

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)
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binaries

Al₈Ni (unstable)

311	aflow:bb3ad6321879429f	$I4/mmm\#139$	$I4/mmm\#139$	0.00	-103	3416	79
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decomposition reaction: $\text{Al}_{0.8889}\text{Ni}_{0.1111} \rightarrow 0.5556 \text{ Al} + 0.4444 \text{ Al}_{0.75}\text{Ni}_{0.25}$

Al₇Ni (unstable)

310	aflow:b9d6f0b4faf76d38	$Fm\bar{3}m\#225$	$Fm\bar{3}m\#225$	0.00	-102	3138	102
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decomposition reaction: $\text{Al}_{0.875}\text{Ni}_{0.125} \rightarrow 0.5 \text{ Al} + 0.5 \text{ Al}_{0.75}\text{Ni}_{0.25}$

Al₅Ni (unstable)

477	aflow:7bc209833bfcf467	$P4/mmm\#123$	$P4/mmm\#123$	0.00	-206	5306	66
480	aflow:c1d8d1f36b3e7b5d	$Cmmm\#65$	$Cmmm\#65$	0.00	-147	3775	126
132	aflow:81a2aba8ffbc5528	$Cm\#8$	$Cm\#8$	0.00	-145	3746	127
145	aflow:cbf1369984f043c1	$Amm2\#38$	$Amm2\#38$	0.00	-101	2605	171
473	aflow:0e79fe3cbcee8a64	$P62m\#189$	$P62m\#189$	0.00	-99	2557	173
253	aflow:5b9235f18029e225	$F43m\#216$	$F43m\#216$	0.00	223	-5736	495
205	aflow:22fb8e50011d5d75	$P6/mmm\#191$	$P6/mmm\#191$	0.00	353	-9080	625

decomposition reaction: $\text{Al}_{0.8333}\text{Ni}_{0.1667} \rightarrow 0.3333 \text{ Al} + 0.6667 \text{ Al}_{0.75}\text{Ni}_{0.25}$

Al₂₄Ni₅ (unstable)

411	aflow:7087154fb5420499	$I\bar{4}3m\#217$	$I\bar{4}3m\#217$	0.00	37	-929	319
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decomposition reaction: $\text{Al}_{0.8276}\text{Ni}_{0.1724} \rightarrow 0.3103 \text{ Al} + 0.6897 \text{ Al}_{0.75}\text{Ni}_{0.25}$

Al₄Ni (unstable)

286	aflow:838d08bd4c1e54d7	$I4/m\#87$	$I4/m\#87$	0.00	-178	4136	149
654.AB	aflow:a028a59883a65c4e	$Im\bar{3}m\#229$	$Im\bar{3}m\#229$	0.00	-92	2130	235
373	aflow:d1d3bea8f906c126	$I23\#197$	$I\bar{4}3m\#217$	0.00	111	-2582	438
203	aflow:5fd464fe4536f54f	$I4/mmm\#139$	$I4/mmm\#139$	0.00	301	-6988	628

decomposition reaction: $\text{Al}_{0.8}\text{Ni}_{0.2} \rightarrow 0.2 \text{ Al} + 0.8 \text{ Al}_{0.75}\text{Ni}_{0.25}$

Al₃Ni (ground-state)

$\Delta H_{\text{sc}} = 24 \text{ meV/atom}$, $\Delta H[2|1] = 409 \text{ meV/atom}$

prototype	auid	original space group	relaxed space group	spin (μ_B /atom)	H_f (meV/atom)	T_S (K)	ΔH_{hull} (meV/atom)
181 ICSD #58040.AB	aflow:077775f1a782c344 aflow:761e3c2131c4eab7	<i>Pnma</i> #62 <i>Pnma</i> #62	<i>Pnma</i> #62 <i>Pnma</i> #62	0.00 0.00	-409 -409	8433 8431	0 0
72	aflow:cdc40f274dca9102	<i>Cmmm</i> #65	<i>P4/mmm</i> #123	0.00	-300	6197	108
541	aflow:54d8ce966dbcd276	<i>Immm</i> #71	<i>Immm</i> #71	0.00	-299	6174	109
81	aflow:f834b7b2a2269e9c	<i>Immm</i> #71	<i>Immm</i> #71	0.00	-299	6174	109
15	aflow:23b16b46c9505206	<i>P4/mmm</i> #123	<i>P4/mmm</i> #123	0.00	-297	6134	111
78	aflow:f37522c2592fe7c2	<i>P4/mmm</i> #123	<i>P4/mmm</i> #123	0.00	-296	6116	112
277	aflow:663411fafdf1eade	<i>Pmmn</i> #59	<i>Pmmn</i> #59	0.00	-261	5382	148
185	aflow:8da38e032f232353	<i>Pm3n</i> #223	<i>Pm3n</i> #223	0.00	-244	5045	164
75	aflow:de55b9e84d4d2027	<i>P2/m</i> #10	<i>Pmmn</i> #47	0.00	-237	4884	172
21	aflow:1f50db9c59fc507d	<i>Pmmm</i> #47	<i>Pmmm</i> #47	0.00	-236	4871	173
243	aflow:0559a9f33381a4c5	<i>Pmmn</i> #59	<i>Pmmn</i> #59	0.00	-235	4842	174
272	aflow:bbfe3b716c04b0b9	<i>Cmcm</i> #63	<i>Cmcm</i> #63	0.00	-235	4842	174
29	aflow:4c964f56246577d2	<i>R3m</i> #166	<i>R3m</i> #166	0.00	-234	4836	174
18	aflow:1435608e51b91828	<i>C2/m</i> #12	<i>C2/m</i> #12	0.00	-224	4627	184
279	aflow:677960de99442e44	<i>I4/mmm</i> #139	<i>I4/mmm</i> #139	0.00	-222	4591	186
124	aflow:cb148c8a5c647bd1	<i>Im2</i> #44	<i>Im2</i> #44	0.00	-222	4586	186
551	aflow:af1b9e4184e43f4c	<i>Im2</i> #44	<i>Im2</i> #44	0.00	-221	4570	187
24	aflow:63b98fe1d5431c1a	<i>I4/mmm</i> #139	<i>I4/mmm</i> #139	0.00	-219	4511	190
83	aflow:ef8a63349e58979b	<i>P4/mmm</i> #123	<i>Pm3m</i> #221	0.00	-219	4509	190
26	aflow:bf8859f97eae501	<i>Pm3m</i> #221	<i>Pm3m</i> #221	0.00	-215	4444	193
239	aflow:96421f256045c61e	<i>P63/mmc</i> #194	<i>P63/mmc</i> #194	0.00	-215	4433	194
471	aflow:27dee68113a5b7ec	<i>Cmcm</i> #63	<i>Cmcm</i> #63	0.00	-213	4393	196
12	aflow:35ea93a4f45b40a9	<i>Cmmm</i> #65	<i>Cmmm</i> #65	0.00	-211	4356	198
187	aflow:66eb2f30e376dda8	<i>P63/mmc</i> #194	<i>P63/mmc</i> #194	0.00	-206	4252	203
244	aflow:97e86b5b22450b11	<i>P63/mmc</i> #194	<i>P63/mmc</i> #194	0.00	-203	4182	206
127	aflow:86a9a9b508906d34	<i>P6m2</i> #187	<i>P6m2</i> #187	0.00	-194	3997	215
121	aflow:444d7bb4596137e5	<i>Pmm2</i> #25	<i>Pmm2</i> #25	0.00	-181	3731	228
86	aflow:db34a37263b28078	<i>Fm3m</i> #225	<i>Fm3m</i> #225	0.00	-85	1759	323
69	aflow:18254da4f94a518c	<i>R3m</i> #166	<i>R3m</i> #166	0.00	-76	1576	332
290	aflow:ca70ca4e46c39b8a	<i>Pm3m</i> #221	<i>Pm3m</i> #221	0.00	0	-2	409

vertex of facets:
(2-phase equilibria)

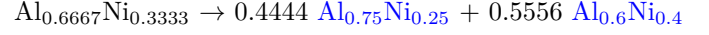
Al–Al₃Ni and Al₃Ni–Al₃Ni₂

Al₂Ni (unstable)

230	aflow:55739447c36ea1f0	<i>I4/mcm</i> #140	<i>I4/mcm</i> #140	0.00	-466	8495	57
235	aflow:a82618a36a4d71a6	<i>I4/mcm</i> #140	<i>I4/mcm</i> #140	0.00	-466	8495	57
210	aflow:8d3692f4c00326c6	<i>Pnma</i> #62	<i>Pnma</i> #62	0.00	-457	8337	66
476	aflow:4836408c19c712d3	<i>C2/m</i> #12	<i>C2/m</i> #12	0.00	-456	8312	67
129	aflow:52ff56b3e9a9247a	<i>C2/m</i> #12	<i>C2/m</i> #12	0.00	-456	8308	68
262	aflow:6e99ded338579900	<i>Fd3m</i> #227	<i>Fd3m</i> #227	0.00	-449	8184	74
584	aflow:99afca1efb37f211	<i>Fm3m</i> #225	<i>Fm3m</i> #225	0.00	-449	8182	74
282	aflow:c3bb4eb05c24f251	<i>Pa3</i> #205	<i>Fm3m</i> #225	0.00	-448	8161	76
209	aflow:a8bcd62c6ee8e617	<i>P62m</i> #189	<i>P62m</i> #189	0.00	-437	7959	87
595	aflow:0a8f123ccd7a77d8	<i>Cmcm</i> #63	<i>Cmcm</i> #63	0.00	-412	7518	111
389	aflow:9784e175e3e0d188	<i>P4/mmm</i> #123	<i>P4/mmm</i> #123	0.00	-405	7380	118
130	aflow:42e7d01d23cefd83	<i>C2/m</i> #12	<i>C2/m</i> #12	0.00	-404	7362	119
539	aflow:28a91cd4b3bfc11a	<i>C2/m</i> #12	<i>C2/m</i> #12	0.00	-403	7352	120
8	aflow:b9a04ecd2948ede3	<i>Immm</i> #71	<i>I4/mmm</i> #139	0.00	-393	7171	130
657.AB	aflow:cf2097eeci1a83ac0	<i>Immm</i> #71	<i>I4/mmm</i> #139	0.00	-393	7169	130
67	aflow:d3c1fbce2a3c1eb2	<i>I4/mmm</i> #139	<i>I4/mmm</i> #139	0.00	-393	7169	130
233	aflow:e1cfff9b26db3d63	<i>I4/mmm</i> #139	<i>I4/mmm</i> #139	0.00	-393	7160	131
258	aflow:c854d3f93b1004c3	<i>Pnnm</i> #58	<i>Pnnm</i> #58	0.00	-387	7057	136
268	aflow:727f4d0cce86efad	<i>Pnnm</i> #58	<i>Pnnm</i> #58	0.00	-387	7057	136
283	aflow:6b16a0e98a0b507c	<i>I4₁/amd</i> #141	<i>I4₁/amd</i> #141	0.00	-385	7026	138
248	aflow:c14fiad6fc0ed3fb	<i>I4₁/amd</i> #141	<i>I4₁/amd</i> #141	0.00	-383	6976	141
547	aflow:b675c8f017d02e18	<i>I4/mmm</i> #139	<i>I4/mmm</i> #139	0.00	-381	6949	142
6	aflow:03e709e726823276	<i>I4/mmm</i> #139	<i>I4/mmm</i> #139	0.00	-381	6948	142
288	aflow:5dcb4543d04c9dff	<i>I4/mmm</i> #139	<i>I4/mmm</i> #139	0.00	-381	6946	142
140	aflow:7be8f8ae545eda5	<i>Cm</i> #8	<i>Cm</i> #8	0.00	-375	6835	148
143	aflow:ede93a806023e4e6	<i>Cmcm</i> #63	<i>Cmcm</i> #63	0.00	-370	6750	153
131	aflow:63860c173e2bd384	<i>C2/m</i> #12	<i>C2/m</i> #12	0.00	-362	6606	161
189	aflow:8526aa4d3cd09da2	<i>Cmcm</i> #63	<i>Cmcm</i> #63	0.00	-348	6351	175
273	aflow:54f706e8c568a9f9	<i>P63/mmc</i> #194	<i>P63/mmc</i> #194	0.00	-327	5958	196
275	aflow:0acb8df64f325dbb	<i>P63/mmc</i> #194	<i>P63/mmc</i> #194	0.00	-327	5958	196
381	aflow:410176f0ca684315	<i>I4₁/amd</i> #141	<i>I4₁/amd</i> #141	0.00	-323	5896	200
142	aflow:27993fe960387778	<i>Cmcm</i> #63	<i>Cmcm</i> #63	0.00	-322	5879	201
10	aflow:be370c278ce1112b	<i>P3m1</i> #164	<i>P3m1</i> #164	0.00	-310	5644	214
191	aflow:8bab8f3c71ca2c01	<i>P3m1</i> #164	<i>P3m1</i> #164	0.00	-309	5631	214
63	aflow:feb453172f33ed7c	<i>P3m1</i> #164	<i>P3m1</i> #164	0.00	-232	4221	292
546	aflow:dfffc53579c1b439	<i>P3m1</i> #164	<i>P3m1</i> #164	0.00	-232	4221	292
269	aflow:0d5d1f80f5af3916	<i>P3m1</i> #164	<i>P3m1</i> #164	0.00	-231	4208	292
217	aflow:8ca96873e9866dd9	<i>P6/mmm</i> #191	<i>P6/mmm</i> #191	0.00	-17	302	507
247	aflow:daa59dc1e53398de	<i>P63/mmc</i> #194	<i>P63/mmc</i> #194	0.00	-16	296	507
179	aflow:05aec1fd8922a79f	<i>P63/mmc</i> #194	<i>P63/mmc</i> #194	0.00	152	-2766	675
316	aflow:b780b6140d2c988c	<i>P63/mmc</i> #194	<i>P63/mmc</i> #194	0.00	156	-2848	679
182	aflow:17419904e04b209	<i>Fd3m</i> #227	<i>Fd3m</i> #227	0.00	176	-3207	699

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



Al_5Ni_3 (unstable)

222	aflow:f3318dc056f67048	$P6_3/mcm\#193$	$P6_3/mcm\#193$	0.00	-486	8518	95
255	aflow:a00432f1b153266c	$Cm\#8$	$I4/mcm\#140$	0.00	-440	7722	140
376	aflow:e174715434bac5c7	$Cmmm\#65$	$Cmmm\#65$	0.00	-426	7466	155

decomposition reaction:

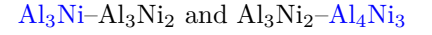


Al_3Ni_2 (ground-state)

$$\Delta H_{\text{sc}} = 21 \text{ meV/atom}, \Delta H[2|1] = 615 \text{ meV/atom}$$

371	aflow:bab26dad8d53e83e	$P3m1\#164$	$P3m1\#164$	0.00	-615	10603	0
ICSD #107713 AB	aflow:458e3729900e23a4	$P3m1\#164$	$P3m1\#164$	0.00	-615	10602	0
259	aflow:5a1a5375b1a8636c	$R3m\#166$	$R3m\#166$	0.00	-351	6056	264
365	aflow:936e2f1983d4c332	$Fdd2\#43$	$Fdd2\#43$	0.00	-345	5948	270

vertex of facets:

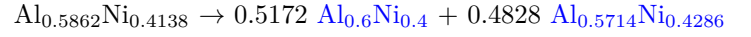


(2-phase equilibria)

$\text{Al}_{17}\text{Ni}_{12}$ (unstable)

560	aflow:398alfcaf3890f63	$I\bar{4}3m\#217$	$I\bar{4}3m\#217$	0.00	-394	6740	228
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decomposition reaction:

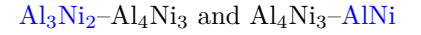


Al_4Ni_3 (ground-state)

$$\Delta H_{\text{sc}} = 2 \text{ meV/atom}, \Delta H[2|1] = 629 \text{ meV/atom}$$

ICSD #55042 AB	aflow:991a1068a704226a	$Ia3d\#230$	$Ia3d\#230$	0.00	-629	10693	0
264	aflow:9c351db34412e5cf	$I4/mmm\#139$	$I4/mmm\#139$	0.00	-444	7542	185
364	aflow:97012146c36992e9	$P6/mmm\#191$	$P6/mmm\#191$	0.00	-336	5712	293

vertex of facets:

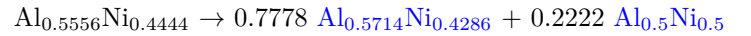


(2-phase equilibria)

Al_5Ni_4 (unstable)

360	aflow:10af6a7bf9e70f56	$P6_3/mcm\#193$	$P6_3/mcm\#193$	0.00	-512	8651	124
314	aflow:1940826c530aa377	$I4/mmm\#139$	$I4/mmm\#139$	0.00	-363	6130	273

decomposition reaction:



Al_7Ni_6 (unstable)

613	aflow:59642cd205ae46d8	$R\bar{3}m\#166$	$R\bar{3}m\#166$	0.00	-120	2017	523
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decomposition reaction:



AlNi (ground-state)

$$\Delta H_{\text{sc}} = 0 \text{ meV/atom}, \Delta H[2|1] = 660 \text{ meV/atom}$$

prototype	auid	original space group	relaxed space group	spin (μ_B /atom)	H_f (meV/atom)	T_S (K)	ΔH_{hull} (meV/atom)
3	aflow:c961031e8d72ff88	$P4/mmm\#123$	$P4/mmm\#123$	0.00	-660	11042	0
447	aflow:bdc29a092e26762b	$P2_1/m\#11$	$P4/mmm\#123$	0.00	-659	11038	0
448	aflow:d861d2e837c5c98c	$P2_1/m\#11$	$P4/mmm\#123$	0.00	-659	11037	0
292	aflow:b564b76f489b68501	$P4/nmm\#129$	$P4/mmm\#123$	0.00	-659	11027	1
291	aflow:94271cc663d9480b	$P4/nmm\#129$	$P4/mmm\#123$	0.00	-659	11027	1
74	aflow:022c8789fcbcd313	$P2_1/m\#11$	$Pm\bar{3}m\#221$	0.00	-659	11038	0
120	aflow:65f3978eb3bfbfad	$Pmma\#51$	$Pm\bar{3}m\#221$	0.00	-659	11036	0
61	aflow:d41dd6c71aac9027	$Pm\bar{3}m\#221$	$Pm\bar{3}m\#221$	0.00	-658	11023	1
60	aflow:72203124e65ecd4b	$Cmmm\#65$	$Pm\bar{3}m\#221$	0.00	-657	11004	2
ICSD #58037.AB	aflow:f25edb875cabb30f	$Pm\bar{3}m\#221$	$Pm\bar{3}m\#221$	0.00	-657	10994	3
195	aflow:045cb438e4d35b12	$P2_13\#198$	$P2_13\#198$	0.00	-635	10627	25
123	aflow:3812d9f54317a664	$C2/m\#12$	$C2/m\#12$	0.00	-584	9773	76
17	aflow:78e6918b17843e22	$C2/m\#12$	$C2/m\#12$	0.00	-584	9772	76
80	aflow:359331e360c25b18	$Imma\#74$	$Imma\#74$	0.00	-577	9662	82
543	aflow:b34eac9da719c87a	$Imma\#74$	$Imma\#74$	0.00	-577	9662	82
23	aflow:9c08125f409b2f65	$I4_1/amd\#141$	$I4_1/amd\#141$	0.00	-576	9636	84
256	aflow:d5f0c67a50c8bb79	$Pnma\#62$	$Pnma\#62$	0.00	-566	9470	94
139	aflow:31b62a26130b2bc2	$Cm\#8$	$Cm\#8$	0.00	-544	9100	116
138	aflow:eb5cf52ae1471d73	$Cm\#8$	$Cm\#8$	0.00	-543	9088	117
198	aflow:4ab66dd14ae21708	$Pbcm\#57$	$Pbcm\#57$	0.00	-504	8440	155
192	aflow:e87d4256ea47f90a	$Cmcm\#63$	$Cmcm\#63$	0.00	-494	8264	166
116	aflow:0fd7494f2657586f	$P6m2\#187$	$P6m2\#187$	0.00	-472	7909	187
193	aflow:d8e65b1295c2de05	$Cmcm\#63$	$Cmcm\#63$	0.00	-450	7528	210
194	aflow:4d741107be61dca8	$Cmcm\#63$	$Cmcm\#63$	0.00	-450	7526	210
20	aflow:b0387c03f8079923	$Pmmn\#59$	$Pmmn\#59$	0.00	-447	7480	213
119	aflow:eeddc9c2f68fe75	$Pmmn\#59$	$Pmmn\#59$	0.00	-444	7440	215
136	aflow:e885af26c7b7e3b5	$C2/m\#12$	$C2/m\#12$	0.00	-442	7392	218
220	aflow:7f2b04fc4a467bf	$P6_3/mmc\#194$	$P6_3/mmc\#194$	0.00	-431	7222	228
77	aflow:524d4faa1210069d0	$P4/nmm\#129$	$P4/nmm\#129$	0.00	-430	7207	229
196	aflow:ba6674cff2e2417c	$P4/nmm\#129$	$P4/nmm\#129$	0.00	-430	7195	230
197	aflow:1fe0e503a1ca7555	$P4/nmm\#129$	$P4/nmm\#129$	0.00	-430	7195	230
14	aflow:fcbcb91e84aff7a7	$P4/nmm\#129$	$P4/nmm\#129$	0.00	-430	7192	230
71	aflow:5d9dbec736c29867	$Cmmc\#67$	$P4/nmm\#129$	0.00	-428	7167	231
4	aflow:261500db22cbfc51	$R3m\#166$	$R3m\#166$	0.00	-417	6982	242
538	aflow:2b7aa2431e702788	$R3m\#166$	$R3m\#166$	0.00	-352	5886	308
405	aflow:c6290defad453df	$R3m\#166$	$R3m\#166$	0.00	-351	5869	309
85	aflow:a698a51ba8baea91	$Fd3m\#227$	$Fd3m\#227$	0.00	-341	5710	318
406	aflow:feb722405bcbf327a	$R3m\#166$	$Fd3m\#227$	0.00	-340	5689	320
537	aflow:3b58fc320412bb9e	$R3m\#166$	$R3m\#166$	0.00	-336	5627	323
221	aflow:a7440b06e608dc96	$P6_3/mmc\#194$	$P6_3/mmc\#194$	0.00	-327	5470	333
407	aflow:8c55af3c125e8ed1	$P6_3/mmc\#194$	$P6_3/mmc\#194$	0.00	-259	4329	401
28	aflow:784266d4965483b8	$R3m\#166$	$R3m\#166$	0.00	-176	2949	483
126	aflow:710a8254bb7f76ba	$P3m1\#164$	$P3m1\#164$	0.00	-175	2935	484
408	aflow:a3d391cf840bc76f	$P6_3/mmc\#194$	$P6_3/mmc\#194$	0.00	-118	1968	542
201	aflow:c4608c08d2caf2ed	$Fm3m\#225$	$Fm3m\#225$	0.00	-109	600	624
219	aflow:15586fdad205415d	$P6_3mc\#186$	$P6_3/mmc\#194$	0.00	36	-1824	768
218	aflow:5e61c60369306e19	$F43m\#216$	$F43m\#216$	0.00	475	-7946	1134

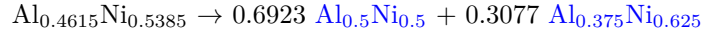
vertex of facets:
(2-phase equilibria)

$\text{Al}_4\text{Ni}_3\text{--AlNi}$ and $\text{AlNi--Al}_3\text{Ni}_5$

Al_6Ni_7 (unstable)

614	aflow:9a25b3b4c22fe29d	$R3m\#166$	$R3m\#166$	0.00	-395	6649	235
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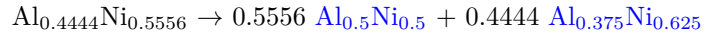
decomposition reaction:



Al_4Ni_5 (unstable)

359	aflow:52c6f87196f67e00	$P6_3/mcm\#193$	$P6_3/mcm\#193$	0.00	-506	8549	112
313	aflow:b3b046171db69436	$I4/mmm\#139$	$I4/mmm\#139$	0.00	-468	7909	150

decomposition reaction:



Al_3Ni_4 (unstable)

263	aflow:c4f5f303a2457891	$I4/mmm\#139$	$I4/mmm\#139$	0.00	-413	7019	193
363	aflow:543629b0c316e9f5	$P6/mmm\#191$	$P6/mmm\#191$	0.00	-71	1202	535

decomposition reaction:



$\text{Al}_{12}\text{Ni}_{17}$ (unstable)

prototype	auid	original space group	relaxed space group	spin (μ_B /atom)	H_f (meV/atom)	T_S (K)	ΔH_{hull} (meV/atom)
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559	aflow:e8516ad20ce75e97	$I\bar{4}3m\#217$	$I\bar{4}3m\#217$	0.00	-327	5594	268
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decomposition reaction:



Al_2Ni_3 (unstable)

366	aflow:d9f55570acd5cc0c	$Fdd2\#43$	$Fdd2\#43$	0.00	-397	6840	188
260	aflow:b1790cbbedfec8ad	$R\bar{3}m\#166$	$R\bar{3}m\#166$	0.00	-308	5316	276
372	aflow:ec8e2f1f2f03d453	$P\bar{3}m1\#164$	$P\bar{3}m1\#164$	0.00	-302	5210	282

decomposition reaction:



Al_3Ni_5 (ground-state)

$$\Delta H_{\text{sc}} = 14 \text{ meV/atom}, \Delta H[2|1] = 566 \text{ meV/atom}$$

375	aflow:d1a94169309817c2	$Cmmm\#65$	$Cmmm\#65$	0.00	-566	9926	0
ICSD #58041: Al	aflow:c5d23b26096ecb5	$Cmmm\#65$	$Cmmm\#65$	0.00	-565	9916	1
223	aflow:14a33bb83f9834fe	$P6_3/mcm\#193$	$P6_3/mcm\#193$	0.00	-434	7617	132
254	aflow:22294f456e4e0a54	$Cm\#8$	$I4/mcm\#140$	0.00	-425	7453	141

vertex of facets:

(2-phase equilibria)

$\text{AlNi}-\text{Al}_3\text{Ni}_5$ and $\text{Al}_3\text{Ni}_5-\text{AlNi}_3$

AlNi_2 (unstable)

211	aflow:becb9db4e88626cf	$Pnma\#62$	$Pnma\#62$	0.00	-516	9413	5
382	aflow:81bd39daa1511250	$I4_1/amd\#141$	$I4_1/amd\#141$	0.00	-499	9097	23
276	aflow:b925e23bf2f9f0ee	$P6_3/mmc\#194$	$P6_3/mmc\#194$	0.00	-480	8757	41
274	aflow:7fd2b3f75c54239	$P6_3/mmc\#194$	$P6_3/mmc\#194$	0.00	-480	8756	41
188	aflow:43a46427cd8c29f3	$Cmcm\#63$	$Cmcm\#63$	0.00	-476	8680	46
150	aflow:2442c533e4304d6a	$Cmcm\#63$	$Cmcm\#63$	0.00	-467	8508	55
540	aflow:3ad0c8fb6b4f522	$C2/m\#12$	$C2/m\#12$	0.00	-453	8264	68
137	aflow:14ab3b7fb8821c99	$C2/m\#12$	$C2/m\#12$	0.00	-453	8263	68
596	aflow:a5a1d0258506c780	$Cmcm\#63$	$Cmcm\#63$	0.00	-453	8255	69
548	aflow:93681f5c3edd954a	$I4/mmm\#139$	$I4/mmm\#139$	0.00	-447	8153	74
5	aflow:315d7be035dd2560	$I4/mmm\#139$	$I4/mmm\#139$	0.00	-447	8150	75
287	aflow:8e1895ce29bf67cb	$I4/mmm\#139$	$I4/mmm\#139$	0.00	-447	8144	75
66	aflow:224c9c7693116fdd	$I4/mmm\#139$	$I4/mmm\#139$	0.00	-447	8143	75
232	aflow:60a0c7caf80f33ef	$I4/mmm\#139$	$I4/mmm\#139$	0.00	-446	8133	76
7	aflow:4dd12e0415162f0b	$Immm\#71$	$Immm\#71$	0.00	-445	8119	76
657: BA	aflow:7831398904927e33	$Immm\#71$	$Immm\#71$	0.00	-445	8111	77
257	aflow:cba2f455ac992913	$Pnnm\#58$	$Immm\#71$	0.00	-442	8057	80
267	aflow:6560f0bacf9e5150	$Pnnm\#58$	$Immm\#71$	0.00	-442	8057	80
208	aflow:9779308add50d025	$P62m\#189$	$P62m\#189$	0.00	-431	7850	91
135	aflow:9bc4ea3876071ffa	$C2/m\#12$	$C2/m\#12$	0.00	-399	7271	123
133	aflow:f3cc23eebf3a35c87	$Cm\#8$	$Cm\#8$	0.00	-396	7216	126
475	aflow:ed8482b591306d7	$C2/m\#12$	$C2/m\#12$	0.00	-394	7189	127
134	aflow:7ccfb9f06004361	$C2/m\#12$	$C2/m\#12$	0.00	-394	7184	128
62	aflow:de3e3898390399de	$P3m1\#164$	$P3m1\#164$	0.00	-390	7103	132
545	aflow:4a945c005ba5934a	$P3m1\#164$	$P3m1\#164$	0.00	-390	7103	132
270	aflow:d16320be51a61750	$P3m1\#164$	$P3m1\#164$	0.00	-389	7100	132
190	aflow:cb7945d5ff0e41c9	$P3m1\#164$	$P3m1\#164$	0.00	-387	7062	134
246	aflow:1062daf63527770b	$P6_3/mmc\#194$	$P6/mmm\#191$	0.00	-322	5870	200
216	aflow:58be1f30cff2faf	$P6/mmm\#191$	$P6/mmm\#191$	0.00	-321	5859	200
261	aflow:82f5472fa079c9d7	$Fd3m\#227$	$Fd3m\#227$	0.00	-300	5467	222
315	aflow:21a275a5af007ea1	$P6_3/mmc\#194$	$P6_3/mmc\#194$	0.00	-292	5320	230
178	aflow:14c6dee95ee789fb	$P6_3/mmc\#194$	$P6_3/mmc\#194$	0.00	-282	5141	240
183	aflow:9fbbbb817d5702c	$Fd3m\#227$	$Fd3m\#227$	0.00	-270	4926	251
284	aflow:a8418c38b0588f4d	$I4_1/amd\#141$	$I4_1/amd\#141$	0.00	-261	4766	260
147	aflow:9c95016eb22dd967	$Cmcm\#63$	$Cmcm\#63$	0.00	-253	4605	269
249	aflow:38c7a5040cfaf3f0	$I4_1/amd\#141$	$I4_1/amd\#141$	0.00	-248	4524	273
9	aflow:904f47aa66edb646	$P3m1\#164$	$P3m1\#164$	0.00	-244	4454	277
234	aflow:594dff9dc0d46c8	$I4/mcm\#140$	$I4/mcm\#140$	0.00	-223	4075	298
231	aflow:8896e2f799c2aad1	$I4/mcm\#140$	$I4/mcm\#140$	0.00	-223	4074	298
583	aflow:c8517b48cdbaaf38	$Fm\bar{3}m\#225$	$Fm\bar{3}m\#225$	0.00	-107	1953	414
390	aflow:632cbf8baa09ef48	$P4/mmm\#123$	$P4/mmm\#123$	0.00	-9	155	513
281	aflow:d479d361145a67c3	$Pa3\#205$	$Pa3\#205$	0.00	242	-4413	764

decomposition reaction:



AlNi_3 (ground-state)

$$\Delta H_{\text{sc}} = 2 \text{ meV/atom}, \Delta H[2|1] = 433 \text{ meV/atom}$$

prototype	auid	original space group	relaxed space group	spin (μ_B /atom)	H_f (meV/atom)	T_S (K)	ΔH_{hull} (meV/atom)
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ICSD #107803.AB	aflow:ff2342ed02b99625	$P4/mmm\#123$	$P4/mmm\#123$	0.19	-433	8937	0
ICSD #58038.AB	aflow:b17d452d976eff96	$Pm\bar{3}m\#221$	$Pm\bar{3}m\#221$	0.19	-431	8894	2
25	aflow:103c03b42470ecc5	$Pm\bar{3}m\#221$	$Pm\bar{3}m\#221$	0.00	-428	8833	5
82	aflow:023a5836d3cba3e8	$P4/mmm\#123$	$Pm\bar{3}m\#221$	0.00	-428	8833	5
238	aflow:6c4dd804499ce8a4	$P6_3/mmc\#194$	$P6_3/mmc\#194$	0.00	-424	8743	9
271	aflow:e91d891d47920583	$Cmcm\#63$	$P6_3/mmc\#194$	0.13	-423	8721	10
280	aflow:4fa3cbb4f781412	$I4/mmm\#139$	$I4/mmm\#139$	0.00	-422	8715	11
186	aflow:bbb5f353fefb9f8a	$P6_3/mmc\#194$	$P6_3/mmc\#194$	0.00	-419	8651	14
245	aflow:9db5dc7660994a2d	$P6_3/mmc\#194$	$P6_3/mmc\#194$	0.00	-411	8491	22
278	aflow:ac36b5273e57b04e	$Pm\bar{m}n\#59$	$Pm\bar{m}n\#59$	0.00	-407	8396	26
242	aflow:98c156c4392e338f	$Pm\bar{m}n\#59$	$Pm\bar{m}n\#59$	0.00	-404	8344	29
118	aflow:ef9aed19ca51e40c	$Pmm2\#25$	$Pmm2\#25$	0.00	-403	8322	30
22	aflow:345f1ff39b76b1cc	$I4/mmm\#139$	$I4/mmm\#139$	0.00	-403	8316	30
542	aflow:b663db2e8f1088e8	$Immm\#71$	$I4/mmm\#139$	0.00	-403	8310	30
79	aflow:4f8752f3f30cacb4	$Immm\#71$	$I4/mmm\#139$	0.00	-403	8309	30
84	aflow:e8e952fc22bf022	$Fm\bar{3}m\#225$	$Fm\bar{3}m\#225$	0.00	-380	7842	53
ICSD #608800.AB	aflow:e58cdd3d2aa2d042	$Fm\bar{3}m\#225$	$Fm\bar{3}m\#225$	0.00	-380	7841	53
11	aflow:5cfce9850745519e	$Cmmm\#65$	$Cmmm\#65$	0.00	-365	7535	68
180	aflow:34b32d0da49f4a47	$Pnma\#62$	$Pnma\#62$	0.00	-361	7457	72
19	aflow:0e2b05b0bf9d3e86	$Pmmm\#47$	$Pmmm\#47$	0.00	-345	7121	88
73	aflow:b6b0d916acfdbf7b	$P2/m\#10$	$Pmmm\#47$	0.00	-345	7117	88
16	aflow:f53a51650fd1fa67	$C2/m\#12$	$C2/m\#12$	0.00	-344	7105	89
122	aflow:f70eafb36ffcf139	$Imm2\#44$	$Imm2\#44$	0.00	-339	7000	94
76	aflow:b5bf4d506b4cb679	$P4/mmm\#123$	$P4/mmm\#123$	0.00	-316	6519	117
13	aflow:27841718e5f0cf1d	$P4/mmm\#123$	$P4/mmm\#123$	0.00	-314	6489	119
70	aflow:efe4ca9f10aa22bf	$Cmmm\#65$	$P4/mmm\#123$	0.00	-314	6471	119
184	aflow:13e7ffec28319c2	$Pm\bar{3}n\#223$	$Pm\bar{3}n\#223$	0.07	-262	5406	171
68	aflow:73fc9224e5d60070	$R\bar{3}m\#166$	$R\bar{3}m\#166$	0.00	-255	5257	178
125	aflow:e98ee1a56847bebe	$P6m2\#187$	$P6m2\#187$	0.00	-162	3335	271
27	aflow:927f88090c4ac3c5	$R\bar{3}m\#166$	$R\bar{3}m\#166$	0.00	-154	3188	279
472	aflow:d36cfd2bec4c2f8	$Cmcm\#63$	$Cmcm\#63$	0.00	-41	856	392
289	aflow:af955b9d78ee2135	$Pm\bar{3}m\#221$	$Pm\bar{3}m\#221$	0.00	1304	-26915	1737

vertex of facets:
(2-phase equilibria)

Al_3Ni_5 – AlNi_3 and AlNi_3 – Ni

AlNi_4 (unstable)

285	aflow:c776751396003d69	$I4/m\#87$	$I4/m\#87$	0.00	-320	7432	26
374	aflow:41d587db1a21609b	$I23\#197$	$I\bar{4}3m\#217$	0.19	60	-1397	407
202	aflow:97f1f911c6a46dbe	$I4/mmm\#139$	$I4/mmm\#139$	0.20	68	-1570	414
654.BA	aflow:2ac1cfeabdda7bdf	$Im\bar{3}m\#229$	$Im\bar{3}m\#229$	0.00	549	-12734	896

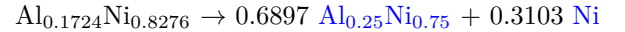
decomposition reaction:



$\text{Al}_5\text{Ni}_{24}$ (unstable)

412	aflow:6c5a6cdcc2fbfed2	$I\bar{4}3m\#217$	$I\bar{4}3m\#217$	0.00	-165	4159	134
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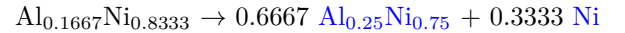
decomposition reaction:



AlNi_5 (unstable)

479	aflow:d1997a8ff268680e	$Cmmm\#65$	$Cmmm\#65$	0.00	-275	7076	14
474	aflow:ef821ceb18b2a705	$P6_2m\#189$	$P6_2m\#189$	0.15	-260	6686	29
141	aflow:6f287ab3ee53ef6f	$Am\bar{m}2\#38$	$Am\bar{m}2\#38$	0.25	-215	5542	74
128	aflow:b2e98be8212c9c84	$Cm\#8$	$Cm\#8$	0.00	-211	5442	77
478	aflow:9e93ecff792db2e	$P4/mmm\#123$	$P4/mmm\#123$	0.32	-187	4812	102
252	aflow:acbc3c2ee275d425	$F43m\#216$	$F43m\#216$	0.00	-93	2406	195
204	aflow:db71fd1d71db7d54	$P6/mmm\#191$	$P6/mmm\#191$	0.17	-13	323	276

decomposition reaction:



AlNi_7 (unstable)

309	aflow:1a5c6483d033a47d	$Fm\bar{3}m\#225$	$Fm\bar{3}m\#225$	0.36	-204	6268	13
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decomposition reaction:



AlNi_8 (unstable)

prototype	auid	original space group	relaxed space group	spin (μ_B /atom)	H_f (meV/atom)	T_S (K)	ΔH_{hull} (meV/atom)
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312	aflow:4d68e3fb62dcb6fe	$I4/mmm\#139$	$I4/mmm\#139$	0.00	-166	5529	26
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decomposition reaction: $\text{Al}_{0.1111}\text{Ni}_{0.8889} \rightarrow 0.4444 \text{Al}_{0.25}\text{Ni}_{0.75} + 0.5556 \text{Ni}$

unaries

Al (ground-state) $\Delta H_{\text{sc}} = 1 \text{ meV/atom}$

A7.A	aflow:f56cb0f7b39a779	$R\bar{3}m\#166$	$R\bar{3}m\#166$	0.00	-2	0	0
A7.A	aflow:532396af4c7eb7c9	$R\bar{3}m\#166$	$R\bar{3}m\#166$	0.00	0	0	2
A7.B	aflow:98341d1381ff1372	$R\bar{3}m\#166$	$R\bar{3}m\#166$	0.00	0	0	2
ICSD #182727	aflow:6914629e1dfa12d4	$Fm\bar{3}m\#225$	$Fm\bar{3}m\#225$	0.00	-1	0	1
ICSD #426922	aflow:ba182066024e73e1	$Fm\bar{3}m\#225$	$Fm\bar{3}m\#225$	0.00	-1	0	1
ICSD #43423	aflow:bf2f7466e5d4b44e	$Fm\bar{3}m\#225$	$Fm\bar{3}m\#225$	0.00	-1	0	1
ICSD #53775	aflow:e336a01f326f9058	$Fm\bar{3}m\#225$	$Fm\bar{3}m\#225$	0.00	-1	0	1
A6	aflow:fdae40be3f9aab33	$I4/mmm\#139$	$Fm\bar{3}m\#225$	0.00	0	0	2
59	aflow:3092a502178b3a34	$Im\bar{3}m\#229$	$Fm\bar{3}m\#225$	0.00	0	0	2
b1	aflow:3638cb56a69e512a	$Im\bar{3}m\#229$	$Fm\bar{3}m\#225$	0.00	0	0	2
1	aflow:e69039ff7bf2ef63	$Fm\bar{3}m\#225$	$Fm\bar{3}m\#225$	0.00	0	0	2
2	aflow:31f9343c80663ca7	$Fm\bar{3}m\#225$	$Fm\bar{3}m\#225$	0.00	0	0	2
f1	aflow:4d38058918ddf31a	$Fm\bar{3}m\#225$	$Fm\bar{3}m\#225$	0.00	0	0	2
f2	aflow:a260bcac010226e7	$Fm\bar{3}m\#225$	$Fm\bar{3}m\#225$	0.00	0	0	2
ICSD #150692	aflow:44926cbc7d08a943	$Fm\bar{3}m\#225$	$Fm\bar{3}m\#225$	0.00	0	0	2
ICSD #166867	aflow:2e6a1db93d1a0997	$Fm\bar{3}m\#225$	$Fm\bar{3}m\#225$	0.00	0	0	2
ICSD #240129	aflow:e9f44f8b8f27ea88	$Fm\bar{3}m\#225$	$Fm\bar{3}m\#225$	0.00	0	0	2
ICSD #43492	aflow:e435482e576f2235	$Fm\bar{3}m\#225$	$Fm\bar{3}m\#225$	0.00	0	0	2
ICSD #44321	aflow:ce0512f7fa3f2069	$Fm\bar{3}m\#225$	$Fm\bar{3}m\#225$	0.00	0	0	2
ICSD #44713	aflow:92bb4fe0216a94f4	$Fm\bar{3}m\#225$	$Fm\bar{3}m\#225$	0.00	0	0	2
ICSD #52255	aflow:aa3e967f17c1165c	$Fm\bar{3}m\#225$	$Fm\bar{3}m\#225$	0.00	0	0	2
ICSD #52611	aflow:22ecd9f427b1b56a8	$Fm\bar{3}m\#225$	$Fm\bar{3}m\#225$	0.00	0	0	2
ICSD #53772	aflow:c21ba7b90b6fc8e2	$Fm\bar{3}m\#225$	$Fm\bar{3}m\#225$	0.00	0	0	2
ICSD #53773	aflow:402c3f2182d191c1	$Fm\bar{3}m\#225$	$Fm\bar{3}m\#225$	0.00	0	0	2
ICSD #53774	aflow:abcd620617024492	$Fm\bar{3}m\#225$	$Fm\bar{3}m\#225$	0.00	0	0	2
ICSD #606000	aflow:28b8bafa661eb8f2	$Fm\bar{3}m\#225$	$Fm\bar{3}m\#225$	0.00	0	0	2
ICSD #606001	aflow:b5676de8e03e74eb	$Fm\bar{3}m\#225$	$Fm\bar{3}m\#225$	0.00	0	0	2
ICSD #606003	aflow:c8e8585fa3b28ad2	$Fm\bar{3}m\#225$	$Fm\bar{3}m\#225$	0.00	0	0	2
ICSD #606004	aflow:4a3a2db4b3bc141c	$Fm\bar{3}m\#225$	$Fm\bar{3}m\#225$	0.00	0	0	2
ICSD #606007	aflow:fd797e42ea534102	$Fm\bar{3}m\#225$	$Fm\bar{3}m\#225$	0.00	0	0	2
ICSD #64700	aflow:33ce30b2715ac575	$Fm\bar{3}m\#225$	$Fm\bar{3}m\#225$	0.00	0	0	2
ICSD #77363	aflow:cf191f6cf619c10c	$Fm\bar{3}m\#225$	$Fm\bar{3}m\#225$	0.00	0	0	2
A1	aflow:c2c7b894cd35ec8a	$Fm\bar{3}m\#225$	$Fm\bar{3}m\#225$	0.00	0	0	2
ICSD #606006	aflow:6856e04bd153f49d	$Fm\bar{3}m\#225$	$Fm\bar{3}m\#225$	0.00	0	0	2
303	aflow:48ffcc78b6ff7ccb	$I4/mmm\#139$	$Fm\bar{3}m\#225$	0.00	0	0	2
304	aflow:b0ab047b9aa5e467	$I4/mmm\#139$	$Fm\bar{3}m\#225$	0.00	0	0	2
324	aflow:dade03313c5797e0	$P3_121\#152$	$Fm\bar{3}m\#225$	0.00	0	0	3
A8	aflow:58e2e44aa505326b	$P3_121\#152$	$Fm\bar{3}m\#225$	0.00	0	0	3
323	aflow:6fae880b087f1b2	$P3_121\#152$	$Fm\bar{3}m\#225$	0.00	0	0	3
A3	aflow:2511f56f9be8af4b	$P6_3/mmc\#194$	$P6_3/mmc\#194$	0.10	11	0	13
115	aflow:ae15567e4b81adee	$P6_3/mmc\#194$	$P6_3/mmc\#194$	0.00	32	0	34
117	aflow:9942e98966b7b08d	$P6_3/mmc\#194$	$P6_3/mmc\#194$	0.00	32	0	34
A3	aflow:b5fb45383c1a4066	$P6_3/mmc\#194$	$P6_3/mmc\#194$	0.00	32	0	34
h1	aflow:44da7901f1894d7b	$P6_3/mmc\#194$	$P6_3/mmc\#194$	0.00	32	0	34
h3	aflow:36b7ca4748a969c9	$P6_3/mmc\#194$	$P6_3/mmc\#194$	0.00	32	0	34
305	aflow:7356f1e3d6c48252	$C2/m\#12$	$C2/m\#12$	0.00	32	0	34
675.A	aflow:d4b5265c7e3e3c2b	$Pm\bar{3}n\#223$	$Pm\bar{3}n\#223$	0.00	78	0	80
58	aflow:10f0f4146438b44b	$Im\bar{3}m\#229$	$Im\bar{3}m\#229$	0.00	96	0	98
59	aflow:1e18ba6b09c5bb35	$Im\bar{3}m\#229$	$Im\bar{3}m\#229$	0.00	96	0	98
b1	aflow:f292baf92e1426fd	$Im\bar{3}m\#229$	$Im\bar{3}m\#229$	0.00	96	0	98
b2	aflow:82ad4024a4126c40	$Im\bar{3}m\#229$	$Im\bar{3}m\#229$	0.00	96	0	98
A2	aflow:ab22f08746e8a248	$Im\bar{3}m\#229$	$Im\bar{3}m\#229$	0.00	96	0	98
ICSD #187080	aflow:88cb361876c0a3b9	$Im\bar{3}m\#229$	$Im\bar{3}m\#229$	0.00	96	0	99
674.A	aflow:de409f81fba91edc	$P6/mmm\#191$	$P6/mmm\#191$	0.00	114	0	116
ICSD #601854.ABC	aflow:a653b04259156354	$Cmcm\#63$	$Cmcm\#63$	0.00	155	0	157
317	aflow:715afe9ecbbaf6b2	$Cmce\#64$	$Cmce\#64$	0.00	181	0	184
318	aflow:f12a9018804788ad	$Cmce\#64$	$Cmce\#64$	0.00	181	0	184
301	aflow:402737964beb1da4	$Fd\bar{3}m\#227$	$P6/mmm\#191$	0.00	218	0	220
305	aflow:8f6db850967dc89d	$I4_1/amd\#141$	$I4_1/amd\#141$	0.00	278	0	281
306	aflow:bd6bfa501314ce0a	$I4_1/amd\#141$	$I4_1/amd\#141$	0.00	278	0	281
A5	aflow:e444ea7c2d798454	$I4_1/amd\#141$	$I4_1/amd\#141$	0.00	278	0	281
A9	aflow:660432436558b3cc	$P6_3/mmc\#194$	$P6_3/mmc\#194$	0.00	499	0	501
A4	aflow:4d4fa955051eeb846	$Fd\bar{3}m\#227$	$Fd\bar{3}m\#227$	0.00	683	0	686
302	aflow:4b73ff47e66a0f5c	$Fd\bar{3}m\#227$	$Fd\bar{3}m\#227$	0.00	746	0	748
A4	aflow:a3766b7e9643c519	$Fd\bar{3}m\#227$	$Fd\bar{3}m\#227$	0.00	746	0	748
301	aflow:9ad5f75943a1ecd3	$Fd\bar{3}m\#227$	$Fd\bar{3}m\#227$	0.00	746	0	748
0	aflow:fbf9c833c51a5b08	$NNN\#0$	$NNN\#0$	1.00	3154	0	3156
0	aflow:3d5c5804ed5c9dfc	$NNN\#0$	$NNN\#0$	1.00	3430	0	3433

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

$\Delta H_{sc} = 0$ meV/atom

A7.B	aflow:c7d7005405b9b047	$R\bar{3}m\#166$	$Fm\bar{3}m\#225$	0.63	0	0	0
2	aflow:f40a0e5ca2872f8e	$Fm\bar{3}m\#225$	$Fm\bar{3}m\#225$	0.63	0	0	0
Q	aflow:579cd607402e32c9	$Fm\bar{3}m\#225$	$Fm\bar{3}m\#225$	0.63	0	0	0
A6	aflow:5db87d4cd52b47a3	$I4/mmm\#139$	$Fm\bar{3}m\#225$	0.63	0	0	0
304	aflow:828468fa9c54f55a	$I4/mmm\#139$	$Fm\bar{3}m\#225$	0.63	0	0	0
1	aflow:d344420fe43bc735	$Fm\bar{3}m\#225$	$Fm\bar{3}m\#225$	0.63	0	0	0
Q2	aflow:2aa2c1163a631a5b	$Fm\bar{3}m\#225$	$Fm\bar{3}m\#225$	0.63	0	0	0
A1	aflow:2d15564b725c7bb1	$Fm\bar{3}m\#225$	$Fm\bar{3}m\#225$	0.62	0	0	0
A7.A	aflow:1e45c99f7a364339	$R\bar{3}m\#166$	$Fm\bar{3}m\#225$	0.64	4	0	4
A7.B	aflow:cbdd6bdf633ab618	$R\bar{3}m\#166$	$Fm\bar{3}m\#225$	0.64	4	0	4
324	aflow:3d642bf743c0b03	$P\bar{3}_121\#152$	$R\bar{3}m\#166$	-0.65	0	0	0
A7	aflow:0fff23eb8d5a920e	$R\bar{3}m\#166$	$R\bar{3}m\#166$	0.63	4	0	4
A3	aflow:6d351fe12ce00965	$P6_3/mmc\#194$	$P6_3/mmc\#194$	0.63	24	0	24
117	aflow:7e9cfd03683673b1	$P6_3/mmc\#194$	$P6_3/mmc\#194$	0.64	24	0	25
h1	aflow:8a5aa1d5f9b5c32b	$P6_3/mmc\#194$	$P6_3/mmc\#194$	0.64	24	0	25
h3	aflow:8a24f83cf8ba3b09	$P6_3/mmc\#194$	$P6_3/mmc\#194$	0.64	25	0	25
115	aflow:6a0d02967f9cf0a0b	$P6_3/mmc\#194$	$P6_3/mmc\#194$	0.64	25	0	25
A7.A	aflow:e0b85bd3ec7eab35	$R\bar{3}m\#166$	$R\bar{3}m\#166$	0.00	62	0	63
A8	aflow:0002cd1136697e3b	$P\bar{3}_121\#152$	$R\bar{3}m\#166$	0.00	62	0	63
324	aflow:c44d9efe905b2bdd	$P\bar{3}_121\#152$	$R\bar{3}m\#166$	0.00	63	0	63
307	aflow:31dbe5785cb25ce0	$P\bar{3}m1\#164$	$R\bar{3}m\#166$	-0.57	86	0	87
308	aflow:93c6f2fa52739577	$P\bar{3}m1\#164$	$R\bar{3}m\#166$	-0.57	86	0	87
A2	aflow:6673e886fa8a7d55	$Im\bar{3}m\#229$	$Im\bar{3}m\#229$	0.55	92	0	92
59	aflow:93963e66c841d429	$Im\bar{3}m\#229$	$Im\bar{3}m\#229$	0.56	97	0	97
b1	aflow:ea485fec603dd262	$Im\bar{3}m\#229$	$Im\bar{3}m\#229$	0.56	97	0	97
58	aflow:c9e66e00c6a2cfd8	$Im\bar{3}m\#229$	$Im\bar{3}m\#229$	0.56	97	0	97
b2	aflow:b38eba20975fb9e4	$Im\bar{3}m\#229$	$Im\bar{3}m\#229$	0.56	97	0	97
308	aflow:490d6cc8983f99d0	$P\bar{3}m1\#164$	$P\bar{3}m1\#164$	0.55	142	0	142
307	aflow:e48f376d78b190b0	$P\bar{3}m1\#164$	$P\bar{3}m1\#164$	0.00	177	0	177
317	aflow:4b0880c9661fc6f4	$Cmce\#64$	$Fmmm\#69$	0.66	337	0	338
318	aflow:8400875169d74571	$Cmce\#64$	$I4/mmm\#139$	0.66	342	0	342
318	aflow:4d826ea3a6ad4625	$Cmce\#64$	$Fmmm\#69$	0.00	376	0	376
317	aflow:864f13154aa80a1f	$Cmce\#64$	$I4/mmm\#139$	0.00	380	0	380
A5	aflow:a6b2363d32233376	$I4_1/amd\#141$	$I4_1/amd\#141$	0.65	451	0	452
306	aflow:d9267191c9320227	$I4_1/amd\#141$	$I4_1/amd\#141$	0.66	467	0	467
305	aflow:620914c6c2f5df17	$I4_1/amd\#141$	$I4_1/amd\#141$	0.67	469	0	469
306	aflow:a9213f3f4a8354ad	$I4_1/amd\#141$	$I4_1/amd\#141$	0.00	482	0	482
308	aflow:c8e5af2e50ef4b25	$P\bar{3}m1\#164$	$C2/m\#12$	0.56	698	0	699
307	aflow:d6c642cbefb24363	$P\bar{3}m1\#164$	$C2/m\#12$	0.57	701	0	702
A4	aflow:98d00e6cef9d7cc2	$Fd\bar{3}m\#227$	$Fd\bar{3}m\#227$	0.79	1191	0	1191
301	aflow:57cdf3f6ee9d2c6c	$Fd\bar{3}m\#227$	$Fd\bar{3}m\#227$	0.79	1197	0	1197
302	aflow:68b37543139df771	$Fd\bar{3}m\#227$	$Fd\bar{3}m\#227$	0.79	1202	0	1202
301	aflow:d27ed13b8a506122	$Fd\bar{3}m\#227$	$Fd\bar{3}m\#227$	0.00	1308	0	1308