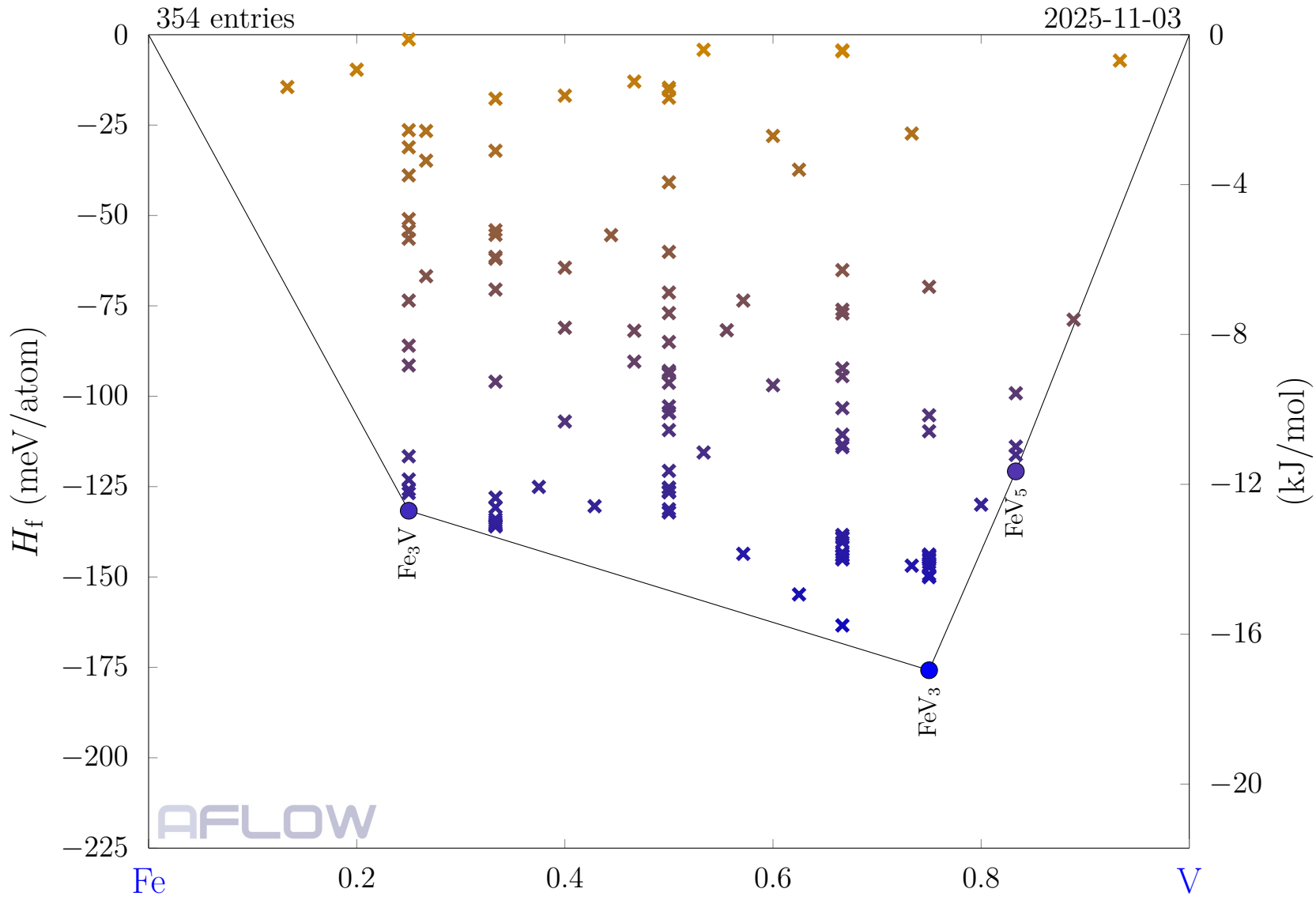
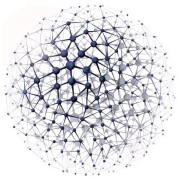

354 entries
2025-11-03
H_f (meV/atom)
(kJ/mol)
0
−25
−50
−75
−100
−125
−150
−175
−200
−225
−4
−8
−12
−16
−20
Fe
V
0.2
0.4
0.6
0.8
Fe_3V
FeV_3
FeV_5
AFLOW



AFLOW
Automatic - FLOW for Materials Discovery

Fe-V summary
354 entries
2025-11-03

Use of this data welcomes reference to the following publication:

C. Oses, E. Gossett, D. Hicks, F. Rose, M. J. Mehl, E. Perim, I. Takeuchi, S. Sanvito, M. Scheffler, Y. Lederer, O. Levy, C. Toher, and S. Curtarolo, *AFLOW-CHULL: Cloud-Oriented Platform for Autonomous Phase Stability Analysis*, J. Chem. Inf. Model. **58**(12), 2477-2490 (2018). doi:10.1021/acs.jcim.8b00393.

prototype	auid	original space group	relaxed space group	spin (μ_B/atom)	H_f (meV/atom)	T_S (K)	ΔH_{hull} (meV/atom)

binaries

$Fe_{22}V$ (unstable)

425	aflow:2ea7f575a72dafb7	$Fd\bar{3}m\#227$	$Fd\bar{3}m\#227$	0.69	190	-12359	213

decomposition reaction: $Fe_{0.9565}V_{0.04348} \rightarrow 0.8261$ Fe + 0.1739 $Fe_{0.75}V_{0.25}$

$Fe_{14}V$ (unstable)

600.BAAAA	aflow:e43e2b39b64ff48b	$P4_2/mnm\#136$	$P4_2/mnm\#136$	2.05	34	-1610	69

decomposition reaction: $Fe_{0.9333}V_{0.06667} \rightarrow 0.7333$ Fe + 0.2667 $Fe_{0.75}V_{0.25}$

$Fe_{13}V$ (unstable)

368	aflow:0d7801a83f445dd5	$Fm\bar{3}c\#226$	$Fm\bar{3}c\#226$	1.97	306	-13819	344

decomposition reaction: $Fe_{0.9286}V_{0.07143} \rightarrow 0.7143$ Fe + 0.2857 $Fe_{0.75}V_{0.25}$

Fe_8V (unstable)

311	aflow:c43d05ab5626daae	$I4/mmm\#139$	$I4/mmm\#139$	1.06	69	-2286	127

decomposition reaction: $Fe_{0.8889}V_{0.1111} \rightarrow 0.5556$ Fe + 0.4444 $Fe_{0.75}V_{0.25}$

Fe_7V (unstable)

310	aflow:0032744816314d4a	$Fm\bar{3}m\#225$	$Fm\bar{3}m\#225$	0.79	63	-1955	129

decomposition reaction: $Fe_{0.875}V_{0.125} \rightarrow 0.5$ Fe + 0.5 $Fe_{0.75}V_{0.25}$

$Fe_{13}V_2$ (unstable)

600.ABAAA	aflow:3b121d6ca524585d	$P4_2/mnm\#136$	$P4_2/mnm\#136$	1.70	-14	428	56

decomposition reaction: $Fe_{0.8667}V_{0.1333} \rightarrow 0.4667$ Fe + 0.5333 $Fe_{0.75}V_{0.25}$

Fe_5V (unstable)

145	aflow:499c8280109483bd	$Amm2\#38$	$Amm2\#38$	0.31	44	-1132	132
132	aflow:849505c0d2c553d6	$Cm\#8$	$Cm\#8$	0.00	46	-1185	134
253	aflow:2a43bfe2de448262	$F\bar{4}3m\#216$	$F\bar{4}3m\#216$	0.70	124	-3181	211
205	aflow:30f5f7314b1894bc	$P6/mmm\#191$	$P6/mmm\#191$	1.12	183	-4720	271

decomposition reaction: $Fe_{0.8333}V_{0.1667} \rightarrow 0.3333$ Fe + 0.6667 $Fe_{0.75}V_{0.25}$

Fe_4V (unstable)

600.BBAAA	aflow:b6baf98a6829de13	$P4_2/mnm\#136$	$P4_2/mnm\#136$	1.45	-10	225	96
286	aflow:8c8cd1439306ee79	$I4/m\#87$	$I4/m\#87$	0.67	35	-813	140
373	aflow:efc51b4ee40354d8	$I23\#197$	$I\bar{4}3m\#217$	0.79	349	-8100	455
203	aflow:b64eaead77292adf	$I4/mmm\#139$	$I4/mmm\#139$	0.00	376	-8713	481
654.AB	aflow:aa7ca684e6212b9c	$Im\bar{3}m\#229$	$Im\bar{3}m\#229$	1.60	921	-21356	1026

prototype	auid	original space group	relaxed space group	spin (μ_B/atom)	H_f (meV/atom)	T_S (K)	ΔH_{hull} (meV/atom)

decomposition reaction: $Fe_{0.8}V_{0.2} \rightarrow 0.2$ Fe + 0.8 $Fe_{0.75}V_{0.25}$

Fe_3V (ground-state) $\Delta H_{sc} = 5$ meV/atom, $\Delta H[2|1] = 132$ meV/atom

86	aflow:05c826cccb796dc0	$Fm\bar{3}m$#225	$Fm\bar{3}m$#225	1.23	-132	2717	0
81	aflow:b78f2d2e4526e0a6	$Immm$#71	$Immm$#71	1.33	-127	2617	5
83	aflow:225a9138bfafb4ec	$P4/mmm$#123	$P4/mmm$#123	1.22	-126	2597	6
272	aflow:44c4a0d7b465a0c8	$Cmcm$#63	$Cmcm$#63	1.23	-123	2539	9
78	aflow:b1b52093363e6cd9	$P4/mmm$#123	$P4/mmm$#123	1.29	-117	2407	15
75	aflow:479cf8f77b7e5111	$P2/m$#10	$P2/m$#10	1.36	-91	1888	40
69	aflow:76cc96a5401b4365	$R\bar{3}m$#166	$R\bar{3}m$#166	1.34	-86	1775	46
185	aflow:6fa0f3f15f16b607	$Pm\bar{3}n$#223	$Pm\bar{3}n$#223	1.29	-74	1518	58
72	aflow:289d5c955e000250	$Cmmm$#65	$Cmmm$#65	1.45	-56	1164	75
26	aflow:c49403d3b6679e07	$Pm\bar{3}m$#221	$Pm\bar{3}m$#221	0.76	-54	1119	77
181	aflow:5d2156e45f35638f	$Pnma$#62	$Pnma$#62	1.16	-51	1052	81
239	aflow:706be9811879c459	$P6_3/mmc$#194	$P6_3/mmc$#194	0.73	-39	803	93
279	aflow:66afa59df31f720f	$I4/mmm$#139	$I4/mmm$#139	0.79	-31	643	101
244	aflow:c84f6452995f5d3b	$P6_3/mmc$#194	$P6_3/mmc$#194	0.71	-26	545	105
187	aflow:5ca85b68056a4c44	$P6_3/mmc$#194	$P6_3/mmc$#194	0.59	-1	27	130
243	aflow:ac1edd50c9e1ee3d	$Pmmn$#59	$Pmmn$#59	0.55	2	-41	134
24	aflow:6b3f216fea1e13f2	$I4/mmm$#139	$I4/mmm$#139	0.63	4	-73	135
277	aflow:aabf7ce2d13b0131	$Pmmn$#59	$Pmmn$#59	0.49	11	-228	143
124	aflow:1bda06ef257b2cc5	$Imm2$#44	$Imm2$#44	0.00	15	-308	147
551	aflow:265fd40ac4fe9d00	$Imm2$#44	$Imm2$#44	0.00	16	-322	147
15	aflow:f314128771a5a1fd	$P4/mmm$#123	$P4/mmm$#123	0.38	30	-625	162
541	aflow:0467231b1164d512	$Immm$#71	$I4/mmm$#139	0.00	39	-799	170
21	aflow:233dcd986f6b157f	$Pmmm$#47	$Pmmm$#47	0.63	41	-845	173
12	aflow:d82036bdf613a22a	$Cmmm$#65	$Cmmm$#65	0.60	44	-918	176
121	aflow:48d1ca7306ea59cc	$Pmm2$#25	$Pmm2$#25	0.23	46	-959	178
18	aflow:47f0b117c17cde3c	$C2/m$#12	$C2/m$#12	0.27	55	-1132	187
127	aflow:dafe00ae79d02ee1	$P\bar{6}m2$#187	$P\bar{6}m2$#187	0.04	109	-2245	240
29	aflow:d0cf549058db1d2f	$R\bar{3}m$#166	$R\bar{3}m$#166	1.38	131	-2711	263
290	aflow:711975dc380ecb2a	$Pm\bar{3}m$#221	$Pm\bar{3}m$#221	1.25	1741	-35932	1873

vertex of facets: Fe–Fe_3V and Fe_3V–FeV_3
(2-phase equilibria)

$Fe_{11}V_4$ (unstable)

600.AABAA	aflow:a712ce95ca6aa8a1	$P4_2/mnm$#136	$P4_2/mnm$#136	1.01	-67	1337	66
600.AAAAB	aflow:13cc64778aa6c824	$P4_2/mnm$#136	$P4_2/mnm$#136	1.10	-35	697	98
600.AAABA	aflow:7be7a304085769b4	$P4_2/mnm$#136	$P4_2/mnm$#136	1.17	-27	533	107

decomposition reaction: $Fe_{0.7333}V_{0.2667} \rightarrow 0.9667$ $Fe_{0.75}V_{0.25}$ + 0.03333 $Fe_{0.25}V_{0.75}$

Fe_2V (unstable)

288	aflow:36c380fb3455f105	$I4/mmm$#139	$I4/mmm$#139	1.09	-136	2479	3
8	aflow:84e385c87f4a32e6	$Immm$#71	$Immm$#71	1.09	-136	2476	3
67	aflow:99295e9674f5848a	$I4/mmm$#139	$I4/mmm$#139	1.09	-136	2471	3
657.AB	aflow:f3fb4b0af18aa4a8	$Immm$#71	$I4/mmm$#139	1.08	-135	2464	4
595	aflow:ba867fdd72ffafd4	$Cmcm$#63	$I4/mmm$#139	1.09	-135	2454	4
143	aflow:1a805fe4a6767b95	$Cmcm$#63	$Cmcm$#63	0.97	-134	2442	5
233	aflow:ec91f16aa89a43d1	$I4/mmm$#139	$I4/mmm$#139	1.09	-131	2384	8
63	aflow:a99790eb5cf193c5	$P\bar{3}m1$#164	$P\bar{3}m1$#164	1.12	-128	2334	11
600.BABAA	aflow:47ff87f2e62d3b3d	$P4_2/mnm$#136	$P4_2/mnm$#136	0.89	-96	1750	43
179	aflow:67d61753bb3e282f	$P6_3/mmc$#194	$P6_3/mmc$#194	0.12	-70	1285	69
381	aflow:d50dc07253c844e0	$I4_1/amd$#141	$I4_1/amd$#141	0.49	-62	1130	77
316	aflow:4bf187413537af82	$P6_3/mmc$#194	$P6_3/mmc$#194	0.27	-61	1120	78
182	aflow:94dba39d07ece166	$Fd\bar{3}m$#227	$Fd\bar{3}m$#227	0.41	-55	1009	84
210	aflow:120534321dbb41b7	$Pnma$#62	$Pnma$#62	0.29	-54	986	85
600.BAAAB	aflow:afb56d0c7f8b9823	$P4_2/mnm$#136	$P4_2/mnm$#136	0.99	-32	585	107
189	aflow:2deec1b41095627f	$Cmcm$#63	$Cmcm$#63	0.56	-18	323	121
6	aflow:f78f79c7ce6fde0a	$I4/mmm$#139	$I4/mmm$#139	0.00	12	-213	151
539	aflow:8729cf868f4ca0d7	$C2/m$#12	$C2/m$#12	0.00	13	-230	152
130	aflow:6e3d8fd01c1109b2	$C2/m$#12	$C2/m$#12	0.00	13	-232	152
547	aflow:10b71c59f5e625de	$I4/mmm$#139	$I4/mmm$#139	0.00	13	-232	152
275	aflow:547a8471bb43d934	$P6_3/mmc$#194	$P6_3/mmc$#194	0.27	14	-252	153
273	aflow:39c6e2f5ba587830	$P6_3/mmc$#194	$P6_3/mmc$#194	0.27	14	-255	153
600.BAABA	aflow:bb8af74f2182076a	$P4_2/mnm$#136	$P4_2/mnm$#136	1.07	16	-298	155
129	aflow:d29d85029c788179	$C2/m$#12	$C2/m$#12	0.01	19	-349	158
476	aflow:a08307320a15b30d	$C2/m$#12	$C2/m$#12	0.00	20	-357	159
140	aflow:082bc8f0658f58a0	Cm#8	Cm#8	0.00	60	-1100	199
131	aflow:8007e8e014cd8198	$C2/m$#12	$C2/m$#12	-0.03	71	-1289	210

prototype	auid	original space group	relaxed space group	spin (μ_B/atom)	H_f (meV/atom)	T_S (K)	ΔH_{hull} (meV/atom)
258	aflow:751bc39743c28cfc	$Pnnm$#58	$Pnnm$#58	0.00	76	-1384	215
268	aflow:4b2886c8f462e285	$Pnnm$#58	$Pnnm$#58	0.00	76	-1384	215
191	aflow:9fdd4950a76d0da1	$P\bar{3}m1$#164	$P\bar{3}m1$#164	0.01	81	-1470	220
262	aflow:97d63f0ddc2f8820	$Fd\bar{3}m$#227	$Fd\bar{3}m$#227	0.85	86	-1564	225
10	aflow:26823bf1bcef18e6	$P\bar{3}m1$#164	$P\bar{3}m1$#164	0.84	111	-2020	250
142	aflow:bedf311cd31912b6	$Cmcm$#63	$Cmcm$#63	0.00	111	-2022	250
269	aflow:f69439d39985b3f4	$P\bar{3}m1$#164	$P\bar{3}m1$#164	0.02	120	-2196	259
217	aflow:dc58ef27c167ccb3	$P6/mmm$#191	$P6/mmm$#191	0.01	121	-2203	260
247	aflow:4b75edb72aa29eba	$P6_3/mmc$#194	$P6/mmm$#191	0.06	123	-2244	262
209	aflow:4425e168da89c2db	$P\bar{6}2m$#189	$P\bar{6}2m$#189	0.67	236	-4312	376
248	aflow:b54941660d8b22cd	$I4_1/amd$#141	$I4_1/amd$#141	0.75	261	-4755	400
283	aflow:7257f34037330342	$Imma$#74	$Imma$#74	0.00	271	-4942	410
230	aflow:ee1c09789ab95568	$I4/mcm$#140	$I4/mcm$#140	0.82	310	-5648	449
235	aflow:1cfe8c6d6e2cae71	$I4/mcm$#140	$I4/mcm$#140	0.82	311	-5665	450
389	aflow:15f0d5e940aa60e6	$P4/mmm$#123	$P4/mmm$#123	0.77	551	-10050	690
282	aflow:204d2ec0a39d6d3d	$Pa\bar{3}$#205	$Pa\bar{3}$#205	0.83	863	-15734	1002

decomposition reaction: $Fe_{0.6667}V_{0.3333} \rightarrow 0.8333\ Fe_{0.75}V_{0.25} + 0.1667\ Fe_{0.25}V_{0.75}$

Fe_5V_3 (unstable)

376	aflow:b2bb95074d35e288	$Cmmm$#65	$Cmmm$#65	0.76	-125	2194	18
222	aflow:f1fee1a3109945ba	$P6_3/mcm$#193	$P6_3/mcm$#193	0.63	110	-1926	253

decomposition reaction: $Fe_{0.625}V_{0.375} \rightarrow 0.75\ Fe_{0.75}V_{0.25} + 0.25\ Fe_{0.25}V_{0.75}$

Fe_3V_2 (unstable)

600.ABAAB	aflow:0ed7d7e2e207a2d2	$P4_2/mnm$#136	$P4_2/mnm$#136	0.74	-107	1845	38
600.ABBAA	aflow:fc8181d1de107f79	$P4_2/mnm$#136	$P4_2/mnm$#136	0.46	-81	1398	64
600.ABABA	aflow:12d293f17fcf4a1c	$P4_2/mnm$#136	$P4_2/mnm$#136	0.70	-64	1111	80
365	aflow:f899a7903f8fa7cd	$Fdd2$#43	$Fdd2$#43	0.00	-17	291	128
259	aflow:fdbe44b5c71fb033	$R\bar{3}m$#166	$R\bar{3}m$#166	0.88	118	-2030	263
371	aflow:c704daf46a6a7a1f	$P\bar{3}m1$#164	$P\bar{3}m1$#164	0.21	262	-4525	407

decomposition reaction: $Fe_{0.6}V_{0.4} \rightarrow 0.7\ Fe_{0.75}V_{0.25} + 0.3\ Fe_{0.25}V_{0.75}$

Fe_4V_3 (unstable)

264	aflow:da0482a6ddd02fe3	$I4/mmm$#139	$I4/mmm$#139	0.87	-130	2216	17
364	aflow:b6c1eab498611823	$P6/mmm$#191	$P6/mmm$#191	1.08	121	-2059	269

decomposition reaction: $Fe_{0.5714}V_{0.4286} \rightarrow 0.6429\ Fe_{0.75}V_{0.25} + 0.3571\ Fe_{0.25}V_{0.75}$

Fe_5V_4 (unstable)

314	aflow:f9baa5fe5a23577c	$I4/mmm$#139	$I4/mmm$#139	0.26	-55	936	93
360	aflow:2972b69dfeda3ad1	$P6_3/mcm$#193	$P6_3/mcm$#193	0.00	3	-53	152

decomposition reaction: $Fe_{0.5556}V_{0.4444} \rightarrow 0.6111\ Fe_{0.75}V_{0.25} + 0.3889\ Fe_{0.25}V_{0.75}$

Fe_8V_7 (unstable)

600.BBBAA	aflow:25b69038716a30f4	$P4_2/mnm$#136	$P4_2/mnm$#136	0.50	-90	1519	60
600.BBAAB	aflow:5f8bd355297cf95a	$P4_2/mnm$#136	$P4_2/mnm$#136	0.53	-82	1375	69
600.BBABA	aflow:7cab53b3075c69b9	$P4_2/mnm$#136	$P4_2/mnm$#136	0.74	-13	218	138

decomposition reaction: $Fe_{0.5333}V_{0.4667} \rightarrow 0.5667\ Fe_{0.75}V_{0.25} + 0.4333\ Fe_{0.25}V_{0.75}$

FeV (unstable)

prototype	auid	original space group	relaxed space group	spin (μ_B/atom)	H_f (meV/atom)	T_S (K)	ΔH_{hull} (meV/atom)
20	aflow:0d6ae9ea39f8f2c1	$Pmmn\#59$	$P4/nmm\#129$	0.71	-132	2212	22
14	aflow:512c8c565e2f41cf	$P4/nmm\#129$	$P4/nmm\#129$	0.72	-132	2209	22
77	aflow:2c0411cbe82dd1d4	$P4/nmm\#129$	$P4/nmm\#129$	0.72	-131	2198	22
61	aflow:d2ba603d72d59264	$Pm\bar{3}m\#221$	$Pm\bar{3}m\#221$	0.41	-127	2119	27
ICSD #103681.AB	aflow:e5deb524c403b17b	$Pm\bar{3}m\#221$	$Pm\bar{3}m\#221$	0.41	-127	2118	27
120	aflow:1ea58b7fb3013b5d	$Pmma\#51$	$Pm\bar{3}m\#221$	0.39	-126	2114	27
291	aflow:d3a356cbd2f08eba	$P4/nmm\#129$	$Pm\bar{3}m\#221$	0.40	-125	2100	28
3	aflow:9505f64ed99f66a8	$P4/mmm\#123$	$P4/mmm\#123$	0.40	-125	2098	28
85	aflow:e700024fdb26b9ab	$Fd\bar{3}m\#227$	$Fd\bar{3}m\#227$	0.55	-121	2020	33
136	aflow:17bbbb99b973d2d1	$Cm\#8$	$C2/m\#12$	0.67	-109	1831	44
60	aflow:8037d2d6e44ce302	$Cmmm\#65$	$Cmmm\#65$	0.64	-105	1752	49
138	aflow:dc41e50160b604aa	$Cm\#8$	$Cm\#8$	0.60	-104	1748	49
119	aflow:16a30aeb950409cc	$Pmmn\#59$	$C2/m\#12$	0.63	-103	1721	51
80	aflow:83b3608c9e1eb36b	$Imma\#74$	$Imma\#74$	0.52	-96	1612	57
123	aflow:7b04444967a27a2c	$C2/m\#12$	$Imma\#74$	0.52	-94	1571	60
17	aflow:18eddf84d10287b5	$C2/m\#12$	$Imma\#74$	0.51	-94	1568	60
448	aflow:a10a45348c783a23	$P2_1/m\#11$	$Pmma\#51$	0.00	-93	1564	60
447	aflow:1d4bad0a63c1370e	$P2_1/m\#11$	$P2_1/m\#11$	0.00	-93	1557	61
74	aflow:5242ecfeffc2ab64	$P2_1/m\#11$	$P2_1/m\#11$	0.58	-85	1423	69
71	aflow:654417e9c7018a1b	$Cmme\#67$	$Cmme\#67$	0.80	-77	1289	77
543	aflow:89afe271dd4270fc	$Imma\#74$	$Imma\#74$	0.00	-71	1194	82
256	aflow:727df76bb66ad3e5	$Pnma\#62$	$Pnma\#62$	0.00	-60	1006	94
139	aflow:3ff9e8ee3eb0f906	$Cm\#8$	$Cm\#8$	0.00	-41	684	113
198	aflow:9d0b22c0dbbb1125	$Pbcm\#57$	$Pbcm\#57$	-0.22	-17	292	136
194	aflow:ab2eb049e925359a	$Cmcm\#63$	$Cmcm\#63$	0.00	-15	256	138
193	aflow:4ddad3bb4e1e4db8	$Cmcm\#63$	$Cmcm\#63$	0.00	-15	245	139
23	aflow:0da54d624f32e95f	$I4_1/amd\#141$	$I4_1/amd\#141$	0.25	8	-126	161
538	aflow:73a0a30687e2c3ae	$R\bar{3}m\#166$	$P\bar{3}m1\#164$	0.00	29	-484	183
406	aflow:70fca6b9aad3fd5f	$R\bar{3}m\#166$	$R\bar{3}m\#166$	0.00	29	-490	183
196	aflow:a88730f3eb5c150f	$P4/nmm\#129$	$P4/nmm\#129$	0.00	31	-520	185
197	aflow:e6dd553f79ad1fb5	$P4/nmm\#129$	$P4/nmm\#129$	0.00	31	-521	185
195	aflow:37b63ecddf58b657	$P2_13\#198$	$P2_13\#198$	0.00	34	-577	188
221	aflow:701facea745999eb	$P6_3/mmc\#194$	$P6_3/mmc\#194$	0.37	116	-1941	270
192	aflow:9d782f556853cbec	$Cmcm\#63$	$Cmcm\#63$	0.24	117	-1966	271
4	aflow:1f8ade7f37bdb875	$R\bar{3}m\#166$	$R\bar{3}m\#166$	0.52	120	-2012	274
28	aflow:732c22c7b6271778	$R\bar{3}m\#166$	$R\bar{3}m\#166$	0.81	143	-2394	297
116	aflow:7605532803346431	$P\bar{6}m2\#187$	$P\bar{6}m2\#187$	0.59	158	-2645	312
126	aflow:f44d8d95425f8df5	$P\bar{3}m1\#164$	$P\bar{3}m1\#164$	0.33	158	-2647	312
220	aflow:c311adb0a50aa130	$P6_3/mmc\#194$	$P6_3/mmc\#194$	-0.12	329	-5508	483
407	aflow:209c0b1da663f00a	$P6_3/mmc\#194$	$P6_3/mmc\#194$	0.00	440	-7360	593
201	aflow:5e2242424ec0ffd1	$Fm\bar{3}m\#225$	$Fm\bar{3}m\#225$	0.00	549	-9195	703
219	aflow:52155a1c6a830f11	$P6_3mc\#186$	$P6_3mc\#186$	0.03	1372	-22967	1526
218	aflow:7670e710fc443ddc	$F\bar{4}3m\#216$	$F\bar{4}3m\#216$	0.00	1414	-23680	1568

decomposition reaction: $Fe_{0.5}V_{0.5} \rightarrow 0.5\ Fe_{0.75}V_{0.25} + 0.5\ Fe_{0.25}V_{0.75}$

Fe_7V_8 (unstable)

600.AABAB	aflow:e7dabf737e1a1b47	$P4_2/mnm\#136$	$P4_2/mnm\#136$	0.13	-116	1941	41
600.AAABB	aflow:1b967439b01a7b57	$P4_2/mnm\#136$	$P4_2/mnm\#136$	0.59	-4	70	152
600.AABBA	aflow:7af24914927e505f	$P4_2/mnm\#136$	$P4_2/mnm\#136$	0.63	21	-354	178

decomposition reaction: $Fe_{0.4667}V_{0.5333} \rightarrow 0.4333\ Fe_{0.75}V_{0.25} + 0.5667\ Fe_{0.25}V_{0.75}$

Fe_6V_7 (unstable)

614	aflow:b954909c0faee06d	$R\bar{3}m\#166$	$R\bar{3}m\#166$	0.87	174	-2923	331

decomposition reaction: $Fe_{0.4615}V_{0.5385} \rightarrow 0.4231\ Fe_{0.75}V_{0.25} + 0.5769\ Fe_{0.25}V_{0.75}$

Fe_4V_5 (unstable)

313	aflow:57636c5acb28320a	$I4/mmm\#139$	$I4/mmm\#139$	0.57	-82	1381	77
359	aflow:07050732e5b32cc3	$P6_3/mcm\#193$	$P6_3/mcm\#193$	-0.01	18	-306	177

decomposition reaction: $Fe_{0.4444}V_{0.5556} \rightarrow 0.3889\ Fe_{0.75}V_{0.25} + 0.6111\ Fe_{0.25}V_{0.75}$

Fe_3V_4 (unstable)

363	aflow:2fd82c935fed6f22	$P6/mmm\#191$	$P6/mmm\#191$	0.45	-144	2440	16
263	aflow:ff55a86637c97890	$I4/mmm\#139$	$I4/mmm\#139$	-0.03	-74	1250	86

decomposition reaction: $Fe_{0.4286}V_{0.5714} \rightarrow 0.3571\ Fe_{0.75}V_{0.25} + 0.6429\ Fe_{0.25}V_{0.75}$

prototype	auid	original space group	relaxed space group	spin (μ_B/atom)	H_f (meV/atom)	T_S (K)	ΔH_{hull} (meV/atom)

Fe_2V_3 (unstable)

600.BABAB	aflow:f8b2a75acbe305b0	$P4_2/mnm\#136$	$P4_2/mnm\#136$	0.00	-97	1672	66
366	aflow:d4c5afa8efed8d31	$Fdd2\#43$	$Fdd2\#43$	-0.05	-28	483	135
600.BAABB	aflow:ab39760ef3c0c889	$P4_2/mnm\#136$	$P4_2/mnm\#136$	0.52	29	-499	192
600.BABBA	aflow:5b4c6c15e91be8d8	$P4_2/mnm\#136$	$P4_2/mnm\#136$	0.56	43	-743	206
372	aflow:9f56f8eb1489abc4	$P\bar{3}m1\#164$	$P\bar{3}m1\#164$	0.00	121	-2081	283
260	aflow:6d6949115376295c	$R\bar{3}m\#166$	$R\bar{3}m\#166$	-0.27	123	-2113	285

decomposition reaction: $Fe_{0.4}V_{0.6} \rightarrow 0.3\ Fe_{0.75}V_{0.25} + 0.7\ Fe_{0.25}V_{0.75}$

Fe_3V_5 (unstable)

375	aflow:393359ffacb736ef	$Cmmm\#65$	$Cmmm\#65$	-0.05	-155	2716	10
223	aflow:172b776452482b35	$P6_3/mcm\#193$	$P6_3/mcm\#193$	0.00	-37	655	127

decomposition reaction: $Fe_{0.375}V_{0.625} \rightarrow 0.25\ Fe_{0.75}V_{0.25} + 0.75\ Fe_{0.25}V_{0.75}$

FeV_2 (unstable)

600.ABBAB	aflow:34e03517de8c7f3b	$P4_2/mnm\#136$	$P4_2/mnm\#136$	0.00	-163	2979	5
5	aflow:fd7115099d49bb44	$I4/mmm\#139$	$I4/mmm\#139$	-0.10	-145	2646	23
137	aflow:b1afdc67bec7348f	$C2/m\#12$	$I4/mmm\#139$	-0.09	-145	2641	24
7	aflow:01237b96a2f2aa76	$Immm\#71$	$I4/mmm\#139$	-0.10	-144	2628	24
66	aflow:cb0b16f179cab6d7	$I4/mmm\#139$	$I4/mmm\#139$	-0.09	-144	2628	24
287	aflow:a3f07418e0ea64f2	$I4/mmm\#139$	$I4/mmm\#139$	-0.10	-144	2625	24
232	aflow:dac28d559ad6a672	$I4/mmm\#139$	$I4/mmm\#139$	-0.09	-143	2612	25
188	aflow:de4d1d954e22a95d	$Cmcm\#63$	$Cmcm\#63$	-0.05	-140	2559	28
657.BA	aflow:dbdf3dfd5f880ea9	$Immm\#71$	$I4/mmm\#139$	0.00	-139	2539	29
150	aflow:ea14d8189487da42	$Cmcm\#63$	$Cmcm\#63$	0.00	-139	2533	29
540	aflow:60fece60d1b40d56	$C2/m\#12$	$C2/m\#12$	0.00	-138	2523	30
135	aflow:dbd7d81bf5e98e38	$C2/m\#12$	$C2/m\#12$	-0.21	-114	2080	54
134	aflow:5b25a5f5d8e8f97a	$C2/m\#12$	$C2/m\#12$	-0.21	-113	2068	55
133	aflow:a58ce7d1d264c27c	$Cm\#8$	$C2/m\#12$	-0.22	-111	2017	58
475	aflow:26355ad57f01a49b	$C2/m\#12$	$C2/m\#12$	0.00	-103	1883	65
147	aflow:a143a7e88da1d4bd	$Cmcm\#63$	$C2/m\#12$	-0.32	-94	1722	74
211	aflow:176d9c687ecb0b4d	$Pnma\#62$	$Pnma\#62$	0.00	-92	1683	76
270	aflow:3f5c48cc9de8cc78	$P\bar{3}m1\#164$	$P\bar{3}m1\#164$	-0.02	-77	1406	91
62	aflow:344c363439b39712	$P\bar{3}m1\#164$	$P\bar{3}m1\#164$	-0.02	-76	1387	92
600.ABABB	aflow:dcff5c042a747b82	$P4_2/mnm\#136$	$P4_2/mnm\#136$	0.26	-65	1187	103
234	aflow:fa9104186e39b889	$I4/mcm\#140$	$I4/mcm\#140$	0.01	-5	83	164
231	aflow:dbb5e15609e75049	$I4/mcm\#140$	$I4/mcm\#140$	0.00	-4	79	164
600.ABBBA	aflow:e43443c69f2985ec	$P4_2/mnm\#136$	$P4_2/mnm\#136$	0.37	6	-110	174
261	aflow:2cf939f13041e461	$Fd\bar{3}m\#227$	$Fd\bar{3}m\#227$	0.00	14	-255	182
382	aflow:6a8d43b324670d9d	$I4_1/amd\#141$	$I4_1/amd\#141$	-0.18	27	-490	195
276	aflow:239c605be2d17acd	$P6_3/mmc\#194$	$P6_3/mmc\#194$	0.00	29	-533	198
274	aflow:29cd4adcd44d551e	$P6_3/mmc\#194$	$P6_3/mmc\#194$	0.00	30	-538	198
208	aflow:d2ba827da249ee44	$P\bar{6}2m\#189$	$P\bar{6}2m\#189$	0.00	59	-1076	227
257	aflow:a506ad129ec38b45	$Pnnm\#58$	$Immm\#71$	0.00	115	-2090	283
267	aflow:3a9297666b7a13d6	$Pnnm\#58$	$Immm\#71$	0.00	115	-2090	283
9	aflow:ea397d09d34301f3	$P\bar{3}m1\#164$	$P\bar{3}m1\#164$	0.04	126	-2304	295
190	aflow:c77fe6b4a172b999	$P\bar{3}m1\#164$	$P\bar{3}m1\#164$	0.00	137	-2506	306
246	aflow:9ba1ce0c350554c2	$P6_3/mmc\#194$	$P6/mmm\#191$	0.69	172	-3141	341
183	aflow:9bca850fcb79e8dc	$Fd\bar{3}m\#227$	$Fd\bar{3}m\#227$	0.71	224	-4081	392
315	aflow:5a7620a03f9797e8	$P6_3/mmc\#194$	$P6_3/mmc\#194$	0.72	243	-4431	411
216	aflow:5a749bedb374650d	$P6/mmm\#191$	$P6/mmm\#191$	0.00	248	-4515	416
178	aflow:06d93406238f4607	$P6_3/mmc\#194$	$P6_3/mmc\#194$	0.75	262	-4782	431
249	aflow:391c7c990c68861b	$I4_1/amd\#141$	$I4_1/amd\#141$	0.00	281	-5129	450
281	aflow:99029b34e4c8bf40	$Pa\bar{3}\#205$	$Pa\bar{3}\#205$	0.00	316	-5760	484
583	aflow:ec7fd97e04a5ac18	$Fm\bar{3}m\#225$	$Fm\bar{3}m\#225$	0.00	317	-5775	485
390	aflow:155b703a1da6844f	$P4/mmm\#123$	$P4/mmm\#123$	0.00	385	-7015	553
284	aflow:b8f6581558913e87	$Imma\#74$	$Imma\#74$	-0.01	401	-7308	569

decomposition reaction: $Fe_{0.3333}V_{0.6667} \rightarrow 0.1667\ Fe_{0.75}V_{0.25} + 0.8333\ Fe_{0.25}V_{0.75}$

Fe_4V_{11} (unstable)

600.BBBAB	aflow:c145f7d267810ad8	$P4_2/mnm\#136$	$P4_2/mnm\#136$	0.00	-147	2939	27
600.BBABB	aflow:2de169ff8090e744	$P4_2/mnm\#136$	$P4_2/mnm\#136$	0.32	-27	547	147
600.BBBBA	aflow:1a9bb3a471f572cc	$P4_2/mnm\#136$	$P4_2/mnm\#136$	0.29	46	-917	220

prototype	auid	original space group	relaxed space group	spin (μ_B/atom)	H_f (meV/atom)	T_S (K)	ΔH_{hull} (meV/atom)

decomposition reaction: $Fe_{0.2667}V_{0.7333} \rightarrow 0.03333\ Fe_{0.75}V_{0.25} + 0.9667\ Fe_{0.25}V_{0.75}$

FeV_3 (ground-state) $\Delta H_{sc} = 26$ meV/atom, $\Delta H[2|1] = 176$ meV/atom

184	aflow:43af6ac464704483	$Pm\bar{3}n\#223$	$Pm\bar{3}n\#223$	0.00	-176	3628	0
118	aflow:ed984aa1a39e3583	$Pmm2\#25$	$Pmmm\#47$	0.00	-150	3096	26
11	aflow:e964fae8df061fbb	$Cmmm\#65$	$P4/mmm\#123$	0.00	-150	3093	26
82	aflow:2586d4dea73e3bb8	$P4/mmm\#123$	$P4/mmm\#123$	0.00	-149	3082	26
19	aflow:710022a91f3d9509	$Pmmm\#47$	$P4/mmm\#123$	0.00	-147	3038	29
271	aflow:ba7c9b19b842fc52	$Cmcm\#63$	$Cmcm\#63$	0.00	-147	3038	29
76	aflow:4cb5da37552e9feb	$P4/mmm\#123$	$P4/mmm\#123$	0.00	-146	3014	30
13	aflow:e7716e6d33bacfa0	$P4/mmm\#123$	$P4/mmm\#123$	0.00	-145	3000	30
84	aflow:cb5a6c0eb4bd0faf	$Fm\bar{3}m\#225$	$Fm\bar{3}m\#225$	0.00	-145	2991	31
16	aflow:f21f551c75a29fe8	$C2/m\#12$	$Immm\#71$	0.00	-144	2978	32
122	aflow:e0dcae4021d305a6	$Imm2\#44$	$Immm\#71$	0.00	-144	2974	32
79	aflow:85fd7e26895e0c11	$Immm\#71$	$Immm\#71$	0.00	-144	2967	32
68	aflow:3f223f2d9bc5978b	$R\bar{3}m\#166$	$R\bar{3}m\#166$	-0.01	-110	2264	66
73	aflow:aa5d41d3951aab3f	$P2/m\#10$	$P2/m\#10$	-0.02	-105	2172	71
70	aflow:553b1d0f7e4bb924	$Cmmm\#65$	$Cmmm\#65$	-0.21	-70	1439	106
22	aflow:bb893e6533c82edd	$I4/mmm\#139$	$I4/mmm\#139$	0.00	33	-684	209
180	aflow:b58175d66245ff17	$Pnma\#62$	$Pnma\#62$	0.00	33	-685	209
280	aflow:fcfcebe4d1e66d5b	$I4/mmm\#139$	$I4/mmm\#139$	-0.07	36	-740	212
242	aflow:08c983ded9950444	$Pmmn\#59$	$Pmmn\#59$	-0.07	36	-753	212
278	aflow:6655e425e574f064	$Pmmn\#59$	$Pmmn\#59$	0.00	53	-1093	229
186	aflow:2cf8bb2e6a193ad9	$P6_3/mmc\#194$	$P6_3/mmc\#194$	0.00	136	-2816	312
245	aflow:2acef4c0bd76af26	$P6_3/mmc\#194$	$P6_3/mmc\#194$	-0.16	142	-2924	318
238	aflow:0029689901a61789	$P6_3/mmc\#194$	$P6_3/mmc\#194$	-0.11	142	-2928	318
27	aflow:a56a6ecd9fe7afac	$R\bar{3}m\#166$	$R\bar{3}m\#166$	-0.09	150	-3090	326
25	aflow:6a8f94bbcf99996b	$Pm\bar{3}m\#221$	$Pm\bar{3}m\#221$	0.31	155	-3192	330
125	aflow:519e8f4147d57514	$P\bar{6}m2\#187$	$P\bar{6}m2\#187$	0.00	202	-4161	377

vertex of facets: Fe_3V–FeV_3 and FeV_3–FeV_5
(2-phase equilibria)

FeV_4 (unstable)

285	aflow:b90389f0a05950a1	$I4/m\#87$	$I4/m\#87$	0.00	-130	3014	13
600.AABBB	aflow:4db6325de8e4379a	$P4_2/mnm\#136$	$P4_2/mnm\#136$	-0.02	45	-1041	188
374	aflow:fdf2d7364b23d035	$I23\#197$	$I\bar{4}3m\#217$	0.00	406	-9422	549
202	aflow:c541cd963c1ee0e3	$I4/mmm\#139$	$I4/mmm\#139$	0.55	669	-15504	811

decomposition reaction: $Fe_{0.2}V_{0.8} \rightarrow 0.4\ Fe_{0.25}V_{0.75} + 0.6\ Fe_{0.1667}V_{0.8333}$

FeV_5 (ground-state) $\Delta H_{sc} = 3$ meV/atom, $\Delta H[2|1] = 121$ meV/atom

128	aflow:1b6ebdf9290ea8f3	$Cm\#8$	$C2/m\#12$	0.00	-121	3111	0
479	aflow:6e037eb24c89bf9b	$Cmmm\#65$	$Cmmm\#65$	0.00	-116	2993	5
141	aflow:25d2e78c9745bf6b	$Amm2\#38$	$Cmmm\#65$	0.00	-114	2934	7
478	aflow:bf4168daa2e00837	$P4/mmm\#123$	$P4/mmm\#123$	0.00	-99	2554	22
252	aflow:0fb22f8e75b7a38b	$F\bar{4}3m\#216$	$F\bar{4}3m\#216$	0.30	190	-4895	311
204	aflow:d0cb0adf53ceaa49	$P6/mmm\#191$	$P6/mmm\#191$	0.35	547	-14097	668

vertex of facets: FeV_3–FeV_5 and FeV_5–V
(2-phase equilibria)

Fe_2V_{13} (unstable)

600.BABBB	aflow:d71897b29444f030	$P4_2/mnm\#136$	$P4_2/mnm\#136$	-0.02	58	-1725	155

decomposition reaction: $Fe_{0.1333}V_{0.8667} \rightarrow 0.8\ Fe_{0.1667}V_{0.8333} + 0.2\ V$

FeV_7 (unstable)

309	aflow:21471afdb5434f0d	$Fm\bar{3}m\#225$	$Fm\bar{3}m\#225$	-0.01	226	-6962	317

prototype	auid	original space group	relaxed space group	spin (μ_B/atom)	H_f (meV/atom)	T_S (K)	ΔH_{hull} (meV/atom)

decomposition reaction: $Fe_{0.125}V_{0.875} \rightarrow 0.75\ Fe_{0.1667}V_{0.8333} + 0.25\ V$

FeV_8 (unstable)

312	aflow:239fbff7746a29c4	$I4/mmm\#139$	$I4/mmm\#139$	0.00	-79	2622	2

decomposition reaction: $Fe_{0.1111}V_{0.8889} \rightarrow 0.6667\ Fe_{0.1667}V_{0.8333} + 0.3333\ V$

FeV_{13} (unstable)

367	aflow:ec09fb46b72e9273	$Fm\bar{3}c\#226$	$Fm\bar{3}c\#226$	0.00	559	-25196	610

decomposition reaction: $Fe_{0.07143}V_{0.9286} \rightarrow 0.4286\ Fe_{0.1667}V_{0.8333} + 0.5714\ V$

FeV_{14} (unstable)

600.ABBBB	aflow:ba3c49d0b45f70a7	$P4_2/mnm\#136$	$P4_2/mnm\#136$	0.00	-7	339	41

decomposition reaction: $Fe_{0.06667}V_{0.9333} \rightarrow 0.4\ Fe_{0.1667}V_{0.8333} + 0.6\ V$

FeV_{22} (unstable)

426	aflow:b84cfc081fdbed95	$Fd\bar{3}m\#227$	$Fd\bar{3}m\#227$	0.09	330	-21432	362

decomposition reaction: $Fe_{0.04348}V_{0.9565} \rightarrow 0.2609\ Fe_{0.1667}V_{0.8333} + 0.7391\ V$

unaries

Fe (ground-state) $\Delta H_{sc} = 6$ meV/atom

A2	aflow:34bb95ea87b4d108	$Im\bar{3}m\#229$	$Im\bar{3}m\#229$	2.20	0	0	0
59	aflow:8e8f948b55e680a2	$Im\bar{3}m\#229$	$Im\bar{3}m\#229$	2.21	0	0	0
58	aflow:22e9902d74212347	$Im\bar{3}m\#229$	$Im\bar{3}m\#229$	2.21	0	0	0
b1	aflow:2172f0ab8c55ec31	$Im\bar{3}m\#229$	$Im\bar{3}m\#229$	2.21	0	0	0
b2	aflow:ab648a3ad39e58d9	$Im\bar{3}m\#229$	$Im\bar{3}m\#229$	2.21	0	0	0
A7.B	aflow:5fcce7c6b295b479	$Im\bar{3}m\#229$	$Im\bar{3}m\#229$	2.20	0	0	0
308	aflow:4a57e93fe4f7dc5b	$P\bar{3}m1\#164$	$I4/mmm\#139$	2.19	6	0	6
A3	aflow:e9fd9bb8cda420c6	$P6_3/mmc\#194$	$P6_3/mmc\#194$	0.00	67	0	67
A3	aflow:a94a08c53b67c204	$P6_3/mmc\#194$	$P6_3/mmc\#194$	0.00	83	0	83
117	aflow:7f1078621a8c1397	$P6_3/mmc\#194$	$P6_3/mmc\#194$	0.00	84	0	84
h1	aflow:a6c125f15fd640ac	$P6_3/mmc\#194$	$P6_3/mmc\#194$	0.00	84	0	84
h3	aflow:c7661ba535d0c133	$P6_3/mmc\#194$	$P6_3/mmc\#194$	0.00	84	0	84
115	aflow:fee4f6b65393fac0	$P6_3/mmc\#194$	$P6_3/mmc\#194$	0.00	84	0	84
A6	aflow:1003a5fb10a4009a	$I4/mmm\#139$	$I4/mmm\#139$	2.39	106	0	106
303	aflow:aa776b5898be7a0d	$I4/mmm\#139$	$I4/mmm\#139$	2.39	107	0	107
304	aflow:b88be86729a74c15	$I4/mmm\#139$	$I4/mmm\#139$	2.40	107	0	107
A1	aflow:72f4a3cca6173583	$Fm\bar{3}m\#225$	$Fm\bar{3}m\#225$	0.61	140	0	140
324	aflow:3c094477b82a2f8f	$P3_121\#152$	$P3_121\#152$	2.60	150	0	150
323	aflow:265ca0ce8d26f696	$P3_121\#152$	$C2/m\#12$	2.60	156	0	156
f1	aflow:f571808c41a5e80b	$Fm\bar{3}m\#225$	$Fm\bar{3}m\#225$	0.92	156	0	156
1	aflow:7cd0996cef2cb410	$Fm\bar{3}m\#225$	$Fm\bar{3}m\#225$	0.92	156	0	156
2	aflow:0ac6dd3d6ba602dc	$Fm\bar{3}m\#225$	$Fm\bar{3}m\#225$	0.92	156	0	156
f2	aflow:a0e6c536ba4711d1	$Fm\bar{3}m\#225$	$Fm\bar{3}m\#225$	0.92	156	0	156
A1	aflow:45269836bb433786	$Fm\bar{3}m\#225$	$Fm\bar{3}m\#225$	1.02	157	0	157
303	aflow:8aa7691c5e900974	$I4/mmm\#139$	$Fm\bar{3}m\#225$	0.00	162	0	162
304	aflow:ded6cc74eae7ea91	$I4/mmm\#139$	$Fm\bar{3}m\#225$	0.00	162	0	162
324	aflow:acefab051a5d8f87	$P3_121\#152$	$Fm\bar{3}m\#225$	0.00	167	0	167
A8	aflow:0aad66fc740e92d7	$P3_121\#152$	$Fm\bar{3}m\#225$	0.00	167	0	167
600.AAAAA	aflow:9fbb8c4c7e07ed94	$P4_2/mnm\#136$	$P4_2/mnm\#136$	-0.31	180	0	180
115	aflow:bf2df0811a2df76f	$P6_3/mmc\#194$	$P6_3/mmc\#194$	2.56	187	0	187
117	aflow:3bad53485637a3a7	$P6_3/mmc\#194$	$P6_3/mmc\#194$	2.56	187	0	187
h1	aflow:7860ecb3bbac844a	$P6_3/mmc\#194$	$P6_3/mmc\#194$	2.56	187	0	187
h3	aflow:0993a7b18f1ed49c	$P6_3/mmc\#194$	$P6_3/mmc\#194$	2.56	187	0	187
A3	aflow:2ac758e8b28d39e7	$P6_3/mmc\#194$	$P6_3/mmc\#194$	2.55	191	0	191
308	aflow:f0670cb72678e389	$P3m1\#156$	$P6/mmm\#191$	0.16	237	0	237
b1	aflow:b6b234cc073058c4	$Im\bar{3}m\#229$	$Im\bar{3}m\#229$	0.00	475	0	475
A7.B	aflow:f7c6adb411bd8f49	$R\bar{3}m\#166$	$Im\bar{3}m\#229$	0.00	479	0	479
A7	aflow:410f2549014815a1	$R\bar{3}m\#166$	$Im\bar{3}m\#229$	0.00	480	0	480
317	aflow:c4354e2c7ac6ffdf	$Cmce\#64$	$I4/mmm\#139$	0.00	491	0	491

prototype	auid	original space group	relaxed space group	spin (μ_B/atom)	H_f (meV/atom)	T_S (K)	ΔH_{hull} (meV/atom)
318	aflow:9df3b66e0dab46e5	$Cmce$#64	$I4/mmm$#139	0.00	492	0	492
318	aflow:314a082e46316381	$I4/mmm$#139	$I4/mmm$#139	2.60	500	0	500
A5	aflow:e35adf09f3c55df9	$I4_1/amd$#141	$I4_1/amd$#141	2.59	510	0	510
306	aflow:2f01918fd7cb19bd	$I4_1/amd$#141	$I4_1/amd$#141	2.57	529	0	529
A5	aflow:4804112fa886606e	$I4_1/amd$#141	$I4_1/amd$#141	2.58	529	0	529
305	aflow:9d6572d5b270bedd	$I4_1/amd$#141	$I4_1/amd$#141	2.58	545	0	545
306	aflow:a74e0e7a7542d696	$I4_1/amd$#141	$I4_1/amd$#141	2.58	545	0	545
305	aflow:7ededf53499905f7	$I4_1/amd$#141	$I4_1/amd$#141	0.00	819	0	819
306	aflow:892e0d2820781af9	$I4_1/amd$#141	$I4_1/amd$#141	0.00	819	0	819
325	aflow:d2867c0d71a592d7	$P6_3/mmc$#194	$P6_3/mmc$#194	0.00	1185	0	1185
326	aflow:c9dc593ba4bc3e98	$P6_3/mmc$#194	$P6_3/mmc$#194	0.00	1185	0	1185
A9	aflow:9b443c3cbf6f0f4d	$P6_3/mmc$#194	$P6_3/mmc$#194	0.00	1201	0	1201
A4	aflow:babe71cd868323d1	$Fd\bar{3}m$#227	$Fd\bar{3}m$#227	0.00	1243	0	1243
301	aflow:c60c00d131a1d750	$Fd\bar{3}m$#227	$Fd\bar{3}m$#227	0.00	1283	0	1283
302	aflow:94e83d3241229150	$Fd\bar{3}m$#227	$Fd\bar{3}m$#227	0.00	1283	0	1283
A4	aflow:67a554c9f20b77b5	$Fd\bar{3}m$#227	$Fd\bar{3}m$#227	0.00	1284	0	1284
0	aflow:2b5c613c7061013d	NNN#0	NNN#0	4.00	4854	0	4854
0	aflow:f3ba5f085734e13a	NNN#0	NNN#0	4.00	4987	0	4987

V (ground-state) $\Delta H_{sc} = 38$ meV/atom

b1	aflow:33980602d79acf54	$Im\bar{3}m$#229	$Im\bar{3}m$#229	0.00	-3	0	0
A2	aflow:9f3c87c3fd786a1d	$Im\bar{3}m$#229	$Im\bar{3}m$#229	0.00	0	0	3
58	aflow:ccad0bcd81e65cf3	$Im\bar{3}m$#229	$Im\bar{3}m$#229	0.00	0	0	4
b2	aflow:92deb5865d72f35c	$Im\bar{3}m$#229	$Im\bar{3}m$#229	0.00	0	0	4
59	aflow:316f97d88f799f53	$Im\bar{3}m$#229	$Im\bar{3}m$#229	0.00	1	0	4
600.BBBBB	aflow:0ebe0581d17d6b71	$P4_2/mnm$#136	$P4_2/mnm$#136	0.00	35	0	38
A6	aflow:210539ec3f7fca00	$I4/mmm$#139	$I4/mmm$#139	0.00	93	0	96
304	aflow:4d45f753057a2b54	$I4/mmm$#139	$I4/mmm$#139	0.00	93	0	96
303	aflow:d6fb5fbe459fbb2f	$I4/mmm$#139	$I4/mmm$#139	0.00	93	0	96
306	aflow:95c11d4def664137	$I4_1/amd$#141	$C2/m$#12	0.00	161	0	165
302	aflow:80094ff701e65e13	$Fd\bar{3}m$#227	$C2/m$#12	0.00	161	0	165
f1	aflow:53cc3fdb56689d43	$Fm\bar{3}m$#225	$Fm\bar{3}m$#225	0.00	241	0	244
307	aflow:90741b0d8d61a7cb	$P\bar{3}m1$#164	$R\bar{3}m$#166	0.00	242	0	245
A1	aflow:e7c3af8393b6c875	$Fm\bar{3}m$#225	$Fm\bar{3}m$#225	0.00	242	0	245
2	aflow:a726df6b49248472	$Fm\bar{3}m$#225	$Fm\bar{3}m$#225	0.00	243	0	246
58	aflow:92fe6f53853c3da6	$Im\bar{3}m$#229	$Fm\bar{3}m$#225	0.00	243	0	246
b2	aflow:26c7a1b6fa99cda6	$Im\bar{3}m$#229	$Fm\bar{3}m$#225	0.00	243	0	246
1	aflow:71fc2f4d2a9bec18	$Fm\bar{3}m$#225	$Fm\bar{3}m$#225	0.00	243	0	246
f2	aflow:35dc453174999f37	$Fm\bar{3}m$#225	$Fm\bar{3}m$#225	0.00	243	0	246
323	aflow:010bb7adfa14cfc6	$P3_121$#152	$R\bar{3}m$#166	0.00	244	0	247
324	aflow:d376ae844427efc5	$P3_121$#152	$R\bar{3}m$#166	0.00	244	0	247
308	aflow:181316b3b270acae	$P\bar{3}m1$#164	$C2/m$#12	0.00	244	0	247
A7	aflow:626356c4148703f3	$R\bar{3}m$#166	$R\bar{3}m$#166	0.00	246	0	249
A7.A	aflow:0954d4b57f9aa490	$R\bar{3}m$#166	$R\bar{3}m$#166	0.00	246	0	249
A7.B	aflow:80852086f278d1e6	$R\bar{3}m$#166	$R\bar{3}m$#166	0.00	246	0	249
A8	aflow:d384fec9272a2f07	$P3_121$#152	$R\bar{3}m$#166	0.00	246	0	249
h1	aflow:956839c6597fb6f3	$P6_3/mmc$#194	$P6_3/mmc$#194	0.00	252	0	256
117	aflow:033dd58526fe4a79	$P6_3/mmc$#194	$P6_3/mmc$#194	0.00	253	0	257
h3	aflow:473b6612cae25b7a	$P6_3/mmc$#194	$P6_3/mmc$#194	0.00	254	0	257
115	aflow:17b04215c36da55e	$P6_3/mmc$#194	$P6_3/mmc$#194	0.00	254	0	257
A1	aflow:820d87da9efd26ab	$Fm\bar{3}m$#225	$Fm\bar{3}m$#225	0.00	258	0	261
317	aflow:f6d437582edc8a5b	$Cmce$#64	$Fmmm$#69	0.00	258	0	261
318	aflow:1259ebe8553156e2	$Cmce$#64	$Fmmm$#69	0.00	258	0	261
A3	aflow:84db5eba4072874c	$P6_3/mmc$#194	$P6_3/mmc$#194	0.00	258	0	262
A5	aflow:4407ce4481816c3d	$I4_1/amd$#141	$I4_1/amd$#141	0.00	438	0	441
A5	aflow:454fed71e7b81950	$I4_1/amd$#141	$I4_1/amd$#141	0.00	466	0	469
305	aflow:b8c0d515c13bf965	$I4_1/amd$#141	$I4_1/amd$#141	0.00	475	0	478
306	aflow:99c90738846197be	$I4_1/amd$#141	$I4_1/amd$#141	0.00	475	0	478
A9	aflow:8b028c4743cabf77	$P6_3/mmc$#194	$P6_3/mmc$#194	0.00	1142	0	1145
325	aflow:89248da2fa974e70	$P6_3/mmc$#194	$P6_3/mmc$#194	0.00	1194	0	1198
326	aflow:e79685027b0c567d	$P6_3/mmc$#194	$P6_3/mmc$#194	0.00	1194	0	1198
301	aflow:a760be0c3e5f5d63	$Fd\bar{3}m$#227	$Fd\bar{3}m$#227	1.92	2294	0	2297
302	aflow:95746e03d7e2f722	$Fd\bar{3}m$#227	$Fd\bar{3}m$#227	1.91	2295	0	2298
A4	aflow:767840beff6bf0ed	$Fd\bar{3}m$#227	$Fd\bar{3}m$#227	0.00	2306	0	2310
A4	aflow:cb2180fd01b2ba30	$Fd\bar{3}m$#227	$Fd\bar{3}m$#227	0.00	2382	0	2385
302	aflow:c3b0c1ec95529fa6	$Fd\bar{3}m$#227	$Fd\bar{3}m$#227	0.00	2390	0	2393