Supplementary Information

Crystal structure and X-ray powder diffraction data of barium copper iodate $Ba_2Cu(IO_3)_6$

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TABLE SI. Indexed X-ray powder diffraction data of $Ba_2Cu(IO_3)_6$. The *d*-values were calculated using Cu Kα_1 radiation (λ = 1.5405981 Å).

Figure S1. Optical microscopy image of as-synthesized $Ba_2Cu(IO_3)_6$ crystals.

Figure S2. The energy-dispersive X-ray spectroscope of the $Ba_2Cu(IO_3)_6$ crystal.

Figure S3. The experimental powder X-ray diffraction pattern and the simulated pattern derived from the single crystal structure.

TABLE SI. Indexed X-ray powder diffraction data of $Ba_2Cu(IO_3)_6$. The *d*-values were calculated using Cu Kα_1 radiation (λ = 1.5405981 Å).

$2\theta_{obs}$ (°)	d_{obs} (Å)	$(I/I_o)_{obs}$	*h*	*k*	*l*	$2\theta_{cal}$ (°)	d_{cal} (Å)	$(I/I_o)_{cal}$	$\Delta 2\theta$ (°)
23.563	3.7726	4.0	1	1	1	23.549	3.7748	2.0	-0.014
23.676	3.7549	33.2	0	0	2	23.687	3.7532	33.8	0.011
24.104	3.6892	57.2	2	0	0	24.095	3.6905	44.3	-0.009
24.192	3.6760	55.6	0	2	0	24.202	3.6745	41.2	0.010
24.723	3.5982	10.5	0	-1	2	24.740	3.5957	12.9	0.017
25.096	3.5456	23.1	0	-2	1	25.112	3.5433	31.1	0.016
25.362	3.5090	57.9	-1	0	2	25.382	3.5063	38.0	0.020
25.671	3.4674	12.8	-2	0	1	25.669	3.4676	11.9	-0.002
26.875	3.3148	43.7	1	-2	1	26.881	3.3140	56.2	0.006
27.184	3.2777	56.3	-1	-1	2	27.198	3.2762	59.3	0.014
27.735	3.2138	45.9	-2	1	1	27.734	3.2140	45.9	-0.001
27.805	3.2059	100.0	1	0	2	27.814	3.2050	100.0	0.009
28.292	3.1518	5.8	2	-1	1	28.291	3.1519	4.6	-0.001
28.620	3.1165	88.4	2	1	0	28.610	3.1175	85.6	-0.010
28.755	3.1022	89.6	0	2	1	28.764	3.1012	87.0	0.009
29.122	3.0639	12.5	-1	1	2	29.125	3.0635	10.6	0.003
31.027	2.8800	6.0	0	-2	2	31.048	2.8780	6.1	0.021
31.683	2.8218	11.8	-2	2	0	31.683	2.8219	9.9	0.000
32.045	2.7908	12.2	-2	0	2	32.046	2.7907	7.5	0.001
33.005	2.7118	19.7	1	-2	2	33.024	2.7103	26.1	0.019
33.404	2.6803	16.2	2	-2	1	33.401	2.6805	17.9	-0.003
33.738	2.6545	18.0	-1	-2	2	33.752	2.6535	19.8	0.014
34.187	2.6206	19.8	-2	-1	2	34.199	2.6198	17.6	0.012
34.415	2.6038	22.1	-2	2	1	34.414	2.6039	19.0	-0.001
34.490	2.5983	28.8	-2	1	2	34.491	2.5982	17.5	0.001
35.405	2.5332	4.4	2	-1	2	35.405	2.5333	4.6	0.000
35.949	2.4961	2.2	2	0	2	35.941	2.4967	1.8	-0.008
36.587	2.4540	6.1	-1	0	3	36.591	2.4538	2.9	0.004
36.690	2.4474	9.5	-2	-2	1	36.692	2.4473	4.9	0.002
36.897	2.4342	8.0	-1	2	2	36.898	2.4341	5.3	0.001
36.975	2.4292	8.2	2	2	0	36.967	2.4297	3.8	-0.008
39.359	2.2874	20.9	3	-1	1	39.341	2.2884	19.4	-0.018
39.789	2.2637	7.0	3	0	1	39.768	2.2648	3.0	-0.021
39.986	2.2530	38.8	-1	-3	1	39.977	2.2534	21.1	-0.009
40.467	2.2273	4.6	1	3	0	40.451	2.2281	2.0	-0.016
40.526	2.2242	7.0	2	1	2	40.517	2.2246	4.6	-0.009
41.013	2.1989	9.4	1	2	2	41.000	2.1995	5.6	-0.013

TABLE SI. Continued

$2\theta_{obs}$ (°)	d_{obs} (Å)	$(I/I_o)_{obs}$	h	k	l	$2\theta_{cal}$ (°)	d_{cal} (Å)	$(I/I_o)_{cal}$	$\Delta 2\theta$ (°)
41.085	2.1952	11.8	2	2	1	41.063	2.1963	6.6	-0.022
41.820	2.1583	3.6	2	-3	1	41.824	2.1581	1.8	0.004
42.000	2.1495	8.5	1	-2	3	42.028	2.1481	10.1	0.028
42.774	2.1123	3.6	3	-2	1	42.762	2.1129	2.7	-0.012
43.019	2.1009	3.4	-3	1	2	43.004	2.1015	2.5	-0.015
43.137	2.0954	3.8	-1	-3	2	43.153	2.0946	2.9	0.016
43.860	2.0625	33.1	-3	-1	2	43.848	2.0631	15.0	-0.012
45.333	1.9989	12.4	3	-1	2	45.319	1.9995	12.3	-0.014
46.685	1.9441	10.6	-2	-3	1	46.669	1.9447	8.1	-0.016
46.788	1.9400	17.0	-1	2	3	46.787	1.9401	8.6	-0.001
47.314	1.9197	6.1	0	-3	3	47.340	1.9187	4.7	0.026
47.445	1.9147	10.0	2	-2	3	47.451	1.9145	7.6	0.006
47.926	1.8966	8.3	0	-1	4	47.940	1.8961	6.7	0.014
48.356	1.8807	4.8	-3	3	0	48.342	1.8812	2.8	-0.014
48.473	1.8765	5.2	0	0	4	48.470	1.8766	2.2	-0.003
48.646	1.8702	19.7	-1	-1	4	48.652	1.8700	14.6	0.006
49.034	1.8563	30.0	1	-4	1	49.027	1.8565	18.6	-0.007
49.264	1.8482	8.9	-1	4	0	49.259	1.8483	3.6	-0.005
49.400	1.8434	26.7	-1	-3	3	49.412	1.8430	9.3	0.012
49.770	1.8306	23.1	-4	1	1	49.743	1.8315	14.7	-0.027
50.588	1.8028	20.5	3	1	2	50.558	1.8039	16.5	-0.030
50.723	1.7984	27.1	-3	1	3	50.726	1.7983	10.3	0.003
50.951	1.7909	25.0	1	2	3	50.934	1.7914	18.5	-0.017
51.423	1.7755	20.3	2	3	1	51.398	1.7763	16.0	-0.025
51.535	1.7719	17.4	1	0	4	51.521	1.7724	8.0	-0.014
51.981	1.7578	6.3	-1	1	4	51.984	1.7577	4.2	0.003
52.175	1.7517	11.4	-1	-4	1	52.178	1.7516	5.5	0.003
52.547	1.7402	4.2	-2	-1	4	52.570	1.7395	2.6	0.023
52.772	1.7333	9.3	-4	0	2	52.754	1.7338	4.3	-0.018
52.913	1.7290	19.8	4	1	0	52.878	1.7300	9.6	-0.035
53.255	1.7187	13.9	0	4	1	53.238	1.7192	10.2	-0.017
53.790	1.7028	2.2	3	-1	3	53.785	1.7030	2.4	-0.005
55.063	1.6665	5.1	-2	4	1	55.051	1.6668	4.5	-0.012
55.161	1.6637	5.3	-4	-1	2	55.131	1.6646	3.4	-0.030
55.534	1.6534	5.6	3	-2	3	55.525	1.6537	5.5	-0.009
55.781	1.6467	5.3	-3	-3	1	55.767	1.6471	3.3	-0.014
55.972	1.6415	5.2	-1	3	3	55.966	1.6417	3.6	-0.006
56.247	1.6342	2.3	4	1	1	56.205	1.6353	1.3	-0.042

TABLE SI. Continued

$2\theta_{obs}$ (°)	d_{obs} (Å)	$(I/I_o)_{obs}$	h	k	l	$2\theta_{cal}$ (°)	d_{cal} (Å)	$(I/I_o)_{cal}$	$\Delta 2\theta$ (°)
56.927	1.6162	3.6	0	-4	3	56.942	1.6158	3.0	0.015
57.471	1.6022	6.8	2	0	4	57.461	1.6025	6.4	-0.010
57.641	1.5979	13.8	-3	-3	2	57.637	1.5980	6.2	-0.004
58.144	1.5853	7.8	-2	3	3	58.123	1.5858	5.5	-0.021
58.415	1.5786	8.1	3	-4	1	58.404	1.5788	4.0	-0.011
59.251	1.5583	10.5	-3	-1	4	59.244	1.5584	7.0	-0.007
59.498	1.5524	11.3	-4	3	1	59.470	1.5530	9.0	-0.028
59.618	1.5495	7.0	0	4	2	59.573	1.5506	4.4	-0.045
59.929	1.5422	3.2	-4	1	3	59.914	1.5426	2.4	-0.015
60.394	1.5315	2.7	-4	-2	2	60.381	1.5318	1.4	-0.013
60.650	1.5256	3.5	3	3	1	60.611	1.5265	1.3	-0.039
61.189	1.5135	3.6	2	-4	3	61.194	1.5134	4.7	0.005
61.733	1.5014	4.0	0	0	5	61.741	1.5013	3.2	0.008
62.238	1.4905	4.7	-3	-3	3	62.233	1.4906	4.3	-0.005
62.376	1.4875	4.5	-2	-3	4	62.371	1.4876	2.5	-0.005
62.954	1.4752	8.9	5	0	0	62.907	1.4762	3.2	-0.047
63.109	1.4720	7.6	-3	3	3	63.068	1.4728	4.9	-0.041
63.230	1.4694	5.7	0	5	0	63.213	1.4698	2.5	-0.017
63.941	1.4548	2.9	-4	2	3	63.914	1.4554	1.5	-0.027
64.682	1.4399	4.3	5	-1	1	64.637	1.4408	3.2	-0.045
64.894	1.4357	3.0	-1	1	5	64.921	1.4352	2.2	0.027
65.424	1.4254	6.3	-1	-5	1	65.407	1.4257	3.4	-0.017
66.756	1.4001	3.5	-4	-3	1	66.713	1.4009	1.6	-0.043
66.832	1.3987	4.3	-1	-5	2	66.807	1.3992	2.5	-0.025
67.123	1.3934	4.5	-2	1	5	67.122	1.3934	3.4	-0.001
67.376	1.3887	3.5	3	-4	3	67.377	1.3887	1.5	0.001
67.980	1.3779	2.6	4	3	0	67.930	1.3788	1.9	-0.050
68.172	1.3745	3.6	0	4	3	68.145	1.3749	1.6	-0.027
69.254	1.3556	2.3	-3	-3	4	69.247	1.3557	1.2	-0.007
69.395	1.3532	3.9	-3	5	0	69.384	1.3534	2.9	-0.011
69.549	1.3506	5.6	2	-2	5	69.568	1.3503	2.6	0.019
69.605	1.3496	5.7	5	-1	2	69.596	1.3498	2.9	-0.009
70.188	1.3398	2.5	3	1	4	70.146	1.3405	1.9	-0.042
70.341	1.3373	4.3	-5	0	3	70.297	1.3380	2.8	-0.044
70.517	1.3344	3.9	-4	3	3	70.476	1.3351	1.2	-0.041
70.654	1.3321	5.2	5	-3	1	70.610	1.3328	5.2	-0.044
70.768	1.3303	4.9	-1	-5	3	70.770	1.3302	4.7	0.002
71.176	1.3236	3.4	-2	-5	1	71.151	1.3240	1.6	-0.025

TABLE SI. Continued

$2\theta_{obs}$ (°)	d_{obs} (Å)	$(I/I_o)_{obs}$	h	k	l	$2\theta_{cal}$ (°)	d_{cal} (Å)	$(I/I_o)_{cal}$	$\Delta 2\theta$ (°)
71.757	1.3143	6.4	4	3	1	71.698	1.3153	2.7	-0.059
71.952	1.3113	8.9	-3	1	5	71.934	1.3115	3.3	-0.018
72.183	1.3076	5.2	-2	-3	5	72.221	1.3070	3.4	0.038
72.684	1.2999	3.0	-3	3	4	72.657	1.3003	2.0	-0.027
72.900	1.2965	4.6	-5	-2	2	72.861	1.2971	3.1	-0.039
73.111	1.2933	4.2	-2	5	2	73.076	1.2938	2.9	-0.035
74.298	1.2756	5.0	4	-1	4	74.254	1.2762	3.0	-0.044
74.725	1.2693	3.9	0	-1	6	74.745	1.2690	3.4	0.020
75.303	1.2610	5.0	5	1	2	75.240	1.2619	3.0	-0.063
75.554	1.2574	8.0	3	3	3	75.497	1.2583	6.9	-0.057
76.001	1.2511	3.3	0	0	6	76.008	1.2511	1.4	0.007
76.638	1.2423	4.2	2	5	1	76.591	1.2430	2.5	-0.047
76.876	1.2391	3.9	5	-1	3	76.892	1.2389	1.5	0.016
76.951	1.2381	6.2	-1	6	0	76.928	1.2384	3.4	-0.023
77.169	1.2351	8.2	-4	-4	1	77.130	1.2356	2.1	-0.039
77.285	1.2335	8.1	-2	-1	6	77.291	1.2335	4.4	0.006
77.359	1.2325	8.8	1	-6	2	77.348	1.2327	4.4	-0.011
77.961	1.2245	2.9	0	6	0	77.938	1.2248	1.6	-0.023
78.584	1.2164	4.3	-6	2	1	78.526	1.2171	4.8	-0.058
79.397	1.2059	5.6	2	-4	5	79.421	1.2056	5.6	0.024
79.940	1.1991	2.3	0	-3	6	79.983	1.1986	1.7	0.043
80.752	1.1891	2.4	4	1	4	80.698	1.1898	2.0	-0.054
81.253	1.1830	2.1	2	2	5	81.213	1.1835	1.9	-0.040
82.983	1.1627	3.1	2	-2	6	82.972	1.1628	2.5	-0.011
83.232	1.1598	5.9	-5	-2	4	83.205	1.1602	4.4	-0.027
83.488	1.1569	5.4	-4	5	2	83.471	1.1571	5.2	-0.017
83.970	1.1515	4.6	0	-5	5	83.997	1.1512	3.7	0.027
84.224	1.1487	3.5	-3	3	5	84.195	1.1490	1.4	-0.029
84.415	1.1466	2.4	2	0	6	84.397	1.1468	2.1	-0.018
86.120	1.1282	4.1	-5	5	0	86.068	1.1287	3.9	-0.052
87.288	1.1161	7.0	-5	0	5	87.268	1.1163	2.8	-0.020
87.869	1.1102	2.2	0	6	2	87.816	1.1107	2.7	-0.053
90.115	1.0883	3.1	2	-6	4	90.112	1.0883	3.2	-0.003
92.637	1.0651	3.5	-4	-2	6	92.636	1.0651	3.1	-0.001
94.208	1.0515	2.8	-3	5	4	94.142	1.0520	2.8	-0.066

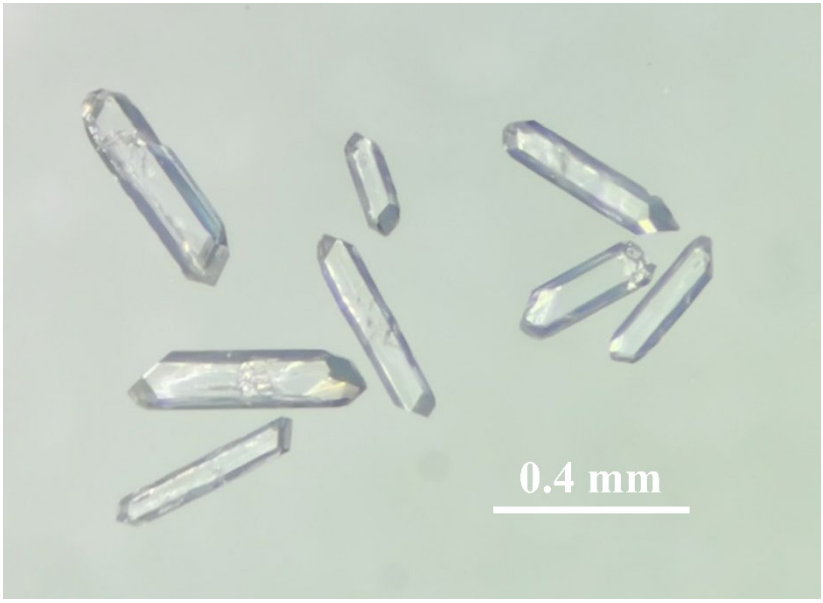

Figure S1. Optical microscopy image of as-synthesized $Ba_2Cu(IO_3)_6$ crystals.

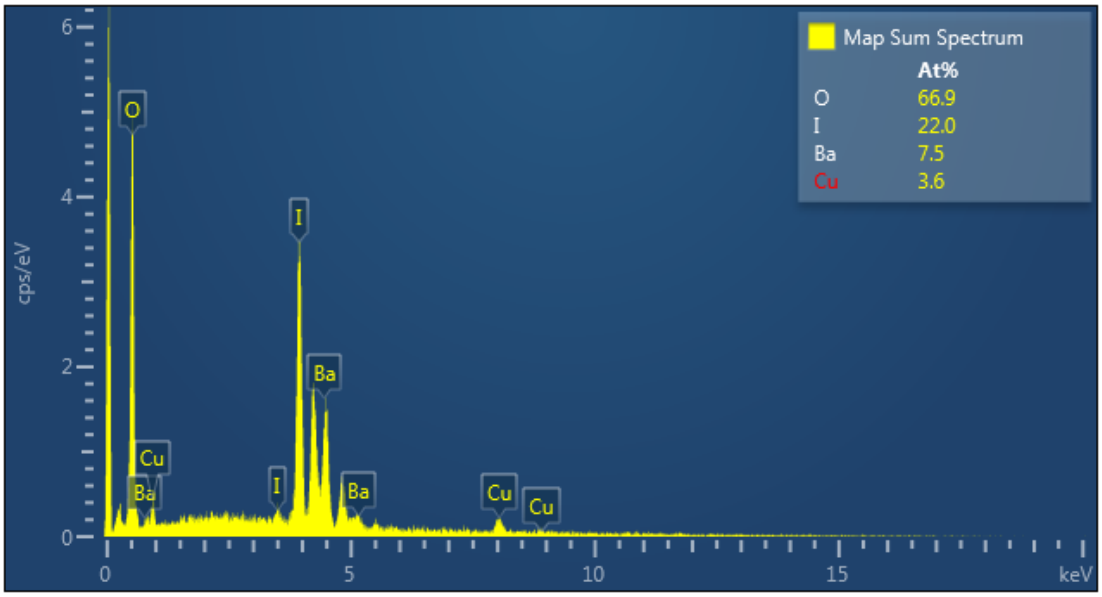

Figure S2. The energy-dispersive X-ray spectroscope of the $Ba_2Cu(IO_3)_6$ crystal.

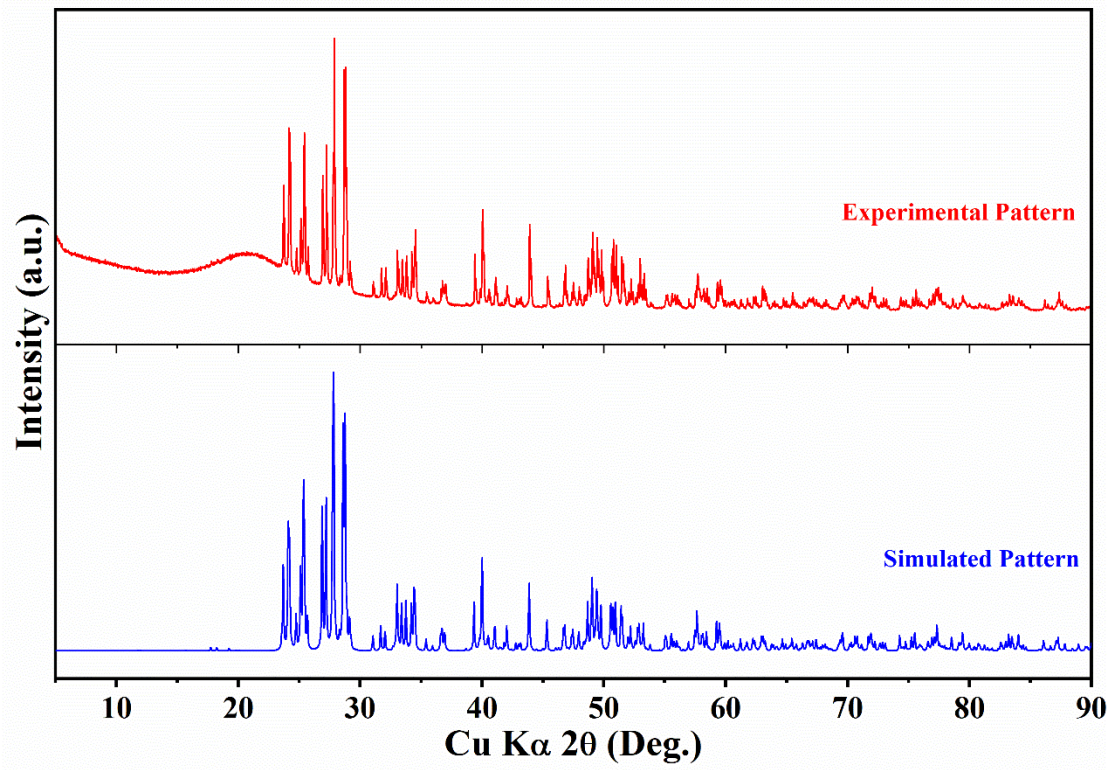

Figure S3. The experimental powder X-ray diffraction pattern and the simulated pattern derived from the single crystal structure.