SUPPORTING INFORMATION

Novel cesium cerium (IV) iodate $Cs_2Ce(IO_3)_6$: hydrothermal synthesis, crystal structure and thermal stability

Oksana P. Grigorieva,[1,] Larisa V. Shvanskaya,*[1] Tatiana B. Shatalova[1], Andrey A. Zolotarev,[2] Peter S. Berdonosov[1] and Valery A. Dolgikh[1]

[1]M.V. Lomonosov Moscow State University, Leninskie Gory 1-3, Moscow 119991 Russia
[2] Institute of Earth Sciences, St. Petersburg State University, Universitetskaya Emb. 7/9, 199034 St. Petersburg, Russia

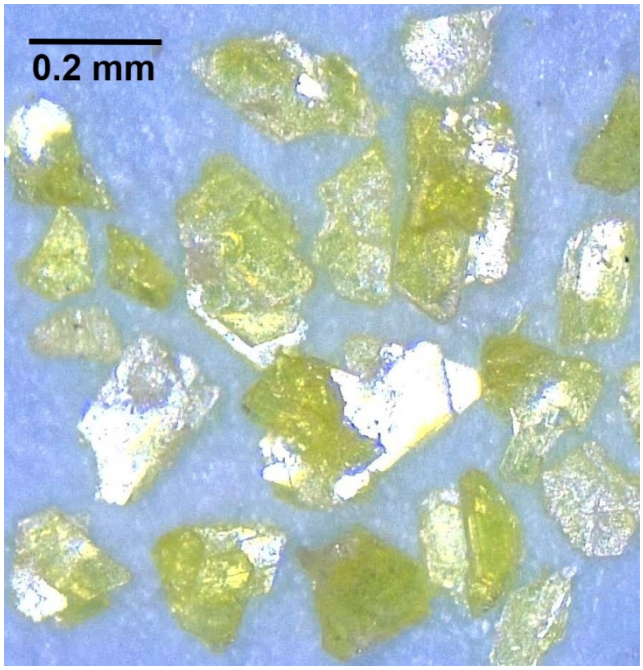

Fig S1. Photo of yellow $Cs_2Ce(IO_3)_6$ crystals with a plate-like habit.

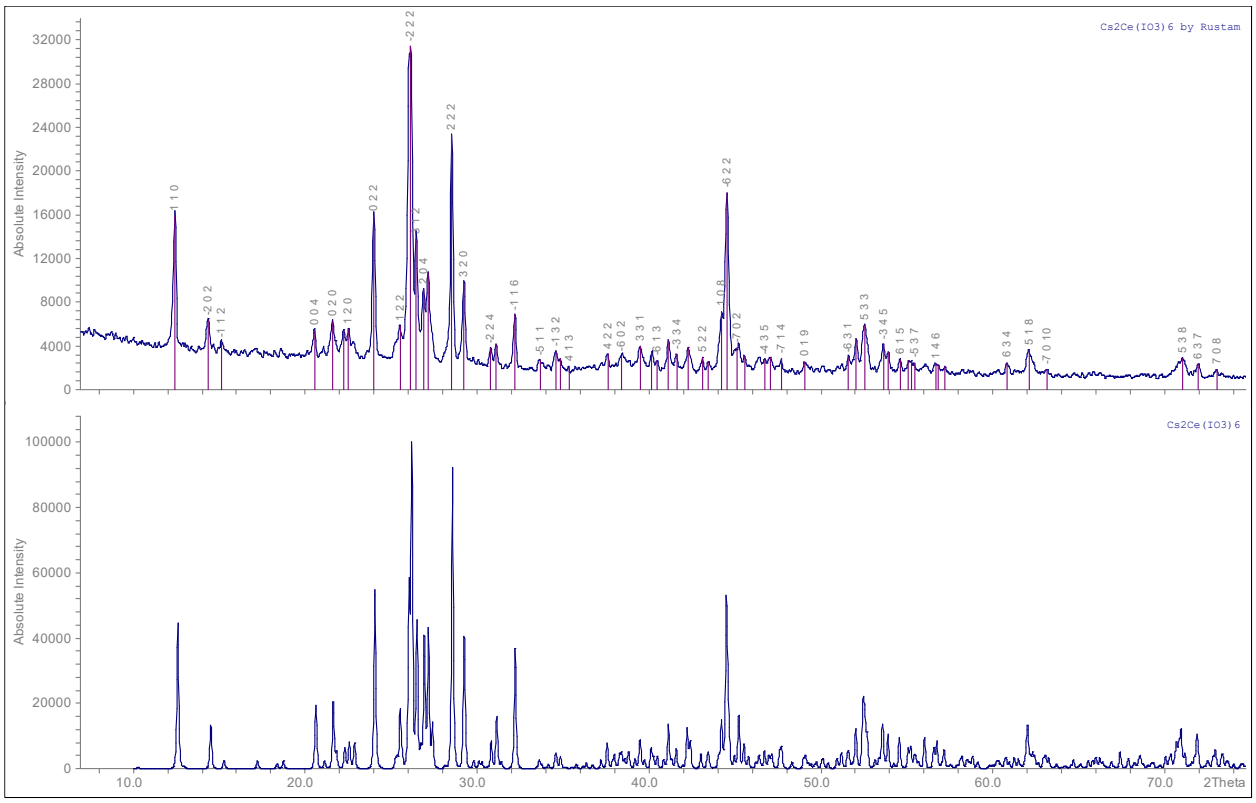

Fig S2. Comparison of PXRD pattern from experimental sample (upper part) and simulated one from single crystal data (low part) for $Cs_2Ce(IO_3)_6$

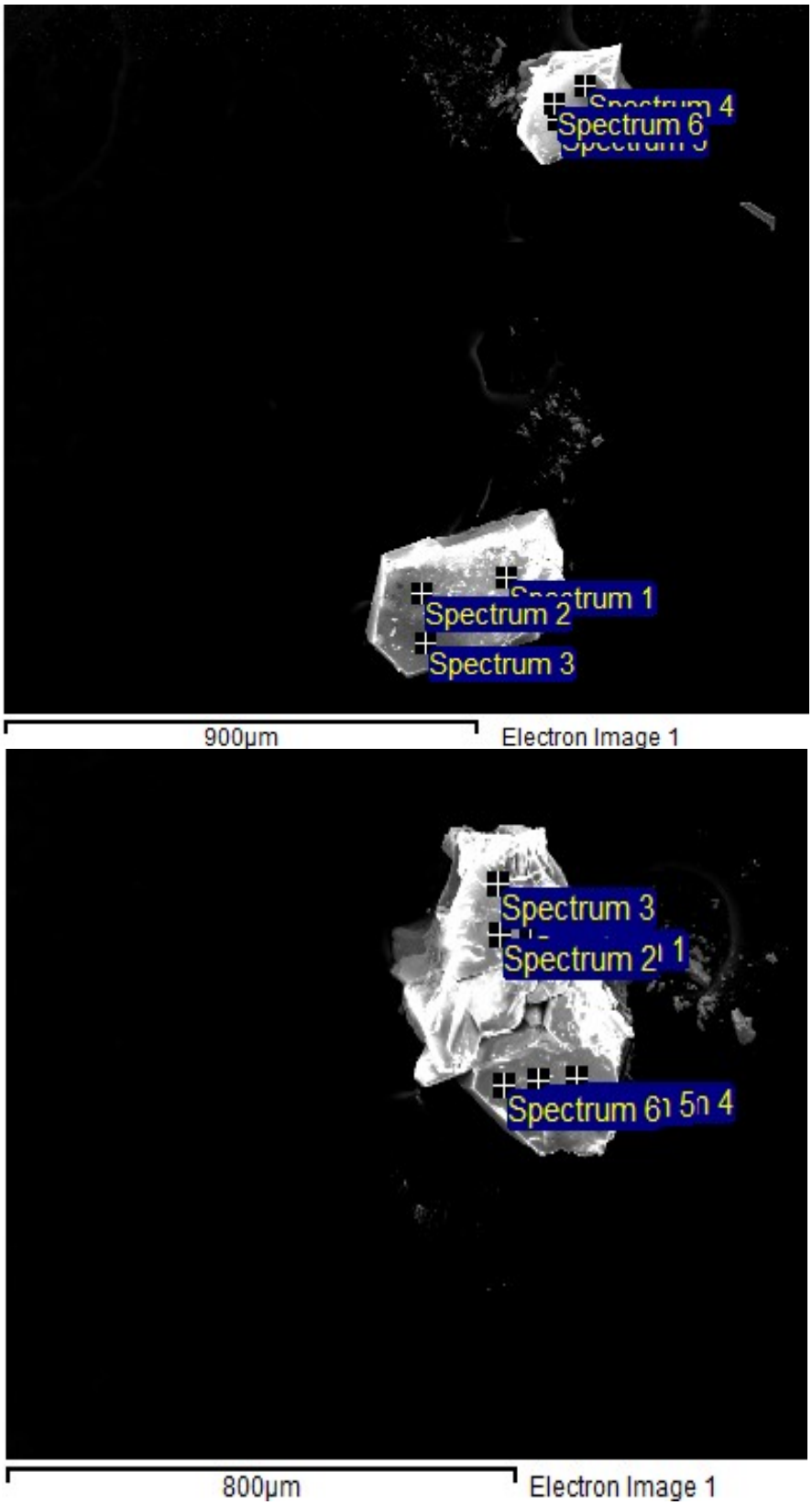

Fig. S3. SEM images of EDX analized crystal samples for $Cs_2Ce(IO_3)_6$ upper -- sample I and lower – sample II

Table S1. Results of EDX elemental analysis for $Cs_2Ce(IO_3)_6$ samples depicted in Fig S2

Sample I					
Spectrum	In stats.	O	I	Cs	Ce
Spectrum 1	Yes	58.44	28.48	8.23	4.86
Spectrum 2	Yes	59.92	27.39	8.24	4.45
Spectrum 3	Yes	54.95	30.73	9.23	5.09
Spectrum 4	Yes	58.91	28.27	8.00	4.82
Spectrum 5	Yes	60.53	27.58	7.67	4.23
Spectrum 6	Yes	56.83	29.78	8.37	5.02
Mean		58.26	28.70	8.29	4.75
Std. deviation		2.07	1.31	0.52	0.34
Max.		60.53	30.73	9.23	5.09
Min.		54.95	27.39	7.67	4.23
Sample II					
Spectrum 1	Yes	58.20	28.63	8.30	4.88
Spectrum 2	Yes	60.30	27.45	7.68	4.57
Spectrum 3	Yes	54.55	31.48	8.91	5.05
Spectrum 4	Yes	47.10	36.31	10.49	6.10
Spectrum 5	Yes	51.80	32.73	9.50	5.97
Spectrum 6	Yes	58.87	28.56	8.04	4.54
Mean		55.14	30.86	8.82	5.18
Std. deviation		5.02	3.33	1.04	0.69
Max.		60.30	36.31	10.49	6.10
Min.		47.10	27.45	7.68	4.54

All results in atomic%

Table S2. Bond valence data for $Cs_2Ce(IO_3)_6$ calculated according formula and parameters from https://www.iucr.org/resources/data/datasets/bond-valence-parameters

atom	atom	R (bond length)		bv	bvs
I1	O8	1.7818		1.818	
	O1	1.8250		1.618	
	O5	1.8635		1.458	**4.89***
	O7	2.4208		0.323	5.22**
I2	O4	1.7860		1.798	
	O7	1.8221		1.631	
	O3	1.8386		1.559	**4.99***
	O5	2.5203		0.247	5.24**
I3	O6	1.8020		1.722	
	O9	1.8080		1.694	
	O2	1.8337		1.580	**5.00**
Ce	O2	2.2325	x2	1.151	
	O3	2.3369	x2	0.868	
	O5	2.3769		0.389	
	O5	2.3770		0.389	
	O1	2.4657	x2	0.613	**3.41**

atom	atom	R (bond length)	bv	bvs
Cs	O1	3.1707	0.130	
	O8	3.2740	0.099	
	O4	3.2800	0.097	
	O8	3.3030	0.091	
	O1	3.3406	0.082	
	O3	3.3741	0.075	
	O3	3.4920	0.054	
	O5	3.5124	0.052	
	O7	3.5570	0.046	
	O4	3.6100	0.040	
	O9	3.6310	0.038	
	O2	3.7070	0.031	**0.84**

* Three nearest I-O distances are taken into account

**Considering the elongated I-O distance, the distorted tetrahedra coordination of I atom