

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 ( $\mu_B$ /atom)	$H_f$ (meV/atom)	$T_S$ (K)	$\Delta H_{\text{hull}}$ (meV/atom)
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## binaries

### Au<sub>22</sub>Cu (unstable)

425	aflow:8dbec6f42967edf4	$Fd\bar{3}m\#227$	$Fd\bar{3}m\#227$	0.00	146	-9461	151
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decomposition reaction:  $\text{Au}_{0.9565}\text{Cu}_{0.04348} \rightarrow 0.8696 \text{ Au} + 0.1304 \text{ Au}_{0.6667}\text{Cu}_{0.3333}$

### Au<sub>13</sub>Cu (unstable)

368	aflow:93622823b404984f	$Fm\bar{3}c\#226$	$Fm\bar{3}c\#226$	0.00	247	-11138	256
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decomposition reaction:  $\text{Au}_{0.9286}\text{Cu}_{0.07143} \rightarrow 0.7857 \text{ Au} + 0.2143 \text{ Au}_{0.6667}\text{Cu}_{0.3333}$

### Au<sub>8</sub>Cu (unstable)

311	aflow:cbcd863690d2a040	$I4/mmm\#139$	$I4/mmm\#139$	0.00	40	-1317	53
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decomposition reaction:  $\text{Au}_{0.8889}\text{Cu}_{0.1111} \rightarrow 0.6667 \text{ Au} + 0.3333 \text{ Au}_{0.6667}\text{Cu}_{0.3333}$

### Au<sub>7</sub>Cu (unstable)

310	aflow:b88ce72ab14ab710	$Fm\bar{3}m\#225$	$Fm\bar{3}m\#225$	0.00	5	-168	21
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decomposition reaction:  $\text{Au}_{0.875}\text{Cu}_{0.125} \rightarrow 0.625 \text{ Au} + 0.375 \text{ Au}_{0.6667}\text{Cu}_{0.3333}$

### Au<sub>5</sub>Cu (unstable)

477	aflow:c81b8d71a097d6df	$P4/mmm\#123$	$P4/mmm\#123$	0.00	-19	495	1
480	aflow:463f06fcc3155db5	$Cmmm\#65$	$Cmmm\#65$	0.00	-10	258	10
132	aflow:634fb49481dbfb2f	$Cm\#8$	$Cm\#8$	0.00	6	-147	26
473	aflow:d51f947c09f7bfaa	$P\bar{6}2m\#189$	$P\bar{6}2m\#189$	0.00	7	-176	27
145	aflow:15e77db01e1b8cf6	$Amm2\#38$	$Amm2\#38$	0.00	8	-197	28
253	aflow:3fa20ce3a96256c8	$F43m\#216$	$F43m\#216$	0.00	243	-6265	263
205	aflow:276d378cf042162c	$P6/mmm\#191$	$P6/mmm\#191$	0.00	246	-6328	266

decomposition reaction:  $\text{Au}_{0.8333}\text{Cu}_{0.1667} \rightarrow 0.5 \text{ Au} + 0.5 \text{ Au}_{0.6667}\text{Cu}_{0.3333}$

### Au<sub>24</sub>Cu<sub>5</sub> (unstable)

411	aflow:cce4ac773e3c6ba9	$I\bar{4}3m\#217$	$I\bar{4}3m\#217$	0.00	105	-2644	126
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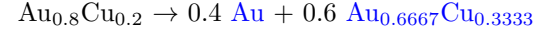
decomposition reaction:  $\text{Au}_{0.8276}\text{Cu}_{0.1724} \rightarrow 0.4828 \text{ Au} + 0.5172 \text{ Au}_{0.6667}\text{Cu}_{0.3333}$

### Au<sub>4</sub>Cu (unstable)

f33	aflow:2c082f6dca0164b2	$I4/mmm\#139$	$I4/mmm\#139$	0.00	-21	496	3
f31	aflow:480783e480e2b732	$Immm\#71$	$Immm\#71$	0.00	-10	227	14
f32	aflow:275e281ae927e78b	$C2/m\#12$	$C2/m\#12$	0.00	-9	205	15
286	aflow:17f7b3c9642e1e39	$I4/m\#87$	$I4/m\#87$	0.00	-8	182	16
f54	aflow:8b0969c86fd331e9	$I4/m\#87$	$I4/m\#87$	0.00	-6	144	18
f30	aflow:1edc987bf6da8762	$R3m\#166$	$R3m\#166$	0.00	3	-66	27
654.AB	aflow:a6c7bdbb9f299d34	$Im\bar{3}m\#229$	$Im\bar{3}m\#229$	0.00	197	-4565	221
373	aflow:361a2cd73756af16	$I23\#197$	$I\bar{4}3m\#217$	0.00	244	-5658	268
203	aflow:5a0834e0e20ea2f5	$I4/mmm\#139$	$I4/mmm\#139$	0.00	270	-6257	294

prototype	auid	original space group	relaxed space group	spin ( $\mu_B$ /atom)	$H_f$ (meV/atom)	$T_S$ (K)	$\Delta H_{\text{hull}}$ (meV/atom)
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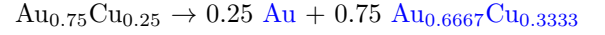
decomposition reaction:



Au<sub>3</sub>Cu (unstable)

15	aflow:1a0ad43f9727b320	<i>P4/mmm</i> #123	<i>P4/mmm</i> #123	0.00	-27	565	3
72	aflow:bbcc0da47a23e16d	<i>Cmmm</i> #65	<i>P4/mmm</i> #123	0.00	-27	565	3
181	aflow:bd04f5caa70fa835	<i>Pnma</i> #62	<i>Pnma</i> #62	0.00	-20	407	11
26	aflow:d5ac175b8fc225fe	<i>Pm3m</i> #221	<i>Pm3m</i> #221	0.00	-19	401	11
83	aflow:911d2b1986546da3	<i>P4/mmm</i> #123	<i>Pm3m</i> #221	0.00	-19	390	11
ICSD #56266.AB	aflow:112269d947c7d6a4	<i>Pm3m</i> #221	<i>Pm3m</i> #221	0.00	-17	354	13
279	aflow:3e41b066f7aa1806	<i>I4/mmm</i> #139	<i>I4/mmm</i> #139	0.00	-15	317	15
239	aflow:02d5a35c592990ec	<i>P63/mmc</i> #194	<i>P63/mmc</i> #194	0.00	-15	308	15
244	aflow:6e78504a71dea087	<i>P63/mmc</i> #194	<i>P63/mmc</i> #194	0.00	-14	287	16
541	aflow:213aa76ef67a2b0f	<i>Immm</i> #71	<i>Immm</i> #71	0.00	-13	271	17
24	aflow:aff311c5ad698ede	<i>I4/mmm</i> #139	<i>I4/mmm</i> #139	0.00	-13	266	17
243	aflow:ea71ca437baec2dd	<i>Pmmn</i> #59	<i>Pmmn</i> #59	0.00	-12	252	18
187	aflow:3f123670737f1fa6	<i>P63/mmc</i> #194	<i>P63/mmc</i> #194	0.00	-11	230	19
272	aflow:e5592c8d8f3f72b5	<i>Cmcm</i> #63	<i>Cmcm</i> #63	0.00	-11	223	20
78	aflow:e1dcbfaf8560d244	<i>P4/mmm</i> #123	<i>P4/mmm</i> #123	0.00	-10	215	20
81	aflow:3f66525e332f3e1b	<i>Immm</i> #71	<i>Immm</i> #71	0.00	-9	194	21
75	aflow:8400d10eea106ead	<i>P2/m</i> #10	<i>P2/m</i> #10	0.00	-7	146	23
21	aflow:0072288e166d1146	<i>Pmmm</i> #47	<i>Pmmm</i> #47	0.00	-7	140	24
277	aflow:70f29ec9ce7524dd	<i>Pmmn</i> #59	<i>Pmmn</i> #59	0.00	-3	65	27
18	aflow:7fd1d2dcac794981	<i>C2/m</i> #12	<i>C2/m</i> #12	0.00	-2	41	28
29	aflow:c11c75a97146f051	<i>R3m</i> #166	<i>R3m</i> #166	0.00	0	-1	30
551	aflow:1083e430ecd595f	<i>Imm2</i> #44	<i>Imm2</i> #44	0.00	7	-148	37
124	aflow:5581703a5ff4c2ee	<i>Imm2</i> #44	<i>Imm2</i> #44	0.00	8	-166	38
127	aflow:6607d12d21475de9	<i>P6m2</i> #187	<i>P6m2</i> #187	0.00	9	-183	39
471	aflow:83c9cf1269751f1d	<i>Cmcm</i> #63	<i>Cmcm</i> #63	0.00	11	-232	42
12	aflow:c5b223874398f662	<i>Cmmm</i> #65	<i>Cmmm</i> #65	0.00	14	-293	44
121	aflow:fb63e35bb53d2677	<i>Pmm2</i> #25	<i>Pmm2</i> #25	0.00	15	-318	46
86	aflow:1c855404b599e390	<i>Fm3m</i> #225	<i>Fm3m</i> #225	0.00	24	-501	55
69	aflow:a6423a3a3f387840	<i>R3m</i> #166	<i>R3m</i> #166	0.00	44	-902	74
185	aflow:b33dc49508a16fb3	<i>Pm3n</i> #223	<i>Pm3n</i> #223	0.00	130	-2692	161
290	aflow:70ea0de0ca41151c	<i>Pm3m</i> #221	<i>Pm3m</i> #221	0.00	801	-16521	831

decomposition reaction:



Au<sub>2</sub>Cu (ground-state)

$$\Delta H_{\text{sc}} = 1 \text{ meV/atom}, \Delta H[2|1] = 40 \text{ meV/atom}$$

6	aflow:2a3dc3024e492067	<i>I4/mmm</i> #139	<i>I4/mmm</i> #139	0.00	-40	736	0
288	aflow:0ba24ec431af6a5f	<i>I4/mmm</i> #139	<i>I4/mmm</i> #139	0.00	-40	726	1
505	aflow:cce1db0bde23bd72	<i>Cmcm</i> #63	<i>I4/mmm</i> #139	0.00	-39	713	1
547	aflow:5adddb8df6d6403f	<i>I4/mmm</i> #139	<i>I4/mmm</i> #139	0.00	-39	703	2
233	aflow:fb5bb81572653498	<i>I4/mmm</i> #139	<i>I4/mmm</i> #139	0.00	-39	717	1
539	aflow:2be0bd6440d6bc77	<i>C2/m</i> #12	<i>Immm</i> #71	0.00	-39	710	1
657.AB	aflow:b68c1704dc0acbb5b	<i>Immm</i> #71	<i>Immm</i> #71	0.00	-31	569	9
130	aflow:05f49758d84dbb6c	<i>C2/m</i> #12	<i>C2/m</i> #12	0.00	-30	556	10
8	aflow:27bd7ceb0c85417a	<i>Immm</i> #71	<i>Immm</i> #71	0.00	-27	492	13
67	aflow:2c388524d02c1f35	<i>I4/mmm</i> #139	<i>I4/mmm</i> #139	0.00	-25	456	15
189	aflow:9a18e1c42a08f45f	<i>Cmcm</i> #63	<i>Cmcm</i> #63	0.00	-23	423	17
210	aflow:29d417f7fc698596	<i>Pnma</i> #62	<i>Pnma</i> #62	0.00	-20	370	20
131	aflow:f71e1915771f4f3d	<i>C2/m</i> #12	<i>C2/m</i> #12	0.00	-20	367	20
209	aflow:f7e07f33d7a8760e	<i>P62m</i> #189	<i>P62m</i> #189	0.00	-18	329	22
381	aflow:5518e5d27fce1923	<i>I41/amd</i> #141	<i>I41/amd</i> #141	0.00	-18	323	23
258	aflow:9f475d6ff5f8511b	<i>Pnnm</i> #58	<i>Pnnm</i> #58	0.00	-16	283	25
268	aflow:a40dd3b31b555b0e	<i>Pnnm</i> #58	<i>Pnnm</i> #58	0.00	-16	283	25
143	aflow:c0eeb213dc89c282	<i>Cmcm</i> #63	<i>Cmcm</i> #63	0.00	-6	116	34
10	aflow:1310c177acc2153f	<i>P3m</i> #164	<i>P3m</i> #164	0.00	0	3	40
476	aflow:3d1a8c6cf1e3a91a	<i>C2/m</i> #12	<i>C2/m</i> #12	0.00	2	-38	42
273	aflow:683f68ad68dccb5f	<i>P63/mmc</i> #194	<i>P63/mmc</i> #194	0.00	2	-40	43
275	aflow:a0649f4a95254ae3	<i>P63/mmc</i> #194	<i>P63/mmc</i> #194	0.00	2	-40	43
129	aflow:798ffea2bb257948	<i>C2/m</i> #12	<i>C2/m</i> #12	0.00	2	-42	43
142	aflow:311f55dc45f7ec14	<i>Cmcm</i> #63	<i>Cmcm</i> #63	0.00	8	-148	49
140	aflow:0963b0dc5e7b2a50	<i>Cm</i> #8	<i>Cm</i> #8	0.00	15	-271	55
269	aflow:ebca0c82e93f0560	<i>P3m</i> #164	<i>P3m</i> #164	0.00	15	-277	56
63	aflow:075416fe1912bd21	<i>P3m</i> #164	<i>P3m</i> #164	0.00	15	-277	56
546	aflow:a3399e2519e87677	<i>P3m</i> #164	<i>P3m</i> #164	0.00	17	-304	57
248	aflow:30c366d38217c3f0	<i>I41/amd</i> #141	<i>I41/amd</i> #141	0.00	28	-505	68
235	aflow:4aba1384ee429d95	<i>I4/mcm</i> #140	<i>I4/mcm</i> #140	0.00	34	-614	74
230	aflow:362af4af6d61b2f4e	<i>I4/mcm</i> #140	<i>I4/mcm</i> #140	0.00	34	-628	75
262	aflow:3288d7e4e9483ca1	<i>Fd3m</i> #227	<i>Fd3m</i> #227	0.00	44	-794	84
283	aflow:00e246d93298ff9	<i>Imma</i> #74	<i>Imma</i> #74	0.00	51	-925	91
389	aflow:48da4e736ed87984	<i>P4/mmm</i> #123	<i>P4/mmm</i> #123	0.00	77	-1397	117
584	aflow:0783eeec8fc82b87	<i>Fm3m</i> #225	<i>Fm3m</i> #225	0.00	109	-1994	150
217	aflow:2432f51e7eaea4a0	<i>P6/mmm</i> #191	<i>P6/mmm</i> #191	0.00	125	-2287	166
247	aflow:711256756af853e5	<i>P63/mmc</i> #194	<i>P6/mmm</i> #191	0.00	134	-2444	174
191	aflow:blb7e98d804dbd0c	<i>P3m</i> #164	<i>P3m</i> #164	0.00	218	-3980	259
179	aflow:ddf19361c679f895	<i>P63/mmc</i> #194	<i>P63/mmc</i> #194	0.00	285	-5203	326

prototype	auid	original space group	relaxed space group	spin ( $\mu_B$ /atom)	$H_f$ (meV/atom)	$T_S$ (K)	$\Delta H_{\text{hull}}$ (meV/atom)
316	aflow:917802d8cf995e8b	$P6_3/mmc\#194$	$P6_3/mmc\#194$	0.00	294	-5359	334
182	aflow:8855919414f46a3e	$Fd3m\#227$	$Fd3m\#227$	0.00	317	-5777	357
282	aflow:8c02d905209b187c	$Pa3\#205$	$Pa3\#205$	0.00	331	-6042	372

vertex of facets:

(2-phase equilibria)

Au–Au<sub>2</sub>Cu and Au<sub>2</sub>Cu–AuCu

Au<sub>5</sub>Cu<sub>3</sub> (unstable)

376	aflow:88e09d861061a653	$Cmmm\#65$	$Cmmm\#65$	0.00	-29	508	14
255	aflow:63917660aa0a6c9a	$Fmm2\#42$	$C2/m\#12$	0.00	44	-767	86
222	aflow:98107a95705b1482	$P6_3/mcm\#193$	$P6_3/mcm\#193$	0.00	51	-889	93

decomposition reaction:



Au<sub>3</sub>Cu<sub>2</sub> (unstable)

f41	aflow:aab64cf2e25924b8	$I4/mmm\#139$	$I4/mmm\#139$	0.00	-43	736	1
f39	aflow:69d67f4cfd81b38	$Immm\#71$	$Immm\#71$	0.00	-37	634	7
f40	aflow:200bd08e2a243dae	$C2/m\#12$	$C2/m\#12$	0.00	-25	435	19
f55	aflow:1efb0327133e9eb5	$C2/m\#12$	$C2/m\#12$	0.00	-23	394	21
f37	aflow:08d606970c048fd2	$I4/mmm\#139$	$I4/mmm\#139$	0.00	-10	174	34
f35	aflow:ba27e0a43a5f0f0f	$Immm\#71$	$Immm\#71$	0.00	-10	167	34
259	aflow:dd3b2744d1d70495	$R3m\#166$	$R3m\#166$	0.00	1	-11	45
365	aflow:2ee47072fb042ed3	$Fdd2\#43$	$Fdd2\#43$	0.00	5	-82	49
f38	aflow:474ccff9f7b3ca50	$R3m\#166$	$R3m\#166$	0.00	7	-113	51
f36	aflow:3ddc5e3b808cd915	$C2/m\#12$	$C2/m\#12$	0.00	7	-114	51
f34	aflow:7d269fbdcccd2d98	$R3m\#166$	$R3m\#166$	0.00	36	-612	80
371	aflow:1046a150b6f38be3	$P3m1\#164$	$P3m1\#164$	0.00	39	-675	83

decomposition reaction:



Au<sub>17</sub>Cu<sub>12</sub> (unstable)

560	aflow:c9bd9f64f9f43552	$I43m\#217$	$I43m\#217$	0.00	4	-72	49
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decomposition reaction:



Au<sub>4</sub>Cu<sub>3</sub> (unstable)

264	aflow:cf7f3988bfa9bfe1	$I4/mmm\#139$	$I4/mmm\#139$	0.00	-25	429	21
364	aflow:715fbec6035c4a9c	$P6/mmm\#191$	$P6/mmm\#191$	0.00	57	-971	103

decomposition reaction:



Au<sub>5</sub>Cu<sub>4</sub> (unstable)

314	aflow:df52a8b748480302	$I4/mmm\#139$	$I4/mmm\#139$	0.00	-4	62	43
360	aflow:2fe82c716ca76e45	$P6_3/mcm\#193$	$P6_3/mcm\#193$	0.00	12	-211	59

decomposition reaction:



Au<sub>7</sub>Cu<sub>6</sub> (unstable)

613	aflow:e38d6b52edc4e2aa	$R3m\#166$	$R3m\#166$	0.00	216	-3632	264
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decomposition reaction:



AuCu (ground-state)

$$\Delta H_{\text{sc}} = 1 \text{ meV/atom}, \Delta H[2|1] = 50 \text{ meV/atom}$$

prototype	auid	original space group	relaxed space group	spin ( $\mu_B$ /atom)	$H_f$ (meV/atom)	$T_S$ (K)	$\Delta H_{\text{hull}}$ (meV/atom)
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90	aflow:4c5e8311267c00ee	<i>Cmmm</i> #65	<i>Cmmm</i> #65	0.00	-50	834	0
291	aflow:6ed221d6611d7ca6	<i>P4/nmm</i> #129	<i>P4/mmm</i> #123	0.00	-49	816	1
292	aflow:f2a7237168e6e4a7	<i>P4/nmm</i> #129	<i>P4/mmm</i> #123	0.00	-48	798	2
447	aflow:7472cdf89358d5e6	<i>P21/m</i> #11	<i>P21/m</i> #11	0.00	-47	781	3
448	aflow:c3f4ab04f81cce5b	<i>P21/m</i> #11	<i>P21/m</i> #11	0.00	-45	757	5
3	aflow:c0614aecf32be432	<i>P4/mmm</i> #123	<i>P4/mmm</i> #123	0.00	-45	752	5
120	aflow:a974fcb1e59b0a35	<i>Pmma</i> #51	<i>Pmma</i> #51	0.00	-44	729	6
ICSD #180861.AB	aflow:3a8fb45b26ce3256	<i>P4/mmm</i> #123	<i>P4/mmm</i> #123	0.00	-42	703	8
ICSD #42574.AB	aflow:a0824585699cf29d	<i>P4/mmm</i> #123	<i>P4/mmm</i> #123	0.00	-42	702	8
61	aflow:bcfdb4a38c43cd22	<i>Pm3m</i> #221	<i>Pm3m</i> #221	0.00	-41	690	9
123	aflow:f4ff58d413a5e8db	<i>C2/m</i> #12	<i>C2/m</i> #12	0.00	-34	562	16
17	aflow:ead3676cf7ce5861	<i>C2/m</i> #12	<i>C2/m</i> #12	0.00	-33	553	17
23	aflow:06e7f61f80e2cad6	<i>I41/amd</i> #141	<i>I41/amd</i> #141	0.00	-31	513	19
543	aflow:3f9731a41d18a38b	<i>Imma</i> #74	<i>I41/amd</i> #141	0.00	-29	484	21
256	aflow:b0be7c80b8bb905d	<i>Pnma</i> #62	<i>Pnma</i> #62	0.00	-22	371	28
192	aflow:0edb7861b3ee7f57	<i>Cmcm</i> #63	<i>Cmcm</i> #63	0.00	-22	370	28
20	aflow:f26cc5280b2a3318	<i>Pmmn</i> #59	<i>Pmmn</i> #59	0.00	-22	363	28
74	aflow:869d973c7e346fcc	<i>P21/m</i> #11	<i>P21/m</i> #11	0.00	-22	360	28
80	aflow:0dce7c6c15b47880	<i>Imma</i> #74	<i>Imma</i> #74	0.00	-19	326	30
138	aflow:ec7ab73e29393f8	<i>Cm</i> #8	<i>Cm</i> #8	0.00	-16	265	34
77	aflow:c9afe272b47ca3cd	<i>P4/nmm</i> #129	<i>P4/nmm</i> #129	0.00	-15	253	35
139	aflow:4e079e8761d95c6e	<i>Cm</i> #8	<i>Cm</i> #8	0.00	-15	252	35
14	aflow:36c87455b9672a5e	<i>P4/nmm</i> #129	<i>P4/nmm</i> #129	0.00	-13	216	37
71	aflow:00a063f574c46a55	<i>Cmmc</i> #67	<i>P4/nmm</i> #129	0.00	-11	182	39
197	aflow:6c01d6fe40e27830	<i>P4/nmm</i> #129	<i>P4/nmm</i> #129	0.00	-10	166	40
196	aflow:8dd63771f1f3fdbb	<i>P4/nmm</i> #129	<i>P4/nmm</i> #129	0.00	-9	153	41
136	aflow:f434b3dfe38a5986	<i>Cm</i> #8	<i>Cm</i> #8	0.00	10	-174	60
119	aflow:024990b371c40524	<i>Pmmn</i> #59	<i>Pmmn</i> #59	0.00	12	-195	61
195	aflow:6981c5847b496a40	<i>P213</i> #198	<i>P213</i> #198	0.00	13	-221	63
198	aflow:a9cd593bcfd6ee1c	<i>Pbcm</i> #57	<i>Pbcm</i> #57	0.00	21	-358	71
4	aflow:c4d2f34e31b7893e	<i>R3m</i> #166	<i>R3m</i> #166	0.00	22	-375	72
28	aflow:9cc6bc3e300ceab6	<i>R3m</i> #166	<i>R3m</i> #166	0.00	34	-571	84
116	aflow:808e9d6ef610b396	<i>P6m2</i> #187	<i>P6m2</i> #187	0.00	36	-597	85
193	aflow:81edce77fefd7bc7	<i>Cmcm</i> #63	<i>Cmcm</i> #63	0.00	40	-671	90
194	aflow:802df5d9ee11b0d1	<i>Cmcm</i> #63	<i>Cmcm</i> #63	0.00	42	-696	91
85	aflow:4b70b21fab9bce03	<i>Fd3m</i> #227	<i>Fd3m</i> #227	0.00	44	-741	94
537	aflow:21dd1aea8336e16d	<i>P3m1</i> #164	<i>R3m</i> #166	0.00	46	-771	96
406	aflow:9dcac19b9dc6f7bc	<i>R3m</i> #166	<i>R3m</i> #166	0.00	47	-781	96
126	aflow:1d50987c9fdfaabf	<i>P3m1</i> #164	<i>P3m1</i> #164	0.00	47	-787	97
538	aflow:1247bba29ace7fa0	<i>R3m</i> #166	<i>R3m</i> #166	0.00	51	-850	101
405	aflow:42c99bd3b54b56f9	<i>R3m</i> #166	<i>R3m</i> #166	0.00	56	-934	106
407	aflow:a7ac5546a19f45ba	<i>P63/mmc</i> #194	<i>P63/mmc</i> #194	0.00	57	-954	107
221	aflow:af3cb3ae9d234841	<i>P63/mmc</i> #194	<i>P63/mmc</i> #194	0.00	170	-2846	220
220	aflow:3fc5bd2750d6cc3e	<i>P63/mmc</i> #194	<i>P63/mmc</i> #194	0.00	205	-3439	255
408	aflow:18084f4aed42304a	<i>P63/mmc</i> #194	<i>P63/mmc</i> #194	0.00	211	-3533	261
201	aflow:46917914822193fe	<i>Fm3m</i> #225	<i>Fm3m</i> #225	0.00	237	-3960	286
219	aflow:fe1c8941049c9dc3	<i>P63mc</i> #186	<i>P63mc</i> #186	0.00	681	-11409	731
218	aflow:9abab2e2184e5839	<i>F43m</i> #216	<i>F43m</i> #216	0.00	688	-11520	738

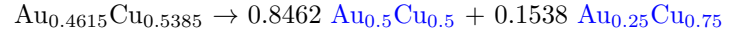
vertex of facets:  
(2-phase equilibria)

$\text{Au}_2\text{Cu}$ – $\text{AuCu}$  and  $\text{AuCu}$ – $\text{AuCu}_3$

$\text{Au}_6\text{Cu}_7$  (unstable)

614	aflow:47cd7a53beb7a8e	<i>R3m</i> #166	<i>R3m</i> #166	0.00	2	-33	50
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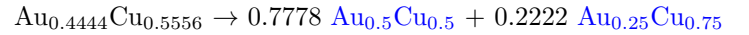
decomposition reaction:



$\text{Au}_4\text{Cu}_5$  (unstable)

313	aflow:310b2a19a1252d54	<i>I4/mmm</i> #139	<i>I4/mmm</i> #139	0.00	-40	681	7
359	aflow:effa94f64a39b9c7	<i>P63/mcm</i> #193	<i>P63/mcm</i> #193	0.00	29	-491	77

decomposition reaction:



$\text{Au}_3\text{Cu}_4$  (unstable)

263	aflow:79dfdcc7d2d26a6f	<i>I4/mmm</i> #139	<i>I4/mmm</i> #139	0.00	-17	294	30
363	aflow:67319b4b7327496e	<i>P6/mmm</i> #191	<i>P6/mmm</i> #191	0.00	247	-4191	294

prototype	auid	original space group	relaxed space group	spin ( $\mu_B$ /atom)	$H_f$ (meV/atom)	$T_S$ (K)	$\Delta H_{\text{hull}}$ (meV/atom)
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decomposition reaction:



$\text{Au}_{12}\text{Cu}_{17}$  (unstable)

559	aflow:7d39f17827558c6b	$I\bar{4}3m\#217$	$I\bar{4}3m\#217$	0.00	111	-1906	158
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decomposition reaction:



$\text{Au}_2\text{Cu}_3$  (unstable)

f47	aflow:89a8ce7ae8c1d0c9	$Immm\#71$	$Immm\#71$	0.00	-38	649	8
f56	aflow:66fbaf66694dc5bc	$C2/m\#12$	$C2/m\#12$	0.00	-30	510	16
f49	aflow:6e1aede47c6b0b4b	$I4/mmm\#139$	$I4/mmm\#139$	0.00	-22	378	24
f44	aflow:40bda952b40c7c93	$C2/m\#12$	$C2/m\#12$	0.00	-15	266	31
f43	aflow:82eb9929aef8cd64	$Immm\#71$	$Immm\#71$	0.00	-8	141	38
f45	aflow:b44a7e3ebbc9f2a9	$I4/mmm\#139$	$I4/mmm\#139$	0.00	-4	76	42
366	aflow:ec85e58e746f4872	$Fdd2\#43$	$Fdd2\#43$	0.00	-4	76	42
f48	aflow:a1cdac1949c7e99c	$C2/m\#12$	$C2/m\#12$	0.00	1	-14	47
260	aflow:37a32686bb5e0698	$R3m\#166$	$R3m\#166$	0.00	33	-575	79
f46	aflow:9158a119f3a24af9	$R3m\#166$	$R3m\#166$	0.00	41	-714	87
f42	aflow:beaa986006ffc59a	$R3m\#166$	$R3m\#166$	0.00	56	-957	102
372	aflow:3b76c915d5d9e4b2	$P3m1\#164$	$P3m1\#164$	0.00	150	-2587	196

decomposition reaction:



$\text{Au}_3\text{Cu}_5$  (unstable)

375	aflow:4d705dbcc826e8cc	$Cmmm\#65$	$Cmmm\#65$	0.00	-37	644	8
223	aflow:d090357ed4c826dc	$P6_3/mcm\#193$	$P6_3/mcm\#193$	0.00	86	-1500	131
254	aflow:95bc65c3121790d0	$C2/m\#12$	$C2/m\#12$	0.00	87	-1519	132

decomposition reaction:



$\text{AuCu}_2$  (unstable)

188	aflow:b554d99a1a47e8ed	$Cmcm\#63$	$Cmcm\#63$	0.00	-37	675	6
382	aflow:e426a6e73906eddff	$I4_1/amd\#141$	$I4_1/amd\#141$	0.00	-37	671	7
211	aflow:9f66d267fa52fc63	$Pnma\#62$	$Pnma\#62$	0.00	-36	658	7
7	aflow:e3e7a0fb8ce2273a	$Immm\#71$	$Immm\#71$	0.00	-30	545	14
657.BA	aflow:851e73256aa6124a	$Immm\#71$	$Immm\#71$	0.00	-28	503	16
257	aflow:bf2b5da1698de45b	$Pnnm\#58$	$Immm\#71$	0.00	-25	448	19
267	aflow:d71eac4326f25ff3	$Pnnm\#58$	$Immm\#71$	0.00	-25	448	19
596	aflow:884c123f5b58ded5	$Cmcm\#63$	$Cmcm\#63$	0.00	-22	393	22
66	aflow:bf0700f2e40159c6	$I4/mmm\#139$	$I4/mmm\#139$	0.00	-20	369	23
150	aflow:1ca4e45a90b47261	$Cmcm\#63$	$Cmcm\#63$	0.00	-17	311	26
232	aflow:91dde1139e5b3996	$I4/mmm\#139$	$I4/mmm\#139$	0.00	-17	310	27
137	aflow:78dbbd3240c2e049	$C2/m\#12$	$C2/m\#12$	0.00	-17	306	27
287	aflow:761ca5ae0622e4ce	$I4/mmm\#139$	$I4/mmm\#139$	0.00	-17	302	27
134	aflow:a9bed1d2947e85e7	$C2/m\#12$	$C2/m\#12$	0.00	-16	283	28
540	aflow:b8a80005b86a59b3	$C2/m\#12$	$C2/m\#12$	0.00	-13	238	30
475	aflow:208ae2a1480399f4	$C2/m\#12$	$C2/m\#12$	0.00	-12	214	32
5	aflow:9a27329dd9325059	$I4/mmm\#139$	$I4/mmm\#139$	0.00	-9	161	35
135	aflow:f08aabe1b6526b45	$C2/m\#12$	$C2/m\#12$	0.00	-8	153	35
548	aflow:14b0d3c4be292eac	$I4/mmm\#139$	$I4/mmm\#139$	0.00	-5	87	39
178	aflow:124194c84818a128	$P6_3/mmc\#194$	$P6_3/mmc\#194$	0.00	5	-85	48
62	aflow:27182dd1c3928a8f	$P3m1\#164$	$P3m1\#164$	0.00	9	-157	52
315	aflow:e55b74aacf2c3309	$P6_3/mmc\#194$	$P6_3/mmc\#194$	0.00	10	-183	54
545	aflow:d911544d7165f346	$P3m1\#164$	$P3m1\#164$	0.00	12	-218	55
216	aflow:431bc08367bd4494	$P6/mmm\#191$	$P6/mmm\#191$	0.00	12	-219	56
270	aflow:ea4b892240a8cfc2	$P3m1\#164$	$P3m1\#164$	0.00	12	-222	56
246	aflow:e2f415523c695f72	$P6_3/mmc\#194$	$P6_3/mmc\#194$	0.00	16	-300	60
133	aflow:4d0a8ecb19696dda	$Cm\#8$	$Cm\#8$	0.00	17	-303	60
183	aflow:4e17dffbf8dc112b0	$Fd3m\#227$	$Fd3m\#227$	0.00	17	-310	61
274	aflow:cdc24b2aed5c4e99	$P6_3/mmc\#194$	$P6_3/mmc\#194$	0.00	36	-653	79
276	aflow:c11d71601bd428d8	$P6_3/mmc\#194$	$P6_3/mmc\#194$	0.00	36	-658	80
208	aflow:ded38bacf03cc819	$P62m\#189$	$P62m\#189$	0.00	36	-659	80
147	aflow:71cd7b9c122365a2	$Cmcm\#63$	$Cmcm\#63$	0.00	40	-736	84
9	aflow:e8edfcd2d5df1570	$P3m1\#164$	$P3m1\#164$	0.00	51	-926	94
284	aflow:04847e8fbef1634c	$Imma\#74$	$Imma\#74$	0.00	116	-2119	160
261	aflow:e1bf7467fcd9e55a	$Fd3m\#227$	$Fd3m\#227$	0.00	144	-2627	188
249	aflow:9dce936fc4f90838	$I4_1/amd\#141$	$I4_1/amd\#141$	0.00	205	-3740	249
231	aflow:2e08c446c8184cad	$I4/mcm\#140$	$I4/mcm\#140$	0.00	216	-3938	260
234	aflow:91300f7e1c582f7d	$I4/mcm\#140$	$I4/mcm\#140$	0.00	216	-3944	260

prototype	auid	original space group	relaxed space group	spin ( $\mu_B$ /atom)	$H_f$ (meV/atom)	$T_S$ (K)	$\Delta H_{\text{hull}}$ (meV/atom)
390	aflow:f3e9f9d885d21ae8	$P4/mmm\#123$	$P4/mmm\#123$	0.00	260	-4748	304
583	aflow:706665bc19bc24fc	$Fm3m\#225$	$Fm3m\#225$	0.00	282	-5146	326
190	aflow:cbb84d97685621f4	$P3m1\#164$	$P3m1\#164$	0.00	308	-5623	352
281	aflow:a8bbf1578155f8dc	$Pa3\#205$	$Pa3\#205$	0.00	509	-9277	552

decomposition reaction:



AuCu<sub>3</sub> (ground-state)

$$\Delta H_{\text{sc}} = 1 \text{ meV/atom}, \Delta H[2|1] = 40 \text{ meV/atom}$$

82	aflow:88cdd0c969ef4d12	$P4/mmm\#123$	$P4/mmm\#123$	0.00	-40	833	0
25	aflow:e816940d150903ac	$Pm3m\#221$	$Pm3m\#221$	0.00	-40	816	1
79	aflow:d39fb2c8b102d201	$Immm\#71$	$Immm\#71$	0.00	-39	815	1
ICSD #40351.AB	aflow:a10f98aa8a8199b7	$Pm3m\#221$	$Pm3m\#221$	0.00	-37	754	4
22	aflow:7ee1256dd88a4fa8	$I4/mmm\#139$	$I4/mmm\#139$	0.00	-37	754	4
238	aflow:d708ef829cc85277	$P63/mmc\#194$	$P63/mmc\#194$	0.00	-36	742	4
280	aflow:b4c9a9f9129b3228	$I4/mmm\#139$	$I4/mmm\#139$	0.00	-36	733	5
245	aflow:22252aee86f6a1f4	$P63/mmc\#194$	$P63/mmc\#194$	0.00	-35	723	5
242	aflow:3e06df2d581f2e68	$Pmnn\#59$	$Pmnn\#59$	0.00	-35	722	5
186	aflow:6105f6d7857babec	$P63/mmc\#194$	$P63/mmc\#194$	0.00	-34	698	7
271	aflow:e8e9fdd83d4ce7d7	$Cmcm\#63$	$Cmcm\#63$	0.00	-33	681	7
542	aflow:78ecc93506ea830c	$Immm\#71$	$I4/mmm\#139$	0.00	-33	674	8
278	aflow:d2f7d873887007a9	$Pmnn\#59$	$Pmnn\#59$	0.00	-31	644	9
73	aflow:56202885c09c6666	$P2/m\#10$	$P2/m\#10$	0.00	-19	392	21
19	aflow:c549a73ff2e51959	$Pmmm\#47$	$Pmmm\#47$	0.00	-17	344	24
16	aflow:29bd19751153c9a7	$C2/m\#12$	$C2/m\#12$	0.00	-3	62	37
13	aflow:e12fe4ab994d5520	$P4/mmm\#123$	$P4/mmm\#123$	0.00	-2	41	38
76	aflow:0e3f8624c8d04894	$P4/mmm\#123$	$P4/mmm\#123$	0.00	0	8	40
180	aflow:abf07ee5490be692	$Pnma\#62$	$Pnma\#62$	0.00	3	-54	43
472	aflow:f68a47556f28d5a4	$Cmcm\#63$	$Cmcm\#63$	0.00	4	-78	44
84	aflow:ab8438914fe47c67	$Fm3m\#225$	$Fm3m\#225$	0.00	5	-100	45
11	aflow:dbe034b67e1b48f2	$Cmmm\#65$	$Cmmm\#65$	0.00	6	-131	47
118	aflow:e889de245081ef9a	$Pmm2\#25$	$Pmm2\#25$	0.00	8	-162	48
122	aflow:f70ed36ae6ffbd75	$Imm2\#44$	$Imm2\#44$	0.00	11	-232	52
70	aflow:07417cfb5ace1a21	$Cmmm\#65$	$Cmmm\#65$	0.00	22	-452	62
184	aflow:d706eed8aef6b53	$Pm3n\#223$	$Pm3n\#223$	0.00	48	-986	88
68	aflow:0e02db91c004f48f	$R3m\#166$	$R3m\#166$	0.00	51	-1049	91
27	aflow:70a5143e6c24493d	$R3m\#166$	$R3m\#166$	0.00	55	-1139	96
125	aflow:f6c52fd263dc74a5	$P6m2\#187$	$P6m2\#187$	0.00	68	-1401	108
289	aflow:7d88e2493c29f696	$Pm3m\#221$	$Pm3m\#221$	0.00	1090	-22500	1131

vertex of facets:

(2-phase equilibria)

AuCu–AuCu<sub>3</sub> and AuCu<sub>3</sub>–Cu

AuCu<sub>4</sub> (unstable)

285	aflow:b725321fe141e71e	$I4/m\#87$	$I4/m\#87$	0.00	-27	616	6
557	aflow:a407190402039c66	$I4/m\#87$	$I4/m\#87$	0.00	-24	567	8
f51	aflow:e1b120f15909f8f8	$Immm\#71$	$Immm\#71$	0.00	-10	234	22
f52	aflow:a712f3662e0616e0	$C2/m\#12$	$C2/m\#12$	0.00	-2	55	30
f53	aflow:26e7c931da2d7b28	$I4/mmm\#139$	$I4/mmm\#139$	0.00	4	-91	36
f50	aflow:38ab356ed9b02a70	$R3m\#166$	$R3m\#166$	0.00	59	-1359	91
374	aflow:015f6c92bb598b06	$I23\#197$	$I43m\#217$	0.00	170	-3941	202
202	aflow:6c4de915c35200e6	$I4/mmm\#139$	$I4/mmm\#139$	0.00	189	-4390	222
654.BA	aflow:f51669ea9453f93c	$Im3m\#229$	$Im3m\#229$	0.00	577	-13372	609

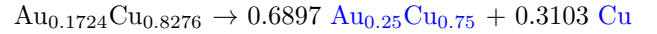
decomposition reaction:



Au<sub>5</sub>Cu<sub>24</sub> (unstable)

412	aflow:ce1a0416a16da439	$I43m\#217$	$I43m\#217$	0.00	26	-664	54
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decomposition reaction:

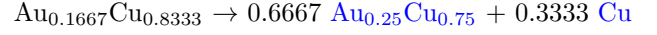


AuCu<sub>5</sub> (unstable)

479	aflow:ed911a9f779e273b	$Cmmm\#65$	$Cmmm\#65$	0.00	-19	502	7
474	aflow:28d4ad4e00061705	$P62m\#189$	$P62m\#189$	0.00	-5	137	22
478	aflow:6d182ae8e93f939d	$P4/mmm\#123$	$P4/mmm\#123$	0.00	7	-184	34
128	aflow:ad82db74e555f500	$Cm\#8$	$Cm\#8$	0.00	11	-296	38
141	aflow:bba4c2f16cc7ccf56	$Am2\#38$	$Am2\#38$	0.00	16	-409	43
252	aflow:cb864365d4ae1ba	$F43m\#216$	$F43m\#216$	0.00	71	-1830	98
204	aflow:3a992a07625695a3	$P6/mmm\#191$	$P6/mmm\#191$	0.00	118	-3038	145

prototype	auid	original space group	relaxed space group	spin ( $\mu_B$ /atom)	$H_f$ (meV/atom)	$T_S$ (K)	$\Delta H_{\text{hull}}$ (meV/atom)
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decomposition reaction:



AuCu<sub>7</sub> (unstable)

309	aflow:fd1d7b4015286364	$Fm\bar{3}m\#225$	$Fm\bar{3}m\#225$	0.00	-3	88	17
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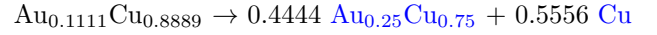
decomposition reaction:



AuCu<sub>8</sub> (unstable)

312	aflow:ca1001bc6033c32a	$I4/mmm\#139$	$I4/mmm\#139$	0.00	857	-28501	875
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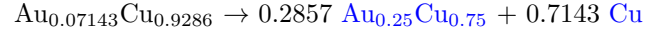
decomposition reaction:



AuCu<sub>13</sub> (unstable)

367	aflow:5bc602bee9a50c6f	$Fm\bar{3}c\#226$	$Fm\bar{3}c\#226$	0.00	184	-8320	196
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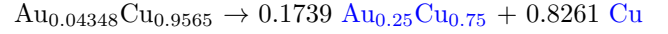
decomposition reaction:



AuCu<sub>22</sub> (unstable)

426	aflow:c60caac643cdf43f	$Fd\bar{3}m\#227$	$Fd\bar{3}m\#227$	0.00	82	-5326	89
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decomposition reaction:



## unaries

Au (ground-state)

$$\Delta H_{\text{sc}} = 4 \text{ meV/atom}$$

324	aflow:aff2afa21f9ff4c2	$P3_121\#152$	$C2/m\#12$	0.00	-5	0	0
A7.B	aflow:3e979e27e5d19925	$R\bar{3}m\#166$	$Fm\bar{3}m\#225$	0.00	-1	0	4
A7	aflow:dd2c29b6fa4bd8e3	$R\bar{3}m\#166$	$Fm\bar{3}m\#225$	0.00	-1	0	4
A7.A	aflow:6d1ed8a51196cdce	$R\bar{3}m\#166$	$Fm\bar{3}m\#225$	0.00	-1	0	5
A8	aflow:efd182804ffef0c3	$P3_121\#152$	$Fm\bar{3}m\#225$	0.00	0	0	5
A1	aflow:fd27d052b14c5203	$Fm\bar{3}m\#225$	$Fm\bar{3}m\#225$	0.00	0	0	5
1	aflow:13372e31f4c850a	$Fm\bar{3}m\#225$	$Fm\bar{3}m\#225$	0.00	0	0	5
2	aflow:ca6394569c4c660f	$Fm\bar{3}m\#225$	$Fm\bar{3}m\#225$	0.00	0	0	5
f1	aflow:307b621b5eb3a7d4	$Fm\bar{3}m\#225$	$Fm\bar{3}m\#225$	0.00	0	0	5
f2	aflow:362fdce9a6a43d79	$Fm\bar{3}m\#225$	$Fm\bar{3}m\#225$	0.00	0	0	5
A7.A	aflow:bd59e41e9692616a	$Fm\bar{3}m\#225$	$Fm\bar{3}m\#225$	0.00	0	0	6
A6	aflow:f8504c6ef9ddfbca	$I4/mmm\#139$	$Fm\bar{3}m\#225$	0.00	0	0	6
303	aflow:3148d330e6399443	$I4/mmm\#139$	$Fm\bar{3}m\#225$	0.00	1	0	6
304	aflow:b54344657841af94	$I4/mmm\#139$	$I4/mmm\#139$	0.00	1	0	6
A3	aflow:1074df487a47535e	$P6_3/mmc\#194$	$P6_3/mmc\#194$	0.00	6	0	11
115	aflow:2088043c87b73668	$P6_3/mmc\#194$	$P6_3/mmc\#194$	0.00	6	0	11
h3	aflow:8cbf0aa6a2f18ea9	$P6_3/mmc\#194$	$P6_3/mmc\#194$	0.00	6	0	11
117	aflow:4b66a87733337b82	$P6_3/mmc\#194$	$P6_3/mmc\#194$	0.00	6	0	11
h1	aflow:324aa867efdf0963	$P6_3/mmc\#194$	$P6_3/mmc\#194$	0.00	6	0	11
317	aflow:5474c00c12bc0bd8	$Cmce\#64$	$I4/mmm\#139$	0.00	14	0	19
318	aflow:7cc1e61d030f7779	$Cmce\#64$	$I4/mmm\#139$	0.00	14	0	19
307	aflow:1963ea8bf251abc1	$P\bar{3}m1\#164$	$R\bar{3}m\#166$	0.00	21	0	27
308	aflow:04e7d87785b478e5	$P\bar{3}m1\#164$	$R\bar{3}m\#166$	0.00	21	0	27
A2	aflow:42d35f144647f73b	$Im\bar{3}m\#229$	$Im\bar{3}m\#229$	0.00	23	0	28
58	aflow:31dd67bb8f65d81c	$Im\bar{3}m\#229$	$Im\bar{3}m\#229$	0.00	23	0	28
59	aflow:0094dbfc4fdb45f2	$Im\bar{3}m\#229$	$Im\bar{3}m\#229$	0.00	23	0	28
b2	aflow:e908e919a44d7806	$Im\bar{3}m\#229$	$Im\bar{3}m\#229$	0.00	23	0	28
b1	aflow:35cf7f959780e51f	$Im\bar{3}m\#229$	$Im\bar{3}m\#229$	0.00	23	0	28
306	aflow:ec28e1972aae4071	$I4_1/amd\#141$	$I4_1/amd\#141$	0.00	148	0	154
305	aflow:68981f8fe574a335	$I4_1/amd\#141$	$I4_1/amd\#141$	0.00	156	0	162
A5	aflow:d870402f19ee3e7	$I4_1/amd\#141$	$I4_1/amd\#141$	0.00	157	0	162
305	aflow:661ba1fbd82e8d39	$I4_1/amd\#141$	$I4_1/amd\#141$	0.00	214	0	219
325	aflow:f3f14882c506f990	$P6_3/mmc\#194$	$P6_3/mmc\#194$	0.00	556	0	561
A9	aflow:ef5ee36cc18cc108	$P6_3/mmc\#194$	$P6_3/mmc\#194$	0.00	565	0	571
301	aflow:939087b9e34b4d34	$Fd\bar{3}m\#227$	$Fd\bar{3}m\#227$	0.00	710	0	716
302	aflow:b3f07c0876be10e	$Fd\bar{3}m\#227$	$Fd\bar{3}m\#227$	0.00	710	0	716
A4	aflow:dde2ca328bbb22f7	$Fd\bar{3}m\#227$	$Fd\bar{3}m\#227$	0.00	714	0	719
0	aflow:70eeb6d5af8a2c8b	$NNN\#0$	$NNN\#0$	1.00	2986	0	2991



prototype	auid	original space group	relaxed space group	spin ( $\mu_B$ /atom)	$H_f$ (meV/atom)	$T_S$ (K)	$\Delta H_{\text{hull}}$ (meV/atom)
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Cu (ground-state)

$\Delta H_{\text{sc}} = 4$  meV/atom

324	aflow:d34bef79cfbf1a1a	$P3_121\#152$	$I4/mmm\#139$	0.00	-5	0	0
304	aflow:186cd42fc850f2b4	$I4/mmm\#139$	$I4/mmm\#139$	0.00	0	0	5
A7.B	aflow:bfe6d927af6631ea	$R\bar{3}m\#166$	$R\bar{3}m\#166$	0.00	0	0	4
A7.A	aflow:c13377b09a507e8a	$R\bar{3}m\#166$	$R\bar{3}m\#166$	0.00	0	0	4
A7.A	aflow:80e862301eea8ed6	$R\bar{3}m\#166$	$Fm\bar{3}m\#225$	0.00	0	0	4
A7.B	aflow:d46f44f5aa2cb0d4f	$R\bar{3}m\#166$	$Fm\bar{3}m\#225$	0.00	0	0	4
A1	aflow:6cd3ec04b89859fb	$Fm\bar{3}m\#225$	$Fm\bar{3}m\#225$	0.00	0	0	5
A6	aflow:3bb5d28f0c05bedd	$I4/mmm\#139$	$Fm\bar{3}m\#225$	0.00	0	0	5
1	aflow:ee9598b295d1f30e	$Fm\bar{3}m\#225$	$Fm\bar{3}m\#225$	0.00	0	0	5
2	aflow:d221bd6a6ef0db74	$Fm\bar{3}m\#225$	$Fm\bar{3}m\#225$	0.00	0	0	5
f1	aflow:cd49ebd39dca1b2c	$Fm\bar{3}m\#225$	$Fm\bar{3}m\#225$	0.00	0	0	5
f2	aflow:53300de18bccfd51	$Fm\bar{3}m\#225$	$Fm\bar{3}m\#225$	0.00	0	0	5
A7	aflow:3e284503257be238	$R\bar{3}m\#166$	$Fm\bar{3}m\#225$	0.00	0	0	5
A8	aflow:d7a563938d27e0ed	$P3_121\#152$	$Fm\bar{3}m\#225$	0.00	1	0	5
A3	aflow:c5f7577f9bd4e8b7	$P6_3/mmc\#194$	$P6_3/mmc\#194$	0.00	8	0	13
h1	aflow:d7d9190d6b88f192	$P6_3/mmc\#194$	$P6_3/mmc\#194$	0.00	8	0	13
h3	aflow:d0730e156256643c	$P6_3/mmc\#194$	$P6_3/mmc\#194$	0.00	8	0	13
115	aflow:973c5f4d3ccf95f	$P6_3/mmc\#194$	$P6_3/mmc\#194$	0.00	8	0	13
117	aflow:b33fe15736eae678	$P6_3/mmc\#194$	$P6_3/mmc\#194$	0.00	8	0	13
A2	aflow:3a8288a412e047ca	$Im\bar{3}m\#229$	$Im\bar{3}m\#229$	0.00	34	0	39
59	aflow:0b423a6aed492759	$Im\bar{3}m\#229$	$Im\bar{3}m\#229$	0.00	35	0	40
b2	aflow:9c5a71303ead7be8	$Im\bar{3}m\#229$	$Im\bar{3}m\#229$	0.00	35	0	40
58	aflow:d891c3801bf66dcf	$Im\bar{3}m\#229$	$Im\bar{3}m\#229$	0.00	35	0	40
b1	aflow:6df4406197842531	$Im\bar{3}m\#229$	$Im\bar{3}m\#229$	0.00	35	0	40
307	aflow:b6d6f5066b25ca24	$P\bar{3}m1\#164$	$P\bar{3}m1\#164$	0.00	39	0	43
308	aflow:ea8668c40e7fa689	$P\bar{3}m1\#164$	$P\bar{3}m1\#164$	0.00	39	0	43
307	aflow:7bfa1066a9b47a01	$P\bar{3}m1\#164$	$C2/m\#12$	0.00	62	0	66
308	aflow:16c1eb270a90ff0c	$P\bar{3}m1\#164$	$C2/m\#12$	0.00	62	0	66
317	aflow:8b7c692bf66bf9f9	$Fm\bar{m}m\#69$	$Fm\bar{m}m\#69$	0.00	161	0	166
317	aflow:1050a71c52c00445	$Cmce\#64$	$Fm\bar{m}m\#69$	0.00	174	0	178
318	aflow:4a9f231dbe21179f	$Cmce\#64$	$Fm\bar{m}m\#69$	0.00	174	0	178
317	aflow:d22d0d6cb59c2e9a	$Cmce\#64$	$Fm\bar{m}m\#69$	0.00	231	0	235
318	aflow:97a64f9fb7cb3e1b	$Cmce\#64$	$Fm\bar{m}m\#69$	0.00	231	0	235
317	aflow:9dc724437000b957	$Cmce\#64$	$I4/mmm\#139$	0.00	247	0	252
318	aflow:44c15e45114bb843	$Cmce\#64$	$Fm\bar{m}m\#69$	0.00	248	0	253
A5	aflow:bc2100b933b9c2e9	$I4_1/amd\#141$	$I4_1/amd\#141$	0.00	321	0	325
305	aflow:4e53ea3edbd452f05	$I4_1/amd\#141$	$I4_1/amd\#141$	0.00	332	0	336
306	aflow:dd084675ee8f73ff	$I4_1/amd\#141$	$I4_1/amd\#141$	0.00	332	0	336
307	aflow:28be870810b1fa44	$P\bar{3}m1\#164$	$R\bar{3}m\#166$	0.00	461	0	466
308	aflow:64a1241cd26d1e2b	$C2/m\#12$	$R\bar{3}m\#166$	0.00	465	0	470
A4	aflow:1d2eec8495b9a047	$Fd\bar{3}m\#227$	$Fd\bar{3}m\#227$	0.00	1026	0	1031
301	aflow:de59b5b38c412a4f	$Fd\bar{3}m\#227$	$Fd\bar{3}m\#227$	0.00	1031	0	1035
302	aflow:3b14f36d0b530892	$Fd\bar{3}m\#227$	$Fd\bar{3}m\#227$	0.00	1031	0	1035
0	aflow:36d2754818b691f9	$NNN\#0$	$NNN\#0$	1.00	3478	0	3482
0	aflow:beb98215b6935fd9	$NNN\#0$	$NNN\#0$	1.00	3497	0	3502