Supporting Information

The subchalcogenides Ir_2In_8Q (Q = S, Se, Te): Dirac semimetal candidates with re-entrant structural modulation

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Refinement Details of Modulated Structure

The displacive distortion of a given atomic position x_4 in the subcell can be expressed by a periodic modulation function $p(x_4)$ in a form of a Fourier expansion:

$$p(k + x_4) = \sum_{n=1}^{m} A_{sn} \sin\left[2\pi\overline{q}_n(k + x_4)\right] + \sum_{n=1}^{m} A_{cn} \cos\left[2\pi\overline{q}_n(k + x_4)\right]$$

in which A_{sn} is the sinusoidal coefficient of the given Fourier term, A_{cn} is the cosine coefficient, n is the number of modulation waves used for the refinement and k is the lattice translation. $\overline{q}_n = \sum_{i=1}^{d} \alpha_{ni} q_i$ where α_{ni} integer numbers for the linear combination of the incommensurate modulation vectors q_i.[1-2] A useful coordinate t that characterizes and describes the real three-dimensional structure constructed as a perpendicular intersection with the fourth dimensional axis is defined as

$$t = x_4 - q \cdot r$$

where r is a vector in the real three-dimensional reciprocal space.[1-2]

The superspace approach includes all methods for solution and refinement of aperiodic crystals. It enables the use of the tools used in structure analysis of regular crystals such as direct methods, Fourier maps, least squares, distance and angle calculations, bond valence summations, maximum entropy method, *etc*. so that they can be used in a similar way like in standard crystallography.

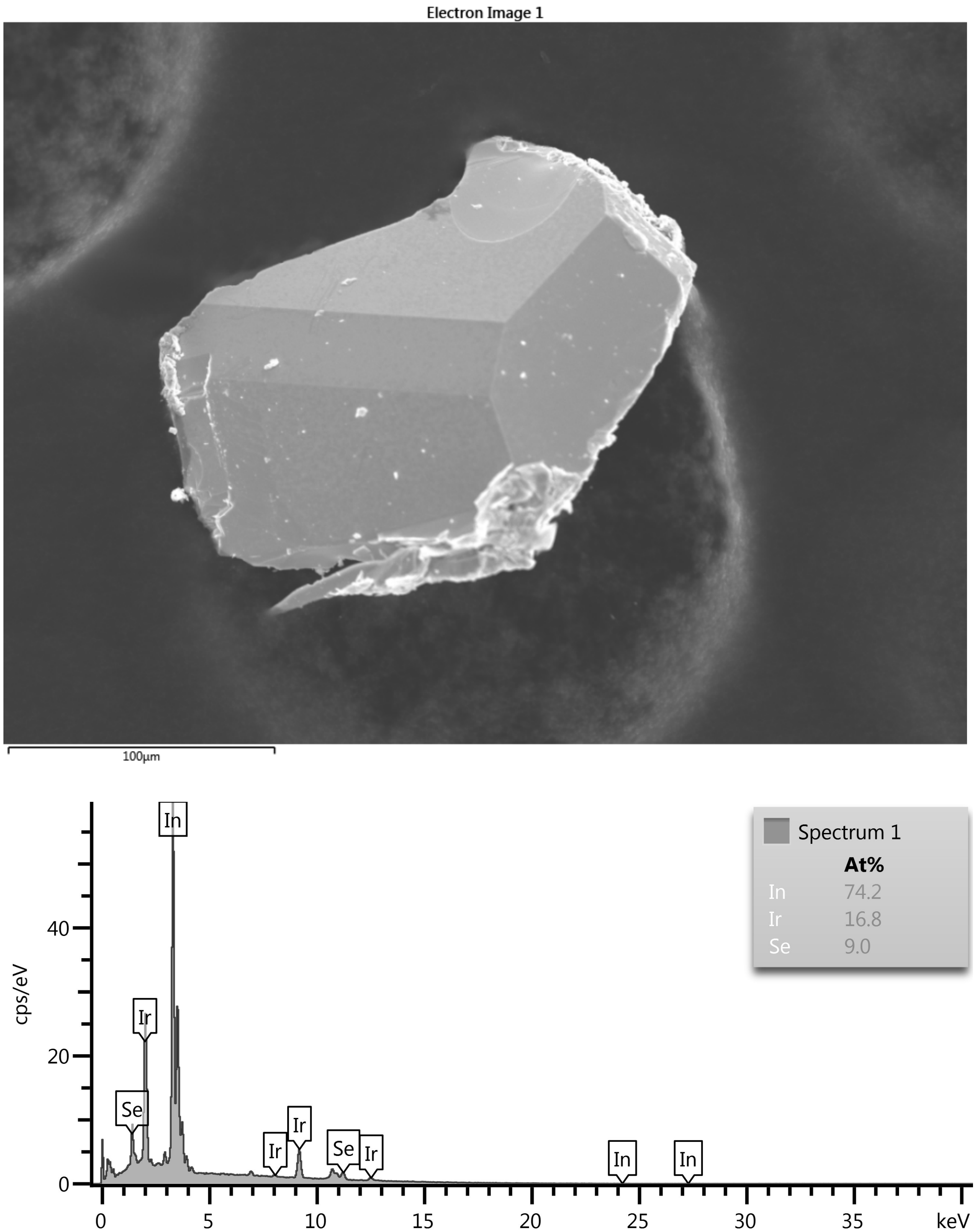


Figure S1: SEM (top) and EDS (bottom) for a single crystal of Ir_2In_8Se. The approximate composition from EDS is $Ir_{1.86}In_{8.24}Se$.

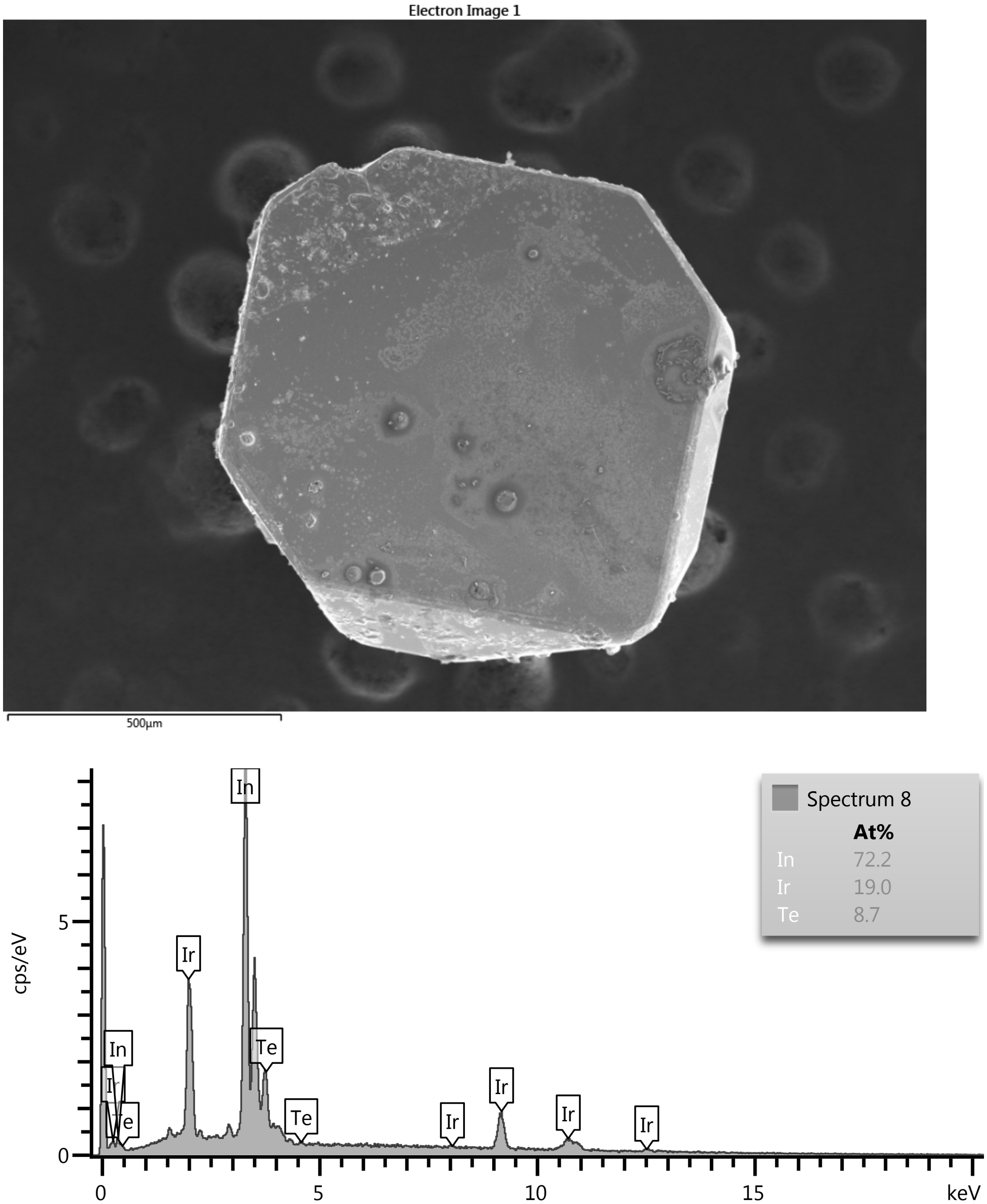


Figure S2: SEM (top) and EDS (bottom) for a single crystal of Ir_2In_8Te. The approximate composition from EDS is $Ir_{2.18}In_{8.29}Te$.

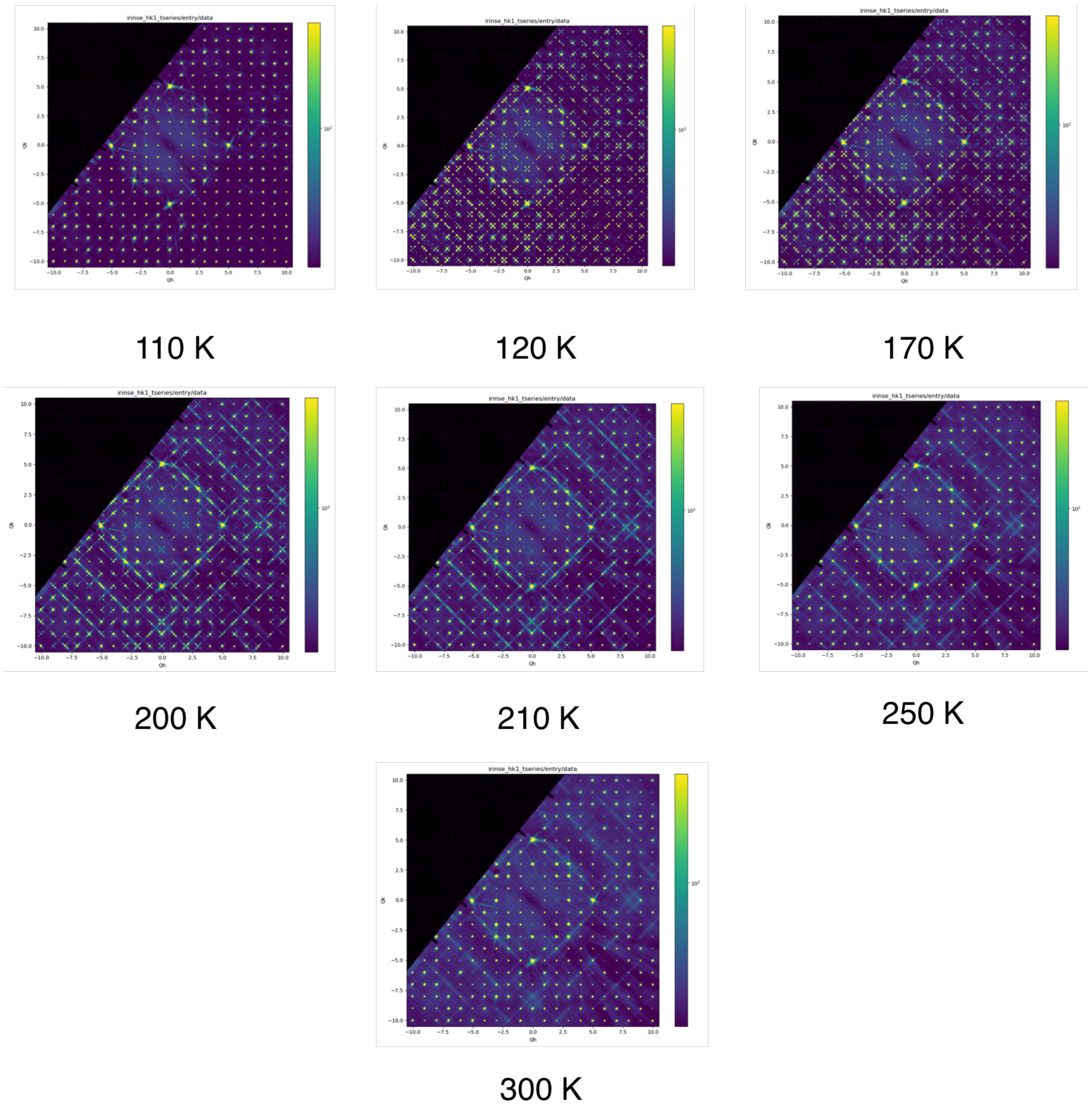


Figure S3: Extended single crystal synchrotron diffraction images of Ir_2In_8Se from 110 – 300 K. The higher temperature regimes show rods of diffuse scattering, the temperatures below the transition temperature (203 K) show supercell ordering, and the temperatures below the second transition temperature (120 K) revert to the original sub-cell with no diffuse scattering.

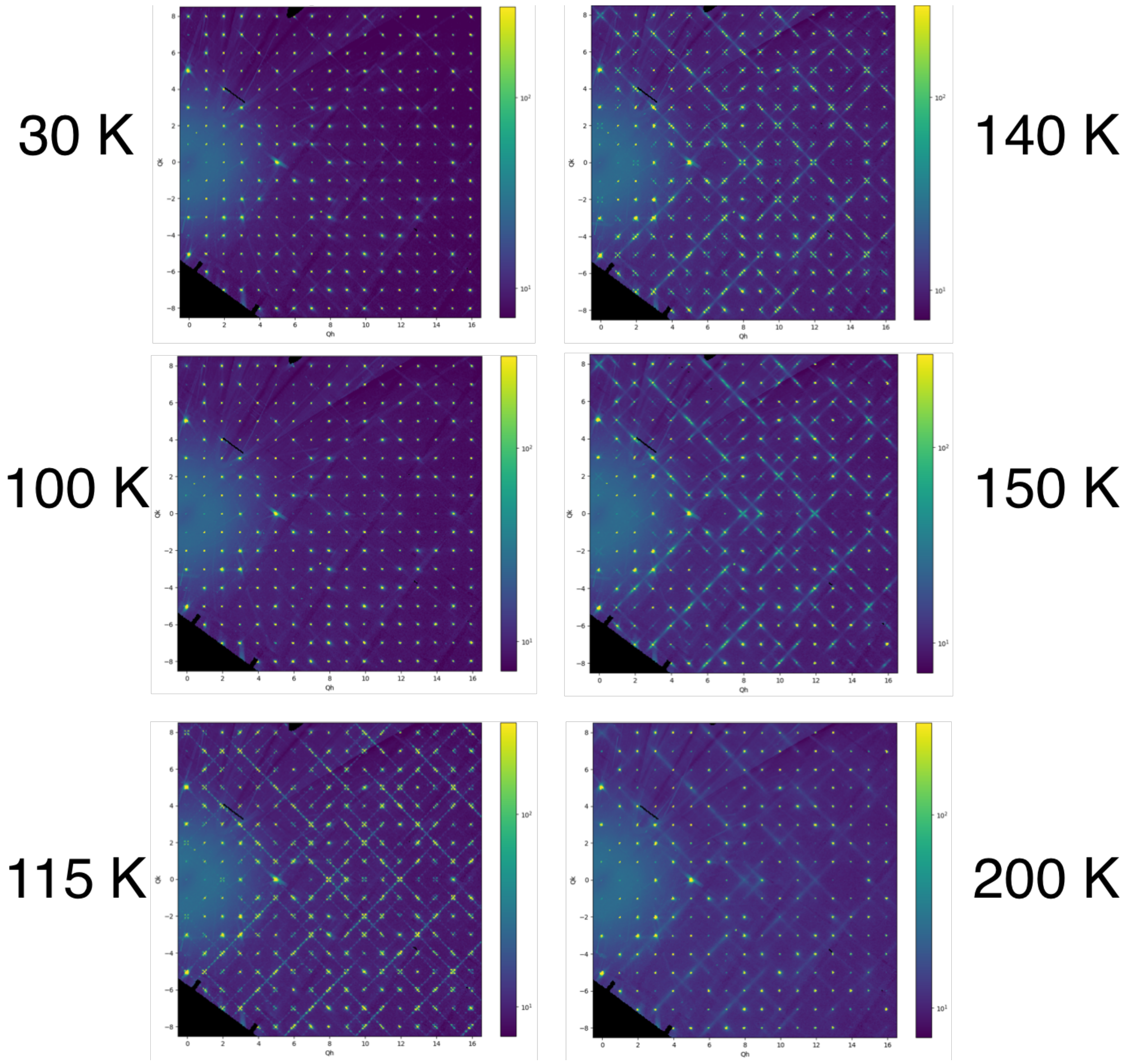
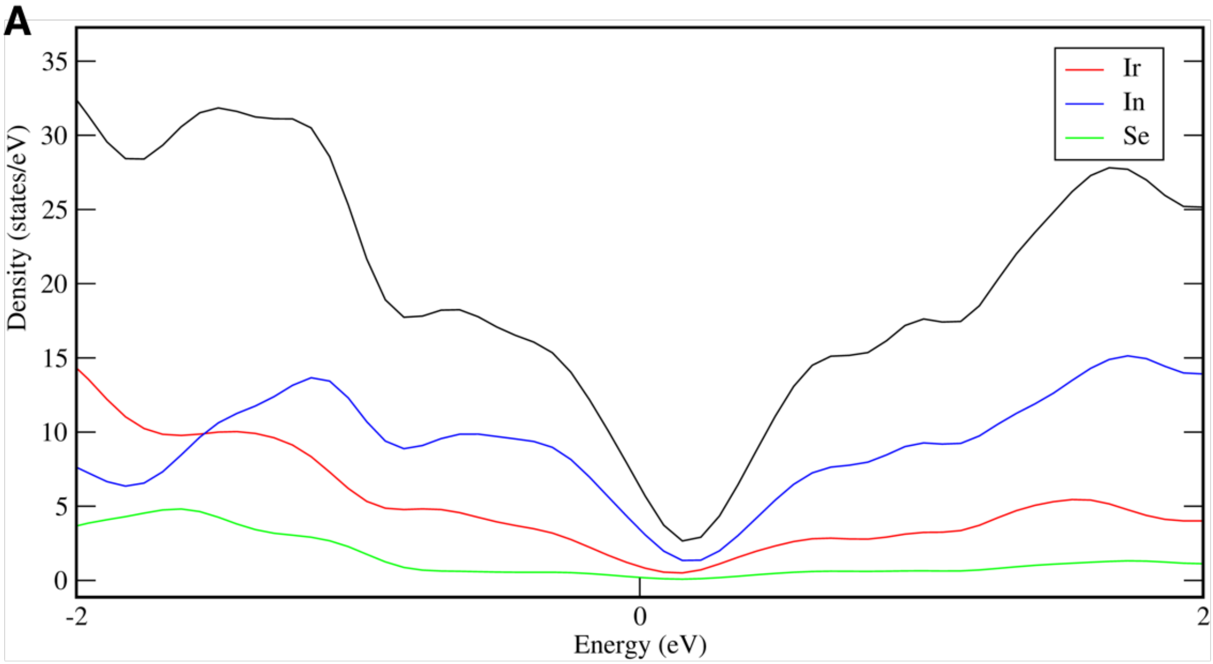


Figure S4: Extended single crystal synchrotron diffraction images of Ir_2In_8Te. The supercell ordering starts to come in below 150 K and reverts to the original sub-cell by 100 K.



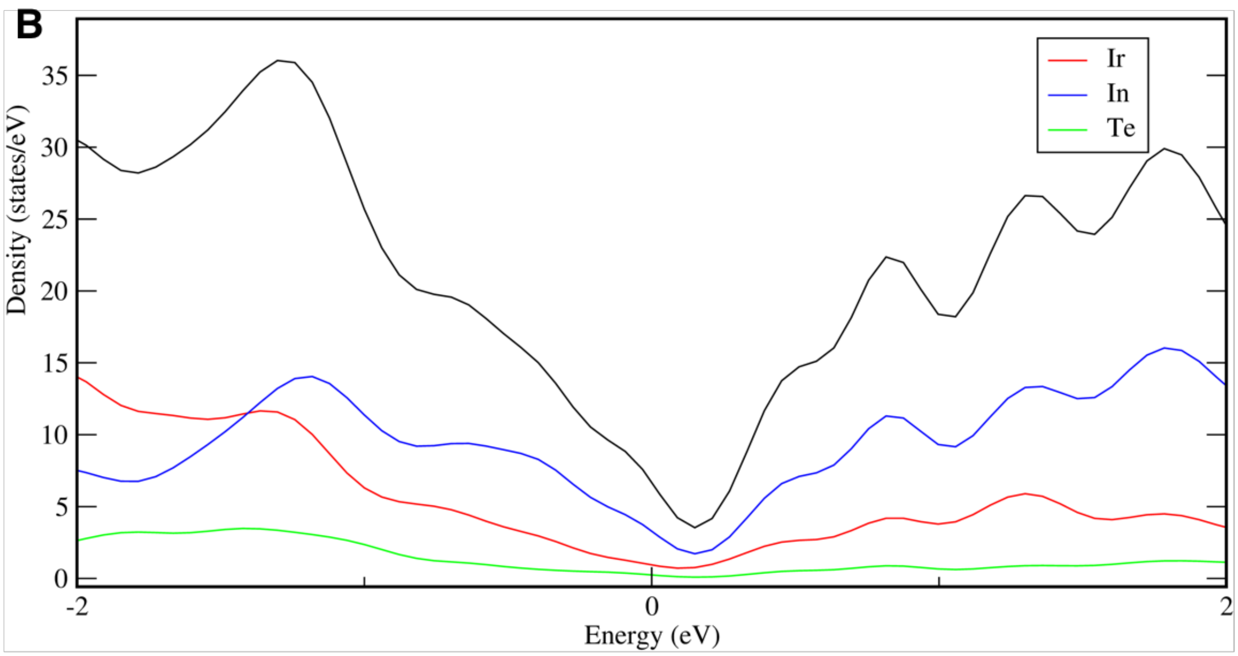


Figure S5: Partial density of states (PDOS) for Ir_2In_8Se (A) and Ir_2In_8Te (B), with the total DOS in black. In both cases, In and Ir orbital contributions are the main contributors to the band structure with minimal contribution from the Q atoms.

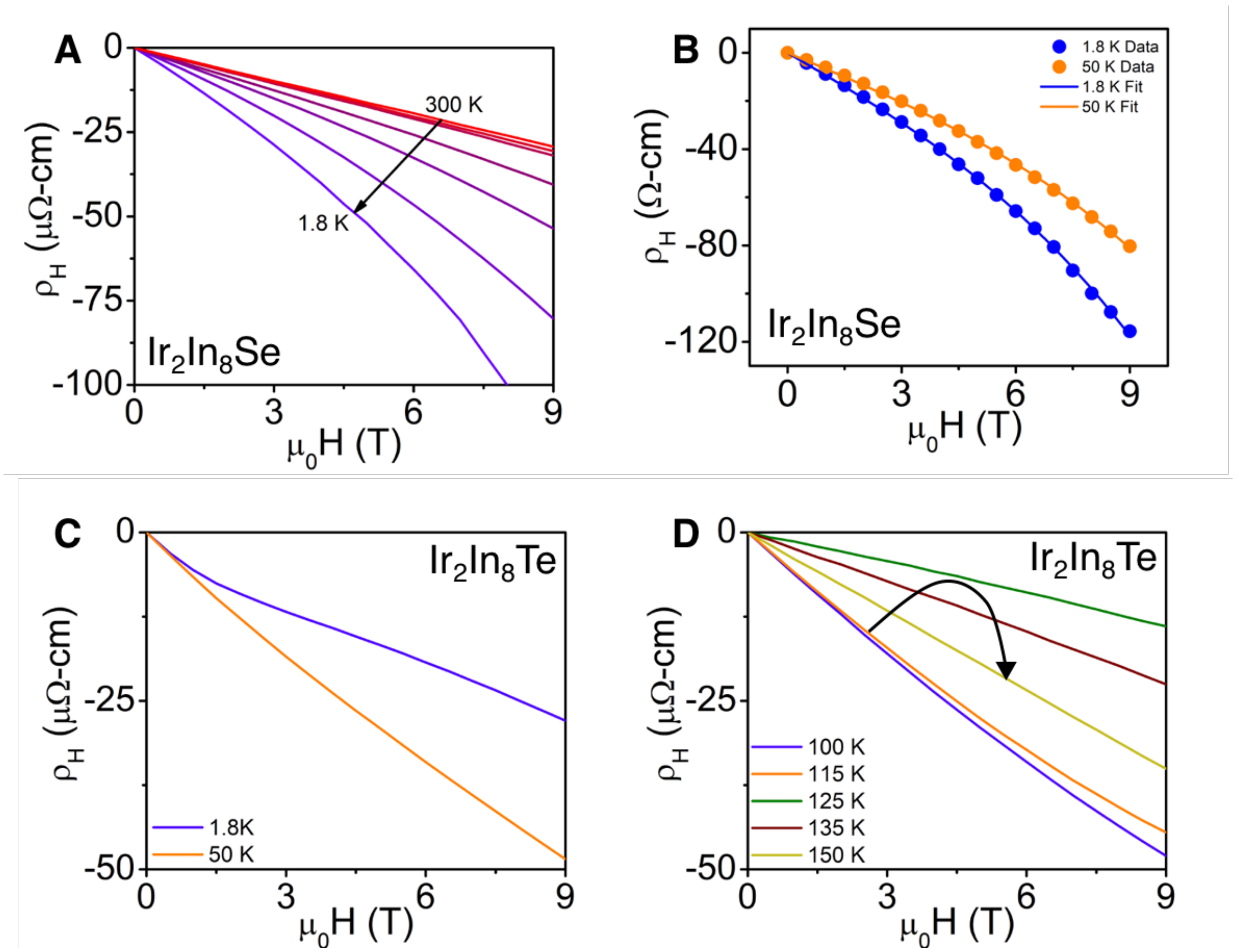


Figure S6: Variable temperature Hall resistivity data for Ir_2In_8Se (A, B) and Ir_2In_8Te (C, D). The multi-band fits in (B) show both electron and hole contribution at low temperatures in Ir_2In_8Se, while the telluride analogue does not fit to a multi-band model. The hole carrier concentration and mobility values are ~900 cm^2/Vs and 5 x 10^{19} cm^{-3} at 1.8 K and ~700 cm^2/Vs and 7 x 10^{18} cm^{-3} at 50 K.

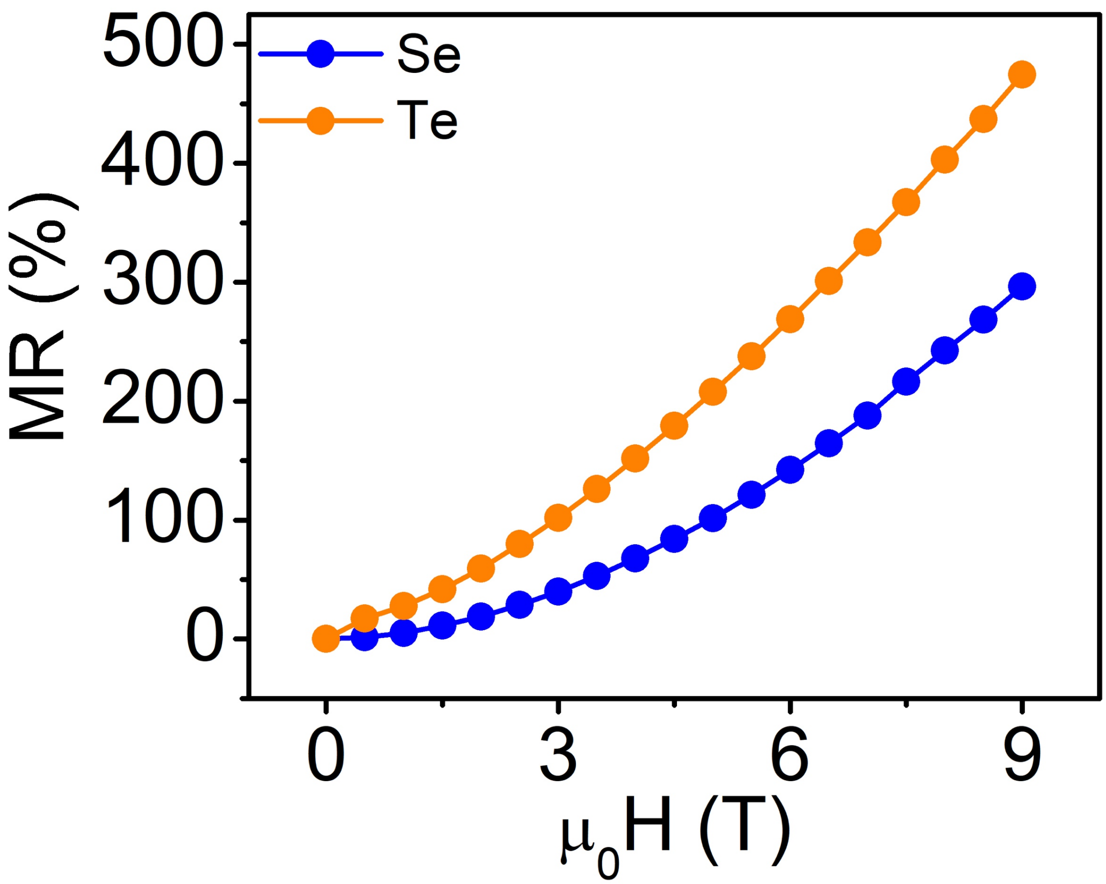


Figure S7: Magnetoresistance data for Ir_2In_8Se and Ir_2In_8Te. Orange and blue lines are guides to the eye.

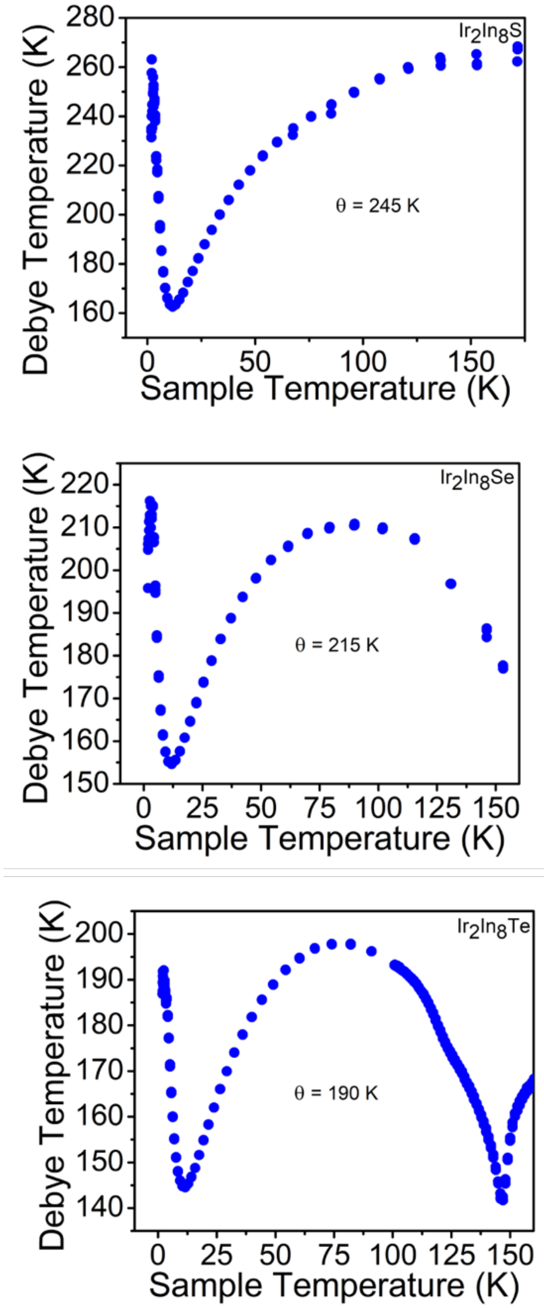


Figure S8: Debye temperature plots and estimated Debye temperature values of Ir_2In_8Q. Ir_2In_8S has the highest Debye temperature due to the more ionic behavior of the sulfide anion, and Ir_2In_8Te has the lowest value due to the softer, more covalent nature of the telluride anion.

Table S1. Atomic coordinates (x10^4) and equivalent isotropic displacement parameters (Å^{2}x10^3) for Ir_2In_8S at 299 K with estimated standard deviations in parentheses.

Label	x	y	z	Occupancy	U_{eq}*
Ir(1)	6876(1)	6876(1)	7399(1)	1	3(1)
In(1)	5957(1)	5957(1)	5000	1	10(1)
In(2)	5000	5000	8340(1)	1	12(1)
In(3)	9478(1)	7009(1)	8046(1)	1	13(1)
In(4)	6841(1)	6841(1)	10000	1	18(1)
In(5)	8003(1)	8003(1)	5000	1	39(1)
S(1)	10000	5000	10000	1	43(2)

*U_{eq} is defined as one third of the trace of the orthogonalized U_{ij} tensor.

Table S2. Anisotropic displacement parameters (Å^{2}x10^3) for Ir_2In_8S at 299 K with estimated standard deviations in parentheses.

Label	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
Ir(1)	2(1)	2(1)	6(1)	0(1)	0(1)	0(1)
In(1)	11(1)	11(1)	7(1)	-6(1)	0	0
In(2)	11(1)	11(1)	14(1)	-8(1)	0	0
In(3)	2(1)	12(1)	24(1)	-3(1)	0(1)	-2(1)
In(4)	24(1)	24(1)	6(1)	-13(1)	0	0
In(5)	55(1)	55(1)	9(1)	-51(1)	0	0
S(1)	104(5)	13(2)	13(2)	22(2)	0	0

The anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U_{11} + ... + 2hka^*b^*U_{12}]$.

Table S3. Bond lengths [Å] for Ir_2In_8S at 299 K with estimated standard deviations in parentheses.

Label	Distances
Ir(1)-In(1)	2.7532(7)
Ir(1)-In(2)	2.7993(6)
Ir(1)-In(3)	2.6668(6)
Ir(1)-In(3)#1	2.6618(6)
Ir(1)-In(3)#2	2.6668(6)
Ir(1)-In(3)#3	2.6618(6)
Ir(1)-In(4)	2.6379(6)
Ir(1)-In(5)	2.9016(8)
In(1)-Ir(1)#4	2.7531(7)
In(1)-In(1)#5	2.6843(19)
In(1)-In(3)#3	3.1858(6)
In(1)-In(3)#6	3.1858(6)
In(1)-In(3)#1	3.1858(6)
In(1)-In(3)#7	3.1858(6)
In(1)-In(5)	2.8711(15)
In(2)-Ir(1)#8	2.7992(6)
In(2)-In(2)#9	3.366(2)
In(2)-In(3)#3	3.3239(8)
In(2)-In(3)#10	3.3239(8)
In(2)-In(3)#11	3.3239(8)
In(2)-In(3)#1	3.3239(8)
In(2)-In(4)	3.0829(11)
In(2)-In(4)#9	3.0829(11)
In(2)-In(5)#11	3.2679(12)
In(2)-In(5)#12	3.2679(12)
In(3)-Ir(1)#13	2.6618(6)
In(3)-In(1)#13	3.1857(6)
In(3)-In(2)#13	3.3239(8)
In(3)-In(3)#1	3.1156(9)
In(3)-In(3)#13	3.1155(9)
In(3)-In(4)	3.2855(9)
In(3)-S(1)	2.8574(6)
In(4)-Ir(1)#14	2.6379(6)

In(4)-In(2)#9	3.0829(11)
In(4)-In(3)#2	3.2855(9)
In(4)-In(3)#14	3.2855(9)
In(4)-In(3)#15	3.2855(9)
In(5)-Ir(1)#4	2.9016(8)
In(5)-In(2)#13	3.2680(12)
In(5)-In(2)#16	3.2680(12)
S(1)-In(3)#17	2.8574(6)
S(1)-In(3)#18	2.8574(6)
S(1)-In(3)#14	2.8574(6)

Symmetry transformations used to generate equivalent atoms:
(1) x-1/2,-y+3/2,-z+3/2 (2) -y+3/2,x-1/2,-z+3/2 (3) y,x,z (4) x,y,-z+1 (5) -x+1,-y+1,-z+1 (6) -y+3/2,x-1/2,z-1/2 (7) x-1/2,-y+3/2,z-1/2 (8) -x+1,-y+1,z (9) -x+1,-y+1,-z+2 (10) y-1/2,-x+3/2,-z+3/2 (11) -x+3/2,y-1/2,-z+3/2 (12) -y+3/2,x-1/2,z+1/2 (13) y+1/2,-x+3/2,-z+3/2 (14) x,y,-z+2 (15) y,x,-z+2 (16) -y+3/2,x+1/2,z-1/2 (17) -x+2,-y+1,-z+2 (18) -x+2,-y+1,z

Table S4. Bond angles [°] for Ir_2In_8S at 299 K with estimated standard deviations in parentheses.

Label	Angles
In(1)-Ir(1)-In(2)	82.01(3)
In(1)-Ir(1)-In(5)	60.96(3)
In(2)-Ir(1)-In(5)	142.97(3)
In(3)#3-Ir(1)-In(1)	72.054(14)
In(3)-Ir(1)-In(1)	123.670(18)
In(3)#2-Ir(1)-In(1)	123.670(18)
In(3)#1-Ir(1)-In(1)	72.054(14)
In(3)#2-Ir(1)-In(2)	126.332(19)
In(3)-Ir(1)-In(2)	126.332(19)
In(3)#1-Ir(1)-In(2)	74.937(14)
In(3)#3-Ir(1)-In(2)	74.937(14)
In(3)#1-Ir(1)-In(3)#2	152.389(11)
In(3)#1-Ir(1)-In(3)	71.56(2)
In(3)#3-Ir(1)-In(3)#1	135.56(3)
In(3)#2-Ir(1)-In(3)	81.00(2)
In(3)#3-Ir(1)-In(3)	152.389(11)
In(3)#3-Ir(1)-In(3)#2	71.56(2)
In(3)#2-Ir(1)-In(5)	79.29(2)
In(3)#3-Ir(1)-In(5)	92.410(16)
In(3)-Ir(1)-In(5)	79.29(2)
In(3)#1-Ir(1)-In(5)	92.410(16)
In(4)-Ir(1)-In(1)	151.02(3)
In(4)-Ir(1)-In(2)	69.01(3)
In(4)-Ir(1)-In(3)#1	99.402(17)
In(4)-Ir(1)-In(3)	76.54(2)
In(4)-Ir(1)-In(3)#2	76.54(2)
In(4)-Ir(1)-In(3)#3	99.402(17)
In(4)-Ir(1)-In(5)	148.02(3)
Ir(1)#4-In(1)-Ir(1)	124.15(4)
Ir(1)-In(1)-In(3)#1	52.645(12)
Ir(1)#4-In(1)-In(3)#1	119.48(2)
Ir(1)#4-In(1)-In(3)#6	52.645(12)
Ir(1)#4-In(1)-In(3)#3	119.48(2)
Ir(1)#4-In(1)-In(3)#7	52.645(12)

Ir(1)-In(1)-In(3)#7	119.48(2)
Ir(1)-In(1)-In(3)#6	119.48(2)
Ir(1)-In(1)-In(3)#3	52.645(12)
Ir(1)#4-In(1)-In(5)	62.074(19)
Ir(1)-In(1)-In(5)	62.074(19)
In(1)#5-In(1)-Ir(1)	117.926(19)
In(1)#5-In(1)-Ir(1)#4	117.926(19)
In(1)#5-In(1)-In(3)#6	97.028(19)
In(1)#5-In(1)-In(3)#3	97.028(19)
In(1)#5-In(1)-In(3)#7	97.028(19)
In(1)#5-In(1)-In(3)#1	97.028(19)
In(1)#5-In(1)-In(5)	180.00(4)
In(3)#3-In(1)-In(3)#7	165.94(4)
In(3)#1-In(1)-In(3)#6	165.94(4)
In(3)#7-In(1)-In(3)#6	101.34(2)
In(3)#3-In(1)-In(3)#1	101.34(2)
In(3)#3-In(1)-In(3)#6	76.91(2)
In(3)#1-In(1)-In(3)#7	76.91(2)
In(5)-In(1)-In(3)#3	82.972(19)
In(5)-In(1)-In(3)#1	82.972(19)
In(5)-In(1)-In(3)#6	82.972(19)
In(5)-In(1)-In(3)#7	82.972(19)
Ir(1)#8-In(2)-Ir(1)	140.13(4)
Ir(1)#8-In(2)-In(2)#9	109.94(2)
Ir(1)-In(2)-In(2)#9	109.94(2)
Ir(1)-In(2)-In(3)#10	110.22(2)
Ir(1)#8-In(2)-In(3)#10	50.651(11)
Ir(1)-In(2)-In(3)#11	110.22(2)
Ir(1)#8-In(2)-In(3)#11	50.651(11)
Ir(1)#8-In(2)-In(3)#1	110.22(2)
Ir(1)#8-In(2)-In(3)#3	110.22(2)
Ir(1)-In(2)-In(3)#1	50.651(11)
Ir(1)-In(2)-In(3)#3	50.651(11)
Ir(1)-In(2)-In(4)	53.022(17)
Ir(1)#8-In(2)-In(4)#9	53.023(17)
Ir(1)#8-In(2)-In(4)	166.85(4)

Ir(1)-In(2)-In(4)#9	166.85(4)
Ir(1)#8-In(2)-In(5)#12	100.114(8)
Ir(1)-In(2)-In(5)#11	100.113(8)
Ir(1)#8-In(2)-In(5)#11	100.114(8)
Ir(1)-In(2)-In(5)#12	100.113(8)
In(3)#1-In(2)-In(2)#9	115.022(19)
In(3)#11-In(2)-In(2)#9	115.02(2)
In(3)#10-In(2)-In(2)#9	115.022(19)
In(3)#3-In(2)-In(2)#9	115.022(19)
In(3)#11-In(2)-In(3)#10	95.69(2)
In(3)#11-In(2)-In(3)#1	129.96(4)
In(3)#10-In(2)-In(3)#3	129.96(4)
In(3)#1-In(2)-In(3)#3	95.69(2)
In(3)#11-In(2)-In(3)#3	62.805(19)
In(3)#10-In(2)-In(3)#1	62.805(19)
In(4)#9-In(2)-In(2)#9	56.91(2)
In(4)-In(2)-In(2)#9	56.91(2)
In(4)-In(2)-In(3)#3	78.131(14)
In(4)#9-In(2)-In(3)#11	78.131(14)
In(4)-In(2)-In(3)#1	78.131(14)
In(4)-In(2)-In(3)#10	131.871(10)
In(4)#9-In(2)-In(3)#3	131.871(10)
In(4)#9-In(2)-In(3)#10	78.131(14)
In(4)#9-In(2)-In(3)#1	131.871(10)
In(4)-In(2)-In(3)#11	131.871(10)
In(4)-In(2)-In(4)#9	113.83(4)
In(4)#9-In(2)-In(5)#11	73.672(17)
In(4)-In(2)-In(5)#11	73.672(17)
In(4)-In(2)-In(5)#12	73.672(17)
In(4)#9-In(2)-In(5)#12	73.672(17)
In(5)#12-In(2)-In(2)#9	59.003(19)
In(5)#11-In(2)-In(2)#9	59.003(19)
In(5)#11-In(2)-In(3)#3	65.313(16)
In(5)#12-In(2)-In(3)#11	148.574(10)
In(5)#11-In(2)-In(3)#10	148.574(10)
In(5)#11-In(2)-In(3)#11	65.313(16)

In(5)#12-In(2)-In(3)#1	65.313(15)
In(5)#11-In(2)-In(3)#1	148.573(10)
In(5)#12-In(2)-In(3)#3	148.574(10)
In(5)#12-In(2)-In(3)#10	65.313(15)
In(5)#11-In(2)-In(5)#12	118.01(4)
Ir(1)#13-In(3)-Ir(1)	147.55(2)
Ir(1)-In(3)-In(1)#13	129.06(2)
Ir(1)#13-In(3)-In(1)#13	55.301(16)
Ir(1)-In(3)-In(2)#13	95.217(17)
Ir(1)#13-In(3)-In(2)#13	54.412(11)
Ir(1)#13-In(3)-In(3)#13	54.296(18)
Ir(1)-In(3)-In(3)#1	54.145(17)
Ir(1)-In(3)-In(3)#13	132.00(2)
Ir(1)#13-In(3)-In(3)#1	134.24(2)
Ir(1)#13-In(3)-In(4)	146.59(3)
Ir(1)-In(3)-In(4)	51.336(17)
Ir(1)-In(3)-S(1)	108.149(17)
Ir(1)#13-In(3)-S(1)	104.214(18)
In(1)#13-In(3)-In(2)#13	68.03(2)
In(1)#13-In(3)-In(4)	91.36(2)
In(3)#13-In(3)-In(1)#13	98.63(3)
In(3)#1-In(3)-In(1)#13	161.73(3)
In(3)#13-In(3)-In(2)#13	98.44(2)
In(3)#1-In(3)-In(2)#13	129.99(3)
In(3)#13-In(3)-In(3)#1	82.737(14)
In(3)#13-In(3)-In(4)	146.30(2)
In(3)#1-In(3)-In(4)	78.27(2)
In(4)-In(3)-In(2)#13	115.11(2)
S(1)-In(3)-In(1)#13	85.83(2)
S(1)-In(3)-In(2)#13	152.58(2)
S(1)-In(3)-In(3)#13	76.718(16)
S(1)-In(3)-In(3)#1	76.718(16)
S(1)-In(3)-In(4)	71.993(15)
Ir(1)-In(4)-Ir(1)#14	177.89(5)
Ir(1)-In(4)-In(2)#9	124.14(4)
Ir(1)#14-In(4)-In(2)	124.14(4)

Ir(1)-In(4)-In(2)	57.97(2)
Ir(1)#14-In(4)-In(2)#9	57.97(2)
Ir(1)-In(4)-In(3)#15	126.29(3)
Ir(1)#14-In(4)-In(3)#2	126.29(3)
Ir(1)-In(4)-In(3)#2	52.128(15)
Ir(1)#14-In(4)-In(3)	126.29(3)
Ir(1)-In(4)-In(3)	52.128(15)
Ir(1)-In(4)-In(3)#14	126.29(3)
Ir(1)#14-In(4)-In(3)#15	52.129(15)
Ir(1)#14-In(4)-In(3)#14	52.129(15)
In(2)-In(4)-In(2)#9	66.17(4)
In(2)-In(4)-In(3)#15	146.186(18)
In(2)-In(4)-In(3)#14	146.186(18)
In(2)#9-In(4)-In(3)#14	99.93(2)
In(2)#9-In(4)-In(3)#15	99.93(2)
In(2)-In(4)-In(3)#2	99.93(2)
In(2)-In(4)-In(3)	99.93(2)
In(2)#9-In(4)-In(3)	146.186(18)
In(2)#9-In(4)-In(3)#2	146.186(18)
In(3)#15-In(4)-In(3)	106.44(4)
In(3)#14-In(4)-In(3)	74.17(3)
In(3)#15-In(4)-In(3)#2	74.17(3)
In(3)#15-In(4)-In(3)#14	63.63(2)
In(3)-In(4)-In(3)#2	63.62(2)
In(3)#14-In(4)-In(3)#2	106.44(4)
Ir(1)-In(5)-Ir(1)#4	113.93(4)
Ir(1)-In(5)-In(2)#16	154.03(3)
Ir(1)#4-In(5)-In(2)#16	92.04(2)
Ir(1)#4-In(5)-In(2)#13	154.03(3)
Ir(1)-In(5)-In(2)#13	92.04(2)
In(1)-In(5)-Ir(1)#4	56.97(2)
In(1)-In(5)-Ir(1)	56.97(2)
In(1)-In(5)-In(2)#13	149.00(2)
In(1)-In(5)-In(2)#16	149.00(2)
In(2)#13-In(5)-In(2)#16	61.99(4)
In(3)#14-S(1)-In(3)#18	92.21(3)

In(3)#17-S(1)-In(3)	92.21(3)
In(3)#18-S(1)-In(3)	180.0
In(3)#17-S(1)-In(3)#18	87.79(3)
In(3)#14-S(1)-In(3)#17	180.0
In(3)#14-S(1)-In(3)	87.79(3)

Symmetry transformations used to generate equivalent atoms:
(1) x-1/2,-y+3/2,-z+3/2 (2) -y+3/2,x-1/2,-z+3/2 (3) y,x,z (4) x,y,-z+1 (5) -x+1,-y+1,-z+1 (6) -y+3/2,x-1/2,z-1/2 (7) x-1/2,-y+3/2,z-1/2 (8) -x+1,-y+1,z (9) -x+1,-y+1,-z+2 (10) y-1/2,-x+3/2,-z+3/2 (11) -x+3/2,y-1/2,-z+3/2 (12) -y+3/2,x-1/2,z+1/2 (13) y+1/2,-x+3/2,-z+3/2 (14) x,y,-z+2 (15) y,x,-z+2 (16) -y+3/2,x+1/2,z-1/2 (17) -x+2,-y+1,-z+2 (18) -x+2,-y+1,z

Table S5. Atomic coordinates (x10^4) and equivalent isotropic displacement parameters (Å^{2}x10^3) for Ir_2In_8Se at 299 K with estimated standard deviations in parentheses.

Label	x	y	z	Occupancy	U_{eq}*
Ir(1)	6863(1)	6863(1)	2405(1)	1	4(1)
In(1)	5953(1)	5953(1)	0	1	13(1)
In(2)	5000	5000	3367(1)	1	12(1)
In(3)	4463(1)	7948(1)	2025(1)	1	15(1)
In(4)	6877(1)	6877(1)	5000	1	19(1)
In(5)	7986(1)	7986(1)	0	1	34(1)
Se(1)	5000	10000	0	1	34(1)

*U_{eq} is defined as one third of the trace of the orthogonalized U_{ij} tensor.

Table S6. Anisotropic displacement parameters (Å^{2}x10^3) for Ir_2In_8Se at 299 K with estimated standard deviations in parentheses.

Label	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
Ir(1)	5(1)	5(1)	4(1)	0(1)	0(1)	0(1)
In(1)	17(1)	17(1)	5(1)	-8(1)	0	0
In(2)	12(1)	12(1)	12(1)	-6(1)	0	0
In(3)	5(1)	15(1)	24(1)	3(1)	1(1)	2(1)
In(4)	28(1)	28(1)	3(1)	-13(1)	0	0
In(5)	47(1)	47(1)	6(1)	-39(1)	0	0
Se(1)	81(2)	12(1)	9(1)	-15(1)	0	0

The anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U_{11} + ... + 2hka^*b^*U_{12}]$.

Table S7. Bond lengths [Å] for Ir_2In_8Se at 299 K with estimated standard deviations in parentheses.

Label	Distances
Ir(1)-In(1)	2.7478(6)
Ir(1)-In(2)	2.7947(5)
Ir(1)-In(3)#1	2.6558(6)
Ir(1)-In(3)#2	2.6472(5)
Ir(1)-In(3)	2.6472(5)
Ir(1)-In(3)#3	2.6558(6)
Ir(1)-In(4)	2.6230(4)
Ir(1)-In(5)	2.8997(7)
In(1)-Ir(1)#4	2.7478(6)
In(1)-In(1)#5	2.6806(18)
In(1)-In(3)#4	3.2131(6)
In(1)-In(3)#2	3.2131(6)
In(1)-In(3)#6	3.2131(6)
In(1)-In(3)	3.2131(6)
In(1)-In(5)	2.8594(14)
In(2)-Ir(1)#7	2.7947(5)
In(2)-In(2)#8	3.3008(19)
In(2)-In(3)	3.2744(7)
In(2)-In(3)#2	3.2744(7)
In(2)-In(3)#9	3.2744(7)
In(2)-In(3)#7	3.2744(7)
In(2)-In(4)	3.1133(10)
In(2)-In(4)#8	3.1133(10)
In(2)-In(5)#10	3.2781(11)
In(2)-In(5)#11	3.2781(11)
In(3)-Ir(1)#11	2.6559(6)
In(3)-In(3)#1	3.1332(8)
In(3)-In(3)#11	3.1333(8)
In(3)-In(4)#11	3.2919(8)
In(3)-Se(1)	2.9394(6)
In(4)-Ir(1)#12	2.6230(4)
In(4)-In(2)#8	3.1133(10)
In(4)-In(3)#13	3.2919(8)

In(4)-In(3)#1	3.2919(8)
In(4)-In(3)#14	3.2919(8)
In(4)-In(3)#3	3.2919(8)
In(5)-Ir(1)#4	2.8997(7)
In(5)-In(2)#15	3.2780(11)
In(5)-In(2)#16	3.2780(11)
Se(1)-In(3)#4	2.9394(6)
Se(1)-In(3)#17	2.9394(6)
Se(1)-In(3)#18	2.9394(6)

Symmetry transformations used to generate equivalent atoms:
(1) y,x,z (2) x+1/2,-y+3/2,-z+1/2 (3) -y+3/2,x+1/2,-z+1/2 (4) x,y,-z (5) -x+1,-y+1,-z (6) y,x,-z (7) -x+1,-y+1,z (8) -x+1,-y+1,-z+1 (9) -y+1,-x+1,z (10) -y+3/2,x-1/2,z+1/2 (11) y-1/2,-x+3/2,-z+1/2 (12) x,y,-z+1 (13) x+1/2,-y+3/2,z+1/2 (14) -y+3/2,x+1/2,z+1/2 (15) y+1/2,-x+3/2,-z+1/2 (16) -y+3/2,x+1/2,z-1/2 (17) -x+1,-y+2,-z (18) -x+1,-y+2,z

Table S8. Bond angles [°] for Ir_2In_8Se at 299 K with estimated standard deviations in parentheses.

Label	Angles
In(1)-Ir(1)-In(2)	82.61(3)
In(1)-Ir(1)-In(5)	60.77(3)
In(2)-Ir(1)-In(5)	143.37(3)
In(3)#2-Ir(1)-In(1)	73.080(13)
In(3)#3-Ir(1)-In(1)	122.390(17)
In(3)#1-Ir(1)-In(1)	122.390(17)
In(3)-Ir(1)-In(1)	73.080(13)
In(3)#1-Ir(1)-In(2)	128.092(17)
In(3)-Ir(1)-In(2)	73.929(13)
In(3)#3-Ir(1)-In(2)	128.092(17)
In(3)#2-Ir(1)-In(2)	73.929(13)
In(3)-Ir(1)-In(3)#2	135.57(2)
In(3)#2-Ir(1)-In(3)#1	151.690(10)
In(3)-Ir(1)-In(3)#1	72.43(2)
In(3)#1-Ir(1)-In(3)#3	79.36(2)
In(3)#2-Ir(1)-In(3)#3	72.43(2)
In(3)-Ir(1)-In(3)#3	151.690(10)
In(3)#3-Ir(1)-In(5)	77.256(19)
In(3)#2-Ir(1)-In(5)	93.928(15)
In(3)#1-Ir(1)-In(5)	77.256(19)
In(3)-Ir(1)-In(5)	93.928(15)
In(4)-Ir(1)-In(1)	152.68(3)
In(4)-Ir(1)-In(2)	70.07(3)
In(4)-Ir(1)-In(3)	98.497(15)
In(4)-Ir(1)-In(3)#2	98.497(15)
In(4)-Ir(1)-In(3)#3	77.16(2)
In(4)-Ir(1)-In(3)#1	77.16(2)
In(4)-Ir(1)-In(5)	146.56(3)
Ir(1)#4-In(1)-Ir(1)	124.49(4)
Ir(1)-In(1)-In(3)#4	120.82(2)
Ir(1)#4-In(1)-In(3)#2	120.82(2)
Ir(1)-In(1)-In(3)	52.018(11)
Ir(1)#4-In(1)-In(3)#4	52.018(11)

Ir(1)-In(1)-In(3)#2	52.018(11)
Ir(1)-In(1)-In(3)#6	120.82(2)
Ir(1)#4-In(1)-In(3)	120.82(2)
Ir(1)#4-In(1)-In(3)#6	52.018(11)
Ir(1)#4-In(1)-In(5)	62.243(18)
Ir(1)-In(1)-In(5)	62.243(18)
In(1)#5-In(1)-Ir(1)	117.757(18)
In(1)#5-In(1)-Ir(1)#4	117.757(18)
In(1)#5-In(1)-In(3)#4	96.351(18)
In(1)#5-In(1)-In(3)#6	96.351(18)
In(1)#5-In(1)-In(3)	96.352(18)
In(1)#5-In(1)-In(3)#2	96.351(18)
In(1)#5-In(1)-In(5)	180.00(4)
In(3)#2-In(1)-In(3)#4	167.30(4)
In(3)-In(1)-In(3)#4	79.17(2)
In(3)#2-In(1)-In(3)#6	79.17(2)
In(3)-In(1)-In(3)#6	167.30(4)
In(3)-In(1)-In(3)#2	99.41(2)
In(3)#4-In(1)-In(3)#6	99.41(2)
In(5)-In(1)-In(3)	83.648(18)
In(5)-In(1)-In(3)#6	83.649(18)
In(5)-In(1)-In(3)#2	83.649(18)
In(5)-In(1)-In(3)#4	83.649(18)
Ir(1)#7-In(2)-Ir(1)	139.27(4)
Ir(1)-In(2)-In(2)#8	110.365(19)
Ir(1)#7-In(2)-In(2)#8	110.365(18)
Ir(1)-In(2)-In(3)#2	50.973(10)
Ir(1)-In(2)-In(3)#7	109.96(2)
Ir(1)-In(2)-In(3)#9	109.96(2)
Ir(1)#7-In(2)-In(3)	109.96(2)
Ir(1)#7-In(2)-In(3)#7	50.972(10)
Ir(1)#7-In(2)-In(3)#2	109.96(2)
Ir(1)-In(2)-In(3)	50.972(10)
Ir(1)#7-In(2)-In(3)#9	50.972(10)
Ir(1)#7-In(2)-In(4)	168.35(3)
Ir(1)#7-In(2)-In(4)#8	52.377(14)

Ir(1)-In(2)-In(4)	52.377(14)
Ir(1)-In(2)-In(4)#8	168.35(3)
Ir(1)#7-In(2)-In(5)#11	100.091(7)
Ir(1)#7-In(2)-In(5)#10	100.091(6)
Ir(1)-In(2)-In(5)#10	100.090(7)
Ir(1)-In(2)-In(5)#11	100.090(7)
In(3)#2-In(2)-In(2)#8	114.478(18)
In(3)#7-In(2)-In(2)#8	114.478(18)
In(3)#9-In(2)-In(2)#8	114.478(17)
In(3)-In(2)-In(2)#8	114.478(18)
In(3)#9-In(2)-In(3)#7	96.91(2)
In(3)-In(2)-In(3)#2	96.91(2)
In(3)-In(2)-In(3)#7	131.04(4)
In(3)#9-In(2)-In(3)#2	131.04(4)
In(3)#7-In(2)-In(3)#2	62.379(17)
In(3)-In(2)-In(3)#9	62.380(17)
In(3)#2-In(2)-In(5)#10	64.021(13)
In(3)#9-In(2)-In(5)#10	148.787(9)
In(3)#2-In(2)-In(5)#11	148.787(9)
In(3)#7-In(2)-In(5)#10	64.021(13)
In(3)#9-In(2)-In(5)#11	64.021(13)
In(3)-In(2)-In(5)#10	148.787(9)
In(3)-In(2)-In(5)#11	64.021(13)
In(3)#7-In(2)-In(5)#11	148.787(9)
In(4)#8-In(2)-In(2)#8	57.988(18)
In(4)-In(2)-In(2)#8	57.988(18)
In(4)#8-In(2)-In(3)#2	131.206(9)
In(4)#8-In(2)-In(3)	131.206(9)
In(4)#8-In(2)-In(3)#7	77.321(12)
In(4)-In(2)-In(3)#2	77.322(12)
In(4)-In(2)-In(3)#9	131.206(9)
In(4)-In(2)-In(3)#7	131.206(9)
In(4)#8-In(2)-In(3)#9	77.321(12)
In(4)-In(2)-In(3)	77.321(12)
In(4)-In(2)-In(4)#8	115.98(4)
In(4)#8-In(2)-In(5)#10	74.521(15)

In(4)-In(2)-In(5)#11	74.521(15)
In(4)#8-In(2)-In(5)#11	74.521(15)
In(4)-In(2)-In(5)#10	74.521(15)
In(5)#10-In(2)-In(2)#8	59.771(17)
In(5)#11-In(2)-In(2)#8	59.771(17)
In(5)#11-In(2)-In(5)#10	119.54(3)
Ir(1)-In(3)-Ir(1)#11	151.06(2)
Ir(1)-In(3)-In(1)	54.903(14)
Ir(1)#11-In(3)-In(1)	129.10(2)
Ir(1)-In(3)-In(2)	55.099(10)
Ir(1)#11-In(3)-In(2)	97.600(16)
Ir(1)#11-In(3)-In(3)#11	53.655(16)
Ir(1)#11-In(3)-In(3)#1	134.39(2)
Ir(1)-In(3)-In(3)#11	136.39(2)
Ir(1)-In(3)-In(3)#1	53.911(17)
Ir(1)-In(3)-In(4)#11	144.70(2)
Ir(1)#11-In(3)-In(4)#11	50.974(15)
Ir(1)-In(3)-Se(1)	102.733(16)
Ir(1)#11-In(3)-Se(1)	106.180(16)
In(1)-In(3)-In(2)	68.65(2)
In(1)-In(3)-In(4)#11	89.80(2)
In(2)-In(3)-In(4)#11	115.614(19)
In(3)#1-In(3)-In(1)	96.51(2)
In(3)#11-In(3)-In(1)	157.55(3)
In(3)#11-In(3)-In(2)	133.40(3)
In(3)#1-In(3)-In(2)	99.77(2)
In(3)#1-In(3)-In(3)#11	84.617(11)
In(3)#1-In(3)-In(4)#11	143.80(2)
In(3)#11-In(3)-In(4)#11	76.79(2)
Se(1)-In(3)-In(1)	84.323(18)
Se(1)-In(3)-In(2)	151.71(2)
Se(1)-In(3)-In(3)#1	74.358(14)
Se(1)-In(3)-In(3)#11	74.357(14)
Se(1)-In(3)-In(4)#11	70.854(13)
Ir(1)-In(4)-Ir(1)#12	179.13(5)
Ir(1)-In(4)-In(2)#8	121.58(4)

Ir(1)-In(4)-In(2)	57.55(2)
Ir(1)#12-In(4)-In(2)	121.58(4)
Ir(1)#12-In(4)-In(2)#8	57.55(2)
Ir(1)-In(4)-In(3)#3	51.867(14)
Ir(1)#12-In(4)-In(3)#13	51.868(14)
Ir(1)-In(4)-In(3)#13	128.79(3)
Ir(1)#12-In(4)-In(3)#14	51.868(14)
Ir(1)-In(4)-In(3)#14	128.79(3)
Ir(1)#12-In(4)-In(3)#1	128.79(3)
Ir(1)#12-In(4)-In(3)#3	128.79(3)
Ir(1)-In(4)-In(3)#1	51.867(14)
In(2)-In(4)-In(2)#8	64.03(4)
In(2)-In(4)-In(3)#13	146.076(18)
In(2)-In(4)-In(3)#14	146.076(18)
In(2)#8-In(4)-In(3)#14	99.809(18)
In(2)#8-In(4)-In(3)#13	99.809(18)
In(2)-In(4)-In(3)#1	99.809(17)
In(2)-In(4)-In(3)#3	99.809(17)
In(2)#8-In(4)-In(3)#3	146.076(18)
In(2)#8-In(4)-In(3)#1	146.076(18)
In(3)#13-In(4)-In(3)#3	76.92(3)
In(3)#14-In(4)-In(3)#3	107.72(3)
In(3)#13-In(4)-In(3)#1	107.72(3)
In(3)#13-In(4)-In(3)#14	62.01(2)
In(3)#3-In(4)-In(3)#1	62.01(2)
In(3)#14-In(4)-In(3)#1	76.92(3)
Ir(1)-In(5)-Ir(1)#4	113.98(4)
Ir(1)-In(5)-In(2)#16	153.24(3)
Ir(1)#4-In(5)-In(2)#16	92.780(19)
Ir(1)#4-In(5)-In(2)#15	153.24(3)
Ir(1)-In(5)-In(2)#15	92.779(19)
In(1)-In(5)-Ir(1)#4	56.990(19)
In(1)-In(5)-Ir(1)	56.991(19)
In(1)-In(5)-In(2)#15	149.770(17)
In(1)-In(5)-In(2)#16	149.770(17)
In(2)#15-In(5)-In(2)#16	60.46(3)

In(3)#4-Se(1)-In(3)	88.30(2)
In(3)#17-Se(1)-In(3)#18	88.30(2)
In(3)-Se(1)-In(3)#18	180.0
In(3)#17-Se(1)-In(3)	91.70(2)
In(3)#4-Se(1)-In(3)#17	180.000(15)
In(3)#4-Se(1)-In(3)#18	91.70(2)

Symmetry transformations used to generate equivalent atoms:
(1) y,x,z (2) x+1/2,-y+3/2,-z+1/2 (3) -y+3/2,x+1/2,-z+1/2 (4) x,y,-z (5) -x+1,-y+1,-z (6) y,x,-z (7) -x+1,-y+1,z (8) -x+1,-y+1,-z+1 (9) -y+1,-x+1,z (10) -y+3/2,x-1/2,z+1/2 (11) y-1/2,-x+3/2,-z+1/2 (12) x,y,-z+1 (13) x+1/2,-y+3/2,z+1/2 (14) -y+3/2,x+1/2,z+1/2 (15) y+1/2,-x+3/2,-z+1/2 (16) -y+3/2,x+1/2,z-1/2 (17) -x+1,-y+2,-z (18) -x+1,-y+2,z

Table S9. Atomic coordinates (x10[4]) and equivalent isotropic displacement parameters ($Å^2$x10^3) for Ir_2In_8Te at 299 K with estimated standard deviations in parentheses.

Label	x	y	z	Occupancy	U_{eq}^*
Ir(1)	6844(1)	3156(1)	7582(1)	1	5(1)
In(2)	5000	5000	6598(1)	1	12(1)
Te(1)	10000	5000	10000	1	20(1)
In(3)	7895(1)	5557(1)	7884(1)	1	16(1)
In(1)	5947(1)	4053(1)	10000	1	14(1)
In(4)	6920(1)	3080(1)	5000	1	18(1)
In(5)	7962(1)	2038(1)	10000	1	23(1)

$^*U_{eq}$ is defined as one third of the trace of the orthogonalized U_{ij} tensor.

Table S10. Anisotropic displacement parameters ($Å^2$x10^3) for Ir_2In_8Te at 299 K with estimated standard deviations in parentheses.

Label	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
Ir(1)	4(1)	4(1)	6(1)	0(1)	0(1)	0(1)
In(2)	11(1)	11(1)	15(1)	5(1)	0	0
Te(1)	10(1)	38(1)	11(1)	7(1)	0	0
In(3)	14(1)	5(1)	28(1)	-2(1)	-4(1)	1(1)
In(1)	17(1)	17(1)	8(1)	9(1)	0	0
In(4)	23(1)	23(1)	6(1)	8(1)	0	0
In(5)	29(1)	29(1)	11(1)	21(1)	0	0

The anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U_{11} + ... + 2hka^*b^*U_{12}]$.

Table S11. Bond lengths [Å] for Ir_2In_8Te at 299 K with estimated standard deviations in parentheses.

Label	Distances
Ir(1)-In(2)	2.827(2)
Ir(1)-In(3)	2.672(2)
Ir(1)-In(3)#1	2.688(2)
Ir(1)-In(3)#2	2.672(2)
Ir(1)-In(3)#3	2.688(2)
Ir(1)-In(1)	2.8002(19)
Ir(1)-In(4)	2.659(2)
Ir(1)-In(5)	2.9590(19)
In(2)-Ir(1)#4	2.827(2)
In(2)-In(2)#5	3.289(3)
In(2)-In(3)	3.265(2)
In(2)-In(3)#6	3.265(2)
In(2)-In(3)#4	3.265(2)
In(2)-In(3)#2	3.265(2)
In(2)-In(4)#5	3.203(2)
In(2)-In(4)	3.203(2)
In(2)-In(5)#7	3.349(2)
In(2)-In(5)#8	3.349(2)
Te(1)-In(3)#9	3.0982(18)
Te(1)-In(3)#10	3.0982(18)
Te(1)-In(3)	3.0982(18)
Te(1)-In(3)#11	3.0982(18)
In(3)-Ir(1)#8	2.688(2)
In(3)-In(3)#8	3.215(2)
In(3)-In(3)#6	3.348(3)
In(3)-In(3)#3	3.215(2)
In(3)-In(1)	3.3091(19)
In(3)-In(4)#8	3.362(2)
In(1)-Ir(1)#9	2.8002(19)
In(1)-In(3)#2	3.3091(19)
In(1)-In(3)#12	3.3091(19)
In(1)-In(3)#9	3.3091(19)
In(1)-In(1)#13	2.712(3)

In(1)-In(5)	2.885(3)
In(4)-Ir(1)#14	2.659(2)
In(4)-In(2)#5	3.203(2)
In(4)-In(3)#15	3.362(2)
In(4)-In(3)#3	3.362(2)
In(4)-In(3)#16	3.362(2)
In(4)-In(3)#1	3.362(2)
In(5)-Ir(1)#9	2.9590(19)
In(5)-In(2)#17	3.349(2)
In(5)-In(2)#18	3.349(2)

Symmetry transformations used to generate equivalent atoms:
(1) -y+1,-x+1,z (2) -y+3/2,x-1/2,-z+3/2 (3) -x+3/2,y-1/2,-z+3/2 (4) -x+1,-y+1,z (5) -x+1,-y+1,-z+1 (6) y,x,z (7) -y+1/2,x-1/2,z-1/2 (8) y+1/2,-x+3/2,-z+3/2 (9) -x+2,-y+1,z (10) x,y,-z+2 (11) -x+2,-y+1,-z+2 (12) -y+1,-x+1,-z+2 (13) -x+1,-y+1,-z+2 (14) x,y,-z+1 (15) -y+3/2,x-1/2,z-1/2 (16) -x+3/2,y-1/2,z-1/2 (17) -y+3/2,x-1/2,z+1/2 (18) y+1/2,-x+1/2,-z+3/2

Table S12. Bond angles [°] for Ir_2In_8Te at 299 K with estimated standard deviations in parentheses.

Label	Angles
In(2)-Ir(1)-In(5)	143.74(2)
In(3)#2-Ir(1)-In(2)	72.790(14)
In(3)-Ir(1)-In(2)	72.789(14)
In(3)#3-Ir(1)-In(2)	130.34(2)
In(3)#1-Ir(1)-In(2)	130.34(2)
In(3)-Ir(1)-In(3)#1	150.733(9)
In(3)#1-Ir(1)-In(3)#3	77.05(2)
In(3)-Ir(1)-In(3)#3	73.74(2)
In(3)#2-Ir(1)-In(3)	135.36(2)
In(3)#2-Ir(1)-In(3)#3	150.732(9)
In(3)#2-Ir(1)-In(3)#1	73.74(2)
In(3)#1-Ir(1)-In(1)	120.521(18)
In(3)#3-Ir(1)-In(1)	120.521(18)
In(3)#2-Ir(1)-In(1)	74.383(12)
In(3)-Ir(1)-In(1)	74.381(12)
In(3)#2-Ir(1)-In(5)	95.61(2)
In(3)#1-Ir(1)-In(5)	74.81(4)
In(3)-Ir(1)-In(5)	95.61(2)
In(3)#3-Ir(1)-In(5)	74.81(4)
In(1)-Ir(1)-In(2)	83.69(5)
In(1)-Ir(1)-In(5)	60.05(6)
In(4)-Ir(1)-In(2)	71.35(3)
In(4)-Ir(1)-In(3)#1	77.92(2)
In(4)-Ir(1)-In(3)#2	97.528(15)
In(4)-Ir(1)-In(3)	97.529(15)
In(4)-Ir(1)-In(3)#3	77.92(2)
In(4)-Ir(1)-In(1)	155.04(4)
In(4)-Ir(1)-In(5)	144.91(4)
Ir(1)#4-In(2)-Ir(1)	138.04(5)
Ir(1)#4-In(2)-In(2)#5	110.98(3)
Ir(1)-In(2)-In(2)#5	110.98(3)
Ir(1)-In(2)-In(3)	51.404(13)
Ir(1)#4-In(2)-In(3)#4	51.403(13)

Ir(1)-In(2)-In(3)#2	51.403(13)
Ir(1)#4-In(2)-In(3)	109.48(3)
Ir(1)-In(2)-In(3)#4	109.49(3)
Ir(1)-In(2)-In(3)#6	109.49(3)
Ir(1)#4-In(2)-In(3)#6	51.403(13)
Ir(1)#4-In(2)-In(3)#2	109.49(3)
Ir(1)-In(2)-In(4)	51.88(5)
Ir(1)#4-In(2)-In(4)#5	51.88(5)
Ir(1)#4-In(2)-In(4)	170.08(3)
Ir(1)-In(2)-In(4)#5	170.08(3)
Ir(1)#4-In(2)-In(5)#8	100.13(2)
Ir(1)#4-In(2)-In(5)#7	100.13(2)
Ir(1)-In(2)-In(5)#8	100.13(2)
Ir(1)-In(2)-In(5)#7	100.13(2)
In(2)#5-In(2)-In(5)#7	60.59(3)
In(2)#5-In(2)-In(5)#8	60.59(3)
In(3)#2-In(2)-In(2)#5	113.91(3)
In(3)#4-In(2)-In(2)#5	113.91(3)
In(3)#6-In(2)-In(2)#5	113.91(3)
In(3)-In(2)-In(2)#5	113.91(3)
In(3)-In(2)-In(3)#4	132.18(6)
In(3)#6-In(2)-In(3)#2	132.18(6)
In(3)#6-In(2)-In(3)#4	98.38(3)
In(3)-In(2)-In(3)#2	98.38(3)
In(3)-In(2)-In(3)#6	61.69(2)
In(3)#4-In(2)-In(3)#2	61.69(2)
In(3)-In(2)-In(5)#7	149.134(11)
In(3)-In(2)-In(5)#8	62.59(4)
In(3)#2-In(2)-In(5)#7	62.59(4)
In(3)#4-In(2)-In(5)#8	149.133(11)
In(3)#4-In(2)-In(5)#7	62.59(4)
In(3)#6-In(2)-In(5)#8	62.59(4)
In(3)#6-In(2)-In(5)#7	149.133(11)
In(3)#2-In(2)-In(5)#8	149.133(11)
In(4)-In(2)-In(2)#5	59.10(3)
In(4)#5-In(2)-In(2)#5	59.10(3)

In(4)-In(2)-In(3)#4	130.396(15)
In(4)#5-In(2)-In(3)#2	130.396(14)
In(4)-In(2)-In(3)	76.60(4)
In(4)#5-In(2)-In(3)	130.396(15)
In(4)#5-In(2)-In(3)#4	76.60(4)
In(4)-In(2)-In(3)#6	130.396(15)
In(4)-In(2)-In(3)#2	76.60(4)
In(4)#5-In(2)-In(3)#6	76.60(4)
In(4)#5-In(2)-In(4)	118.20(6)
In(4)#5-In(2)-In(5)#8	75.39(3)
In(4)-In(2)-In(5)#7	75.39(3)
In(4)#5-In(2)-In(5)#7	75.39(3)
In(4)-In(2)-In(5)#8	75.39(3)
In(5)#7-In(2)-In(5)#8	121.18(6)
In(3)#10-Te(1)-In(3)	180.0
In(3)-Te(1)-In(3)#11	90.69(7)
In(3)#10-Te(1)-In(3)#9	90.69(7)
In(3)#9-Te(1)-In(3)#11	180.0
In(3)#10-Te(1)-In(3)#11	89.31(7)
In(3)-Te(1)-In(3)#9	89.31(7)
Ir(1)-In(3)-Ir(1)#8	155.37(2)
Ir(1)#8-In(3)-In(2)	100.653(18)
Ir(1)-In(3)-In(2)	55.807(10)
Ir(1)#8-In(3)-Te(1)	103.655(16)
Ir(1)-In(3)-Te(1)	100.969(15)
Ir(1)#8-In(3)-In(3)#3	136.77(2)
Ir(1)-In(3)-In(3)#3	53.361(16)
Ir(1)-In(3)-In(3)#8	138.47(2)
Ir(1)-In(3)-In(3)#6	111.195(11)
Ir(1)#8-In(3)-In(3)#6	51.475(10)
Ir(1)#8-In(3)-In(3)#8	52.901(16)
Ir(1)-In(3)-In(1)	54.58(4)
Ir(1)#8-In(3)-In(1)	128.79(2)
Ir(1)-In(3)-In(4)#8	142.08(3)
Ir(1)#8-In(3)-In(4)#8	50.67(4)
In(2)-In(3)-In(3)#6	59.156(10)

In(2)-In(3)-In(1)	69.64(5)
In(2)-In(3)-In(4)#8	116.34(3)
Te(1)-In(3)-In(2)	150.551(18)
Te(1)-In(3)-In(3)#3	71.65(4)
Te(1)-In(3)-In(3)#6	127.95(3)
Te(1)-In(3)-In(3)#8	71.65(4)
Te(1)-In(3)-In(1)	82.17(5)
Te(1)-In(3)-In(4)#8	69.19(4)
In(3)#8-In(3)-In(2)	137.45(4)
In(3)#3-In(3)-In(2)	101.13(2)
In(3)#8-In(3)-In(3)#3	86.533(11)
In(3)#8-In(3)-In(3)#6	104.357(10)
In(3)#3-In(3)-In(3)#6	159.562(17)
In(3)#3-In(3)-In(1)	93.82(3)
In(3)#8-In(3)-In(1)	152.31(3)
In(3)#8-In(3)-In(4)#8	75.07(4)
In(3)#3-In(3)-In(4)#8	140.248(19)
In(3)#6-In(3)-In(4)#8	60.138(18)
In(1)-In(3)-In(3)#6	84.483(16)
In(1)-In(3)-In(4)#8	87.52(6)
Ir(1)#9-In(1)-Ir(1)	125.41(6)
Ir(1)-In(1)-In(3)#9	122.73(4)
Ir(1)-In(1)-In(3)#12	122.73(4)
Ir(1)#9-In(1)-In(3)	122.73(4)
Ir(1)#9-In(1)-In(3)#2	122.73(4)
Ir(1)-In(1)-In(3)	51.03(3)
Ir(1)#9-In(1)-In(3)#9	51.03(3)
Ir(1)#9-In(1)-In(3)#12	51.03(3)
Ir(1)-In(1)-In(3)#2	51.03(3)
Ir(1)#9-In(1)-In(5)	62.71(3)
Ir(1)-In(1)-In(5)	62.71(3)
In(3)-In(1)-In(3)#12	168.97(3)
In(3)-In(1)-In(3)#9	82.30(7)
In(3)#2-In(1)-In(3)#12	82.30(7)
In(3)-In(1)-In(3)#2	96.63(6)
In(3)#9-In(1)-In(3)#12	96.63(6)

In(3)#9-In(1)-In(3)#2	168.96(3)
In(1)#13-In(1)-Ir(1)	117.29(3)
In(1)#13-In(1)-Ir(1)#9	117.29(3)
In(1)#13-In(1)-In(3)	95.518(16)
In(1)#13-In(1)-In(3)#12	95.517(16)
In(1)#13-In(1)-In(3)#9	95.518(16)
In(1)#13-In(1)-In(3)#2	95.517(16)
In(1)#13-In(1)-In(5)	180.0
In(5)-In(1)-In(3)#2	84.482(16)
In(5)-In(1)-In(3)	84.483(16)
In(5)-In(1)-In(3)#12	84.482(16)
In(5)-In(1)-In(3)#9	84.482(16)
Ir(1)-In(4)-Ir(1)#14	175.33(4)
Ir(1)#14-In(4)-In(2)	118.57(4)
Ir(1)-In(4)-In(2)	56.77(3)
Ir(1)#14-In(4)-In(2)#5	56.77(3)
Ir(1)-In(4)-In(2)#5	118.57(4)
Ir(1)#14-In(4)-In(3)#16	51.42(4)
Ir(1)#14-In(4)-In(3)#3	132.12(4)
Ir(1)#14-In(4)-In(3)#1	132.12(4)
Ir(1)-In(4)-In(3)#15	132.11(4)
Ir(1)-In(4)-In(3)#16	132.11(4)
Ir(1)-In(4)-In(3)#3	51.42(4)
Ir(1)#14-In(4)-In(3)#15	51.42(4)
Ir(1)-In(4)-In(3)#1	51.42(4)
In(2)-In(4)-In(2)#5	61.80(6)
In(2)-In(4)-In(3)#1	99.34(5)
In(2)-In(4)-In(3)#3	99.34(5)
In(2)-In(4)-In(3)#16	145.84(2)
In(2)#5-In(4)-In(3)#15	99.34(5)
In(2)#5-In(4)-In(3)#16	99.34(5)
In(2)#5-In(4)-In(3)#3	145.84(2)
In(2)-In(4)-In(3)#15	145.84(2)
In(2)#5-In(4)-In(3)#1	145.84(2)
In(3)#16-In(4)-In(3)#3	109.56(5)
In(3)#15-In(4)-In(3)#1	109.56(5)

In(3)#16-In(4)-In(3)#15	59.73(4)
In(3)#3-In(4)-In(3)#1	59.73(4)
In(3)#16-In(4)-In(3)#1	80.73(7)
In(3)#3-In(4)-In(3)#15	80.73(7)
Ir(1)#9-In(5)-Ir(1)	114.48(7)
Ir(1)-In(5)-In(2)#18	152.17(3)
Ir(1)#9-In(5)-In(2)#17	152.17(3)
Ir(1)-In(5)-In(2)#17	93.35(6)
Ir(1)#9-In(5)-In(2)#18	93.35(6)
In(2)#17-In(5)-In(2)#18	58.82(6)
In(1)-In(5)-Ir(1)#9	57.24(3)
In(1)-In(5)-Ir(1)	57.24(3)
In(1)-In(5)-In(2)#18	150.59(3)
In(1)-In(5)-In(2)#17	150.59(3)

Symmetry transformations used to generate equivalent atoms:
(1) -y+1,-x+1,z (2) -y+3/2,x-1/2,-z+3/2 (3) -x+3/2,y-1/2,-z+3/2 (4) -x+1,-y+1,z (5) -x+1,-y+1,-z+1 (6) y,x,z (7) -y+1/2,x-1/2,z-1/2 (8) y+1/2,-x+3/2,-z+3/2 (9) -x+2,-y+1,z (10) x,y,-z+2 (11) -x+2,-y+1,-z+2 (12) -y+1,-x+1,-z+2 (13) -x+1,-y+1,-z+2 (14) x,y,-z+1 (15) -y+3/2,x-1/2,z-1/2 (16) -x+3/2,y-1/2,z-1/2 (17) -y+3/2,x-1/2,z+1/2 (18) y+1/2,-x+1/2,-z+3/2

Table S13. Crystal data and structure refinement for Ir_2In_8Se at 120 K.

Empirical formula	Ir_2In_8Se
Formula weight	1382
Temperature	120 K
Wavelength	0.71073 Å
Crystal system	monoclinic
Space group	Pm(αβ0)0
Unit cell dimensions	a = 9.9200(6) Å, α = 90° b = 9.9262(6) Å, β = 90° c = 10.1092(6) Å, γ = 89.9995°
q-vector(1)	$0.166667a^* + 0.166667b^* + 0.000000c^*$
Volume	995.43(10) $Å^3$
Z	4
Density (calculated)	9.2213 g/cm^3
Absorption coefficient	48.361 mm^{-1}
F(000)	2320
Crystal size	0.278 x 0.246 x 0.225 mm^3
θ range for data collection	3.78 to 29.98°
Index ranges	-14<=h<=12, -7<=k<=14, -14<=l<=11, -1<=m<=1
Reflections collected	13783
Independent reflections	9179 [R_{int} = 0.095]
Completeness to θ = 22.14°	90%
Refinement method	Full-matrix least-squares on F^2
Data / constrains / restraints / parameters	9179 / 3 / 0 / 669
Goodness-of-fit on F^2	2.45
Final R indices [I>2σ(I)]	R_{obs} = 0.0513, wR_{obs} = 0.1085
R indices [all data]	R_{all} = 0.0749, wR_{all} = 0.1101
T_{min} and T_{max} coefficients	0.0927 and 0.5796
Largest diff. peak and hole	9.29 and -10.15 e·$Å^{-3}$

$R = \Sigma||F_o|-|F_c|| / \Sigma|F_o|$, $wR = \{\Sigma[w(|F_o|^2 - |F_c|^2)^2] / \Sigma[w(|F_o|^4)]\}^{1/2}$ and $w=1/(\sigma^2(I)+0.0004I^2)$

Table S14. Atomic coordinates (x10^4), occupancy and equivalent isotropic displacement parameters (Å^{2}x10^3) for Ir_2In_8Se at 120 K with estimated standard deviations in parentheses.

Label	x	y	z	Occupancy	U_{eq}*
Ir(1)	1867(7)	1868(8)	2381(2)	1	4(1)
Ir(2)	-1865(7)	-1868(8)	-2418(2)	1	4(1)
Ir(3)	6860(7)	3138(8)	2587(2)	1	5(1)
Ir(4)	-6871(7)	-3141(8)	-2596(2)	1	6(1)
In(1)	5919(8)	4002(9)	5000	1	6(1)
In(2)	-5981(8)	-4075(9)	-5000	1	8(1)
In(3)	937(8)	933(9)	0	1	6(1)
In(4)	-979(8)	-966(9)	0	1	9(1)
In(5)	4979(7)	5003(9)	1644(2)	1	9(1)
In(6)	8169(8)	2156(9)	5000	1	12(1)
In(7)	-7814(8)	-1861(9)	-5000	1	10(1)
In(8)	2032(7)	4467(9)	2991(3)	1	8(1)
In(9)	-2063(7)	-4459(9)	-2964(2)	1	7(1)
In(10)	16(7)	10(9)	3405(2)	1	7(1)
In(11)	2949(7)	-543(9)	1955(2)	1	8(1)
In(12)	-2935(7)	538(8)	-2063(2)	1	9(1)
In(13)	4464(7)	2035(9)	2969(3)	1	9(1)
In(14)	-4458(7)	-2061(9)	-2998(3)	1	9(1)
In(15)	-522(7)	2949(9)	1970(3)	1	8(1)
In(16)	535(7)	-2949(9)	-2073(3)	1	8(1)
In(17)	1880(8)	1900(9)	5000	1	10(1)
In(18)	-1830(8)	-1876(9)	-5000	1	12(1)
In(19)	6859(8)	3118(9)	0	1	10(1)
In(20)	-6943(8)	-3183(9)	0	1	11(2)
In(21)	2968(8)	3003(9)	0	1	2(2)
In(22)	-3019(8)	-2979(10)	0	1	4(2)
Se(1)	5021(9)	-31(12)	0	1	2(2)
Se(2)	4763(9)	-42(10)	5000	1	15(2)
Se(3)	6(10)	5001(10)	0	1	1(2)
Se(4)	-72(9)	4750(11)	5000	1	14(2)

*U_{eq} is defined as one third of the trace of the orthogonalized U_{ij} tensor.

Table S15. Anisotropic displacement parameters (Å^{2}x10^3) for Ir_2In_8Se at 120 K with estimated standard deviations in parentheses.

Label	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
Ir(1)	1(1)	5(1)	4(1)	7(1)	0(1)	2(1)
Ir(2)	2(1)	10(1)	2(1)	7(1)	-1(1)	1(1)
Ir(3)	3(1)	10(1)	2(1)	7(1)	0(1)	-2(1)
Ir(4)	4(1)	10(1)	4(1)	8(1)	0(1)	-1(1)
In(1)	0(2)	12(2)	6(2)	7(2)	0	0
In(2)	2(2)	12(2)	9(2)	4(2)	0	0
In(3)	9(2)	10(2)	0(2)	5(2)	0	0
In(4)	8(2)	18(2)	2(2)	-2(2)	0	0
In(5)	4(1)	15(2)	8(2)	11(1)	0(1)	-4(2)
In(6)	10(2)	23(2)	2(2)	10(2)	0	0
In(7)	9(2)	21(2)	-1(2)	8(2)	0	0
In(8)	6(2)	11(1)	9(2)	6(2)	0(1)	-1(2)
In(9)	7(2)	11(2)	4(2)	2(2)	1(1)	1(1)
In(10)	6(1)	11(2)	4(1)	6(1)	0(1)	-2(1)
In(11)	7(2)	8(1)	11(2)	8(2)	1(1)	2(1)
In(12)	5(2)	5(1)	16(2)	6(2)	0(1)	-1(1)
In(13)	1(1)	17(2)	10(2)	5(2)	-2(1)	2(2)
In(14)	0(1)	18(2)	8(2)	7(2)	1(1)	1(2)
In(15)	3(1)	11(2)	10(2)	10(1)	1(1)	2(1)
In(16)	6(1)	8(2)	11(2)	7(2)	0(1)	-2(1)
In(17)	10(2)	14(2)	5(2)	2(2)	0	0
In(18)	6(2)	12(2)	17(2)	-8(2)	0	0
In(19)	12(2)	22(2)	-5(2)	8(2)	0	0
In(20)	8(2)	21(2)	4(2)	5(2)	0	0
In(21)	-10(2)	1(2)	14(2)	6(2)	0	0
In(22)	-4(2)	8(3)	10(2)	5(2)	0	0
Se(1)	0(2)	-3(2)	8(2)	-1(2)	0	0
Se(2)	19(2)	19(3)	7(2)	12(2)	0	0
Se(3)	-13(2)	9(2)	8(2)	2(2)	0	0
Se(4)	7(2)	28(3)	6(2)	1(2)	0	0

Table S16. Crystal data and structure refinement for Ir_2In_8Te at 115 K.

Empirical formula	Ir_2In_8Te
Formula weight	1430.6
Temperature	115 K
Wavelength	0.71073 Å
Crystal system	monoclinic
Space group	Pm(αβ0)0
Unit cell dimensions	a = 10.005(4) Å, α = 90° b = 10.007(4) Å, β = 90° c = 10.196(4) Å, γ = 89.991(8)°
q-vector(1)	$0.100000a^{*} + -0.100000b^{*} + 0.000000c^{*}$
Volume	1020.8(7) $Å^3$
Z	4
Density (calculated)	9.3091 g/cm^3
Absorption coefficient	46.397 mm^{-1}
F(000)	2392
Crystal size	0.278 x 0.246 x 0.225 mm^3
θ range for data collection	2 to 30.9°
Index ranges	-7<=h<=13, -8<=k<=14, -5<=l<=13, -1<=m<=1
Reflections collected	9321
Independent reflections	5402 [R_{int} = 0.0509]
Completeness to θ = 20.59°	80%
Refinement method	Full-matrix least-squares on F^2
Data / constrains / restraints / parameters	5402 / 3 / 0 / 667
Goodness-of-fit on F^2	2.37
Final R indices [I>3σ(I)]	R_{obs} = 0.0747, wR_{obs} = 0.1218
R indices [all data]	R_{all} = 0.1237, wR_{all} = 0.1314
T_{min} and T_{max} coefficients	0.0101 and 0.1629
Largest diff. peak and hole	14.82 and -17.22 $e \cdot Å^{-3}$

$R = \Sigma||F_o|-|F_c|| / \Sigma|F_o|$, $wR = \{\Sigma[w(|F_o|^2 - |F_c|^2)^2] / \Sigma[w(|F_o|^4)]\}^{1/2}$ and $w=1/(\sigma^2(I)+0.0004I^2)$

Table S17. Atomic coordinates (x10^4), occupancy and equivalent isotropic displacement parameters (Å^{2}x10^3) for Ir_2In_8Te at 115 K with estimated standard deviations in parentheses.

Label	x	y	z	Occupancy	U_{eq}*
Ir(1)	83(12)	-5287(9)	2579(5)	1	13(2)
Ir(2)	-4907(13)	-6598(9)	2412(5)	1	12(2)
Ir(3)	-1222(12)	-298(10)	2422(4)	1	14(2)
Ir(4)	3771(12)	-1606(10)	2590(4)	1	13(2)
Te(1)	6884(16)	-3446(14)	0	1	4(3)
Te(2)	7040(20)	-3420(20)	5000	1	27(4)
In(1)	-5885(11)	-8993(10)	2076(8)	1	18(3)
Te(3)	1900(30)	-8445(17)	5000	1	34(4)
In(2)	6420(13)	-1324(12)	2152(7)	1	12(3)
In(3)	1957(16)	-3433(13)	1598(6)	1	16(3)
In(4)	1040(18)	-4435(16)	5000	1	16(4)
In(5)	-999(19)	-6440(17)	5000	1	27(5)
In(6)	1418(13)	-536(12)	2898(8)	1	15(3)
In(7)	-1206(17)	-369(16)	5000	1	13(4)
Te(4)	1949(19)	-8515(16)	0	1	13(3)
In(8)	4930(20)	-490(17)	5000	1	35(5)
In(9)	-4015(19)	-7519(15)	0	1	16(4)
In(10)	-3063(15)	-8435(13)	3411(6)	1	15(2)
In(11)	4892(16)	-3990(11)	2872(9)	1	17(3)
In(12)	2506(15)	-6333(13)	2906(8)	1	19(3)
In(13)	-4994(17)	-6542(16)	5000	1	11(4)
In(14)	2909(18)	-2517(15)	5000	1	12(4)
In(15)	-46(18)	-5375(16)	0	1	19(4)
In(16)	-2467(14)	-5537(13)	2073(9)	1	24(3)
In(17)	-2095(18)	-9403(16)	0	1	15(4)
In(18)	3835(18)	-1521(16)	0	1	15(4)
In(19)	13(16)	-11397(16)	0	1	14(4)
In(20)	-976(12)	-2886(13)	2880(8)	1	16(3)
In(21)	-5918(17)	-5488(16)	0	1	21(4)
In(22)	0(2000)	-10000(200)	2116(8)	1	16(3)

*U_{eq} is defined as one third of the trace of the orthogonalized U_{ij} tensor.

Table S18. Anisotropic displacement parameters (Å^{2}x10^3) for Ir_2In_8Te at 115 K with estimated standard deviations in parentheses.

Label	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
Ir(1)	22(3)	5(3)	11(3)	10(3)	4(2)	3(2)
Ir(2)	27(4)	-2(2)	10(2)	8(2)	0(2)	0(2)
Ir(3)	23(4)	9(3)	12(3)	11(3)	2(2)	-8(2)
Ir(4)	21(3)	8(2)	11(2)	13(2)	9(2)	10(2)
Te(1)	-4(5)	5(5)	12(4)	0(4)	0	0
Te(2)	24(8)	43(8)	14(5)	-5(6)	0	0
In(1)	21(6)	11(4)	21(5)	5(5)	-4(4)	-1(4)
Te(3)	78(11)	8(6)	16(5)	-6(6)	0	0
In(2)	16(5)	6(4)	15(4)	9(4)	-1(3)	-7(3)
In(3)	29(5)	4(4)	16(4)	5(4)	6(5)	-4(4)
In(4)	23(9)	13(7)	11(6)	4(7)	0	0
In(5)	46(12)	25(8)	9(6)	-18(8)	0	0
In(6)	15(6)	9(5)	20(5)	12(4)	-2(4)	4(4)
In(7)	13(8)	1(6)	24(7)	8(6)	0	0
Te(4)	19(7)	10(6)	10(5)	2(5)	0	0
In(8)	86(13)	18(7)	2(6)	-49(8)	0	0
In(9)	31(9)	2(6)	14(6)	11(6)	0	0
In(10)	21(5)	12(4)	13(3)	6(4)	12(4)	-1(4)
In(11)	20(6)	12(5)	19(5)	6(5)	2(4)	-7(4)
In(12)	33(7)	13(5)	11(4)	9(5)	-8(4)	8(4)
In(13)	13(7)	16(7)	3(5)	4(7)	0	0
In(14)	26(9)	1(6)	10(6)	7(6)	0	0
In(15)	26(9)	12(7)	20(7)	-4(7)	0	0
In(16)	32(7)	6(4)	33(6)	7(5)	-11(5)	-4(4)
In(17)	14(8)	17(7)	13(7)	8(6)	0	0
In(18)	32(9)	10(6)	4(5)	7(7)	0	0
In(19)	16(7)	10(7)	16(6)	0(6)	0	0
In(20)	27(7)	0(4)	20(5)	6(4)	13(4)	-7(3)
In(21)	11(7)	31(9)	20(6)	2(6)	0	0
In(22)	27(6)	-3(4)	23(5)	6(4)	-11(4)	-5(3)

Table S19. Fermi velocity and tilt fit values for Ir_2In_8Se (A) and Ir_2In_8Te (B). All quantities are in units of 10^5 m/s. The reduced *k* coordinates denote the crossing.

A	Ir_2In_8Se		
k = (0, 0, 0.225)			
$\vec{w}_0$	w_0^x	w_0^y	w_0^z
	0.00	0.00	1.18918
$\vec{v}_F$	v_F^x	v_F^y	v_F^z
	0.31259	0.31259	0.86652
k = (0, 0, 0.296)			
$\vec{w}_0$	w_0^x	w_0^y	w_0^z
	0.00	0.00	1.02907
$\vec{v}_F$	v_F^x	v_F^y	v_F^z
	1.71689	1.71689	1.43972

B	Ir_2In_8Te		
k = (0, 0, 0.188)			
$\vec{w}_0$	w_0^x	w_0^y	w_0^z
	0.00	0.00	0.99534
$\vec{v}_F$	v_F^x	v_F^y	v_F^z
	0.35250	0.35250	0.61711
k = (0, 0, 0.235)			
$\vec{w}_0$	w_0^x	w_0^y	w_0^z
	0.00	0.00	2.14744
$\vec{v}_F$	v_F^x	v_F^y	v_F^z
	1.88943	1.88943	2.05040

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