Electronic Supplementary Material (ESI) for Dalton Transactions.

Supporting Information

New iodate fluoride $Rb_2Ce(IO_3)_5F$ with nonlinear optical properties

Oksana P. Grigorieva[a] , Tatiana B. Shatalova[a], Alexey N. Kuznetsov[a], Peter S. Berdonosov[a]*, Sergey Yu. Stefanovich[a], Konstantin A. Lyssenko[a], Valery A. Dolgikh[a]

a Lomonosov Moscow State University, Moscow 119991, Russia.

* Corresponding Author: berdonosov@inorg.chem.msu.ru

Table S1. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (Å^{2}x 10^3) for $Rb_2Ce(IO_3)_5F$. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
Ce(1)	10000	4531(1)	6240(1)	14(1)
Rb(1)	5000	5022(3)	3498(1)	18(1)
Rb(2)	10000	-331(3)	6034(1)	18(1)
I(1)	7627(1)	2487(2)	4743(1)	27(1)
I(2)	10000	4693(2)	8666(1)	15(1)
I(3)	7346(1)	2129(1)	7315(1)	14(1)
O(1)	8306(11)	-160(20)	4760(8)	63(5)
O(2)	8751(10)	3261(13)	5405(6)	24(2)
O(3)	8443(10)	2907(12)	3879(5)	19(2)
O(4)	8760(9)	3241(12)	8596(6)	20(2)
O(5)	10000	5549(16)	7670(7)	17(3)
O(6)	6576(9)	1386(12)	6431(5)	19(2)
O(7)	6684(8)	4147(11)	7313(6)	19(2)
O(8)	8812(8)	2589(12)	6907(6)	17(2)
F(1)	10000	6250(13)	5257(6)	21(2)

Table S2. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for $Rb_2Ce(IO_3)_5F$. The anisotropic displacement factor exponent takes the form: $-2p^2[\ h^2\ a^{*2}U^{11} + \ldots + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Ce(1)	14(1)	14(1)	15(1)	-1(1)	0	0
Rb(1)	18(1)	18(1)	20(1)	0(1)	0	0
Rb(2)	18(1)	17(1)	18(1)	0(1)	0	0
I(1)	31(1)	35(1)	14(1)	-1(1)	-2(1)	-19(1)
I(2)	15(1)	15(1)	14(1)	1(1)	0	0
I(3)	15(1)	13(1)	15(1)	1(1)	1(1)	-1(1)
O(1)	23(7)	139(15)	27(7)	18(8)	-7(5)	-22(9)
O(2)	26(6)	27(5)	20(5)	1(4)	-3(4)	-10(4)
O(3)	22(6)	22(5)	13(4)	0(4)	6(4)	0(4)
O(4)	24(6)	19(5)	18(4)	3(4)	-2(4)	-2(4)
O(5)	16(7)	21(6)	14(6)	3(5)	0	0
O(6)	21(5)	21(5)	14(4)	-4(4)	0(3)	-2(4)
O(7)	21(5)	13(4)	25(5)	-3(4)	0(4)	4(4)
O(8)	9(5)	18(4)	23(4)	-3(4)	7(4)	-1(4)
F(1)	28(7)	14(5)	22(5)	3(4)	0	0

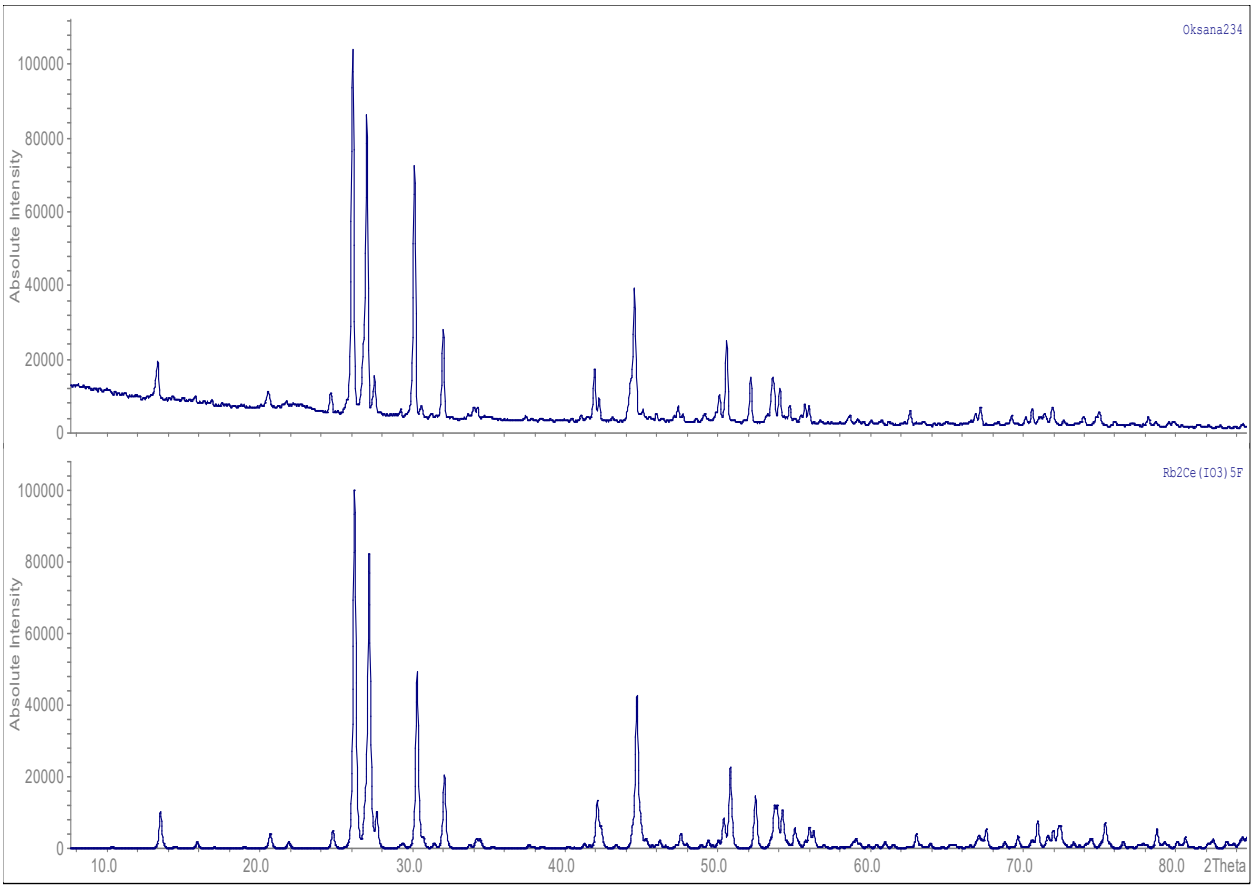

Fig S1. Powder XRD pattern from manually selected orange crystals (upper panel) and simulated pattern from structural refinement of $Rb_2Ce(IO_3)_5F$ on single crystal data (low panel)

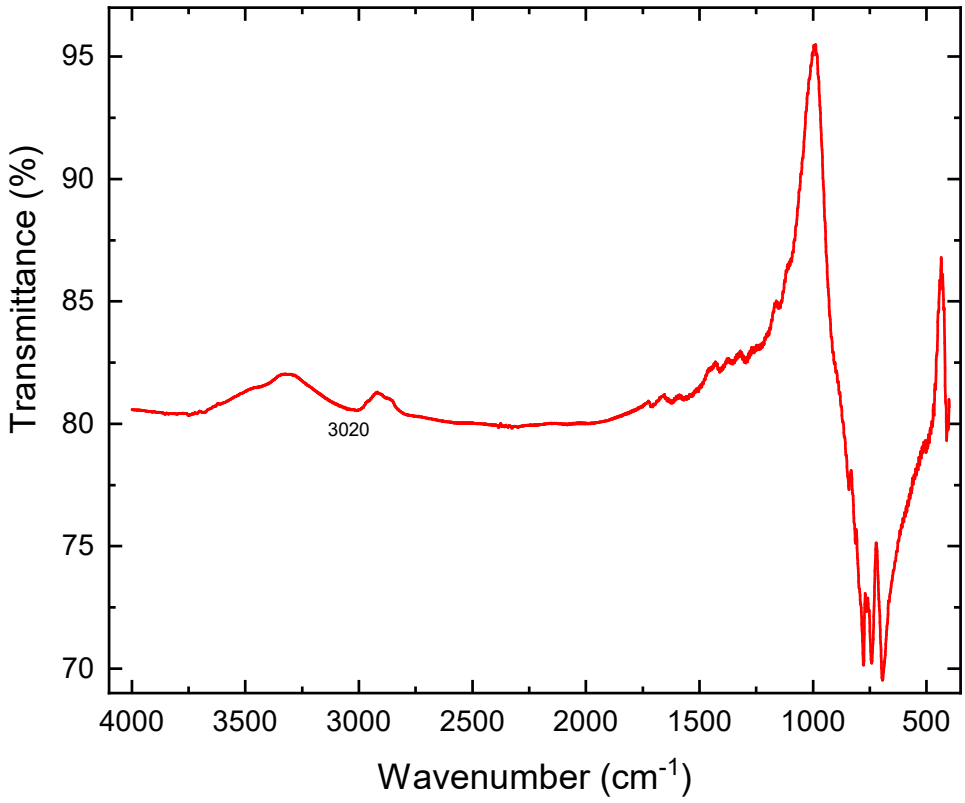

Fig S2. The registered IR spectrum for $Rb_2Ce(IO_3)_5F$ crashed crystals 4000-400 cm^{-1} range