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Superconductivity in structurally disordered $\text{Y}_5\text{Ir}_6\text{Sn}_{18}$

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Supporting Information

Table S1 Selected interatomic distances d together with their contractions (-) or elongation (+) in comparison with the sums of atomic radii of the elements (in %) in the crystal structure of $\text{Y}_5\text{Ir}_6\text{Sn}_{18}$. (Self-excluding pairs appearing due to the partial site occupancies are not presented here.)

Atom	$d, \text{Å}$	$\frac{d - \sum r_i}{\sum r_i} \times 100\%$
Y1 - 24Sn4	3.423(2)	+6.3 %
- 6Ir	3.508(1)	+10.7 %
Y2 - 3Sn3	2.99(2)	-7.1 %
- 3Sn2	3.02(1)	-6.2 %
- 3Ir	3.060(4)	-3.5 %
- 6Sn4	3.137(4)	-2.6 %
- 3Sn1	3.248(5)	+0.9 %
- 6Sn4	3.349(4)	+4.0 %
- 3Y2	3.784(5)	+4.5 %
Ir - 8Sn4	2.658(2)	-4.0 %
- 4Sn1	2.762(3)	-0.3 %
- 4Y2	3.060(4)	-3.5 %
- 1Y1	3.508(1)	+10.7 %
Sn1 - 3Sn1	2.421(4)	-14.1 %
- 3Ir	2.762(3)	-0.3 %
- 1Sn2	3.11(2)	+10.3 %
- 3Y2	3.248(5)	+0.9 %
Sn2 - 3Y2	3.02(1)	-6.2 %
- 1Sn1	3.11(2)	+10.3 %
- 6Sn4	3.24(2)	+14.9 %
Sn3 - 2Y2	2.99(2)	-7.1 %
- 2Sn4	3.14(2)	+11.3 %
Sn4 - 2Ir	2.658(2)	-4.0 %
- 1Sn4	2.902(2)	+2.9 %
- 1Sn4	2.924(2)	+3.7 %
- 2Y2	3.137(4)	-2.6 %
- 1Sn3	3.14(2)	+11.3 %
- 2Sn4	3.162(3)	+12.1 %
- 2Sn2	3.24(2)	+14.9 %
- 2Y2*	3.349(4)	+4.0 %
- 1Y1	3.423(2)	+6.3 %

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Table S2 Theoretically optimized atomic coordinates for the idealized $\text{Y}_5\text{Ir}_6\text{Sn}_{18}$ structure [space group $F\bar{4}3m$, $a = 13.7706(1)$ Å].

Atom	Site	x	y	z
Y1	$4a$	0	0	0
Y2	$16e$	0.36918	x	x
Ir	$24f$	0.74551	0	0
Sn1	$4c$	1/4	1/4	1/4
Sn2	$4d$	3/4	3/4	3/4
Sn3	$16e$	0.58733	x	x
Sn4	$48h$	0.17615	x	0.98835

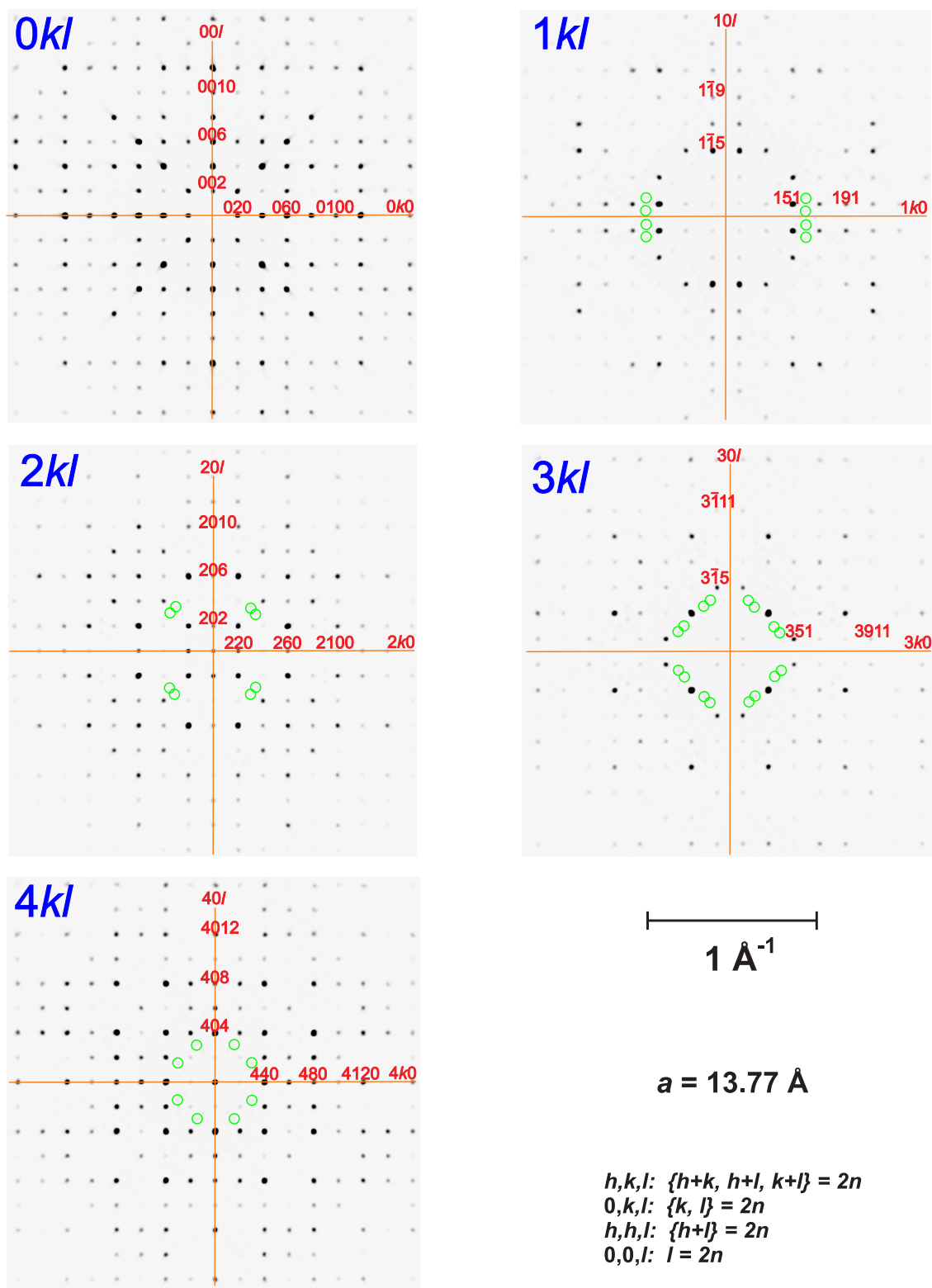


Fig. S1 Selected unwarped pictures of the single crystal XRD pattern of $\text{Y}_5\text{Ir}_6\text{Sn}_{18}$ proving the extinction group $F\text{---}$. Unsystematic weak satellite peaks breaking the given reflection conditions are marked with green circles.