

Supporting Information for:

Synthesis, structure and electrical properties of single-crystal Ba₈Cu₁₆As₃₀

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Table S1. Anisotropic atomic displacement parameters* ($\text{\AA}^2$) for $\text{Ba}_8\text{Cu}_{16}\text{As}_{30}$

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
Ba1	0.00713(8)	0.00713(8)	0.00713(8)	0.000	0.000	0.000
Ba2	0.0239(7)	0.0102(7)	0.0228(8)	0.0005(7)	0.000	0.000
As3/Cu3	0.0084(2)	0.00583(14)	0.00583(14)	0.000	0.000	0.000
As4/Cu4	0.00813(13)	0.00813(13)	0.00813(13)	-0.00128(11)	-0.00128(11)	-0.00128(11)
As5/Cu5	0.00845(9)	0.0063(3)	0.00669(13)	-0.0009(2)	0.000	0.000

* The anisotropic atomic displacement factor exponent takes the form: $-2\pi^2 [h^2 a^{*2} U_{11} + \dots + 2hka^*b^*U_{12}]$

Table S2. Selected atomic distances (Å) and their average values for Ba₈Cu₁₆As₃₀. The distances listed on the left-hand column involved the disordered ‘As’ and those in the right-hand column involve the disordered ‘Cu’ sites.

As-sites			Cu-sites			Ave _{As-Cu} (Å)
Atoms	Distances(Å)	Ave(Å)	Atoms	Distances(Å)	Ave(Å)	
Ba1-As4	3.365(4) x8	3.412	Ba1-Cu4	3.311(5) x8	3.424	3.418
-As5	3.443(4) x12		-Cu5	3.499(9) x12		
Ba2-As3	3.530(5) x2	3.733	Ba2-Cu3	3.530(5) x2	3.728	3.731
-As3	3.737(4) x2		-Cu3	3.737(4) x2		
-As4	3.965(3) x2		-Cu4	3.979(3) x2		
-As4	4.045(3) x2		-Cu4	4.062(3) x2		
-As4	3.776(3) x2		-Cu4	3.794(4) x2		
-As4	3.737(4) x2		-Cu4	3.743(4) x2		
-As5	3.840(4) x2		-Cu5	3.875(4) x2		
-As5	3.560(5) x2		-Cu5	3.512(5) x2		
-As5	3.427(5) x2		-Cu5	3.379(5) x2		
-As5	3.460(5) x2		-Cu5	3.416(5) x2		
-As5	3.673(5) x2		-Cu5	3.624(5) x2		
-As5	4.046(3) x2		-Cu5	4.081(3) x2		
As3-As5	2.440(3) x4	2.428	As3-Cu5	2.397(9) x4	2.424	2.426
As4-As4	2.327(8)		As4-Cu4	2.380(6)		
-As5	2.425(2) x3		-Cu5	2.469(5) x3		
As5-As3	2.440(3)		As5-Cu3	2.440(3)		
-As4	2.425(2) x2		-Cu4	2.408(3) x2		
-As5	2.478(6)		-Cu5	2.455(6)		
			Cu3-As5	2.440(3) x4	2.425	
			Cu4-As4	2.327(8)		
			-As5	2.408(3) x3		
			Cu5-As3	2.397(9)		
			-As4	2.469(3) x2		
			-As5	2.455(6)		
			Cu3-Cu5	2.397(9) x4	2.426	
			Cu4-Cu4	2.43(2)		
			-Cu5	2.453(6) x3		
			Cu5-Cu3	2.397(9)		
			-Cu4	2.453(6) x2		
			-Cu5	2.43(2)		

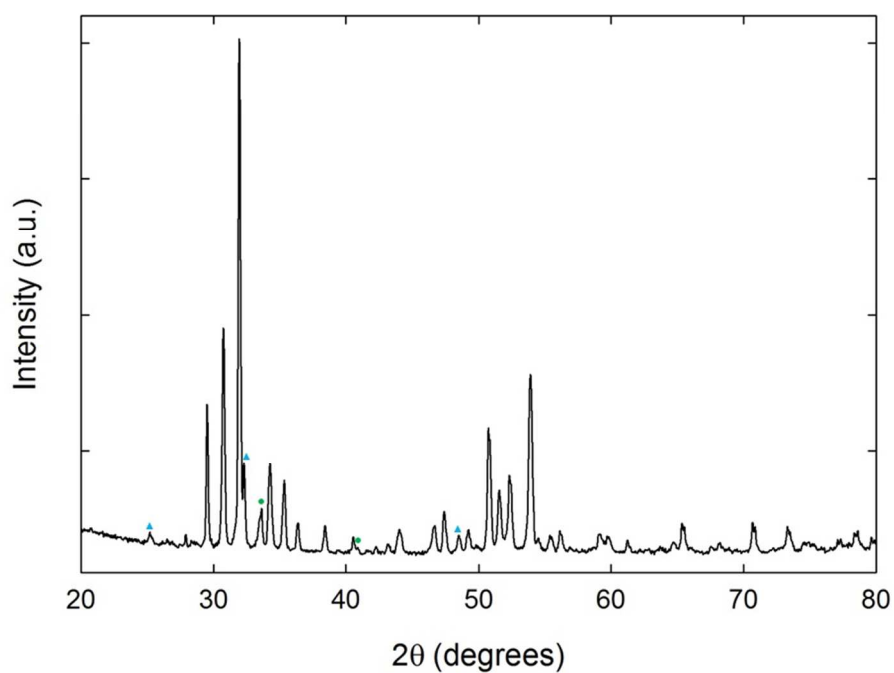


Figure S1. Powder X-ray diffraction pattern of the microcrystalline synthetic product indicating primarily clathrate-I $\text{Ba}_8\text{Cu}_{16}\text{As}_{30}$ with As (triangle) and BaCu_2As_2 (circle) as impurity phases. These impurities represent less than 5% of the total yield when considering that the single-crystals were not ground and used in taking these data.

Coordinate file (xyz format) for the Ba₈Cu₁₆As₃₀ (C1) structure:

```

213
Ba8Cu16As30_C1
As 2.691492 0.000000 5.382984
As 2.691492 10.765968 5.382984
As 8.074476 0.000000 5.382984
As 8.074476 10.765968 5.382984
As 5.382984 2.691492 0.000000
As 5.382984 2.691492 10.765968
As 5.382984 8.074476 0.000000
As 5.382984 8.074476 10.765968
As 0.000000 5.382984 2.691492
As 10.765968 5.382984 2.691492
As 0.000000 5.382984 8.074476
As 10.765968 5.382984 8.074476
As 0.000000 3.219694 1.311966
As 10.765968 3.219694 1.311966
As 0.000000 7.546275 9.454002
As 10.765968 7.546275 9.454002
As 0.000000 7.546275 1.311966
As 10.765968 7.546275 1.311966
As 0.000000 3.219694 9.454002
As 10.765968 3.219694 9.454002
As 1.311966 0.000000 3.219694
As 1.311966 10.765968 3.219694
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As 9.454002 10.765968 7.546275
As 1.311966 0.000000 7.546275
As 1.311966 10.765968 7.546275
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As 9.454002 10.765968 3.219694
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As 3.219694 1.311966 10.765968
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As 7.546275 9.454002 10.765968
As 7.546275 1.311966 0.000000
As 7.546275 1.311966 10.765968
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As 3.219694 9.454002 10.765968
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As 2.163291 5.382984 6.694951
As 2.163291 5.382984 4.071018
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As 5.382984 6.694951 8.602677
As 5.382984 4.071018 2.163291
As 6.694951 8.602677 5.382984
As 4.071018 2.163291 5.382984
As 6.694951 2.163291 5.382984
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Cu 8.797357 8.797357 1.968612
Cu 1.968612 1.968612 8.797357
Cu 8.797357 1.968612 8.797357
Cu 1.968612 8.797357 1.968612
Cu 1.968612 8.797357 8.797357
Cu 8.797357 1.968612 1.968612
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Cu 3.414372 3.414372 7.351596
Cu 3.414372 3.414372 3.414372

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Cu	7.351596	3.414372	3.414372
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Ba	5.382984	10.765968	8.074476
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Ba	2.691492	5.382984	10.765968
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Ba	10.765968	2.691492	5.382984
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As	7.546275	-1.311966	0.000000

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Coordinate file (xyz format) for the Ba₈Cu₁₆As₃₀ (C2) structure:

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Ba 3.200810 5.571548 0.117212
Ba 8.228022 4.535957 10.426970
Ba 10.287051 2.270965 5.924329
Ba 0.186684 7.881132 5.010854
As 2.360696 10.461679 5.224073
As 4.805440 2.418010 10.278143
As 5.833545 8.291276 0.032727
As 0.163827 5.481334 7.571872
As 2.102120 1.655926 2.190088
As 9.313114 9.318634 2.040393
As 8.449978 1.323116 8.707850
As 1.810945 7.825665 9.099594
As 8.102255 7.415360 3.197928
As 3.450016 2.783495 4.013366
As 6.945592 2.312576 7.119157
As 4.207157 7.027760 3.410083
As 3.917677 7.386150 7.164259
As 8.190048 3.544908 2.821191
As 0.754095 3.575012 1.276162
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As 0.017247 2.745632 9.540688
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As	7.320933	9.230841	10.640576
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As	6.121727	4.309060	1.640264
As	2.659142	1.828217	6.233916
As	7.038198	1.219002	4.936584
As	5.559123	7.971282	5.371863
Cu	8.537614	9.916904	5.483915
Cu	0.984412	5.708714	2.510223
Cu	8.731490	8.228358	8.898079
Cu	1.596129	1.034703	8.902332
Cu	2.300039	8.059666	2.388389
Cu	10.126002	2.264753	2.368910
Cu	1.734088	3.502160	7.929290
Cu	7.427863	6.378234	7.753836
Cu	11.133155	7.732285	1.434318
Cu	0.354639	0.367160	3.455179
Cu	8.925474	0.444151	3.475260
Cu	6.661849	0.881812	10.239896
Cu	2.405794	5.572962	6.553569
Cu	6.142010	6.749740	1.885824
Cu	7.904028	7.521983	5.653012
As	10.642898	-3.271356	-1.061521
As	9.748322	-0.243986	-3.193079
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As	4.762564	4.342720	-2.696888
As	5.387552	3.021833	-0.447272
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As	7.607937	2.941084	13.546606
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As	-1.343735	5.510046	3.073293
As	-1.952334	5.432702	6.296801
As	-1.338064	9.929220	7.532337
As	0.730755	-0.821368	7.548834
As	2.983446	0.419209	10.824169
As	11.816691	3.575012	1.276162
As	11.201220	7.505673	-1.061521
As	1.802374	-0.315350	5.224073
As	6.762611	-1.546188	10.640576
Ba	8.810133	5.139780	-0.298446
Cu	7.979292	-0.860125	5.483915

Cu	10.574833	-3.044744	1.434318
Cu	9.483796	11.221180	3.475260

Coordinate file (xyz format) for the Ba₈CuAs₃₀ (C3) structure:

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Ba 5.329104 -0.087591 7.837046
Ba 5.327656 10.555068 2.762663
Ba 8.172301 5.121236 10.570117
Ba 10.622919 8.130925 5.243287
Ba 0.150304 2.405200 5.622988
As 1.983925 1.838076 1.967740
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As 3.463814 3.197714 7.321358
As 7.448329 1.212872 10.596996
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As 8.736255 5.278733 6.643800
As 3.550010 7.268243 7.232683
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As 7.372081 3.310008 7.391527
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As 9.396766 -0.035699 3.241671
As 3.353678 1.066410 0.004080
As 6.755516 8.605617 5.338996
As 6.632829 1.938874 5.319193
As 5.395806 6.486320 8.732832
As 0.116339 5.061624 3.085984
As 5.364215 4.103436 2.085353
As 0.177169 3.148800 9.419322
As 9.441393 -0.104659 7.397505
Cu 8.675921 5.157384 4.250203
Cu 4.177200 1.967014 5.324644
Cu 5.383094 4.104805 8.542188
Cu 4.295133 8.586092 5.358610
Cu 1.508657 10.557944 7.234128
Cu 0.172200 5.227710 8.089268
Cu 2.245788 5.254370 4.132264
Cu 8.806511 8.732718 8.726233
Cu 1.469774 10.632219 3.372395
Cu 8.796144 1.875825 8.660727
Cu 5.403876 7.860325 10.703624
Cu 2.220184 1.959229 8.920280
Cu 8.047940 -0.083026 5.342430
Cu 1.930683 8.402953 1.947564
Cu 8.544636 1.817292 1.950457
Cu 7.294934 7.290803 3.397453

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As	7.634967	11.914248	10.596996
As	10.618502	7.112217	11.812303
As	8.705237	8.487936	12.723926
As	9.628031	10.596717	7.397505
As	9.643179	10.491195	13.954437
As	10.702750	13.753872	12.076918
As	12.712349	8.734282	8.645305
As	12.790895	12.364970	12.680506
As	10.924363	13.850176	9.419322
As	13.854179	9.005523	10.831231
As	14.160647	11.593304	10.716846
As	-0.104219	3.226978	1.364152
As	0.057914	7.494421	-1.420099
As	-0.001830	7.286700	1.099537
As	0.117393	3.323283	-1.293444
As	3.413453	0.891928	10.716846
As	6.568878	-2.095759	5.338996
As	7.228624	-1.452549	10.638922
As	3.540315	11.767786	0.004080
As	2.949329	10.643786	5.291376
As	7.355486	9.423309	-0.073844
As	6.819467	12.640249	5.319193
As	10.516112	3.052495	12.076918
As	10.737725	3.148800	9.419322
As	9.583404	10.665677	3.241671
As	-1.163791	-0.035699	3.241671
As	-1.119164	-0.104659	7.397505
As	-1.824302	5.278733	6.643800
As	10.676895	5.061624	3.085984
As	-0.932526	10.596717	7.397505
As	0.117689	7.319938	9.292666
As	-0.977153	10.665677	3.241671
As	2.170562	12.539453	1.967740
As	5.441518	6.540812	12.770370
As	3.293623	9.005523	10.831231
As	7.388554	1.387354	-0.115769
Ba	-0.124275	-2.570451	5.243287
Ba	0.062363	8.130925	5.243287
Ba	10.436281	-2.570451	5.243287
Cu	1.283136	-0.069157	3.372395
Cu	8.234578	10.618350	5.342430

Coordinate file (xyz format) for the As₄₆ structure:

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64
As46
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As 2.845709 11.382835 5.691418
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As 8.537127 11.382835 5.691418
As 5.691418 2.845709 0.000000
As 5.691418 2.845709 11.382835
As 5.691418 8.537127 0.000000
As 5.691418 8.537127 11.382835
As 0.000000 5.691418 2.845709
As 11.382835 5.691418 2.845709
As 0.000000 5.691418 8.537127
As 11.382835 5.691418 8.537127
As 1.980025 1.980025 1.980025
As 9.402810 9.402810 9.402810
As 9.402810 9.402810 1.980025

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As	9.402810	1.980025	1.980025
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As	3.711393	7.671443	7.671443
As	7.671443	3.711393	3.711393
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As	0.000000	7.964440	1.373589
As	11.382835	7.964440	1.373589
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As	10.009247	0.000000	3.418395
As	10.009247	11.382835	3.418395
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As	7.964440	10.009247	11.382835
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As	2.273023	5.691418	7.065006
As	2.273023	5.691418	4.317829
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As	5.691418	7.065006	9.109813
As	5.691418	4.317829	2.273023
As	7.065006	9.109813	5.691418
As	4.317829	2.273023	5.691418
As	7.065006	2.273023	5.691418
As	4.317829	9.109813	5.691418