Cr0.375Fe1.625O4	-1.69	-1.40	-0.88	-0.44	2.34
252	Ca0.75Cd0.25Ga0.5Fe1.5O4	-1.70	-1.41	-0.86	-0.32	2.36
253	Ca0.875Cd0.125Ga0.5Fe1.5O4	-1.65	-1.63	-0.92	-0.40	2.36
254	Ca0.625Mg0.375Ga0.375Fe1.625O4	-2.09	-1.81	-1.67	-1.22	2.36
255	Ca0.75Mg0.25Ga0.375Fe1.625O4	-2.12	-1.89	-1.69	-1.27	2.36
256	Ca0.875Cd0.125Ga0.375Fe1.625O4	-1.62	-1.64	-0.92	-0.40	2.39

257	Ca0.75Cd0.25Ga0.375Fe1.625O4	-1.70	-1.39	-0.86	-0.33	2.39
258	Ca0.625Cd0.375Ga0.5Fe1.5O4	-1.70	-1.40	-0.89	-0.42	2.41
259	Ca0.5Cd0.5Ga0.5Fe1.5O4	-1.54	-1.21	-0.81	-0.23	2.44
260	Ca0.625Ni0.375Ga0.25Fe1.75O4	-1.44	-1.11	-0.83	-0.39	2.44
261	Ca0.625Mg0.375Ga0.25Fe1.75O4	-2.06	-1.86	-1.70	-1.22	2.45
262	Ca0.5Mg0.5Ga0.25Fe1.75O4	-2.04	-1.24	-0.97	-0.43	2.45
263	Ca0.625Cd0.375Ga0.375Fe1.625O4	-1.70	-1.42	-0.92	-0.42	2.46
264	Ca0.5Mg0.5Ga0.375Fe1.625O4	-2.05	-1.23	-0.97	-0.44	2.46
265	Ca0.75Cd0.25Ga0.25Fe1.75O4	-1.69	-1.39	-0.87	-0.35	2.48
266	Ca0.875Ni0.125Cr0.25Fe1.75O4	-1.89	-1.88	-1.38	-1.22	2.51
267	Ca0.5Cd0.5Ga0.25Fe1.75O4	-1.55	-1.34	-0.86	-0.25	2.55
268	Ca0.5Cd0.5Ga0.375Fe1.625O4	-1.56	-1.22	-0.80	-0.23	2.55
269	Ca0.625Cd0.375Ga0.25Fe1.75O4	-1.71	-1.42	-0.92	-0.41	2.57
270	Ca0.625Mg0.375Cr0.25Fe1.75O4	-2.04	-1.85	-1.67	-1.19	2.58
271	Ca0.875Mg0.125Cr0.25Fe1.75O4	-2.08	-1.91	-1.69	-1.27	2.58
272	Ca0.75Ni0.25Cr0.375Fe1.625O4	-1.80	-1.48	-1.17	-0.36	2.58
273	Ca0.75Mg0.25Cr0.25Fe1.75O4	-2.04	-1.86	-1.70	-1.25	2.59
274	Ca0.75Ni0.25Cr0.25Fe1.75O4	-1.79	-1.45	-1.16	-0.36	2.59
275	Ca0.625Cd0.375Cr0.25Fe1.75O4	-1.68	-1.40	-0.85	-0.34	2.60
276	Ca0.75Ni0.25Cr0.5Fe1.5O4	-1.79	-1.46	-1.18	-0.41	2.60
277	Ca0.5Mg0.5Cr0.25Fe1.75O4	-2.05	-1.56	-1.23	-1.08	2.60
278	Ca0.75Cd0.25Cr0.25Fe1.75O4	-1.60	-1.38	-0.82	-0.41	2.60
279	Ca0.75Mg0.25Ga0.25Fe1.75O4	-2.10	-1.87	-1.70	-1.27	2.62
280	Ca0.875Cd0.125Cr0.25Fe1.75O4	-1.83	-1.66	-1.11	-0.61	2.62
281	Ca0.875Cd0.125Ga0.25Fe1.75O4	-1.80	-1.76	-1.12	-0.57	2.63
282	Ca0.5Cd0.5Cr0.25Fe1.75O4	-1.56	-1.39	-0.90	-0.46	2.63
283	Ca0.625Ni0.375Mn0.375Fe1.625O4	-1.97	-1.24	-0.96	-0.41	2.63
284	Ca0.875Ni0.125Cr0.5Fe1.5O4	-1.97	-1.86	-1.63	-1.22	2.64
285	Ca0.875Ni0.125Cr0.375Fe1.625O4	-2.04	-1.94	-1.69	-1.22	2.64
286	Ca0.875Mg0.125Ga0.25Fe1.75O4	-2.09	-1.96	-1.69	-1.25	2.65
287	Ca0.625Ni0.375Mn0.25Fe1.75O4	-1.92	-1.25	-0.97	-0.40	2.68

288	Ca0.5Cd0.5Mn0.5Fe1.5O4	-1.64	-1.41	-0.89	-0.43	2.86
289	Ca0.5Cd0.5Mn0.375Fe1.625O4	-1.63	-1.37	-0.87	-0.44	2.88
290	Ca0.5Cd0.5Mn0.25Fe1.75O4	-1.64	-1.38	-0.88	-0.45	2.88
291	Ca0.75Ni0.25Mn0.25Fe1.75O4	-1.93	-1.51	-1.17	-0.45	2.88
292	Ca0.625Ni0.375Cr0.25Fe1.75O4	-1.83	-1.22	-0.93	-0.40	3.04
293	Ca0.5Mg0.5Mn0.25Fe1.75O4	-1.94	-1.58	-1.20	-1.02	3.07
294	Ca0.5Mg0.5Mn0.375Fe1.625O4	-1.94	-1.60	-1.23	-1.08	3.07
295	Ca0.5Mg0.5Mn0.5Fe1.5O4	-1.95	-1.62	-1.24	-1.15	3.07
296	Ca0.625Ni0.375Cr0.375Fe1.625O4	-1.74	-1.15	-0.89	-0.37	3.08
297	Ca0.625Mg0.375Mn0.25Fe1.75O4	-1.94	-1.85	-1.68	-1.24	3.08
298	Ca0.625Mg0.375Mn0.375Fe1.625O4	-1.94	-1.85	-1.68	-1.26	3.08
299	Ca0.625Mg0.375Mn0.5Fe1.5O4	-1.94	-1.89	-1.69	-1.26	3.08
300	Ca0.875Mg0.125Mn0.25Fe1.75O4	-1.98	-1.90	-1.67	-1.27	3.08
301	Ca0.875Mg0.125Mn0.375Fe1.625O4	-1.99	-1.90	-1.67	-1.27	3.08
302	Ca0.875Mg0.125Mn0.5Fe1.5O4	-1.99	-1.91	-1.68	-1.27	3.08
303	Ca0.75Mg0.25Mn0.25Fe1.75O4	-1.95	-1.88	-1.68	-1.27	3.09
304	Ca0.75Mg0.25Mn0.375Fe1.625O4	-1.95	-1.86	-1.67	-1.27	3.09
305	Ca0.75Mg0.25Mn0.5Fe1.5O4	-1.96	-1.89	-1.69	-1.27	3.09
306	Ca0.625Cd0.375Mn0.375Fe1.625O4	-1.60	-1.35	-0.81	-0.32	3.09
307	Ca0.625Cd0.375Mn0.5Fe1.5O4	-1.61	-1.64	-0.85	-0.46	3.09
308	Ca0.5Ni0.5Mn0.5Fe1.5O4	-1.61	-1.30	-0.94	-0.36	3.09
309	Ca0.75Cd0.25Mn0.25Fe1.75O4	-1.58	-1.60	-0.88	-0.50	3.10
310	Ca0.75Cd0.25Mn0.375Fe1.625O4	-1.54	-1.58	-0.87	-0.52	3.10
311	Ca0.75Cd0.25Mn0.5Fe1.5O4	-1.54	-1.60	-0.87	-0.52	3.10
312	Ca0.5Ni0.5Mn0.375Fe1.625O4	-1.59	-1.28	-0.93	-0.35	3.10
313	Ca0.875Cd0.125Mn0.5Fe1.5O4	-1.79	-1.66	-1.10	-0.67	3.10
314	Ca0.625Ni0.375Cr0.5Fe1.5O4	-1.88	-1.20	-1.02	-0.38	3.12
315	Ca0.875Cd0.125Mn0.25Fe1.75O4	-1.73	-1.65	-1.11	-0.67	3.12
316	Ca0.875Cd0.125Mn0.375Fe1.625O4	-1.70	-1.63	-1.08	-0.67	3.12
317	Ca0.625Ni0.375Mn0.5Fe1.5O4	-1.95	-1.21	-0.96	-0.40	2.26
318	Ca0.5Ni0.5Mn0.25Fe1.75O4	-1.41	-1.19	-0.83	-0.35	2.28

319	Ca0.875Ni0.125Mn0.25Fe1.75O4	-1.92	-1.93	-1.40	-0.67	2.25
320	Ca0.5Ni0.5Cr0.25Fe1.75O4	-1.48	-1.27	-0.87	-0.29	3.26
321	Ca0.75Ni0.25Mn0.375Fe1.625O4	-1.91	-1.61	-1.17	-0.60	2.32
322	Ca0.875Ni0.125Mn0.375Fe1.625O4	-1.89	-1.93	-1.40	-1.15	2.29
323	Ca0.875Ni0.125Mn0.5Fe1.5O4	-1.91	-1.92	-1.38	-1.27	2.30
324	Ca0.75Ni0.25Mn0.5Fe1.5O4	-1.87	-1.91	-1.39	-0.60	2.24
325	Cd0.5Mg0.5Cr0.25Fe1.75O4	-1.24	-1.12	-0.73	-0.22	2.80
326	Cd0.5Mg0.5Cr0.375Fe1.625O4	-1.24	-1.10	-0.73	-0.26	2.50
327	Cd0.5Mg0.5Cr0.5Fe1.5O4	-1.26	-1.08	-0.75	-0.29	2.50
328	Cd0.625Mg0.375Cr0.25Fe1.75O4	-1.33	-1.15	-0.85	-0.33	2.79
329	Cd0.625Mg0.375Cr0.375Fe1.625O4	-1.33	-1.15	-0.86	-0.32	2.54
330	Cd0.625Mg0.375Cr0.5Fe1.5O4	-1.34	-1.12	-0.85	-0.35	2.52
331	Cd0.75Mg0.25Cr0.25Fe1.75O4	-1.33	-1.06	-0.70	-0.05	2.77
332	Cd0.75Mg0.25Cr0.375Fe1.625O4	-1.30	-1.05	-0.69	-0.05	2.55
333	Cd0.75Mg0.25Cr0.5Fe1.5O4	-1.29	-1.02	-0.68	-0.01	2.54
334	Cd0.5Mg0.5Ga0.25Fe1.75O4	-1.33	-1.15	-0.87	-0.33	2.70
335	Cd0.5Mg0.5Ga0.375Fe1.625O4	-1.30	-1.14	-0.86	-0.33	2.71
336	Cd0.5Mg0.5Ga0.5Fe1.5O4	-1.29	-1.18	-0.86	-0.33	2.62
337	Cd0.625Mg0.375Ga0.25Fe1.75O4	-1.36	-1.16	-0.82	-0.06	2.67
338	Cd0.625Mg0.375Ga0.375Fe1.625O4	-1.33	-1.14	-0.82	-0.05	2.67
339	Cd0.625Mg0.375Ga0.5Fe1.5O4	-1.06	-1.07	-0.75	-0.05	2.59
340	Cd0.75Mg0.25Ga0.25Fe1.75O4	-1.09	-1.10	-0.77	-0.07	2.67
341	Cd0.75Mg0.25Ga0.375Fe1.625O4	-1.09	-1.08	-0.76	-0.07	2.67
342	Cd0.75Mg0.25Ga0.5Fe1.5O4	-1.06	-1.07	-0.75	-0.05	2.59
343	Cd0.5Mg0.5V0.25Fe1.75O4	-1.20	-1.12	-0.74	-0.22	2.84
344	Cd0.5Mg0.5V0.375Fe1.625O4	-1.17	-1.10	-0.74	-0.29	2.82
345	Cd0.5Mg0.5V0.5Fe1.5O4	-1.16	-1.07	-0.74	-0.29	2.66
346	Cd0.625Mg0.375V0.25Fe1.75O4	-1.34	-1.15	-0.88	-0.34	2.82
347	Cd0.625Mg0.375V0.375Fe1.625O4	-1.32	-1.14	-0.86	-0.32	2.76
348	Cd0.625Mg0.375V0.5Fe1.5O4	-1.28	-1.14	-0.84	-0.36	2.64
349	Cd0.75Mg0.25V0.25Fe1.75O4	-1.06	-1.06	-0.75	-0.05	2.83

350	Cd0.75Mg0.25V0.375Fe1.625O4	-1.07	-1.06	-0.73	-0.04	2.76
351	Cd0.75Mg0.25V0.5Fe1.5O4	-1.07	-1.05	-0.75	-0.03	2.63
352	Cd0.5Ca0.5Cr0.25Fe1.75O4	-1.58	-1.39	-0.90	-0.46	2.63
353	Cd0.5Ca0.5Cr0.375Fe1.625O4	-1.69	-1.40	-0.88	-0.44	2.34
354	Cd0.5Ca0.5Cr0.5Fe1.5O4	-1.67	-1.39	-0.85	-0.47	2.32
355	Cd0.625Ca0.375Cr0.25Fe1.75O4	-1.43	-1.09	-0.68	-0.18	2.71
356	Cd0.625Ca0.375Cr0.375Fe1.625O4	-1.53	-1.13	-0.75	-0.18	2.44
357	Cd0.625Ca0.375Cr0.5Fe1.5O4	-1.52	-1.19	-0.76	-0.19	2.32
358	Cd0.75Ca0.25Cr0.25Fe1.75O4	-1.35	-1.04	-0.70	0.04	2.70
359	Cd0.75Ca0.25Cr0.375Fe1.625O4	-1.33	-1.03	-0.70	0.04	2.44
360	Cd0.75Ca0.25Cr0.5Fe1.5O4	-1.31	-1.01	-0.65	-0.03	2.43
361	Cd0.5Ca0.5Ga0.25Fe1.75O4	-1.57	-1.34	-0.86	-0.25	2.55
362	Cd0.5Ca0.5Ga0.375Fe1.625O4	-1.56	-1.22	-0.81	-0.23	2.55
363	Cd0.5Ca0.5Ga0.5Fe1.5O4	-1.54	-1.21	-0.81	-0.23	2.44
364	Cd0.625Ca0.375Ga0.25Fe1.75O4	-1.36	-1.09	-0.76	-0.14	2.59
365	Cd0.625Ca0.375Ga0.375Fe1.625O4	-1.37	-1.08	-0.76	-0.14	2.59
366	Cd0.625Ca0.375Ga0.5Fe1.5O4	-1.37	-1.07	-0.75	-0.14	2.49
367	Cd0.75Ca0.25Ga0.25Fe1.75O4	-1.36	-1.09	-0.76	-0.02	2.59
368	Cd0.75Ca0.25Ga0.375Fe1.625O4	-1.36	-1.09	-0.76	-0.05	2.59
369	Cd0.75Ca0.25Ga0.5Fe1.5O4	-1.36	-1.08	-0.76	-0.07	2.51
370	Cd0.5Ca0.5V0.25Fe1.75O4	-1.68	-1.34	-0.86	-0.45	2.73
371	Cd0.5Ca0.5V0.375Fe1.625O4	-1.69	-1.21	-0.80	-0.41	2.61
372	Cd0.5Ca0.5V0.5Fe1.5O4	-1.69	-1.20	-0.80	-0.42	2.30
373	Cd0.625Ca0.375V0.25Fe1.75O4	-1.46	-1.06	-0.74	-0.15	2.78
374	Cd0.625Ca0.375V0.375Fe1.625O4	-1.55	-1.19	-0.77	-0.14	2.66
375	Cd0.625Ca0.375V0.5Fe1.5O4	-1.50	-1.18	-0.76	-0.14	2.33
376	Cd0.75Ca0.25V0.25Fe1.75O4	-1.35	-1.05	-0.70	0.04	2.77
377	Cd0.75Ca0.25V0.375Fe1.625O4	-1.36	-1.05	-0.71	-0.08	2.66
378	Cd0.75Ca0.25V0.5Fe1.5O4	-1.32	-1.03	-0.70	-0.14	2.43
379	Cd0.5Cu0.5Cr0.25Fe1.75O4	-0.79	-0.78	-0.52	0.17	2.63
380	Cd0.5Cu0.5Cr0.375Fe1.625O4	-0.88	-0.74	-0.48	0.09	2.56

381	Cd0.5Cu0.5Cr0.5Fe1.5O4	-0.89	-0.79	-0.50	0.07	2.43
382	Cd0.625Cu0.375Cr0.25Fe1.75O4	-0.81	-0.76	-0.47	0.14	2.64
383	Cd0.625Cu0.375Cr0.375Fe1.625O4	-0.80	-0.75	-0.47	0.13	2.64
384	Cd0.625Cu0.375Cr0.5Fe1.5O4	-0.81	-0.74	-0.51	0.06	2.69
385	Cd0.75Cu0.25Cr0.25Fe1.75O4	-0.80	-0.81	-0.49	0.14	2.58
386	Cd0.75Cu0.25Cr0.375Fe1.625O4	-0.90	-0.84	-0.48	0.10	2.58
387	Cd0.75Cu0.25Cr0.5Fe1.5O4	-0.93	-0.86	-0.59	0.10	2.60
388	Cd0.5Cu0.5Ga0.25Fe1.75O4	-0.79	-0.78	-0.51	0.18	2.49
389	Cd0.5Cu0.5Ga0.375Fe1.625O4	-0.84	-0.79	-0.52	0.16	2.52
390	Cd0.5Cu0.5Ga0.5Fe1.5O4	-0.84	-0.78	-0.52	0.16	2.43
391	Cd0.625Cu0.375Ga0.25Fe1.75O4	-0.81	-0.81	-0.49	0.13	2.43
392	Cd0.625Cu0.375Ga0.375Fe1.625O4	-0.85	-0.79	-0.49	0.13	2.42
393	Cd0.625Cu0.375Ga0.5Fe1.5O4	-0.85	-0.80	-0.48	0.10	2.49
394	Cd0.75Cu0.25Ga0.25Fe1.75O4	-0.83	-0.80	-0.52	0.01	2.42
395	Cd0.75Cu0.25Ga0.375Fe1.625O4	-0.83	-0.81	-0.52	0.01	2.42
396	Cd0.75Cu0.25Ga0.5Fe1.5O4	-0.82	-0.81	-0.53	0.01	2.43
397	Cd0.5Cu0.5V0.25Fe1.75O4	-0.80	-0.76	-0.51	0.15	2.74
398	Cd0.5Cu0.5V0.375Fe1.625O4	-0.80	-0.75	-0.49	0.15	2.67
399	Cd0.5Cu0.5V0.5Fe1.5O4	-0.79	-0.73	-0.49	0.09	2.59
400	Cd0.625Cu0.375V0.25Fe1.75O4	-0.81	-0.76	-0.46	0.15	2.60
401	Cd0.625Cu0.375V0.375Fe1.625O4	-0.82	-0.76	-0.46	0.14	2.59
402	Cd0.625Cu0.375V0.5Fe1.5O4	-0.90	-0.81	-0.56	0.09	2.61
403	Cd0.75Cu0.25V0.25Fe1.75O4	-0.80	-0.77	-0.47	0.10	2.54
404	Cd0.75Cu0.25V0.375Fe1.625O4	-0.92	-0.82	-0.58	0.06	2.58
405	Cd0.75Cu0.25V0.5Fe1.5O4	-0.91	-0.82	-0.57	0.09	2.59
406	Cd0.875Mg0.125Cr0.25Fe1.75O4	-1.36	-1.06	-0.73	-0.10	2.68
407	Cd0.875Mg0.125Cr0.375Fe1.625O4	-1.31	-1.05	-0.70	-0.06	2.50
408	Cd0.875Mg0.125Cr0.5Fe1.5O4	-1.30	-1.04	-0.70	-0.06	2.48
409	Cd0.875Mg0.125Ga0.25Fe1.75O4	-1.24	-1.11	-0.78	-0.04	2.67
410	Cd0.875Mg0.125Ga0.375Fe1.625O4	-1.10	-1.09	-0.77	-0.04	2.67
411	Cd0.875Mg0.125Ga0.5Fe1.5O4	-1.08	-1.07	-0.75	-0.04	2.59

412	Cd0.875Mg0.125V0.25Fe1.75O4	-1.21	-1.06	-0.75	-0.09	2.83
413	Cd0.875Mg0.125V0.375Fe1.625O4	-1.07	-1.06	-0.75	-0.06	2.76
414	Cd0.875Mg0.125V0.5Fe1.5O4	-1.07	-1.05	-0.75	-0.04	2.63
415	Cd0.875Cu0.125Cr0.25Fe1.75O4	-1.08	-1.03	-0.69	0.02	2.54
416	Cd0.875Cu0.125Cr0.375Fe1.625O4	-1.02	-0.99	-0.64	0.08	2.54
417	Cd0.875Cu0.125Cr0.5Fe1.5O4	-1.02	-0.94	-0.61	0.07	2.55
418	Cd0.875Cu0.125Ga0.25Fe1.75O4	-0.90	-0.97	-0.66	-0.03	2.42
419	Cd0.875Cu0.125Ga0.375Fe1.625O4	-0.87	-0.97	-0.64	-0.02	2.42
420	Cd0.875Cu0.125Ga0.5Fe1.5O4	-0.86	-0.96	-0.64	-0.02	2.42
421	Cd0.875Cu0.125V0.25Fe1.75O4	-1.02	-1.05	-0.69	-0.01	2.54
422	Cd0.875Cu0.125V0.375Fe1.625O4	-0.95	-1.05	-0.63	0.00	2.55
423	Cd0.875Cu0.125V0.5Fe1.5O4	-0.92	-0.93	-0.63	0.00	2.55
424	Cd0.875Ca0.125Cr0.25Fe1.75O4	-1.35	-1.06	-0.69	-0.08	2.70
425	Cd0.875Ca0.125Cr0.375Fe1.625O4	-1.33	-1.03	-0.69	0.00	2.47
426	Cd0.875Ca0.125Cr0.5Fe1.5O4	-1.31	-1.02	-0.69	0.01	2.46
427	Cd0.875Ca0.125Ga0.25Fe1.75O4	-1.37	-1.09	-0.78	-0.11	2.59
428	Cd0.875Ca0.125Ga0.375Fe1.625O4	-1.37	-1.08	-0.77	-0.13	2.59
429	Cd0.875Ca0.125Ga0.5Fe1.5O4	-1.37	-1.08	-0.76	-0.13	2.51
430	Cd0.875Ca0.125V0.25Fe1.75O4	-1.35	-1.06	-0.71	-0.07	2.74
431	Cd0.875Ca0.125V0.375Fe1.625O4	-1.35	-1.06	-0.71	-0.07	2.64
432	Cd0.875Ca0.125V0.5Fe1.5O4	-1.33	-1.06	-0.70	-0.06	2.58
433	Mg0.625Zn0.375Al0.375Fe1.625O4	-0.99	-0.87	-0.64	-0.24	2.71
434	Mg0.625Zn0.375Al0.5Fe1.5O4	-1.03	-0.88	-0.69	-0.26	2.35
435	Mg0.75Zn0.25Al0.25Fe1.75O4	-0.92	-0.80	-0.53	-0.05	2.75
436	Mg0.75Zn0.25Al0.375Fe1.625O4	-1.04	-0.88	-0.68	-0.15	2.40
437	Mg0.75Zn0.25Al0.5Fe1.5O4	-1.10	-0.94	-0.75	-0.23	2.22
438	Mg0.5Zn0.5Mn0.25Fe1.75O4	-0.92	-0.78	-0.54	-0.13	3.11
439	Mg0.5Zn0.5Mn0.375Fe1.625O4	-1.13	-0.92	-0.64	-0.15	3.11
440	Mg0.5Zn0.5Mn0.5Fe1.5O4	-1.13	-0.97	-0.71	-0.15	3.07
441	Mg0.625Zn0.375Mn0.25Fe1.75O4	-0.92	-0.81	-0.53	-0.13	3.11
442	Mg0.625Zn0.375Mn0.375Fe1.625O4	-0.93	-0.80	-0.53	-0.13	3.07

443	Mg0.625Zn0.375Mn0.5Fe1.5O4	-1.11	-0.95	-0.66	-0.16	3.08
444	Mg0.75Zn0.25Mn0.25Fe1.75O4	-1.01	-0.86	-0.58	-0.14	3.03
445	Mg0.75Zn0.25Mn0.375Fe1.625O4	-1.00	-0.87	-0.59	-0.16	3.02
446	Mg0.75Zn0.25Mn0.5Fe1.5O4	-1.01	-0.88	-0.61	-0.17	3.02
447	Mg0.5Zn0.5In0.25Fe1.75O4	-1.17	-1.01	-0.70	0.11	2.75
448	Mg0.5Zn0.5In0.375Fe1.625O4	-0.87	-0.77	-0.50	0.15	2.75
449	Mg0.5Zn0.5In0.5Fe1.5O4	-0.87	-0.80	-0.54	0.13	2.81
450	Mg0.625Zn0.375In0.25Fe1.75O4	-1.14	-1.01	-0.70	0.16	2.75
451	Mg0.625Zn0.375In0.375Fe1.625O4	-0.84	-0.80	-0.53	0.15	2.75
452	Mg0.625Zn0.375In0.5Fe1.5O4	-0.85	-0.78	-0.52	0.16	2.77
453	Mg0.75Zn0.25In0.25Fe1.75O4	-1.19	-1.05	-0.72	0.17	2.73
454	Mg0.75Zn0.25In0.375Fe1.625O4	-0.80	-0.77	-0.52	0.13	2.68
455	Mg0.75Zn0.25In0.5Fe1.5O4	-0.84	-0.78	-0.52	0.14	2.77
456	Mg0.5Ni0.5Al0.25Fe1.75O4	-1.12	-1.06	-0.64	-0.09	2.75
457	Mg0.5Ni0.5Al0.375Fe1.625O4	-1.13	-1.03	-0.70	-0.15	2.65
458	Mg0.5Ni0.5Al0.5Fe1.5O4	-1.18	-1.08	-0.69	-0.21	2.58
459	Mg0.625Ni0.375Al0.25Fe1.75O4	-1.18	-1.04	-0.60	-0.09	2.65
460	Mg0.625Ni0.375Al0.375Fe1.625O4	-1.15	-1.04	-0.65	-0.15	2.57
461	Mg0.625Ni0.375Al0.5Fe1.5O4	-1.11	-1.01	-0.69	-0.19	1.89
462	Mg0.75Ni0.25Al0.25Fe1.75O4	-1.16	-1.08	-0.60	-0.08	2.54
463	Mg0.75Ni0.25Al0.375Fe1.625O4	-1.13	-1.04	-0.64	-0.16	1.97
464	Mg0.75Ni0.25Al0.5Fe1.5O4	-1.10	-0.92	-0.69	-0.19	1.91
465	Mg0.5Ni0.5Mn0.25Fe1.75O4	-0.91	-0.68	-0.50	-0.04	3.03
466	Mg0.5Ni0.5Mn0.375Fe1.625O4	-0.88	-0.70	-0.49	-0.06	3.03
467	Mg0.5Ni0.5Mn0.5Fe1.5O4	-0.86	-0.68	-0.44	-0.03	3.03
468	Mg0.625Ni0.375Mn0.25Fe1.75O4	-0.86	-0.69	-0.45	0.04	2.66
469	Mg0.625Ni0.375Mn0.375Fe1.625O4	-0.89	-0.69	-0.49	0.03	2.76
470	Mg0.625Ni0.375Mn0.5Fe1.5O4	-0.87	-0.68	-0.46	-0.04	3.08
471	Mg0.75Ni0.25Mn0.25Fe1.75O4	-0.86	-0.66	-0.46	-0.02	2.89
472	Mg0.75Ni0.25Mn0.375Fe1.625O4	-0.88	-0.71	-0.50	-0.02	3.01
473	Mg0.75Ni0.25Mn0.5Fe1.5O4	-1.09	-0.90	-0.65	-0.07	3.12

474	Mg0.5Ni0.5In0.375Fe1.625O4	-0.78	-0.62	-0.37	0.24	2.61
475	Mg0.5Ni0.5In0.5Fe1.5O4	-0.83	-0.67	-0.37	0.22	2.49
476	Mg0.625Ni0.375In0.25Fe1.75O4	-1.25	-1.11	-0.78	0.23	2.55
477	Mg0.625Ni0.375In0.375Fe1.625O4	-0.78	-0.63	-0.35	0.27	2.45
478	Mg0.625Ni0.375In0.5Fe1.5O4	-0.82	-0.63	-0.38	0.26	2.43
479	Mg0.75Ni0.25In0.25Fe1.75O4	-1.14	-0.97	-0.72	0.22	2.31
480	Mg0.75Ni0.25In0.375Fe1.625O4	-0.81	-0.64	-0.34	0.27	2.28
481	Mg0.75Ni0.25In0.5Fe1.5O4	-0.84	-0.64	-0.39	0.22	2.38
482	Mg0.5Co0.5Al0.25Fe1.75O4	-1.02	-0.86	-0.61	-0.14	1.70
483	Mg0.5Co0.5Al0.375Fe1.625O4	-1.02	-0.82	-0.60	-0.10	1.70
484	Mg0.5Co0.5Al0.5Fe1.5O4	-1.07	-0.87	-0.68	-0.10	1.68
485	Mg0.625Co0.375Al0.25Fe1.75O4	-0.95	-0.76	-0.55	-0.10	1.67
486	Mg0.625Co0.375Al0.375Fe1.625O4	-1.03	-0.84	-0.66	-0.12	1.77
487	Mg0.625Co0.375Al0.5Fe1.5O4	-1.09	-0.90	-0.70	-0.20	1.96
488	Mg0.75Co0.25Al0.25Fe1.75O4	-0.95	-0.77	-0.56	-0.09	1.72
489	Mg0.75Co0.25Al0.375Fe1.625O4	-1.03	-0.84	-0.63	-0.15	1.99
490	Mg0.75Co0.25Al0.5Fe1.5O4	-1.14	-0.95	-0.76	-0.29	1.91
491	Mg0.5Co0.5Mn0.25Fe1.75O4	-0.88	-0.70	-0.47	-0.06	3.24
492	Mg0.5Co0.5Mn0.375Fe1.625O4	-0.88	-0.70	-0.48	-0.06	3.53
493	Mg0.5Co0.5Mn0.5Fe1.5O4	-0.88	-0.70	-0.50	-0.07	3.77
494	Mg0.625Co0.375Mn0.25Fe1.75O4	-0.88	-0.71	-0.49	-0.09	3.58
495	Mg0.625Co0.375Mn0.375Fe1.625O4	-0.88	-0.70	-0.49	-0.08	4.12
496	Mg0.625Co0.375Mn0.5Fe1.5O4	-0.92	-0.72	-0.51	-0.09	4.65
497	Mg0.75Co0.25Mn0.25Fe1.75O4	-0.97	-0.71	-0.50	-0.04	3.18
498	Mg0.75Co0.25Mn0.375Fe1.625O4	-0.88	-0.69	-0.48	-0.07	3.21
499	Mg0.75Co0.25Mn0.5Fe1.5O4	-0.89	-0.70	-0.51	-0.08	3.21
500	Mg0.5Co0.5In0.5Fe1.5O4	-0.84	-0.79	-0.51	0.16	2.57
501	Mg0.625Co0.375In0.375Fe1.625O4	-1.09	-0.96	-0.60	0.10	2.68
502	Mg0.625Co0.375In0.5Fe1.5O4	-0.86	-0.78	-0.41	0.19	2.56
503	Mg0.75Co0.25In0.375Fe1.625O4	-0.82	-0.70	-0.36	0.19	2.68
504	Mg0.75Co0.25In0.5Fe1.5O4	-0.84	-0.73	-0.44	0.20	2.67

505	Mg0.875Zn0.125Mn0.25Fe1.75O4	-1.02	-0.87	-0.61	-0.14	3.02
506	Mg0.875Zn0.125Mn0.375Fe1.625O4	-1.01	-0.84	-0.56	-0.14	3.02
507	Mg0.875Zn0.125Mn0.5Fe1.5O4	-0.96	-0.84	-0.57	-0.16	3.00
508	Mg0.875Zn0.125In0.25Fe1.75O4	-1.21	-1.06	-0.70	0.21	2.71
509	Mg0.875Zn0.125In0.375Fe1.625O4	-0.89	-0.78	-0.51	0.14	2.71
510	Mg0.875Zn0.125In0.5Fe1.5O4	-0.89	-0.77	-0.48	0.14	2.67
511	Mg0.875Ni0.125Al0.25Fe1.75O4	-1.24	-1.15	-0.80	-0.08	1.86
512	Mg0.875Ni0.125Al0.375Fe1.625O4	-1.25	-1.18	-0.75	-0.18	1.90
513	Mg0.875Ni0.125Al0.5Fe1.5O4	-1.10	-0.93	-0.71	-0.22	1.84
514	Mg0.875Ni0.125Mn0.25Fe1.75O4	-0.91	-0.75	-0.52	-0.14	2.98
515	Mg0.875Ni0.125Mn0.375Fe1.625O4	-0.96	-0.82	-0.55	-0.10	3.03
516	Mg0.875Ni0.125Mn0.5Fe1.5O4	-0.95	-0.79	-0.55	-0.15	3.09
517	Mg0.875Ni0.125In0.25Fe1.75O4	-1.11	-0.96	-0.69	0.22	2.64
518	Mg0.875Ni0.125In0.375Fe1.625O4	-0.79	-0.65	-0.35	0.26	2.65
519	Mg0.875Ni0.125In0.5Fe1.5O4	-0.85	-0.67	-0.41	0.18	2.59
520	Mg0.875Co0.125Al0.25Fe1.75O4	-0.89	-0.72	-0.57	-0.11	1.50
521	Mg0.875Co0.125Al0.375Fe1.625O4	-1.03	-0.82	-0.64	-0.15	1.64
522	Mg0.875Co0.125Al0.5Fe1.5O4	-1.10	-0.90	-0.72	-0.24	1.68
523	Mg0.875Co0.125Mn0.25Fe1.75O4	-0.89	-0.72	-0.48	-0.03	3.17
524	Mg0.875Co0.125Mn0.375Fe1.625O4	-0.87	-0.71	-0.48	-0.06	3.21
525	Mg0.875Co0.125Mn0.5Fe1.5O4	-0.90	-0.74	-0.51	-0.07	3.34
526	Mg0.875Co0.125In0.25Fe1.75O4	-1.12	-0.95	-0.69	0.22	2.64
527	Mg0.875Co0.125In0.375Fe1.625O4	-0.80	-0.63	-0.34	0.26	2.64
528	Mg0.875Co0.125In0.5Fe1.5O4	-0.87	-0.67	-0.44	0.15	2.64
529	Mg0.5Zn0.5Al0.5Fe1.5O4	-1.23	-0.99	-0.78	-0.24	2.34
530	Mg0.625Co0.375In0.25Fe1.75O4	-1.61	-1.46	-1.08	-0.48	2.58
531	Mg0.5Zn0.5Al0.375Fe1.625O4	-1.03	-0.96	-0.67	-0.22	2.59
532	Mg0.5Co0.5In0.25Fe1.75O4	-1.62	-1.42	-1.05	-0.56	2.59
533	Mg0.5Co0.5In0.375Fe1.625O4	-1.48	-1.33	-0.85	-0.01	2.60
534	Mg0.625Zn0.375Al0.25Fe1.75O4	-0.94	-0.80	-0.58	-0.14	2.62
535	Mg0.5Ni0.5In0.25Fe1.75O4	-1.51	-1.36	-1.06	-0.35	2.64

536	Mg0.5Zn0.5Al0.25Fe1.75O4	-0.88	-0.81	-0.53	-0.14	2.64
537	Mg0.75Co0.25In0.25Fe1.75O4	-1.57	-1.46	-1.08	-0.40	2.80
538	Mg0.875Zn0.125Al0.25Fe1.75O4	-0.92	-0.79	-0.54	-0.10	3.35
539	Mg0.875Zn0.125Al0.375Fe1.625O4	-1.02	-0.86	-0.61	-0.18	3.36
540	Mg0.875Zn0.125Al0.5Fe1.5O4	-1.18	-1.00	-0.79	-0.25	3.44
541	Ni0.5Cd0.5Co0.25Fe1.75O4	-0.90	-0.83	-0.51	0.21	2.73
542	Ni0.5Cd0.5Co0.375Fe1.625O4	-0.85	-0.74	-0.44	0.21	2.57
543	Ni0.5Cd0.5Co0.5Fe1.5O4	-0.81	-0.77	-0.45	0.20	2.59
544	Ni0.5Co0.5Co0.25Fe1.75O4	-0.82	-0.62	-0.39	0.51	2.43
545	Ni0.5Co0.5Co0.375Fe1.625O4	-0.80	-0.54	-0.39	0.52	2.47
546	Ni0.5Co0.5Co0.5Fe1.5O4	-0.77	-0.49	-0.40	0.57	2.45
547	Ni0.5Co0.5Mn0.5Fe1.5O4	-0.89	-0.70	-0.50	0.05	3.35
548	Ni0.625Cd0.375Co0.25Fe1.75O4	-1.46	-1.36	-0.91	0.03	2.74
549	Ni0.625Cd0.375Co0.375Fe1.625O4	-1.51	-1.41	-1.01	0.01	2.52
550	Ni0.625Co0.375Mn0.25Fe1.75O4	-0.87	-0.69	-0.47	0.15	3.03
551	Ni0.75Cd0.25Ga0.5Fe1.5O4	-1.14	-1.04	-0.67	0.14	2.29
552	Ni0.75Co0.25Ga0.375Fe1.625O4	-1.08	-0.95	-0.65	-0.13	2.38
553	Ni0.75Co0.25Ga0.5Fe1.5O4	-1.08	-0.96	-0.66	-0.09	2.36
554	Ni0.875Cd0.125Mn0.375Fe1.625O4	-0.95	-0.78	-0.59	-0.18	3.33
555	Ni0.875Mg0.125Co0.375Fe1.625O4	-1.04	-0.99	-0.63	-0.02	2.27
556	Ni0.875Mg0.125Mn0.375Fe1.625O4	-0.88	-0.73	-0.47	-0.14	3.16
557	Ni0.875Cd0.125Ga0.5Fe1.5O4	-1.13	-0.96	-0.74	-0.27	1.90
558	Ni0.875Co0.125Co0.5Fe1.5O4	-0.84	-0.45	-0.43	0.34	2.00
559	Ni0.625Cd0.375Co0.5Fe1.5O4	-1.63	-1.51	-1.05	0.00	2.03
560	Ni0.875Co0.125Ga0.5Fe1.5O4	-1.04	-1.03	-0.65	-0.07	2.08
561	Ni0.75Cd0.25Co0.5Fe1.5O4	-1.54	-1.35	-1.06	-0.39	2.10
562	Ni0.875Mg0.125Ga0.5Fe1.5O4	-0.96	-0.83	-0.55	-0.07	2.10
563	Ni0.75Cd0.25Co0.375Fe1.625O4	-1.59	-1.44	-1.08	-0.50	2.10
564	Ni0.625Cd0.375Ga0.5Fe1.5O4	-0.80	-0.77	-0.52	0.12	2.11
565	Ni0.625Co0.375Ga0.5Fe1.5O4	-1.08	-0.98	-0.66	-0.11	2.12
566	Ni0.875Cd0.125Co0.25Fe1.75O4	-1.13	-1.20	-0.90	-0.20	2.12

567	Ni0.875Co0.125Mn0.25Fe1.75O4	-0.88	-0.72	-0.49	-0.08	2.12
568	Ni0.875Mg0.125Co0.5Fe1.5O4	-1.24	-1.13	-0.76	-0.11	2.13
569	Ni0.75Cd0.25Ga0.25Fe1.75O4	-1.53	-1.45	-1.11	-0.47	2.13
570	Ni0.75Mg0.25Ga0.25Fe1.75O4	-1.00	-0.80	-0.61	-0.17	2.13
571	Ni0.875Co0.125Ga0.375Fe1.625O4	-1.06	-0.93	-0.65	-0.10	2.13
572	Ni0.875Mg0.125Co0.25Fe1.75O4	-1.07	-0.90	-0.66	-0.14	2.14
573	Ni0.75Cd0.25Ga0.375Fe1.625O4	-1.17	-1.07	-0.78	0.16	2.15
574	Ni0.75Co0.25Mn0.25Fe1.75O4	-0.87	-0.71	-0.49	0.04	2.15
575	Ni0.875Mg0.125Ga0.375Fe1.625O4	-0.99	-0.83	-0.53	-0.05	2.16
576	Ni0.75Cd0.25Co0.25Fe1.75O4	-1.58	-1.48	-1.07	-0.52	2.17
577	Ni0.625Co0.375Ga0.375Fe1.625O4	-1.14	-0.98	-0.66	-0.15	2.17
578	Ni0.75Co0.25Ga0.25Fe1.75O4	-0.98	-0.84	-0.58	-0.03	2.18
579	Ni0.5Cd0.5Ga0.5Fe1.5O4	-0.83	-0.78	-0.52	0.16	2.19
580	Ni0.75Mg0.25Ga0.375Fe1.625O4	-0.89	-0.75	-0.59	-0.14	2.19
581	Ni0.75Mg0.25Ga0.5Fe1.5O4	-0.87	-0.74	-0.59	-0.11	2.20
582	Ni0.875Cd0.125Ga0.375Fe1.625O4	-1.35	-1.01	-0.75	-0.35	2.20
583	Ni0.875Co0.125Co0.25Fe1.75O4	-0.96	-0.74	-0.48	0.26	2.20
584	Ni0.625Mg0.375Co0.5Fe1.5O4	-1.12	-0.97	-0.72	-0.25	2.21
585	Ni0.75Co0.25Co0.25Fe1.75O4	-0.86	-0.61	-0.43	0.38	2.23
586	Ni0.625Co0.375Ga0.25Fe1.75O4	-1.02	-0.87	-0.59	-0.10	2.24
587	Ni0.625Mg0.375Co0.375Fe1.625O4	-1.06	-0.93	-0.71	-0.31	2.25
588	Ni0.5Co0.5Ga0.5Fe1.5O4	-1.09	-1.01	-0.65	-0.15	2.25
589	Ni0.875Cd0.125Co0.375Fe1.625O4	-1.94	-1.76	-1.40	-0.49	2.27
590	Ni0.5Mg0.5Co0.375Fe1.625O4	-1.11	-0.98	-0.70	-0.32	2.28
591	Ni0.5Cd0.5Ga0.375Fe1.625O4	-0.80	-0.78	-0.50	0.18	2.29
592	Ni0.625Cd0.375Ga0.375Fe1.625O4	-0.77	-0.75	-0.45	0.17	2.29
593	Ni0.75Mg0.25Co0.5Fe1.5O4	-1.07	-0.85	-0.69	-0.17	2.30
594	Ni0.5Mg0.5Co0.5Fe1.5O4	-1.11	-0.91	-0.70	-0.37	2.31
595	Ni0.875Co0.125Ga0.25Fe1.75O4	-1.42	-1.34	-1.08	-0.19	2.32
596	Ni0.875Mg0.125Ga0.25Fe1.75O4	-1.03	-0.88	-0.63	-0.05	2.32
597	Ni0.5Co0.5Ga0.375Fe1.625O4	-1.11	-0.95	-0.58	-0.14	2.32

598	Ni0.875Cd0.125Co0.5Fe1.5O4	-1.79	-1.48	-1.23	-0.50	2.33
599	Ni0.625Co0.375Co0.25Fe1.75O4	-0.85	-0.64	-0.50	0.52	2.35
600	Ni0.875Cd0.125Ga0.25Fe1.75O4	-1.57	-1.38	-1.04	-0.42	2.35
601	Ni0.625Co0.375Co0.5Fe1.5O4	-0.82	-0.52	-0.41	0.57	2.36
602	Ni0.75Mg0.25Co0.375Fe1.625O4	-1.05	-0.83	-0.67	-0.15	2.36
603	Ni0.5Cd0.5Ga0.25Fe1.75O4	-0.79	-0.76	-0.45	0.25	2.37
604	Ni0.625Cd0.375Ga0.25Fe1.75O4	-1.08	-0.97	-0.62	0.14	2.37
605	Ni0.75Co0.25Co0.5Fe1.5O4	-0.83	-0.45	-0.44	0.54	2.40
606	Ni0.5Co0.5Ga0.25Fe1.75O4	-1.02	-0.86	-0.59	-0.14	2.44
607	Ni0.875Co0.125Mn0.5Fe1.5O4	-0.85	-0.68	-0.46	0.14	2.46
608	Ni0.5Mg0.5Co0.25Fe1.75O4	-1.14	-1.01	-0.73	-0.32	2.46
609	Ni0.75Mg0.25Co0.25Fe1.75O4	-0.98	-0.80	-0.58	-0.17	2.47
610	Ni0.5Cd0.5Mn0.375Fe1.625O4	-1.13	-1.12	-0.76	0.06	2.51
611	Ni0.5Cd0.5Mn0.25Fe1.75O4	-1.11	-1.09	-0.72	0.08	2.51
612	Ni0.5Cd0.5Mn0.5Fe1.5O4	-1.14	-1.13	-0.85	0.01	2.52
613	Ni0.875Co0.125Co0.375Fe1.625O4	-0.89	-0.53	-0.43	0.29	2.59
614	Ni0.875Co0.125Mn0.375Fe1.625O4	-0.87	-0.70	-0.50	-0.01	2.59
615	Ni0.625Cd0.375Mn0.5Fe1.5O4	-1.37	-1.19	-0.85	0.10	2.62
616	Ni0.625Mg0.375Co0.25Fe1.75O4	-1.03	-0.87	-0.68	-0.32	2.64
617	Ni0.625Cd0.375Mn0.25Fe1.75O4	-1.41	-1.23	-0.86	0.13	2.65
618	Ni0.625Cd0.375Mn0.375Fe1.625O4	-1.37	-1.23	-0.87	0.10	2.65
619	Ni0.75Co0.25Mn0.5Fe1.5O4	-0.86	-0.68	-0.47	0.19	2.67
620	Ni0.75Co0.25Mn0.375Fe1.625O4	-0.87	-0.69	-0.48	0.16	2.68
621	Ni0.75Co0.25Co0.375Fe1.625O4	-0.84	-0.52	-0.41	0.40	2.84
622	Ni0.5Co0.5Mn0.25Fe1.75O4	-0.90	-0.68	-0.48	0.15	2.85
623	Ni0.625Co0.375Mn0.375Fe1.625O4	-0.87	-0.69	-0.48	0.16	2.85
624	Ni0.75Cd0.25Mn0.375Fe1.625O4	-1.34	-1.07	-0.92	-0.46	2.90
625	Ni0.875Mg0.125Mn0.25Fe1.75O4	-0.88	-0.72	-0.46	-0.06	2.94
626	Ni0.625Co0.375Co0.375Fe1.625O4	-0.86	-0.58	-0.41	0.53	2.97
627	Ni0.875Mg0.125Mn0.5Fe1.5O4	-0.87	-0.73	-0.47	-0.14	3.06
628	Ni0.5Co0.5Mn0.375Fe1.625O4	-0.85	-0.68	-0.48	0.15	3.08

629	Ni0.75Cd0.25Mn0.5Fe1.5O4	-1.30	-1.06	-0.88	-0.44	3.08
630	Ni0.875Cd0.125Mn0.5Fe1.5O4	-0.93	-0.77	-0.57	-0.19	3.11
631	Ni0.75Cd0.25Mn0.25Fe1.75O4	-1.37	-1.15	-0.95	-0.45	3.14
632	Ni0.625Co0.375Mn0.5Fe1.5O4	-0.86	-0.67	-0.47	0.17	3.18
633	Ni0.875Cd0.125Mn0.25Fe1.75O4	-0.94	-0.80	-0.59	-0.19	3.54
634	Ni0.5Mg0.5Ga0.25Fe1.75O4	-1.09	-0.92	-0.70	-0.18	2.73
635	Ni0.5Mg0.5Ga0.375Fe1.625O4	-1.08	-0.94	-0.72	-0.31	2.68
636	Ni0.5Mg0.5Ga0.5Fe1.5O4	-1.20	-0.98	-0.78	-0.32	2.50
637	Ni0.5Mg0.5Mn0.25Fe1.75O4	-1.16	-0.97	-0.71	-0.23	3.03
638	Ni0.5Mg0.5Mn0.375Fe1.625O4	-1.15	-0.97	-0.72	-0.23	3.03
639	Ni0.5Mg0.5Mn0.5Fe1.5O4	-1.18	-0.99	-0.74	-0.23	3.03
640	Ni0.625Mg0.375Ga0.25Fe1.75O4	-1.08	-0.87	-0.63	-0.26	2.75
641	Ni0.625Mg0.375Ga0.375Fe1.625O4	-1.12	-0.93	-0.64	-0.24	2.63
642	Ni0.625Mg0.375Ga0.5Fe1.5O4	-1.14	-0.94	-0.69	-0.25	2.55
643	Ni0.625Mg0.375Mn0.25Fe1.75O4	-1.12	-0.95	-0.72	-0.29	3.23
644	Ni0.625Mg0.375Mn0.375Fe1.625O4	-1.13	-0.94	-0.75	-0.32	3.28
645	Ni0.625Mg0.375Mn0.5Fe1.5O4	-1.10	-0.88	-0.71	-0.19	3.21
646	Ni0.75Mg0.25Mn0.25Fe1.75O4	-0.96	-0.80	-0.49	-0.19	3.33
647	Ni0.75Mg0.25Mn0.375Fe1.625O4	-1.10	-0.92	-0.62	-0.23	3.28
648	Ni0.75Mg0.25Mn0.5Fe1.5O4	-1.09	-0.90	-0.63	-0.23	3.30
649	Zn0.5Ca0.5Cr0.375Fe1.625O4	-1.80	-1.15	-0.86	-0.41	2.37
650	Zn0.625Ni0.375Ti0.25Fe1.75O4	-1.11	-0.92	-0.65	-0.15	2.68
651	Zn0.625Co0.375Ti0.375Fe1.625O4	-1.22	-1.05	-0.77	-0.12	2.68
652	Zn0.5Co0.5V0.25Fe1.75O4	-0.93	-0.78	-0.51	-0.11	3.20
653	Zn0.875Ca0.125Ti0.5Fe1.5O4	-1.18	-1.01	-0.79	-0.34	2.79
654	Zn0.875Co0.125Ti0.375Fe1.625O4	-1.17	-1.01	-0.78	-0.21	2.95
655	Zn0.5Ca0.5V0.5Fe1.5O4	-1.80	-1.15	-0.84	-0.38	2.23
656	Zn0.5Ca0.5Cr0.5Fe1.5O4	-1.77	-1.14	-0.83	-0.41	2.28
657	Zn0.625Ca0.375V0.5Fe1.5O4	-1.52	-1.18	-0.84	-0.38	2.39
658	Zn0.625Ca0.375Cr0.5Fe1.5O4	-1.32	-1.09	-0.77	-0.31	2.40
659	Zn0.625Ca0.375Cr0.375Fe1.625O4	-1.32	-1.11	-0.79	-0.31	2.44

660	Zn0.75Ca0.25Cr0.375Fe1.625O4	-1.10	-0.99	-0.71	-0.28	2.54
661	Zn0.75Ca0.25Cr0.5Fe1.5O4	-1.10	-0.97	-0.68	-0.28	2.56
662	Zn0.875Ni0.125V0.375Fe1.625O4	-1.15	-0.98	-0.69	-0.14	2.60
663	Zn0.875Ni0.125V0.5Fe1.5O4	-1.13	-0.98	-0.76	-0.17	2.60
664	Zn0.875Ni0.125V0.25Fe1.75O4	-1.20	-1.01	-0.69	-0.13	2.60
665	Zn0.875Co0.125V0.375Fe1.625O4	-1.16	-0.99	-0.75	-0.17	2.62
666	Zn0.875Co0.125V0.5Fe1.5O4	-1.16	-0.98	-0.75	-0.17	2.62
667	Zn0.75Ca0.25V0.5Fe1.5O4	-1.12	-0.98	-0.70	-0.28	2.62
668	Zn0.75Ni0.25V0.25Fe1.75O4	-1.13	-0.92	-0.67	-0.15	2.63
669	Zn0.75Co0.25V0.25Fe1.75O4	-1.14	-0.99	-0.72	-0.15	2.63
670	Zn0.875Ni0.125Cr0.25Fe1.75O4	-1.18	-1.00	-0.70	-0.12	2.64
671	Zn0.5Ca0.5V0.375Fe1.625O4	-1.80	-1.15	-0.83	-0.39	2.65
672	Zn0.75Co0.25V0.375Fe1.625O4	-1.10	-0.98	-0.69	-0.15	2.65
673	Zn0.75Ni0.25Ti0.375Fe1.625O4	-1.16	-0.98	-0.71	-0.13	2.65
674	Zn0.75Ni0.25Ti0.5Fe1.5O4	-1.17	-1.01	-0.75	-0.17	2.65
675	Zn0.75Co0.25V0.5Fe1.5O4	-1.14	-0.98	-0.74	-0.15	2.66
676	Zn0.75Ni0.25V0.375Fe1.625O4	-1.11	-0.93	-0.66	-0.14	2.66
677	Zn0.875Ca0.125Cr0.375Fe1.625O4	-1.16	-1.00	-0.72	-0.24	2.66
678	Zn0.875Ca0.125Cr0.5Fe1.5O4	-1.15	-0.99	-0.71	-0.22	2.66
679	Zn0.625Ca0.375V0.375Fe1.625O4	-1.24	-1.08	-0.75	-0.30	2.67
680	Zn0.625Ni0.375V0.375Fe1.625O4	-1.15	-0.97	-0.68	-0.15	2.67
681	Zn0.75Ni0.25Ti0.25Fe1.75O4	-1.14	-0.98	-0.71	-0.13	2.67
682	Zn0.625Ni0.375V0.25Fe1.75O4	-0.93	-0.84	-0.56	-0.13	2.67
683	Zn0.875Ni0.125Cr0.375Fe1.625O4	-1.14	-0.97	-0.72	-0.13	2.67
684	Zn0.75Co0.25Cr0.25Fe1.75O4	-1.19	-1.00	-0.71	-0.16	2.68
685	Zn0.75Ni0.25Cr0.25Fe1.75O4	-1.13	-0.92	-0.65	-0.15	2.68
686	Zn0.5Ni0.5Ti0.375Fe1.625O4	-1.18	-0.99	-0.74	-0.19	2.69
687	Zn0.75Ni0.25V0.5Fe1.5O4	-1.12	-0.93	-0.67	-0.15	2.69
688	Zn0.75Co0.25Cr0.5Fe1.5O4	-1.20	-0.98	-0.71	-0.19	2.69
689	Zn0.625Co0.375Ti0.25Fe1.75O4	-1.25	-1.07	-0.77	-0.19	2.69
690	Zn0.5Ni0.5Ti0.25Fe1.75O4	-0.99	-0.87	-0.59	-0.17	2.69

691	Zn0.625Ni0.375V0.5Fe1.5O4	-1.14	-0.98	-0.71	-0.18	2.69
692	Zn0.875Co0.125Cr0.25Fe1.75O4	-1.20	-1.02	-0.70	-0.13	2.70
693	Zn0.625Ni0.375Ti0.375Fe1.625O4	-1.10	-0.92	-0.67	-0.15	2.70
694	Zn0.75Co0.25Cr0.375Fe1.625O4	-1.14	-0.97	-0.75	-0.18	2.70
695	Zn0.625Ni0.375Ti0.5Fe1.5O4	-1.07	-0.89	-0.68	-0.14	2.71
696	Zn0.625Co0.375Ti0.5Fe1.5O4	-1.22	-1.03	-0.80	-0.20	2.71
697	Zn0.875Ni0.125Cr0.5Fe1.5O4	-1.12	-0.92	-0.68	-0.17	2.71
698	Zn0.875Co0.125Cr0.375Fe1.625O4	-1.17	-0.98	-0.70	-0.13	2.71
699	Zn0.875Co0.125Cr0.5Fe1.5O4	-1.11	-0.96	-0.77	-0.19	2.71
700	Zn0.625Ni0.375Cr0.25Fe1.75O4	-0.97	-0.87	-0.56	-0.17	2.72
701	Zn0.75Ni0.25Cr0.375Fe1.625O4	-1.12	-0.92	-0.66	-0.15	2.72
702	Zn0.5Ca0.5Cr0.25Fe1.75O4	-1.78	-1.16	-0.82	-0.38	2.72
703	Zn0.625Ni0.375Cr0.375Fe1.625O4	-1.02	-0.85	-0.61	-0.18	2.72
704	Zn0.875Ca0.125V0.5Fe1.5O4	-1.18	-0.97	-0.73	-0.17	2.73
705	Zn0.5Ni0.5Ti0.5Fe1.5O4	-1.07	-0.93	-0.68	-0.16	2.74
706	Zn0.875Co0.125V0.25Fe1.75O4	-1.19	-1.01	-0.70	-0.13	2.74
707	Zn0.5Ca0.5V0.25Fe1.75O4	-1.80	-1.16	-0.83	-0.39	2.74
708	Zn0.75Ni0.25Cr0.5Fe1.5O4	-1.06	-0.92	-0.66	-0.15	2.75
709	Zn0.5Ca0.5Ti0.5Fe1.5O4	-1.77	-1.13	-0.85	-0.40	2.81
710	Zn0.625Co0.375V0.25Fe1.75O4	-1.05	-0.92	-0.70	-0.16	2.81
711	Zn0.625Ca0.375Cr0.25Fe1.75O4	-1.35	-1.13	-0.79	-0.30	2.82
712	Zn0.5Ca0.5Ti0.375Fe1.625O4	-1.75	-1.15	-0.83	-0.41	2.83
713	Zn0.875Ca0.125V0.375Fe1.625O4	-1.20	-1.00	-0.75	-0.23	2.83
714	Zn0.75Ca0.25Cr0.25Fe1.75O4	-1.11	-1.00	-0.70	-0.25	2.84
715	Zn0.5Ca0.5Ti0.25Fe1.75O4	-1.76	-1.15	-0.83	-0.40	2.84
716	Zn0.75Ca0.25V0.375Fe1.625O4	-1.11	-0.98	-0.68	-0.28	2.85
717	Zn0.5Ni0.5V0.25Fe1.75O4	-0.99	-0.87	-0.61	-0.16	2.86
718	Zn0.5Ni0.5Cr0.5Fe1.5O4	-0.98	-0.87	-0.60	-0.21	2.87
719	Zn0.875Ni0.125Ti0.25Fe1.75O4	-1.19	-1.00	-0.69	-0.15	2.88
720	Zn0.875Ni0.125Ti0.375Fe1.625O4	-1.16	-1.03	-0.75	-0.19	2.88
721	Zn0.875Ca0.125Cr0.25Fe1.75O4	-1.16	-1.00	-0.71	-0.23	2.89

722	Zn0.625Ca0.375Ti0.25Fe1.75O4	-1.32	-1.10	-0.78	-0.33	2.90
723	Zn0.625Ca0.375Ti0.375Fe1.625O4	-1.58	-1.21	-0.86	-0.40	2.90
724	Zn0.625Ca0.375V0.25Fe1.75O4	-1.25	-1.13	-0.78	-0.30	2.90
725	Zn0.75Co0.25Ti0.25Fe1.75O4	-1.19	-1.01	-0.72	-0.15	2.91
726	Zn0.625Ni0.375Cr0.5Fe1.5O4	-1.16	-0.99	-0.71	-0.18	2.91
727	Zn0.5Ni0.5Cr0.375Fe1.625O4	-0.96	-0.84	-0.57	-0.16	2.92
728	Zn0.75Ca0.25V0.25Fe1.75O4	-1.10	-1.00	-0.70	-0.26	2.94
729	Zn0.75Ca0.25Ti0.5Fe1.5O4	-1.20	-1.06	-0.77	-0.34	2.94
730	Zn0.5Co0.5Ti0.25Fe1.75O4	-1.02	-0.93	-0.66	-0.20	2.94
731	Zn0.5Co0.5Ti0.375Fe1.625O4	-1.18	-1.00	-0.72	-0.17	2.94
732	Zn0.625Co0.375V0.375Fe1.625O4	-1.19	-0.98	-0.69	-0.19	2.94
733	Zn0.75Co0.25Ti0.375Fe1.625O4	-1.18	-1.00	-0.76	-0.18	2.94
734	Zn0.625Ca0.375Ti0.5Fe1.5O4	-1.60	-1.17	-0.85	-0.41	2.94
735	Zn0.875Ni0.125Ti0.5Fe1.5O4	-1.16	-0.99	-0.76	-0.20	2.95
736	Zn0.875Co0.125Ti0.5Fe1.5O4	-1.17	-1.01	-0.78	-0.23	2.95
737	Zn0.75Co0.25Ti0.5Fe1.5O4	-1.13	-0.98	-0.74	-0.12	2.96
738	Zn0.875Co0.125Ti0.25Fe1.75O4	-1.17	-1.00	-0.71	-0.16	2.96
739	Zn0.875Ca0.125V0.25Fe1.75O4	-1.18	-1.00	-0.71	-0.25	2.96
740	Zn0.625Co0.375V0.5Fe1.5O4	-1.17	-0.97	-0.67	-0.11	2.97
741	Zn0.5Ni0.5V0.375Fe1.625O4	-0.99	-0.87	-0.57	-0.16	2.98
742	Zn0.75Ca0.25Ti0.375Fe1.625O4	-1.12	-1.01	-0.73	-0.33	2.98
743	Zn0.75Ca0.25Ti0.25Fe1.75O4	-1.11	-1.02	-0.70	-0.32	2.99
744	Zn0.875Ca0.125Ti0.25Fe1.75O4	-1.19	-1.04	-0.76	-0.27	2.99
745	Zn0.875Ca0.125Ti0.375Fe1.625O4	-1.18	-1.02	-0.74	-0.22	2.99
746	Zn0.625Co0.375Cr0.5Fe1.5O4	-1.14	-0.96	-0.70	-0.21	2.99
747	Zn0.625Co0.375Cr0.25Fe1.75O4	-0.96	-0.83	-0.61	-0.17	3.01
748	Zn0.625Co0.375Cr0.375Fe1.625O4	-1.16	-0.96	-0.70	-0.19	3.02
749	Zn0.5Ni0.5V0.5Fe1.5O4	-1.15	-0.94	-0.61	-0.18	3.03
750	Zn0.5Co0.5Ti0.5Fe1.5O4	-1.17	-0.97	-0.71	-0.17	3.04
751	Zn0.5Ni0.5Cr0.25Fe1.75O4	-0.94	-0.82	-0.56	-0.16	3.06
752	Zn0.5Co0.5V0.375Fe1.625O4	-0.94	-0.78	-0.53	-0.04	3.22

753	Zn0.5Co0.5V0.5Fe1.5O4	-1.08	-0.87	-0.62	-0.10	3.25
754	Zn0.5Co0.5Cr0.5Fe1.5O4	-1.03	-0.80	-0.51	-0.08	3.27
755	Zn0.5Co0.5Cr0.375Fe1.625O4	-1.06	-0.96	-0.64	-0.12	3.41
756	Zn0.5Co0.5Cr0.25Fe1.75O4	-1.08	-0.92	-0.64	-0.12	3.52

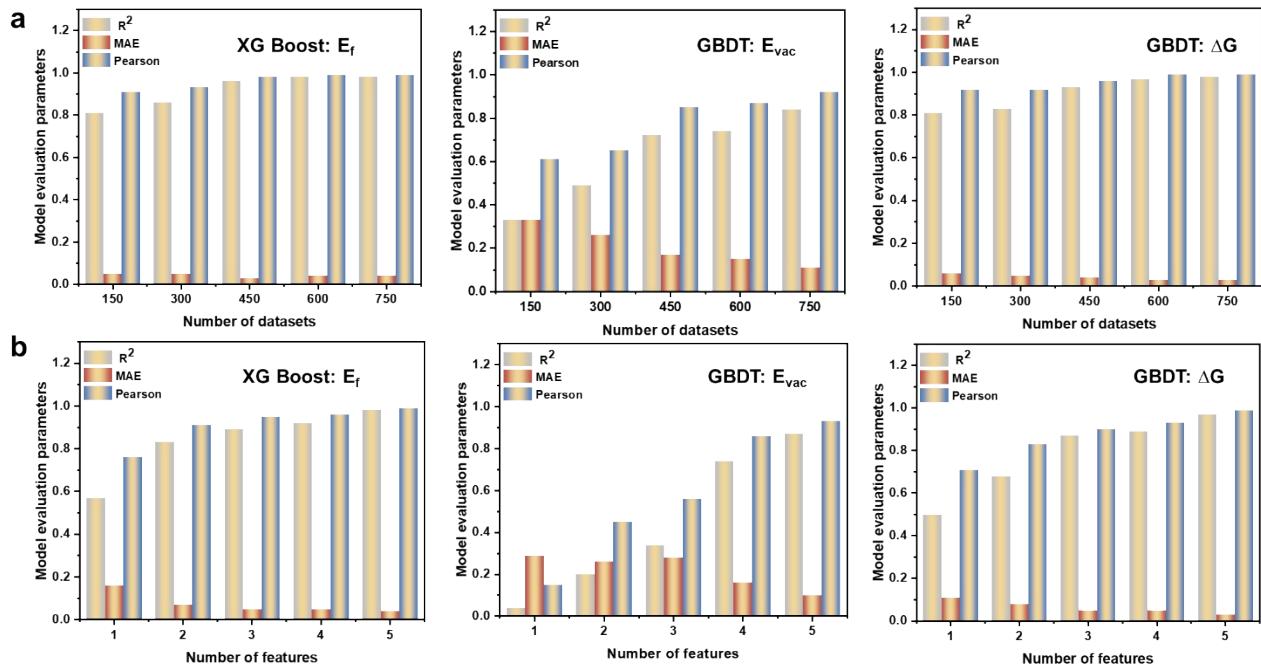


Fig. S2. Effect of data sample size and feature size on model prediction accuracy. (a) Model prediction accuracy for different database sizes (200,350,500,650,800). (b) Model prediction accuracy for different number of feature quantities.

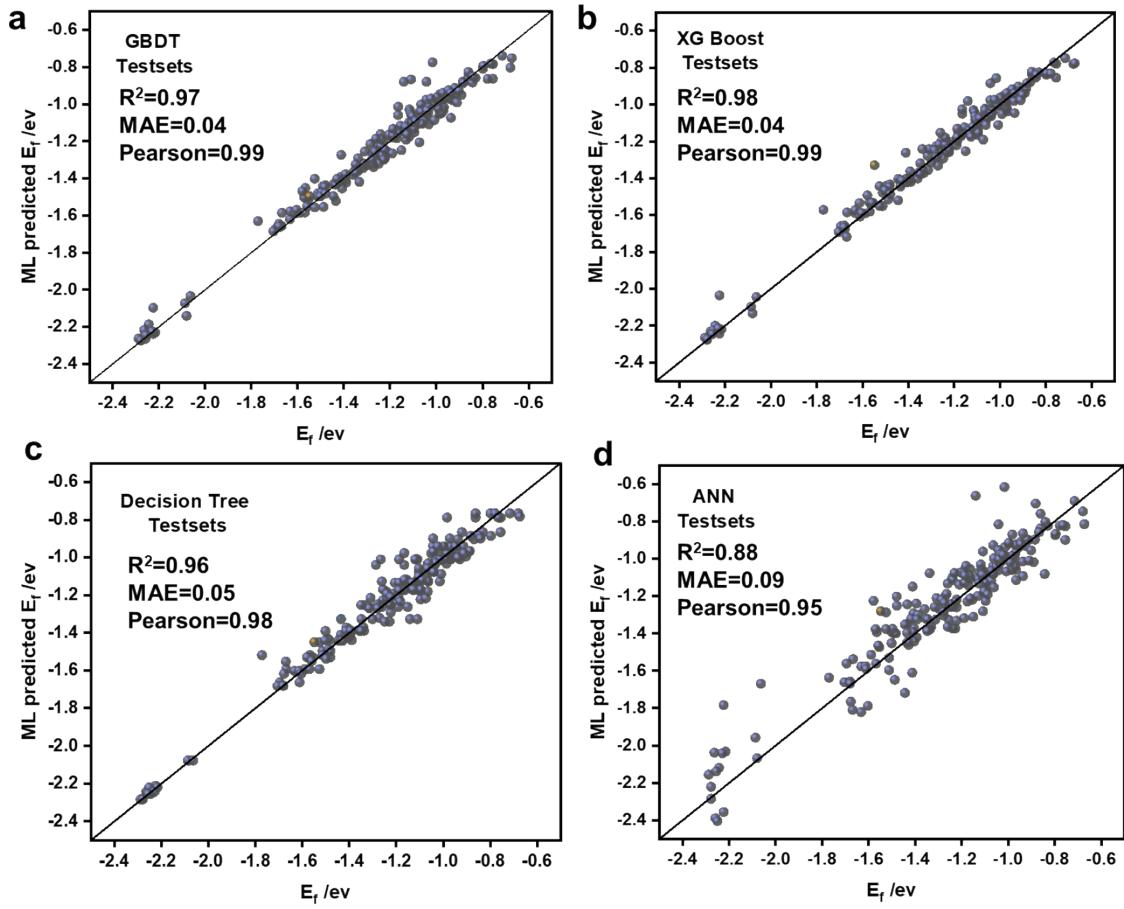


Fig. S3. Comparison of the correlation between the predictions of machine learning models about formation energy and the results of DFT calculations. (a) GBDT model. (b) XG Boost model. (c) Decision tree model. (d) ANN model.

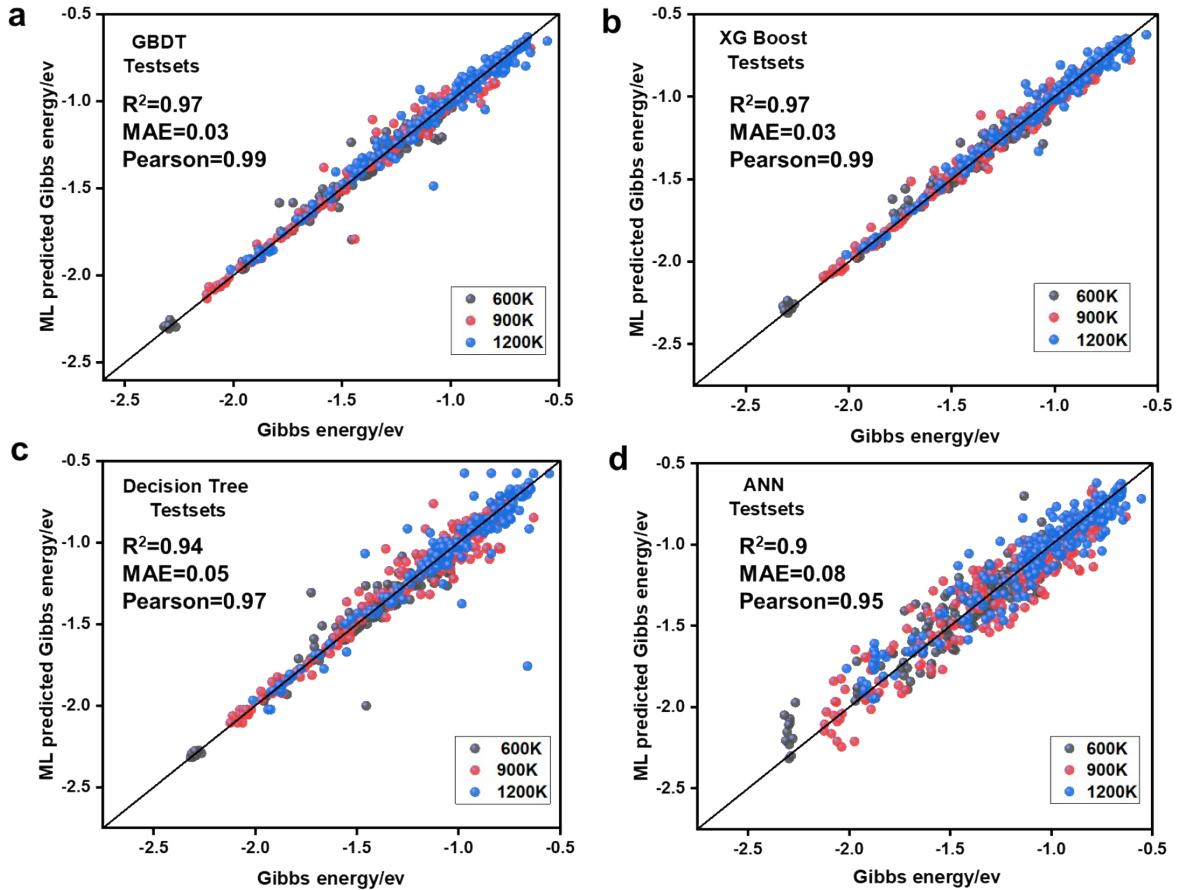


Fig. S4. Comparison of the correlation between the predictions of machine learning models about Gibbs formation energy and the results of DFT calculations. (a) GBDT model. (b) XG Boost model. (c) Decision tree model. (d) ANN model.

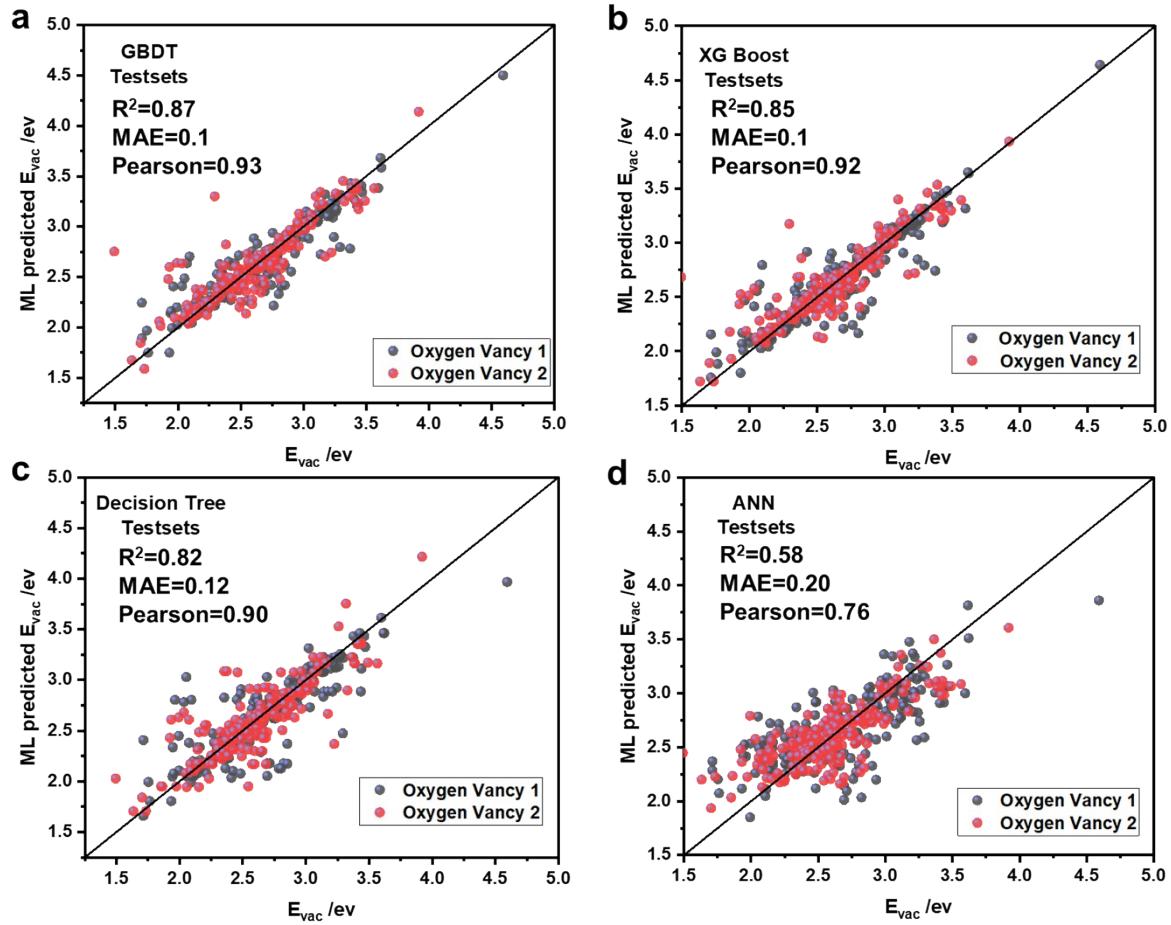


Fig. S5. Comparison of the correlation between the predictions of machine learning models about oxygen vacancy formation energy and the results of DFT calculations. (a) GBDT model. (b) XG Boost model. (c) Decision tree model. (d) ANN model.

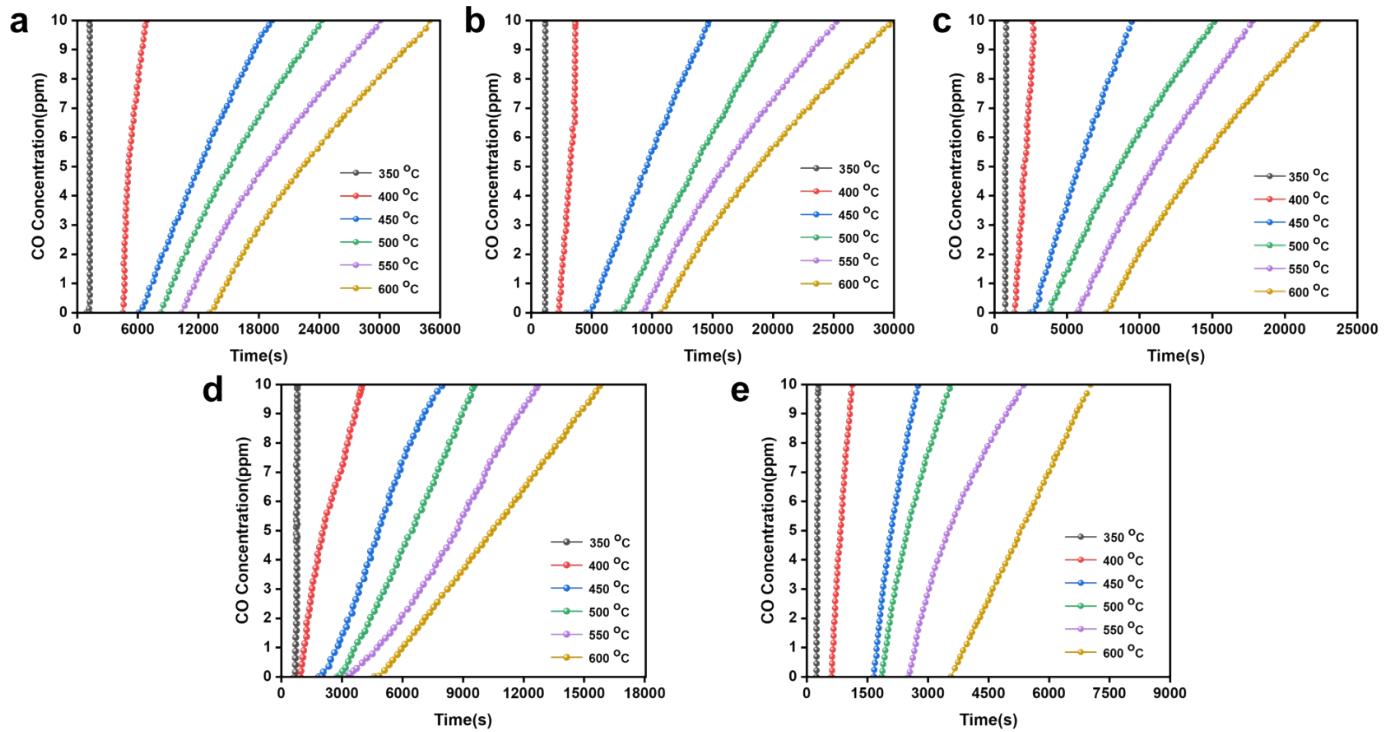


Fig. S6. Effect of removing CO from oxygen carriers at different temperatures. (a) $\text{Cu}_{0.875}\text{Ni}_{0.125}\text{Al}_{0.5}\text{Fe}_{1.5}\text{O}_4$. (b) $\text{Cu}_{0.625}\text{Co}_{0.375}\text{Co}_{0.25}\text{Fe}_{1.75}\text{O}_4$. (c) $\text{Cu}_{0.625}\text{Mg}_{0.375}\text{Al}_{0.25}\text{Fe}_{1.75}\text{O}_4$. (d) $\text{Cu}_{0.875}\text{Ca}_{0.1-25}\text{Mn}_{0.375}\text{Fe}_{1.625}\text{O}_4$. (e) Fe_2O_3 . (100 ppm CO)

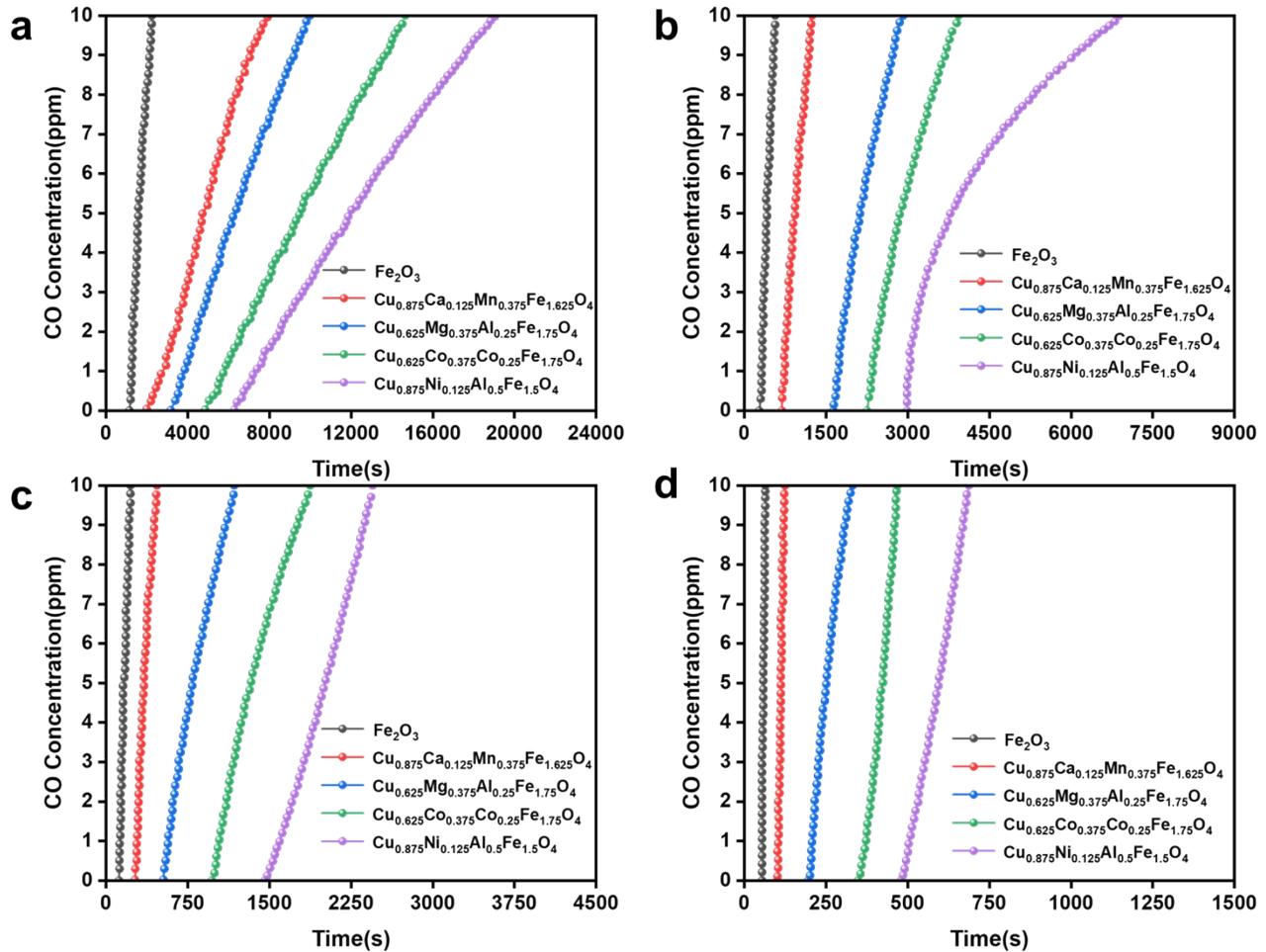


Fig. S7. Effect of different CO concentrations on the performance of oxygen carriers at 500 °C. (a) 100ppm. (b) 500ppm. (c) 1000ppm. (d) 2000ppm.