Table S1. Crystal data and structure refinement for $Cs_3Ta(IO_3)_8$

Formula	$Cs_3Ta(IO_3)_8$
Formula weight	1978.88
Crystal system	trigonal
Space group, Z	$P31c$, 2
a, Å	8.0774(1)
c, Å	23.4262(3)
V, Å^3	1323.67(3)
D_x, г/см^3	4.965
μ, мм$^{-1}$	17.642
Wavelength, Å	0.71073
Θ range/degree	2.91- 30.87
Refl. collected/unique/$R_{int.}$	21164 / 2644 / 0.0481
Completeness to Θ, %	0.961
Parameters	110
GOF (S)	1.133
R_{all}, R_{gt}, R_{wgt}	0.0384, 0.0361, 0.0873
$\Delta\rho_{min}/\Delta\rho_{max}$, э/Å^3	-7.066/ 1.682

[1] $R_{gt} = \Sigma. \ ||F_o|-|F_c||/ = \Sigma |F_o|$ and $R_{wgt} = [\Sigma w (F_o^2 - F_c^2)^2 / \Sigma w (F_o^2)^2]^{1/2}$ for $F_o^2 > 2\sigma (F_o^2)$.

Table S2. Atomic coordinates and equivalent displacement parameters for $Cs_3Ta(IO_3)_8$.

Atom	x/a	y/b	z/c	U_{equ}, Å^2
I1	0.6667	0.3333	0.13162(5)	0.0196(2)
I2	0.88012(7)	0.67265(7)	0.26158(2)	0.0116(1)
I3	0.45888(8)	0.00075(7)	0.00020(2)	0.0124(1)
I4	0.0000	0.0000	0.12891(5)	0.0206(2)
Ta	0.6667	0.3333	0.38072(3)	0.0101(1)
Cs1	0.3333	0.6667	0.35321(6)	0.0290(3)
Cs2	0.3333	0.6667	0.15339(7)	0.0330(3)
Cs3	0.0000	0.0000	-0.08599(6)	0.0300(3)
O1	0.175(1)	0.214(1)	0.1656(3)	0.030(2)
O2	0.774(1)	0.565(1)	0.3326(3)	0.018(1)
O3	0.457(1)	-0.102(1)	-0.0728(3)	0.015(1)
O4	0.934(1)	0.494(1)	0.2369(4)	0.023(1)
O5	0.659(1)	0.529(1)	0.0964(4)	0.037(2)
O6	0.410(1)	0.177(1)	-0.0290(3)	0.022(1)
O7	0.228(1)	-0.177(1)	0.0242(3)	0.024(2)
O8	0.105(1)	0.845(1)	0.2931(3)	0.022(2)

Table S3. Interatomic distances for $Cs_3Ta(IO_3)_8$.

Bond	Distance, Å	Bond	Distance, Å
I1 – O5 (x3)	1.812(8)	I4 – O1 (x3)	1.810(8)
Average I1 – O	1.812	Average I5 – O	1.810
I2 – O4	1.800(7)	I3 – O7	1.784(7)
I2 – O8	1.803(8)	I3 – O6	1.792(7)
I2 – O2	1.874(7)	I3 – O3	1.896(6)
Average I2 – O	1.826	Average I3 – O	1.824
Ta – O3 (x3)	1.952(6)	Cs1 – O8 (x3)	3.178(8)
Ta – O2 (x3)	1.978(6)	Cs1 – O6 (x3)	3.299(8)
		Cs1 – O3 (x3)	3.504(6)
Average Ta – O	1.965	Average Cs1 – O	3.327
Cs2 – O1 (x3)	3.230(8)	Cs3 – O6 (x3)	3.173(7)
Cs2 – O4 (x3)	3.417(7)	Cs3 – O8 (x3)	3.373(8)
Cs2 – O7 (x3)	3.541(8)	Cs3 – O2 (x3)	3.589(7)
Average Cs2 – O	3.396	Average Cs3 – O	3.378