AFLOW
Automatic - FLOW for Materials Discovery

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

unaries

S (ground-state) $\Delta H_{sc} = 19432$ 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)
ICSD #391460	aflow:e346a17500727d92	$Fddd\#70$	$Fddd\#70$	0.00	-19432	0	0
ICSD #66517	aflow:476a068c8e1d1ab5	$P2/c\#13$	$P2/c\#13$	0.00	0	0	19432
A16	aflow:c40fbde5833b2825	$Fddd\#70$	$Fddd\#70$	0.00	0	0	19432
ICSD #26463	aflow:dfc991d36a12d5af	$Pnnm\#58$	$Pnnm\#58$	0.00	13	0	19446
ICSD #408504	aflow:d73df7bd41e54345	$P\bar{1}\#2$	$P\bar{1}\#2$	0.00	16	0	19449
ICSD #6002	aflow:eef658df76bf8231	$P2_1/c\#14$	$P2_1/c\#14$	0.00	18	0	19451
ICSD #38263	aflow:1f45617ded5839bf	$C2/c\#15$	$C2/c\#15$	0.00	30	0	19463
ICSD #16469	aflow:472fe28b3c52f1cf	$P2_1/c\#14$	$P2_1/c\#14$	0.00	39	0	19471
ICSD #281124	aflow:4af81c5605a2812d	$P3_221\#154$	$P3_221\#154$	0.00	39	0	19472
323	aflow:43554f6bd8b161d9	$P3_121\#152$	$P3_121\#152$	0.00	42	0	19475
324	aflow:414f4f60ed0d637d	$P3_121\#152$	$P3_121\#152$	0.00	42	0	19475
A8	aflow:40c9a341a80206e5	$P3_121\#152$	$P3_121\#152$	0.00	42	0	19475
ICSD #40021	aflow:2435279d9d7c313b	$R\bar{3}\#148$	$R\bar{3}\#148$	0.00	64	0	19497
ICSD #27495	aflow:d782323bad02f963	$R\bar{3}\#148$	$R\bar{3}\#148$	0.00	65	0	19497
ICSD #650792	aflow:27f69873894ce7b9	$R\bar{3}\#148$	$R\bar{3}\#148$	0.00	65	0	19497
ICSD #37090	aflow:64017e38a4380498	$R\bar{3}\#148$	$R\bar{3}\#148$	0.00	65	0	19497
ICSD #38264	aflow:fda46f8a968593cd	$C2/c\#15$	$C2/c\#15$	0.00	108	0	19541
ICSD #20710	aflow:7b12ac4ee692a308	$P3\#143$	$P3\#143$	0.00	124	0	19556
ICSD #27840	aflow:96c1056a41ab9e0e	$Fddd\#70$	$Fddd\#70$	0.00	159	0	19592
317	aflow:2ed030ba40fbfbf9	$Cmce\#64$	$Fmmm\#69$	0.00	196	0	19628
318	aflow:4b16930a80d65871	$Cmce\#64$	$Fmmm\#69$	0.00	196	0	19628
ICSD #38147	aflow:16bed904776afc56	$Fddd\#70$	$Fddd\#70$	0.00	263	0	19695
ICSD #43251	aflow:131ca8900221aad9	$Fddd\#70$	$Fddd\#70$	0.00	486	0	19919
A6	aflow:371b6c4f17a8664f	$I4/mmm\#139$	$I4/mmm\#139$	0.00	493	0	19926
303	aflow:cbdf50d27a670c5f	$I4/mmm\#139$	$I4/mmm\#139$	0.00	505	0	19938
304	aflow:37ea4e5bfe892559	$I4/mmm\#139$	$I4/mmm\#139$	0.00	505	0	19938
A7	aflow:8a915c04b6b1fd31	$R\bar{3}m\#166$	$Pm\bar{3}m\#221$	0.00	616	0	20048
A7.A	aflow:825eeeed1f7cd01c	$R\bar{3}m\#166$	$Pm\bar{3}m\#221$	0.00	618	0	20050
A7.B	aflow:350d48e61f48c23b	$R\bar{3}m\#166$	$Pm\bar{3}m\#221$	0.00	618	0	20050
ICSD #57164	aflow:cc57f09f2501838d	$R\bar{3}m\#166$	$R\bar{3}m\#166$	0.00	619	0	20052
A5	aflow:eebe8a58086c645f	$I4_1/amd\#141$	$I4_1/amd\#141$	0.00	710	0	20143
305	aflow:4b504f5f39d9e361	$I4_1/amd\#141$	$I4_1/amd\#141$	0.00	712	0	20145
306	aflow:b04f8baa4351202d	$I4_1/amd\#141$	$I4_1/amd\#141$	0.00	712	0	20145
A9	aflow:de5c09945cbd9df3	$P6_3/mmc\#194$	$P6_3/mmc\#194$	0.00	812	0	20245
A3	aflow:6851b71520bf32ec	$P6_3/mmc\#194$	$P6_3/mmc\#194$	0.00	849	0	20281
115	aflow:1a397079ff4fbcca	$P6_3/mmc\#194$	$P6_3/mmc\#194$	0.00	850	0	20283
117	aflow:301aebbe8efdce37	$P6_3/mmc\#194$	$P6_3/mmc\#194$	0.00	850	0	20283
h1	aflow:e3380000c220e330	$P6_3/mmc\#194$	$P6_3/mmc\#194$	0.00	850	0	20283
h3	aflow:f1badea8c9307465	$P6_3/mmc\#194$	$P6_3/mmc\#194$	0.00	850	0	20283
A4	aflow:d91ffc62c6dc4017	$Fd\bar{3}m\#227$	$Fd\bar{3}m\#227$	0.00	1002	0	20435
301	aflow:4431ae97e0b80a21	$Fd\bar{3}m\#227$	$Fd\bar{3}m\#227$	0.00	1003	0	20435
302	aflow:c19d7e0066e38ac8	$Fd\bar{3}m\#227$	$Fd\bar{3}m\#227$	0.00	1003	0	20435
58	aflow:0372a5924d8b34b0	$Im\bar{3}m\#229$	$Im\bar{3}m\#229$	0.00	1121	0	20553
59	aflow:a136f2e34d1bca08	$Im\bar{3}m\#229$	$Im\bar{3}m\#229$	0.00	1121	0	20553
b1	aflow:39fa51d69d416557	$Im\bar{3}m\#229$	$Im\bar{3}m\#229$	0.00	1121	0	20553
b2	aflow:f952d15070c41f99	$Im\bar{3}m\#229$	$Im\bar{3}m\#229$	0.00	1121	0	20553
A2	aflow:e786dc4b859dccda	$Im\bar{3}m\#229$	$Im\bar{3}m\#229$	0.00	1123	0	20555
1	aflow:8a50b7a60e13f707	$Fm\bar{3}m\#225$	$Fm\bar{3}m\#225$	0.00	1296	0	20728
2	aflow:18f275b3b0cb1707	$Fm\bar{3}m\#225$	$Fm\bar{3}m\#225$	0.00	1296	0	20728
f1	aflow:a94f2282888e4c85	$Fm\bar{3}m\#225$	$Fm\bar{3}m\#225$	0.00	1296	0	20728
f2	aflow:cf336b7347cabf93	$Fm\bar{3}m\#225$	$Fm\bar{3}m\#225$	0.00	1296	0	20728
A1	aflow:aef23df622ddb939	$Fm\bar{3}m\#225$	$Fm\bar{3}m\#225$	0.00	1296	0	20729
0	aflow:9c6d8ab7e954c66d	$NNN\#0$	$NNN\#0$	2.00	3047	0	22479

Zn (ground-state) $\Delta H_{sc} = 20$ 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)
h1	aflow:880cb7454966ab58	$P6_3/mmc\#194$	$P6_3/mmc\#194$	0.00	-1	0	0
A3	aflow:b7a826ee350bbb3d	$P6_3/mmc\#194$	$P6_3/mmc\#194$	0.00	0	0	0
h3	aflow:229461b8628bdbbf	$P6_3/mmc\#194$	$P6_3/mmc\#194$	0.00	0	0	1
115	aflow:e9d55d43f797e596	$P6_3/mmc\#194$	$P6_3/mmc\#194$	0.00	1	0	1
117	aflow:fdb5fe544f7493fd	$P6_3/mmc\#194$	$P6_3/mmc\#194$	0.00	1	0	1
323	aflow:b01dc7aea574f736	$P3_121\#152$	$R\bar{3}m\#166$	0.00	20	0	20
324	aflow:c19541d14c542600	$P3_121\#152$	$R\bar{3}m\#166$	0.00	20	0	20

prototype	auid	original space group	relaxed space group	spin $(\mu_{\rm B}/{\rm atom})$	$H_{\rm f}$ (meV/atom)	$T_{\rm S}$ (K)	$\Delta H_{\rm hull}$ (meV/atom)
A7.B	aflow:3ecd4e77f36156b8	$R\bar{3}m\#166$	$R\bar{3}m\#166$	0.00	22	0	23
A7.A	aflow:d335e8b06e520fa0	$R\bar{3}m\#166$	$R\bar{3}m\#166$	0.00	22	0	23
A7	aflow:09462457781b4a68	$R\bar{3}m\#166$	$R\bar{3}m\#166$	0.00	22	0	23
1	aflow:6d89a906cff9bead	$Fm\bar{3}m\#225$	$Fm\bar{3}m\#225$	0.00	22	0	23
f2	aflow:9821d7e8c7be4ea2	$Fm\bar{3}m\#225$	$Fm\bar{3}m\#225$	0.00	22	0	23
2	aflow:bc413e1e81f4048f	$Fm\bar{3}m\#225$	$Fm\bar{3}m\#225$	0.00	22	0	23
A6	aflow:2f90799dd11afc87	$I4/mmm\#139$	$Fm\bar{3}m\#225$	0.00	22	0	23
A1	aflow:33bae93e4a9477fb	$Fm\bar{3}m\#225$	$Fm\bar{3}m\#225$	0.00	22	0	23
A8	aflow:927eaaab6d6e1e69	$P3_121\#152$	$R\bar{3}m\#166$	0.00	23	0	23
303	aflow:daf0ab70776c1338	$I4/mmm\#139$	$R\bar{3}m\#166$	0.00	23	0	23
304	aflow:8762640e13a6847c	$I4/mmm\#139$	$R\bar{3}m\#166$	0.00	23	0	23
f1	aflow:4f03676ebf0610e1	$Fm\bar{3}m\#225$	$Fm\bar{3}m\#225$	0.00	23	0	23
b1	aflow:d9d62b17dac139e4	$Im\bar{3}m\#229$	$Im\bar{3}m\#229$	0.00	81	0	82
58	aflow:806d8a6f4dc0f1bc	$Im\bar{3}m\#229$	$Im\bar{3}m\#229$	0.00	83	0	83
b2	aflow:9c7d8e119c022823	$Im\bar{3}m\#229$	$Im\bar{3}m\#229$	0.00	83	0	84
59	aflow:de034b2cd771ce5a	$Im\bar{3}m\#229$	$Im\bar{3}m\#229$	0.00	83	0	84
A2	aflow:b59a35f4590074ea	$Im\bar{3}m\#229$	$Im\bar{3}m\#229$	0.00	85	0	85
308	aflow:d7c006e5f72c04f1	$P\bar{3}m1\#164$	$P\bar{3}m1\#164$	0.00	86	0	86
307	aflow:19e86c6fefd832cb	$P\bar{3}m1\#164$	$C2/m\#12$	0.00	89	0	90
318	aflow:943af330db5deb0c	$Cmce\#64$	$Fmmm\#69$	0.00	105	0	106
A5	aflow:e256de0918a5a174	$I4_1/amd\#141$	$I4_1/amd\#141$	0.00	182	0	182
305	aflow:cdc88913cb9253b6	$I4_1/amd\#141$	$I4_1/amd\#141$	0.00	184	0	185
306	aflow:33b27ea0f7e72474	$I4_1/amd\#141$	$I4_1/amd\#141$	0.00	184	0	185
317	aflow:7dfa6a4d6a08ee23	$Cmce\#64$	$Cmce\#64$	0.00	187	0	188
318	aflow:d2e3339b190f6859	$Cmce\#64$	$Cmce\#64$	0.00	187	0	188
308	aflow:2e1fe7d785d6828f	$P\bar{3}m1\#164$	$R\bar{3}m\#166$	0.00	222	0	222
307	aflow:fb53fe8a5c75a7aa	$P\bar{3}m1\#164$	$C2/m\#12$	0.00	222	0	222
A9	aflow:00b8960c80015660	$P6_3/mmc\#194$	$P6_3/mmc\#194$	0.00	323	0	324
326	aflow:7fa82ade94fa26fa	$P6_3/mmc\#194$	$P6_3/mmc\#194$	0.00	406	0	406
302	aflow:6eb6611eafb84067	$Fd\bar{3}m\#227$	$Fd\bar{3}m\#227$	0.00	468	0	469
301	aflow:46a4d83f5d0f2d22	$Fd\bar{3}m\#227$	$Fd\bar{3}m\#227$	0.00	470	0	470
A4	aflow:d56d6b43d13c35d7	$Fd\bar{3}m\#227$	$Fd\bar{3}m\#227$	0.00	471	0	471
0	aflow:6f4a035f7b34f99a	$NNN\#0$	$NNN\#0$	0.00	1102	0	1103