

Supporting Information

Evolution of fractal patterns in lead-free, zero-dimensional perovskite $\text{Cs}_2\text{InBr}_5(\text{H}_2\text{O})$

Wanyin Ge^{a,*}, Maohao Yang^a, Masaki Saruyama², Kenshi Matsumoto², Ryota Sato²,
Haruka Takekuma², Ryo Takahata², and Toshiharu Teranishi^{2,*}

^a School of Materials Science and Engineering, Shaanxi University of Science and Technology, Xi'an, Shaanxi 710021, P. R. China.

^b Institute for Chemical Research, Kyoto University, Gokasho, Uji, Kyoto 611-0011, Japan

* Email: gewanyin@sust.edu.cn; teranisi@scl.kyoto-u.ac.jp.

The standard card information of $\text{Cs}_2\text{InBr}_5(\text{H}_2\text{O})$

Compound name: Cesium Indium Bromide Hydrate
Common name: Dicaesium indium pentabromide hydrate
PDF index name: Cesium Indium Bromide Hydrate
Chemical formula: $\text{Cs}_2\text{InBr}_5(\text{H}_2\text{O})$
PDF: 01-087-4184

Structure: Orthorhombic
Space group: Pnma
Space group No.: 62
a (Å): 14.8763
b (Å): 10.8116
c (Å): 7.6437
Alpha (°): 90.0000
Beta (°): 90.0000
Gamma (°): 90.0000
Volume of cell (10^6 pm^3): 1229.39
Z: 4.00
RIR: 2.71

Reference: Zhou, Lei; Liao, Jin-Feng; Huang, Zeng-Guang; Wei, Jun-Hua; Wang, Xu-Dong; Li, Wen-Guang; Chen, Hong-Yan; Kuang, Dai-Bin; Su, Cheng-Yong, *Angew. Chem.*,

Peak lists

No.	h	k	l	d [Å]	2Theta [°]	I [%]
1	2	0	0	7.43815	11.888	5.0
2	1	0	1	6.79874	13.011	4.4
3	0	1	1	6.24140	14.179	42.5
4	2	1	0	6.12798	14.443	43.2
5	1	1	1	5.75537	15.383	2.6
6	0	2	0	5.40580	16.384	1.3
7	2	0	1	5.33075	16.617	1.3
8	2	1	1	4.78117	18.543	1.2
9	2	2	0	4.37292	20.291	1.2
10	1	2	1	4.23128	20.978	0.3
11	3	0	1	4.16004	21.342	0.6
12	3	1	1	3.88255	22.887	1.3
13	0	0	2	3.82185	23.255	7.6
14	2	2	1	3.79567	23.418	42.2
15	4	0	0	3.71907	23.907	18.9
16	1	0	2	3.70164	24.022	18.8
17	4	1	0	3.51682	25.304	0.1
18	1	1	2	3.50207	25.413	0.2
19	2	0	2	3.39937	26.194	0.3
20	4	0	1	3.34423	26.634	20.8
21	3	2	1	3.29684	27.024	37.5
22	0	3	1	3.25972	27.338	8.7
23	2	1	2	3.24324	27.479	12.4
24	2	3	0	3.24324	27.479	12.4
25	4	1	1	3.19488	27.903	5.7
26	0	2	2	3.12070	28.581	38.3
27	4	2	0	3.06399	29.121	100.0
28	1	2	2	3.05422	29.216	88.7
29	3	0	2	3.02710	29.484	56.3
30	2	3	1	2.98560	29.903	0.9
31	3	1	2	2.91500	30.645	2.9
32	2	2	2	2.87769	31.052	0.3
33	4	2	1	2.84401	31.430	9.4
34	5	0	1	2.77262	32.261	1.9
35	0	4	0	2.70290	33.116	79.5
36	4	0	2	2.66538	33.596	51.3
37	3	2	2	2.64119	33.913	1.4
38	4	1	2	2.58789	34.634	0.7
39	4	3	0	2.58789	34.634	0.7
40	2	4	0	2.54037	35.303	0.7
41	1	0	3	2.51133	35.724	2.0
42	1	4	1	2.51133	35.724	2.0

43	2	3	2	2.47285	36.300	1.8
44	1	1	3	2.45138	36.629	2.4
45	4	3	1	2.45138	36.629	2.4
46	6	1	0	2.41665	37.174	1.1
47	2	0	3	2.41041	37.274	3.0
48	2	4	1	2.41041	37.274	3.0
49	4	2	2	2.39059	37.595	1.7
50	5	0	2	2.34772	38.308	24.1
51	3	3	2	2.31791	38.820	1.1
52	6	1	1	2.30423	39.060	0.7
53	5	1	2	2.29425	39.237	5.5
54	1	2	3	2.27756	39.536	6.8
55	3	0	3	2.26625	39.742	4.4
56	3	4	1	2.26625	39.742	4.4
57	6	2	0	2.25365	39.973	1.9
58	3	1	3	2.21804	40.643	3.3
59	0	4	2	2.20679	40.859	2.9
60	2	2	3	2.20147	40.963	1.4
61	5	3	1	2.19752	41.040	1.1
62	4	4	0	2.18646	41.257	9.4
63	1	4	2	2.18290	41.327	9.2
64	6	2	1	2.16165	41.752	12.0
65	5	2	2	2.15341	41.919	1.9
66	4	3	2	2.14296	42.134	0.4
67	4	0	3	2.10215	42.992	10.1
68	4	4	1	2.10215	42.992	10.1
69	3	2	3	2.09002	43.254	7.6
70	6	0	2	2.08067	43.458	3.2
71	0	5	1	2.08067	43.458	3.2
72	2	5	0	2.07636	43.553	3.7
73	1	3	3	2.06331	43.842	3.9
74	4	1	3	2.06331	43.842	3.9
75	7	0	1	2.04752	44.198	7.0
76	6	1	2	2.04256	44.311	4.5
77	6	3	0	2.04256	44.311	4.5
78	3	4	2	2.01615	44.923	29.8
79	2	3	3	2.00357	45.221	0.9
80	2	5	1	2.00357	45.221	0.9
81	5	3	2	1.96713	46.106	2.4
82	4	2	3	1.95906	46.307	0.6
83	6	2	2	1.94127	46.757	0.5
84	5	0	3	1.93526	46.911	3.0
85	5	4	1	1.93526	46.911	3.0
86	3	3	3	1.91846	47.346	2.0
87	3	5	1	1.91846	47.346	2.0
88	0	0	4	1.91093	47.544	1.3

89	1	0	4	1.89783	47.893	36.9
90	4	4	2	1.89783	47.893	36.9
91	1	1	4	1.86688	48.738	4.3
92	1	5	2	1.86688	48.738	4.3
93	7	0	2	1.85954	48.943	11.5
94	8	0	0	1.85954	48.943	11.5
95	2	0	4	1.85082	49.189	1.4
96	1	4	3	1.83978	49.504	1.1
97	7	1	2	1.83263	49.710	0.7
98	8	1	0	1.83263	49.710	0.7
99	5	2	3	1.82449	49.947	1.7
100	2	5	2	1.82449	49.947	1.7
101	4	3	3	1.81568	50.206	3.4
102	4	5	1	1.81568	50.206	3.4
103	8	0	1	1.80684	50.469	6.2
104	2	4	3	1.80167	50.624	5.3
105	0	2	4	1.80167	50.624	5.3
106	7	3	1	1.78212	51.219	4.7
107	8	1	1	1.78212	51.219	4.7
108	5	4	2	1.77246	51.519	17.9
109	7	2	2	1.75656	52.020	3.3
110	8	2	0	1.75656	52.020	3.3
111	2	2	4	1.75104	52.196	1.2
112	2	6	0	1.75104	52.196	1.2
113	3	4	3	1.73660	52.663	3.1
114	8	2	1	1.71365	53.424	8.9
115	5	3	3	1.70705	53.647	4.0
116	2	6	1	1.70705	53.647	4.0
117	4	0	4	1.69969	53.898	1.2
118	3	2	4	1.69336	54.116	8.0
119	1	3	4	1.67750	54.670	2.1
120	4	1	4	1.67750	54.670	2.1
121	8	0	2	1.67212	54.861	0.3
122	8	3	0	1.65348	55.532	4.2
123	3	6	1	1.65348	55.532	4.2
124	2	3	4	1.64640	55.792	0.3
125	1	5	3	1.63861	56.081	0.5
126	7	0	3	1.63210	56.324	7.9
127	7	4	1	1.63210	56.324	7.9
128	6	5	0	1.62986	56.409	5.8
129	0	6	2	1.62986	56.409	5.8
130	1	6	2	1.62162	56.721	16.4
131	4	6	0	1.62162	56.721	16.4
132	7	1	3	1.61520	56.967	3.4
133	8	3	1	1.61520	56.967	3.4
134	5	0	4	1.60786	57.251	1.2

135	2	5	3	1.60786	57.251	1.2
136	8	2	2	1.59744	57.659	3.0
137	9	1	1	1.59744	57.659	3.0
138	6	3	3	1.59382	57.803	0.7
139	6	5	1	1.59382	57.803	0.7
140	5	5	2	1.59050	57.935	1.9
141	2	6	2	1.59050	57.935	1.9
142	4	6	1	1.58631	58.102	1.4
143	5	4	3	1.57351	58.621	1.7
144	0	4	4	1.56236	59.081	11.4
145	7	2	3	1.56236	59.081	11.4
146	1	4	4	1.55184	59.521	16.8
147	5	2	4	1.54113	59.977	6.4
148	7	4	2	1.53199	60.372	10.8
149	8	4	0	1.53199	60.372	10.8
150	2	4	4	1.52711	60.585	1.4
151	1	0	5	1.52073	60.866	0.4
152	9	0	2	1.51711	61.027	0.5
153	2	7	0	1.51392	61.169	0.8
154	0	7	1	1.51392	61.169	0.8
155	1	1	5	1.50719	61.472	1.6
156	4	5	3	1.50719	61.472	1.6
157	8	0	3	1.50212	61.702	6.3
158	8	4	1	1.50212	61.702	6.3
159	2	0	5	1.49905	61.842	1.8
160	6	5	2	1.49905	61.842	1.8
161	4	6	2	1.49280	62.130	0.4
162	7	3	3	1.48840	62.334	2.3
163	3	4	4	1.48840	62.334	2.3
164	2	1	5	1.48328	62.573	0.6
165	6	4	3	1.48328	62.573	0.6
166	10	1	0	1.47374	63.025	1.0
167	9	3	1	1.47374	63.025	1.0
168	1	2	5	1.46405	63.490	1.7
169	1	6	3	1.46405	63.490	1.7
170	9	2	2	1.46068	63.654	3.1
171	6	2	4	1.45750	63.809	1.6
172	6	6	0	1.45750	63.809	1.6
173	10	1	1	1.44722	64.317	0.8
174	8	2	3	1.44722	64.317	0.8
175	5	5	3	1.44310	64.523	1.4
176	2	2	5	1.44310	64.523	1.4
177	4	4	4	1.43884	64.737	1.0
178	10	2	0	1.43431	64.966	0.7
179	6	6	1	1.43184	65.092	2.6
180	1	5	4	1.42531	65.428	1.8

181	1	7	2	1.42531	65.428	1.8
182	7	0	4	1.42096	65.653	3.4
183	8	4	2	1.42096	65.653	3.4
184	4	0	5	1.41395	66.020	0.5
185	10	2	1	1.41043	66.206	3.3
186	3	6	3	1.41043	66.206	3.3
187	1	3	5	1.40110	66.704	0.8
188	4	1	5	1.40110	66.704	0.8
189	6	3	4	1.39709	66.921	1.5
190	7	4	3	1.39709	66.921	1.5
191	8	5	1	1.38668	67.490	3.9
192	9	0	3	1.38668	67.490	3.9
193	5	4	4	1.38185	67.758	1.3
194	2	3	5	1.38185	67.758	1.3
195	7	2	4	1.37508	68.137	1.0
196	10	3	0	1.37508	68.137	1.0
197	4	6	3	1.36793	68.543	1.5
198	4	2	5	1.36793	68.543	1.5

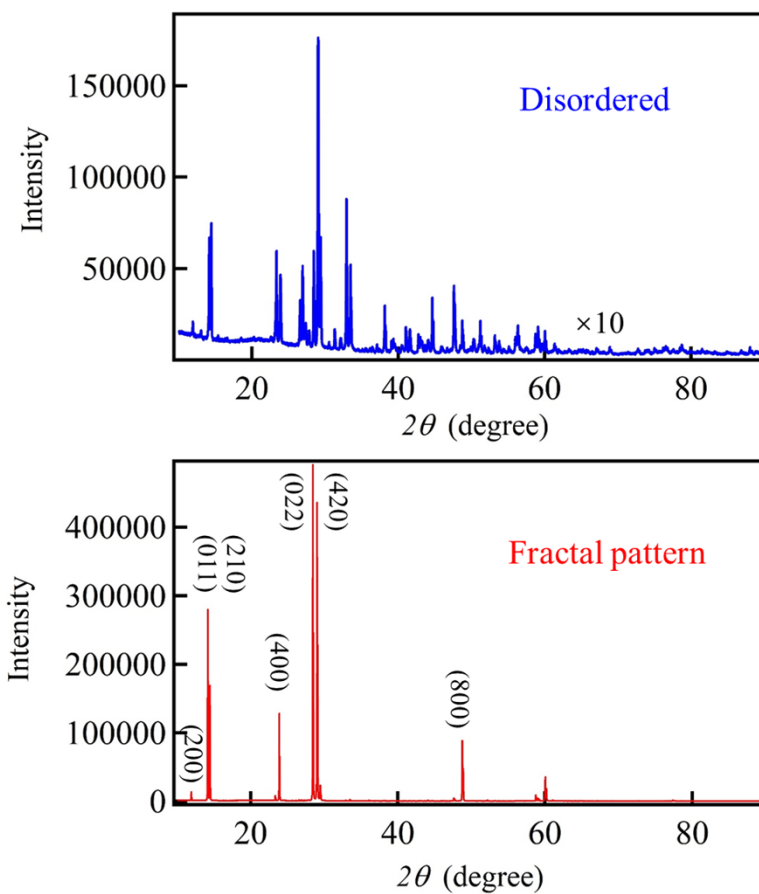


Fig. S1 XRD patterns of disordered sample and fractal patterns of $\text{Cs}_2\text{InBr}_5(\text{H}_2\text{O})\text{:Sb}$