Supplementary Material

Single crystal diffraction data were collected on an Oxford Diffraction SuperNova Diffractometer equipped with an Atlas CCD-detector at *T*=220 K, using an Oxford Instruments Cryojet HT cooler. Data collection, cell refinement, and data reduction were carried out using CrysAlisPro [1]. Superflip software [2] was used for structure solution and space-group assignment, and JANA2006 [3] for structure refinement. Figures were generated using VESTA [4]. The absorption correction was done analytically using a multifaceted crystal model [5]. No extinction corrections were necessary. From the total number (23429) of measured intensities, we obtained 6068 unique reflections (reflections related by symmetry are merged together), out of which 2523 reflections are satisfying $F^2>3\sigma(F^2)$. The calculated vs. observed structure factors are shown in Fig. S2.

Table I. Crystal Data

Empirical Formula	$IrTe_2$
Formula weight	447.4
Crystal system	Triclinic
Space Group	P-1 (No. 2)
Unit Cell Parameters	
a = 3.9548(2) Å	$\alpha = 98.129(5)^o$
b = 6.6542(4) Å	$\beta = 92.571(4)^o$
c = 14.4345(7) Å	$\gamma = 107.119(5)^o$
Volume	357.88(4) $Å^3$
Z	5
Density (calculated)	10.3767 g/cm^3
Absorption coef.	65.937 mm^{-1}
F(000)	905
Crystal Size	101.6x32.8x17.2 μm
Max. and Min. transmission factors	0.027 and 0.348
Absorption correction	Analytical
Min. and Max. theta angles	3.23 and 45.42

Table II. Experimental Data

Temperature	220K
Radiation type	Mo K_α
Wavelength	0.7107 Å
Detector resolution	10.362 pix./mm.
Measurement method	ω scans
Measured Intensities	23429
Unique reflections	6068 [R_{int}=0.1105]
Strong reflections	2523
Index ranges	$-7 \le h \le 7$ $-13 \le k \le 13$ $-28 \le l \le 28$
Counting time	10 s/frame

Table III. Refinement Data

Data/parameters	2523 / 70
Refinement Method	Full-matrix least-squares on F^2
R1 / wR2 [2523]	0.0571 / 0.1083
Goodness-of-fit [2523]	1.44
R1 / wR2 [6068]	0.1340 / 0.1386
Goodness-of-fit [6068]	1.19

$$R_1 = \frac{\sum|F_{obs} - F_{calc}|}{\sum|F_{obs}|} \qquad wR_2 = \sqrt{\frac{\sum w(F_{obs}^2 - F_{calc}^2)^2}{\sum w(F_{obs}^2)^2}}$$

$$w = \frac{1}{(\sigma(F_{obs}^2)^2 + 0.0004\,(F_{obs}^2)^2)} \qquad S = \sqrt{\frac{\sum w(F_{obs}^2 - F_{calc}^2)^2}{N_{ref} - N_{param}}}$$

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S - Goodness-of-fit

N_{ref} – the number of reflections used in the refinement

N_{param} - the number of refined parameters

Table IV. Anisotropic atomic displacement factors U_{ij}(Å^2).

Atom	U_{11}	U_{22}`	U_{33}	U_{12}	U_{13}	U_{23}
Ir(1)	0.0087(3)	0.0123(3)	0.0078(3)	0.0039(2)	0.00103(19)	0.0047(2)
Ir(2)	0.00821(19)	0.0123(2)	0.00788(18)	0.00386(15)	0.00092(14)	0.00474(14)
Ir(3)	0.0087(2)	0.0130(2)	0.00803(19)	0.00401(16)	0.00096(14)	0.00464(15)
Te(1)	0.0085(3)	0.0127(4)	0.0104(3)	0.0037(3)	0.0008(2)	0.0049(3)
Te(2)	0.0087(3)	0.0123(4)	0.0082(3)	0.0041(3)	0.0008(2)	0.0041(2)
Te(3)	0.0089(3)	0.0119(3)	0.0080(3)	0.0038(3)	0.0006(2)	0.0042(2)
Te(4)	0.0089(3)	0.0127(3)	0.0087(3)	0.0038(3)	0.0008(2)	0.0043(3)
Te(5)	0.0094(3)	0.0122(3)	0.0076(3)	0.0036(3)	0.0004(2)	0.0041(2)

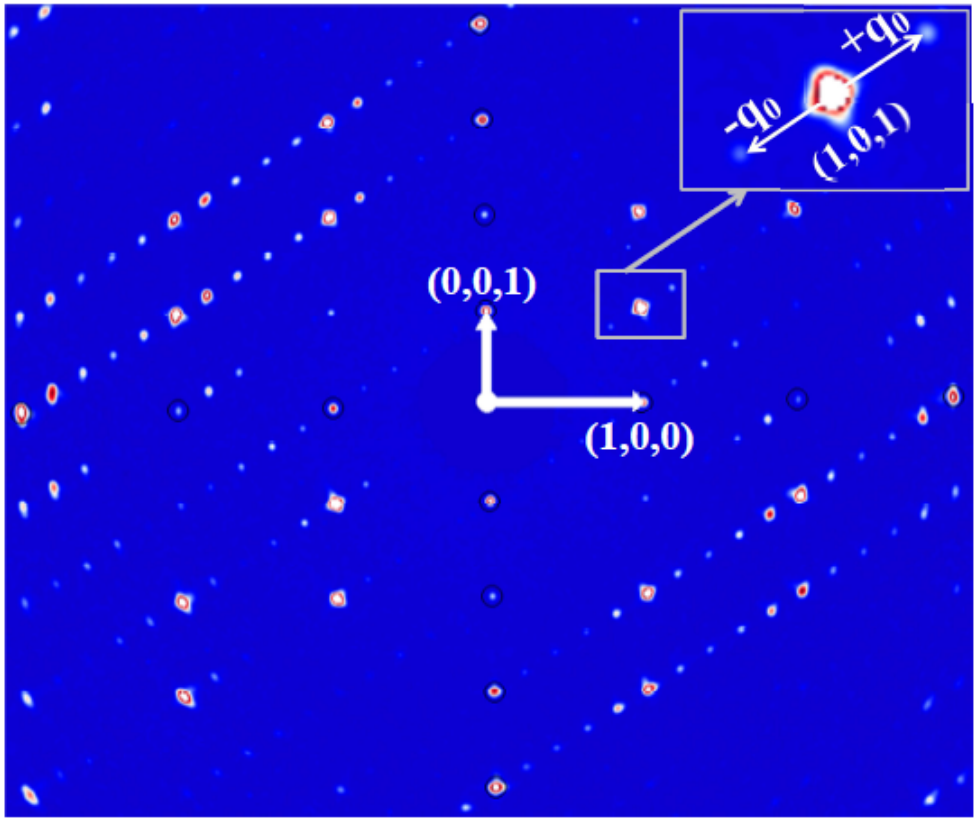

Figure S1. X-ray diffraction pattern in the (H 0 L) reciprocal plane (high-temperature notation) at T=220 K. The high-temperature a_0* and c_0* directions are given by the (1,0,0) and (0,0,1) Bragg peaks, respectively. The inset shows the structural modulation peaks with $\boldsymbol{q_0}$=(1/5, 0, 1/5).

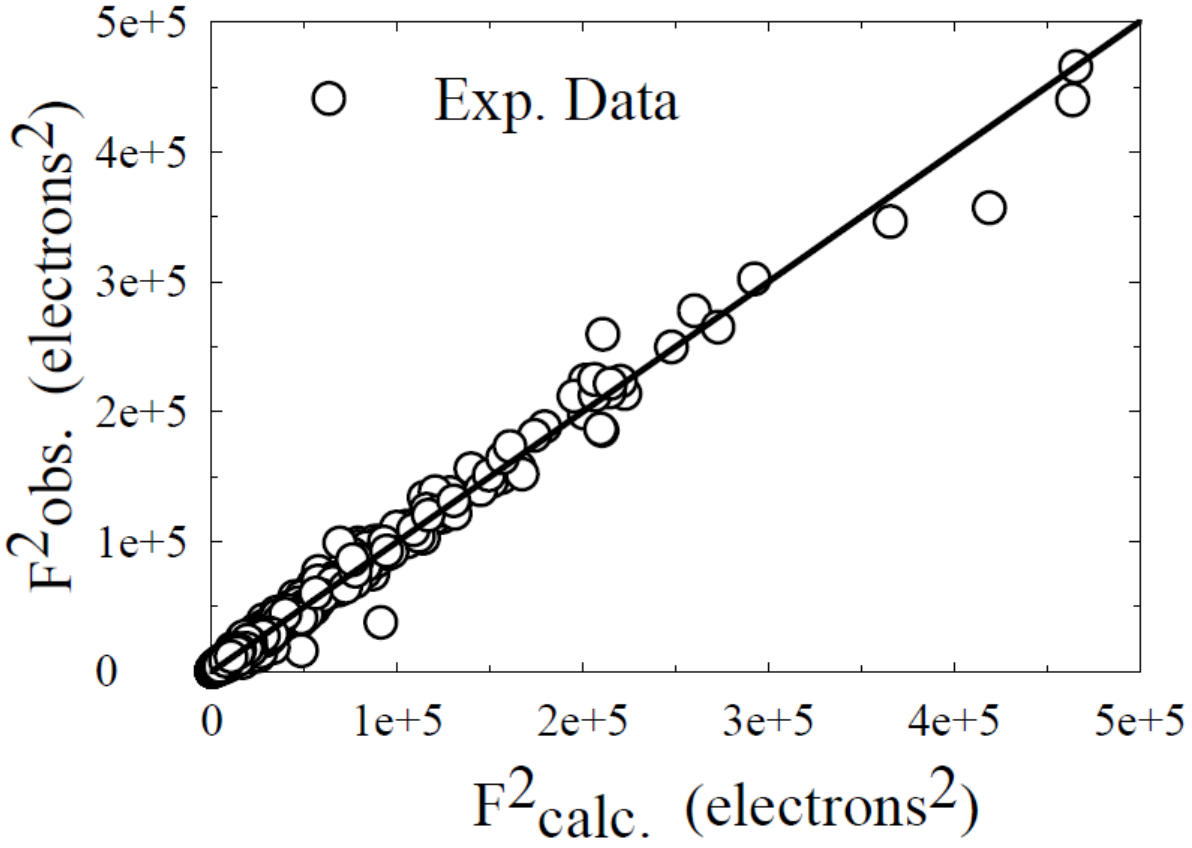

Figure S2. Observed vs. calculated structure factors squared, F^2 satisfying $F^2>3\sigma(F^2)$. Statistical error bars are smaller than the symbol size.

References

[1]. CrysAlisPro, Oxford Diffraction Ltd., Version 1.171.36.21 (release 14-08-2012 CrysAlis171.NET).

[2]. Superflip - a computer program for the solution of crystal structures by charge flipping in arbitrary dimensions; L. Palatinus, G. J. Chapuis, Appl. Cryst. **40**, 786-790 (2007).

[3]. Jana2006 - Structure Determination Software Programs (Institute of Physics, Prague, Czech Republic) V. Petricek , M. Dusek and L. Palatinus (2006).

[4]. VESTA – a computer program for three-dimensional visualization of crystal, volumetric and morphology data; K. Momma and F. Izumi, J. Appl. Crystallogr. **44**, 1272-1276 (2011).

[5]. Analytical numeric absorption correction using a multifaceted crystal model based on expressions derived by R.C. Clark and J.S. Reid; R.C. Clark and J.S. Reid, Acta Cryst. A**51**, 887-897 (1995).