Structural Evolution during Reversible Halogen Intercalation in WTe_2: Commensurate–Incommensurate WTe_2I and Multistage WTe_2Br_x (x = 0.5, 1.0 and 1.25)

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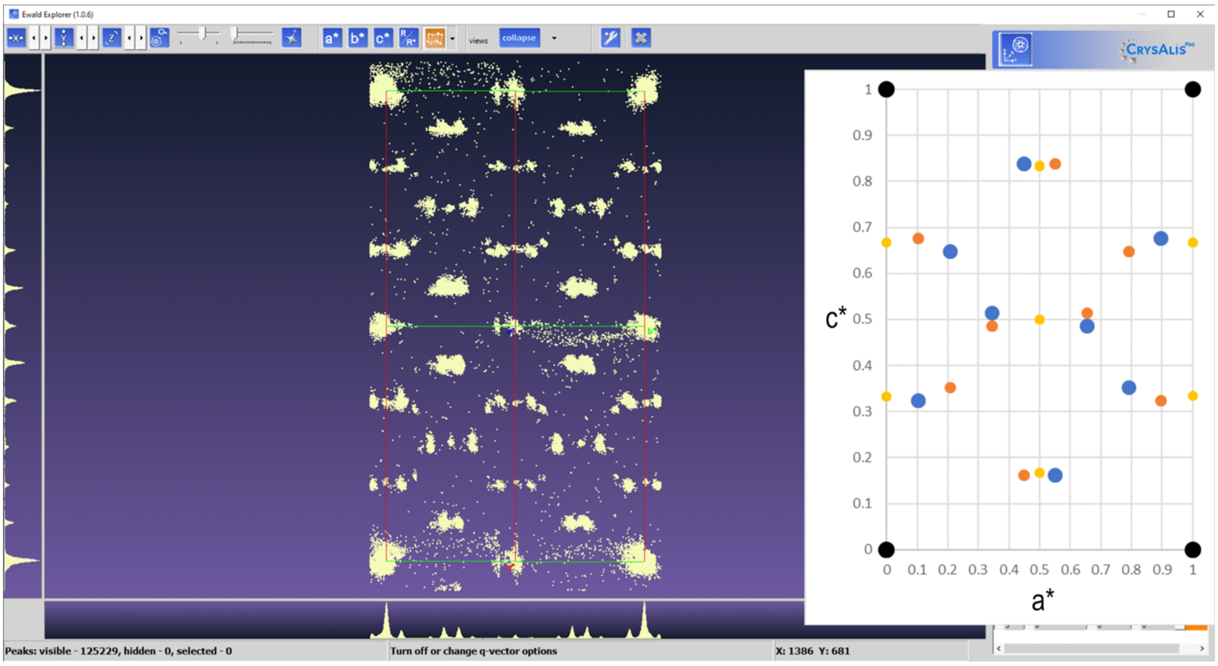


Figure S1. Screenshot from the Ewald Explorer in CrysalisPro showing the collapsed reciprocal lattice, with a simulated satellite pattern on the right (with m≤|±4|). Black dots mark the main reflections, while red and blue dots indicate incommensurate, twinned satellite reflections. Yellow dots denote the commensurate case.

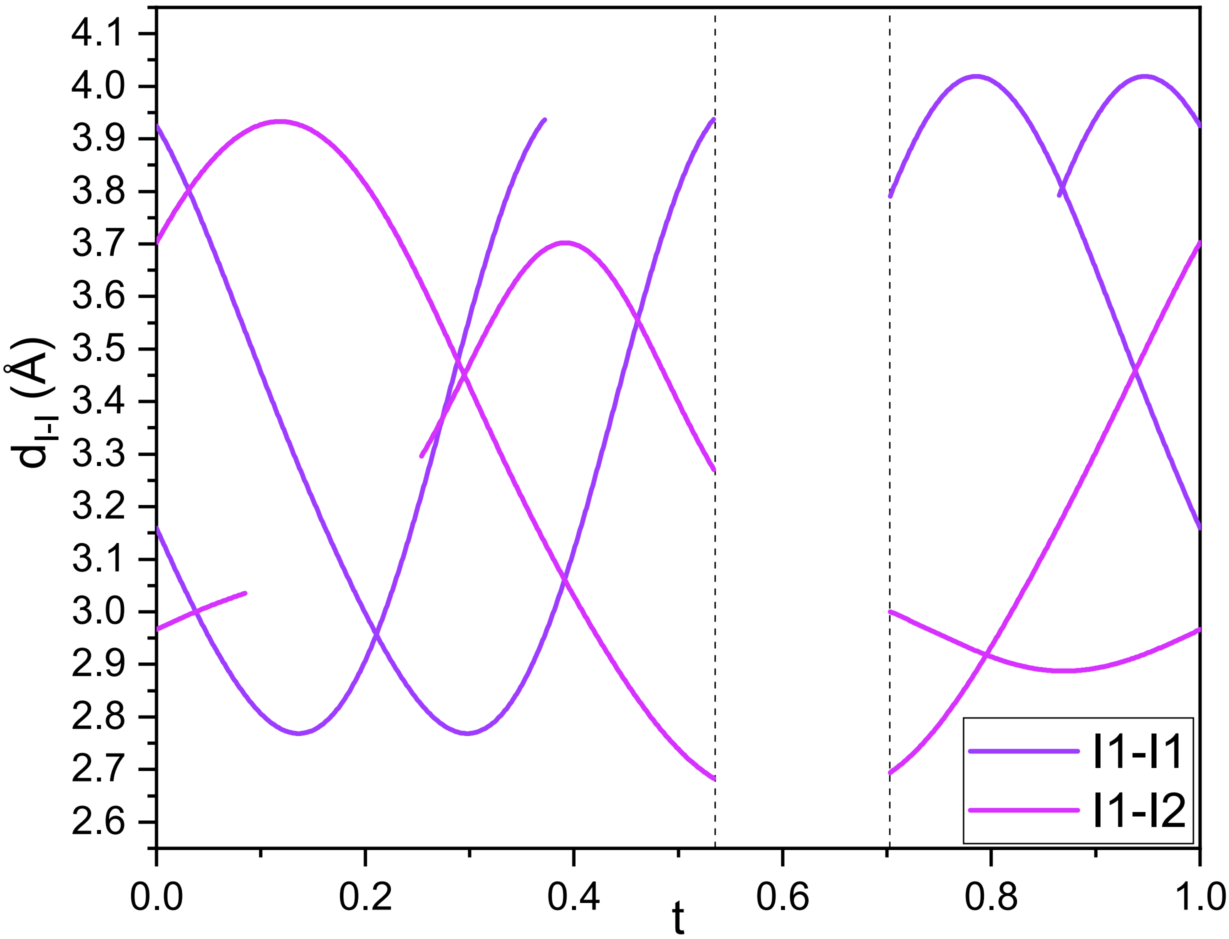


Figure S2. *t* plots of the distances for I1-I1 and I1-I2 in grey with crenel limits marked as dashed vertical line.

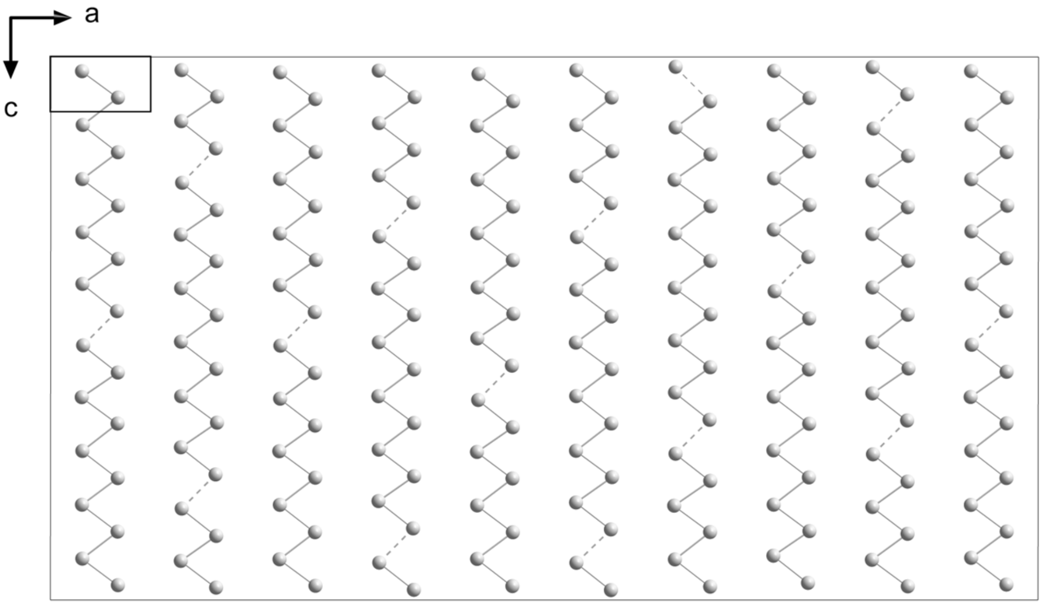


Figure S3. Section of the incommensurate WTe_2I structure showing only one layer of tungsten atoms with long bonds indicated as dashed lines. The unit cell is highlighted in the top left corner.

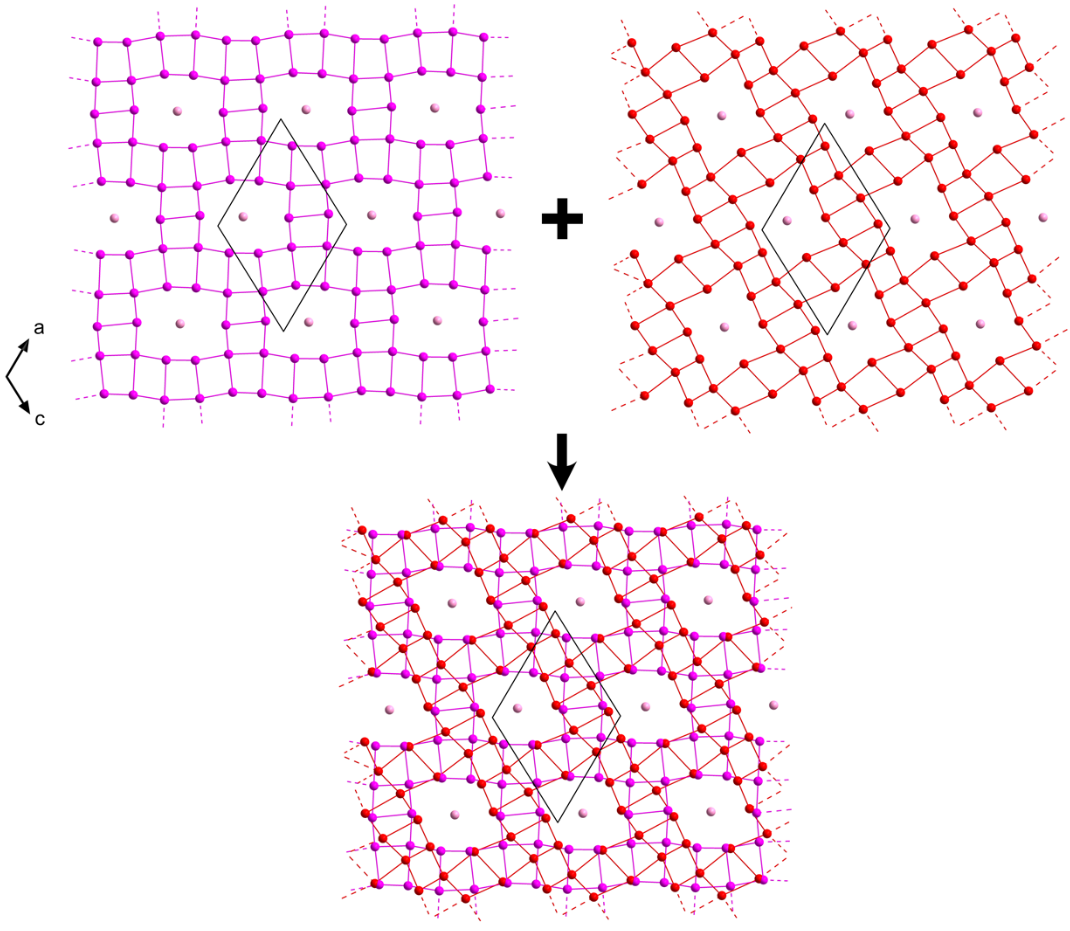


Figure S4. Sections of the WTe_2I supercell structure illustrating the iodine-layer disorder model. The top panels show the two disorder components separately (part a, purple; part b, red), while the bottom panel displays the combined iodine layer. Out-of-plane iodine atoms are highlighted in light purple. The structure is viewed along the *b*-axis, with the unit cell outlined.

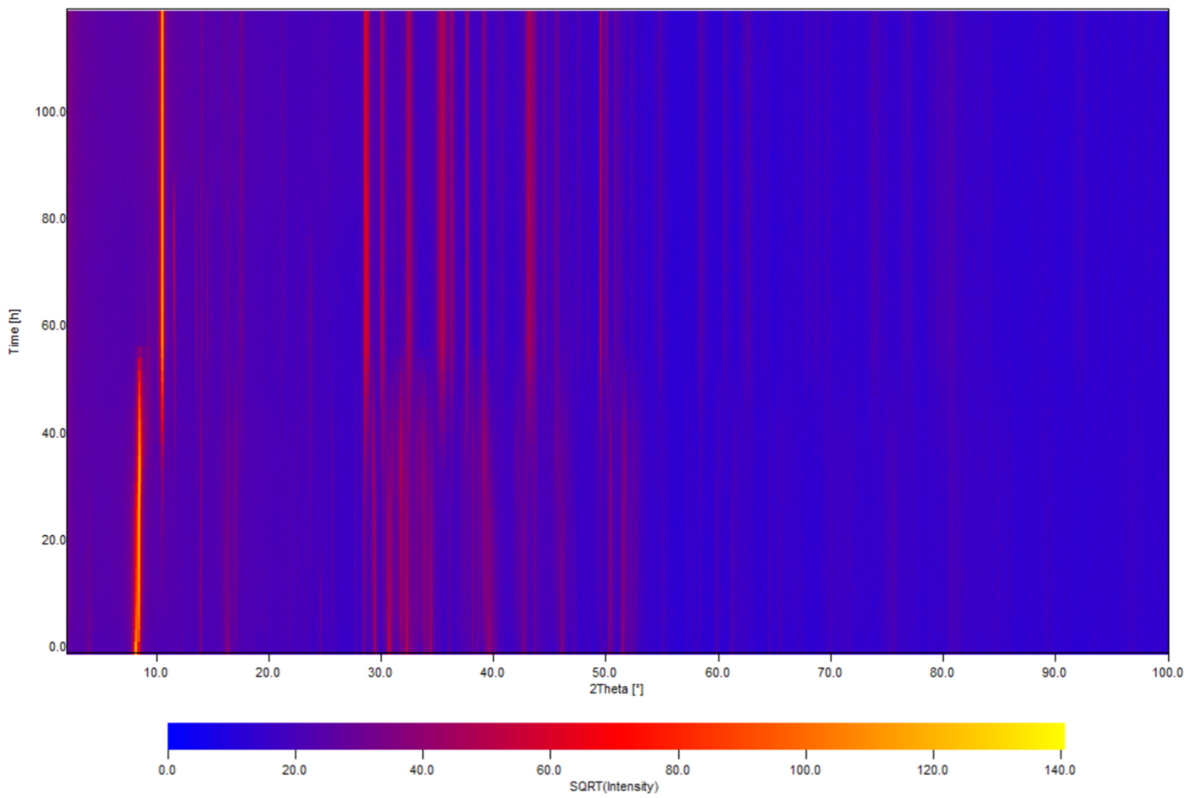


Figure S5. Time resolved PXRD analysis of WTe_2Br_x showing structural evolution while bromine deintercalation.

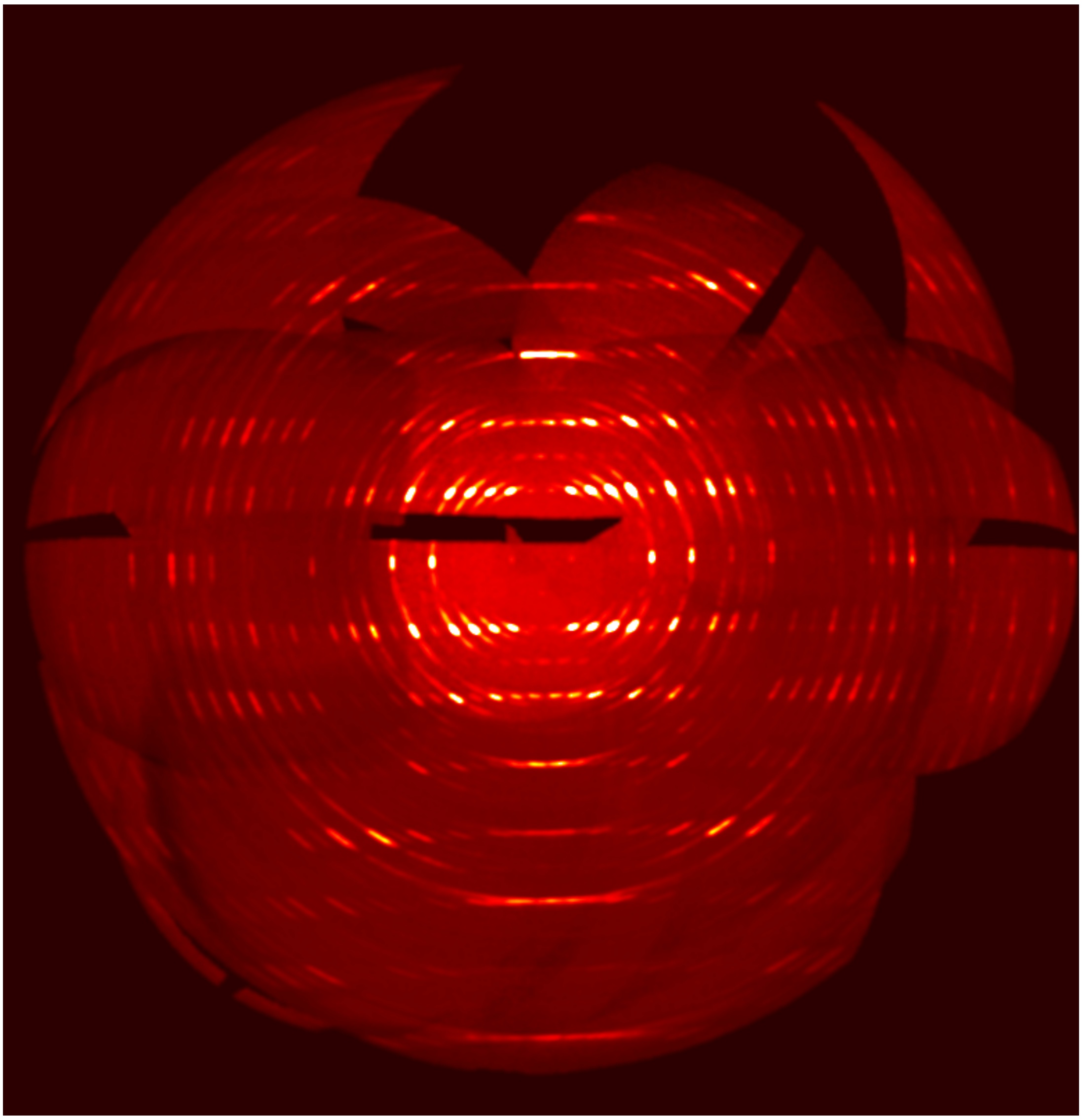


Figure S6. Reconstruction of the (-3*kn*) of the reciprocal-space plane of $WTe_2Br_{1.25}$, highlighting reduced crystallinity due to multiple phase transitions.

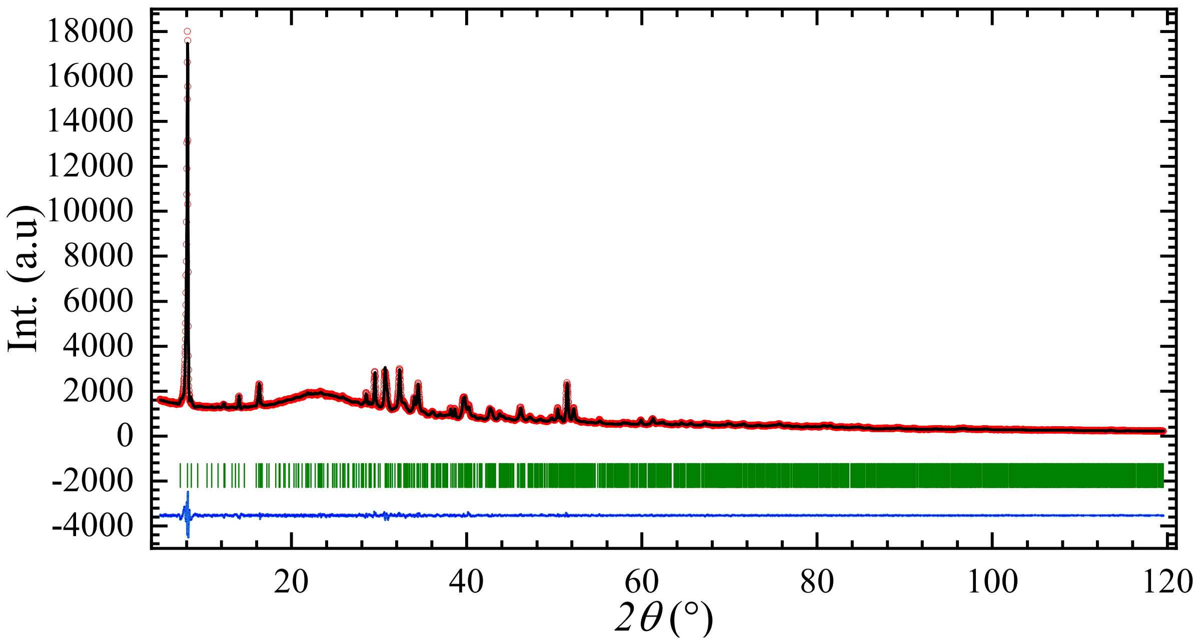


Figure S7. Rietveld refinement of $WTe_2Br_{1.25}$ using SXRD results for lattice and position parameters. The refinement shows a good agreement of PXRD and SXRD results.

Specialized Transmission Sample Holder

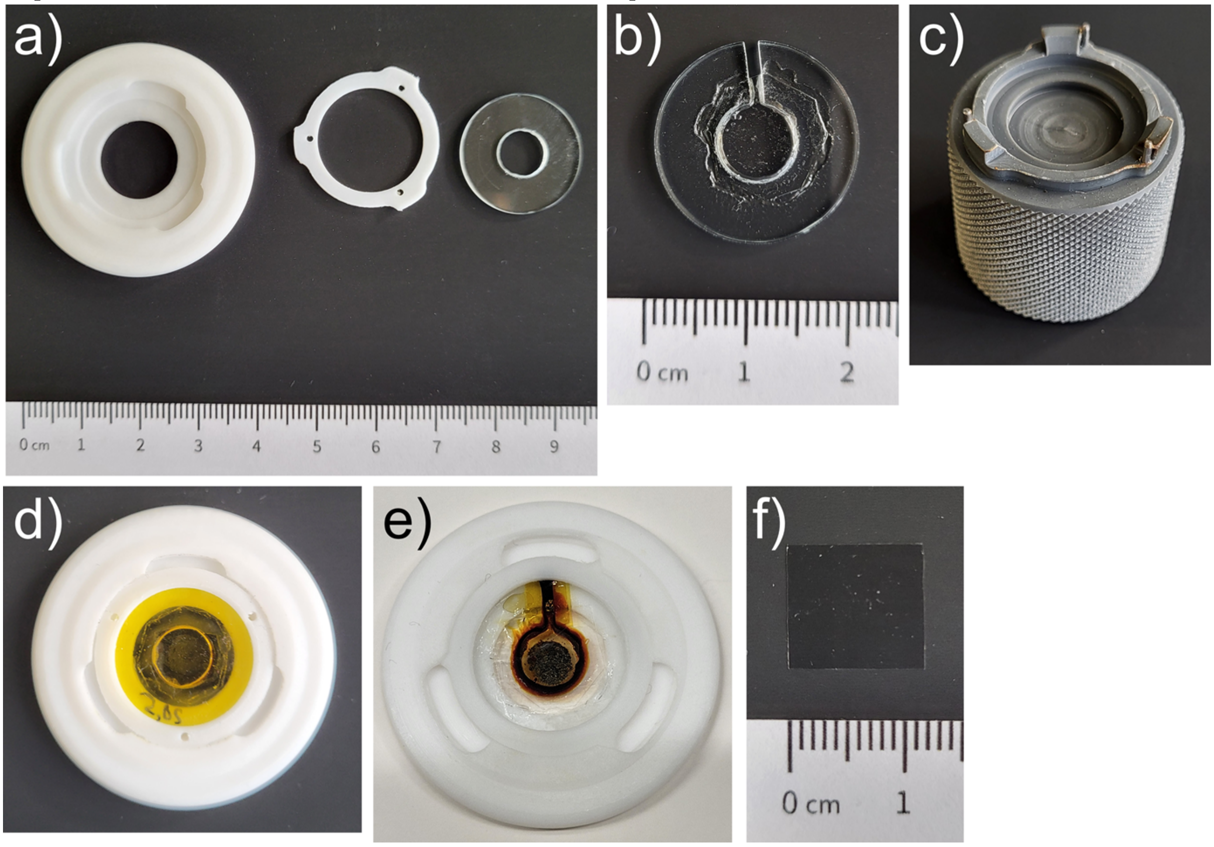
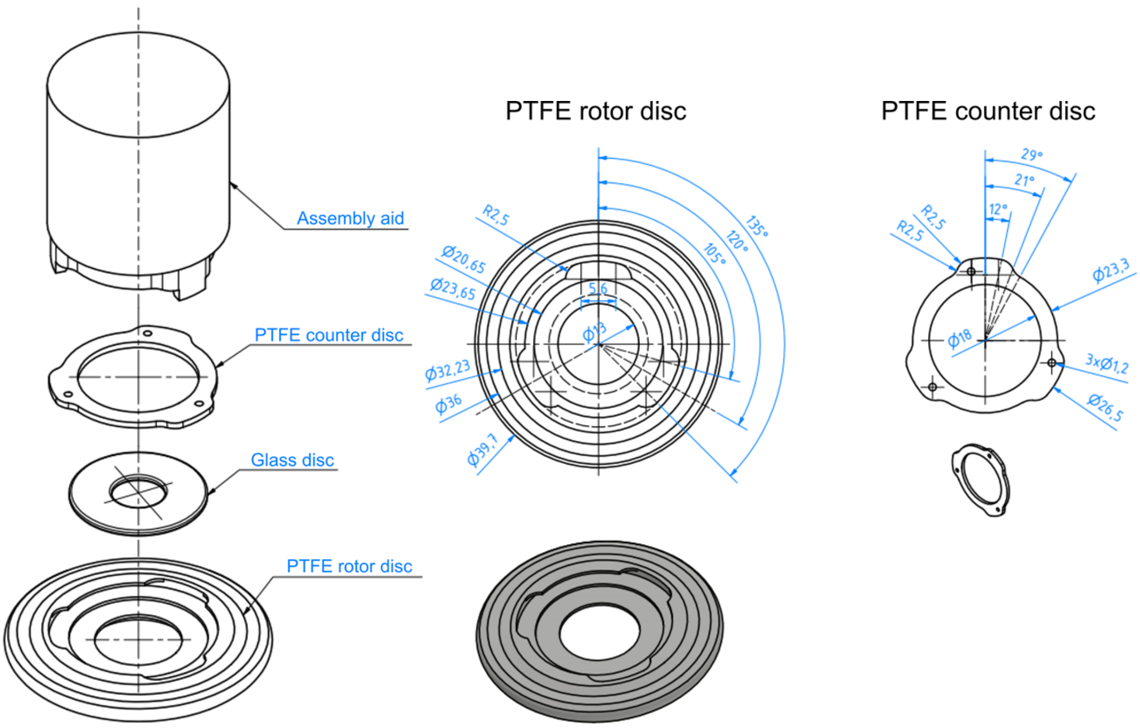


Figure S8. Components and assembly of the redesigned transmission sample holder. (a) PTFE rotor disc, PTFE counter disc, and glass disc. (b) Glass disc with an insertion slit and an ultrathin-glass window bonded to one side. (c) Assembly aid. (d) Transmission holder equipped with an assembled rotor disc (ultrathin glass on one side and Kapton on the other). (e) Examples of assembled rotor discs prepared for bromine-containing samples; for experiments with excess bromine, both sides were sealed with ultrathin glass and the perimeter was sealed with wax and cyanoacrylate under argon. (f) Ultrathin-glass window (Schott AF 32®).

Exploded view drawing



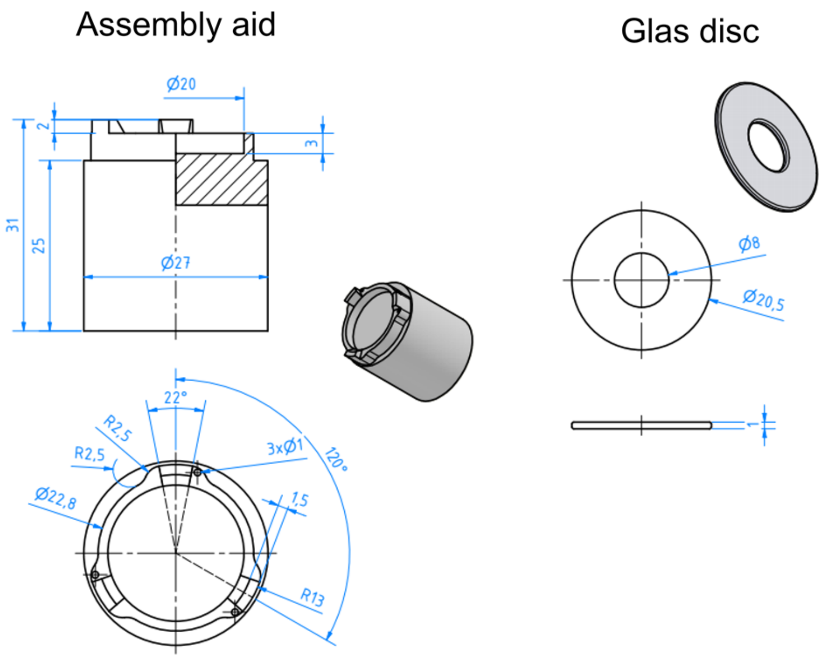


Figure S9. Engineering drawing of the redesigned transmission holder components (PTFE rotor disc, PTFE counter disc, glass disc, and assembly aid), including an exploded view and key dimensions (mm).

Crystallographic details for WTe_2I (supercell)

Table S1: Fractional Atomic Coordinates (×10⁴) and Equivalent Isotropic Displacement Parameters (Å²×10³) for **WTe_2I (supercell)**. U_{eq} is defined as 1/3 of the trace of the orthogonalised U_{ij}.

Atom	x	y	z	U_{eq}
W1	10340.8(7)	10074.9(3)	11376.4(7)	7.57(13)
W2	12243.8(8)	10053.4(4)	9537.5(8)	8.11(14)
W3	18784.5(7)	10050.7(4)	13031.9(8)	7.03(13)
W4	16172.5(7)	9956.1(4)	12038.8(8)	7.31(13)
W5	17157.2(7)	10038.2(4)	14661.4(8)	7.08(13)
W6	14525.4(6)	9978.7(3)	13694.4(6)	6.94(11)
Te1	9174.9(11)	9090.6(5)	10028.2(11)	8.51(18)
Te2	12484.8(13)	10971.8(6)	8234.0(12)	9.0(2)
Te3	15801.4(13)	9057.9(6)	13340.0(12)	8.5(2)
Te4	14134.7(11)	9056.6(5)	14952.2(11)	7.95(18)
Te5	17459.0(13)	10958.6(6)	13354.1(12)	8.2(2)
Te6	9010.4(12)	10972.9(6)	11644.3(12)	7.4(2)
Te7	10862.9(11)	9332.5(6)	13394.7(12)	7.9(2)
Te8	20758.1(12)	10691.9(6)	14936.8(12)	7.6(2)
Te9	17602.7(11)	9298.0(5)	16706.1(11)	7.33(18)
Te10	14124.3(12)	10697.7(6)	11583.2(12)	8.0(2)
Te11	14260.3(12)	9310.0(6)	10046.9(12)	7.9(2)
Te12	12502.9(11)	9513.6(5)	11682.9(11)	8.48(17)
I1	12390.5(13)	8251.2(5)	11550.8(13)	17.6(2)
I2A	17522(5)	7500	13841(6)	52.0(13)
I3A	15352(3)	7500	11151(4)	31.9(8)
I4A	13166(6)	7500	8826(6)	36.5(11)
I5A	10319(5)	7500	6530(4)	40.1(10)
I6A	15867(6)	7500	15192(6)	58.0(14)
I7A	9118(7)	7500	8110(8)	73.7(18)
I8A	14665(5)	7500	16743(4)	39.4(10)
I9A	11810(6)	7500	14423(6)	40.6(12)
I10A	9570(4)	7500	12122(4)	34.9(8)
I11A	7449(5)	7500	9458(6)	56.5(14)
I2B	13600(20)	12500	10224(16)	58(5)
I4B	14321(17)	12500	13021(15)	44(4)
I3B	11067(17)	12500	8914(17)	44(4)
I5B	10720(20)	12500	11142(12)	50(5)
I6B	14478(12)	12500	15563(13)	29(3)
I7B	10810(20)	12500	13717(12)	50(5)
I8B	14046(17)	12500	17773(14)	38(3)
I9B	11430(20)	12500	16481(16)	51(4)
I10B	12130(30)	7500	14788(16)	50(8)
I11B	12890(30)	7500	8436(15)	43(7)

Table S2: Anisotropic Displacement Parameters (×10^4) for **WTe_2I (supercell)**. The anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2} \times U_{11} + ... + 2hka^* \times b^* \times U_{12}]$

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
W1	5.7(3)	10.2(3)	6.0(3)	-0.1(2)	2.0(2)	-0.5(2)
W2	6.4(3)	10.8(3)	6.0(4)	0.4(3)	1.9(3)	-1.0(3)
W3	4.9(3)	10.9(3)	5.3(3)	0.4(3)	2.3(2)	-1.1(3)
W4	5.1(3)	11.3(3)	5.7(4)	0.5(3)	2.7(2)	-1.2(3)
W5	4.8(3)	11.1(3)	5.3(4)	0.8(3)	2.3(2)	-1.3(3)
W6	4.7(4)	10.6(3)	5.4(4)	0.9(2)	2.3(2)	-1.4(2)
Te1	9.9(6)	11.5(4)	3.9(5)	1.0(4)	3.1(3)	-2.5(4)
Te2	10.5(6)	11.3(6)	6.0(6)	0.5(4)	4.5(5)	-1.7(4)
Te3	11.2(6)	11.0(5)	3.9(5)	1.0(4)	4.0(4)	-1.8(4)
Te4	11.0(6)	10.6(4)	3.3(5)	1.0(4)	4.3(3)	-1.7(4)
Te5	10.5(6)	10.9(5)	4.1(5)	1.0(4)	4.1(5)	-1.6(4)
Te6	8.7(5)	10.2(5)	5.0(5)	0.4(4)	4.6(4)	-1.0(4)
Te7	3.5(5)	13.3(5)	6.6(5)	0.2(4)	2.2(4)	-1.9(4)
Te8	3.2(5)	12.1(5)	7.8(6)	0.5(4)	2.8(4)	-1.7(4)
Te9	3.4(5)	11.4(4)	7.4(5)	0.9(4)	2.7(3)	-1.3(4)
Te10	3.7(5)	11.8(5)	8.4(6)	0.9(4)	2.8(4)	-1.4(4)
Te11	3.5(5)	12.6(5)	8.1(6)	1.3(5)	3.0(4)	-0.7(4)
Te12	4.2(5)	14.5(4)	7.7(5)	0.0(4)	3.6(3)	-1.5(4)
I1	20.0(6)	12.4(5)	20.0(7)	-1.0(5)	9.0(4)	-0.2(4)
I2A	62(3)	26.7(18)	92(4)	0	57(3)	0
I3A	39.1(19)	16.2(13)	49(2)	0	27.0(17)	0
I4A	49(3)	21.2(17)	44(3)	0	25(3)	0
I5A	63(3)	17.9(14)	49(2)	0	34(2)	0
I6A	91(4)	17.1(14)	79(4)	0	50(3)	0
I7A	100(5)	16.6(16)	110(6)	0	53(4)	0
I8A	65(3)	19.7(14)	49(2)	0	40(2)	0
I9A	53(3)	22.1(18)	52(4)	0	29(3)	0
I10A	46(2)	17.4(13)	54(2)	0	34.1(18)	0
I11A	64(3)	29.3(19)	99(4)	0	58(3)	0
I2B	91(15)	53(10)	29(8)	0	26(9)	0
I4B	55(10)	29(6)	34(7)	0	9(7)	0
I3B	56(10)	27(7)	51(10)	0	27(8)	0
I5B	97(13)	11(5)	10(5)	0	-2(7)	0
I6B	31(3)	25(3)	26(3)	0	10(2)	0
I7B	85(14)	37(7)	10(5)	0	6(6)	0
I8B	67(10)	18(5)	33(7)	0	27(7)	0
I9B	86(14)	43(8)	39(8)	0	42(9)	0
I10B	73(16)	26(8)	7(6)	0	-19(7)	0
I11B	70(15)	19(7)	5(7)	0	-13(7)	0

Table S3: Bond Lengths in Å for **WTe$_2$I (supercell)**.

Atom	Atom	Length / Å
W1	W1[1]	3.0734(14)
W1	W2[1]	2.8219(10)
W1	Te1	2.6803(13)
W1	Te1[1]	2.7458(15)
W1	Te6	2.6604(15)
W1	Te7	2.7622(14)
W1	Te9[2]	2.8591(13)
W1	Te12	2.7676(14)
W2	W3[3]	2.7874(10)
W2	Te1[1]	2.7594(16)
W2	Te2	2.6596(15)
W2	Te6[1]	2.7211(16)
W2	Te10	2.8528(16)
W2	Te11	2.7641(15)
W2	Te12	2.7478(15)
W3	W4	2.8361(11)
W3	Te2[3]	2.7492(16)
W3	Te5	2.6997(16)
W3	Te6[4]	2.7259(15)
W3	Te7[4]	2.8329(15)
W3	Te8[5]	2.7905(15)
W3	Te8	2.8190(15)
W4	W5	2.8479(10)
W4	Te2[3]	2.7213(16)
W4	Te3	2.6904(15)
W4	Te5	2.7388(16)
W4	Te10	2.8055(15)
W4	Te11	2.8387(16)
W4	Te11[3]	2.8393(15)
W5	W6	2.8572(11)
W5	Te3	2.7292(16)
W5	Te4[2]	2.7022(16)

Atom	Atom	Length / Å
W5	Te5	2.6953(15)
W5	Te7[2]	2.8304(15)
W5	Te8[5]	2.8419(15)
W5	Te9	2.8035(14)
W6	W6[2]	2.8355(14)
W6	Te3	2.6978(16)
W6	Te4	2.7049(14)
W6	Te4[2]	2.7085(13)
W6	Te9[2]	2.8771(14)
W6	Te10	2.8554(14)
W6	Te12	2.7383(12)
Te12	I1	2.7663(15)
I2A	I3A	3.111(8)
I2A	I6A	3.136(8)
I3A	I4A	2.846(7)
I5A	I7A	2.906(9)
I6A	I8A	2.875(7)
I7A	I11A	3.148(10)
I9A	I10A	2.863(8)
I10A	I11A	3.068(8)
I2B	I4B	3.10(2)
I2B	I3B	2.73(3)
I4B	I6B	3.01(2)
I3B	I5B	2.93(3)
I5B	I7B	3.09(2)
I6B	I8B	2.97(2)
I7B	I9B	3.09(2)
I8B	I9B	2.82(3)

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[1]2-x,2-y,2-z; [2]3-x,2-y,3-z; [3]3-x,2-y,2-z; [4]1+x,+y,+z; [5]4-x,2-y,3-z

Table S4: Atomic Occupancies for all atoms that are not fully occupied in **WTe_2I (supercell)**.

Atom	Occupancy
I2A	0.803(4)
I3A	0.803(4)
I4A	0.803(4)
I5A	0.803(4)
I6A	0.803(4)
I7A	0.803(4)
I8A	0.803(4)
I9A	0.803(4)
I10A	0.803(4)
I11A	0.803(4)

Atom	Occupancy
I2B	0.197(4)
I4B	0.197(4)
I3B	0.197(4)
I5B	0.197(4)
I6B	0.197(4)
I7B	0.197(4)
I8B	0.197(4)
I9B	0.197(4)
I10B	0.197(4)
I11B	0.197(4)

Crystallographic details for incommensurate WTe_2I

Table S5: Occupational waves for incommensurate WTe_2I.

Atom	Wave/Parameter	Occ
Te2	delta	0.8318(8)
	x40	0.2710(4)
Te3	delta	0.1682(8)
	x40	0.7754(5)
I1	delta	0.8318(8)
	x40	0.3929(4)
I2	delta	0.8318(8)
	x40	0.1633(4)
I3	delta	0.1682(8)
	x40	0.7865(4)

Table S6: Positional parameters for incommensurate WTe_2I.

Atom	Occ	Wave	x	y	z	Ueq/Uiso
W1	1		0.32142(3)	0.495374(9)	0.25174(13)	0.00479(7)
		s,1	-0.00194(5)	0.001783(16)	-0.0072(12)	
		c,1	0.00190(5)	-0.001740(16)	-0.0085(10)	
		s,2	-0.00203(5)	-0.000332(16)	0.0046(2)	
		c,2	0.00211(5)	-0.000476(16)	0.0091(8)	
		s,3	-0.0010(3)	0.00067(8)	-0.0068(9)	
		c,3	0.0032(2)	-0.00036(7)	0.0057(11)	
		s,4	0	0	-0.067(2)	
		c,4	0.3826(5)	1	0	
Te1	1		0.57919(5)	0.595074(13)	0.24836(18)	0.00651(7)
		s,1	-0.00264(8)	0.00038(3)	0.02596(15)	
		c,1	-0.01089(8)	-0.00028(3)	-0.01238(15)	
		s,2	0.00422(8)	-0.00187(3)	0.00920(15)	
		c,2	0.00324(8)	-0.00144(3)	-0.00400(16)	
Te2	0.8318(8)		0.07022(7)	0.56927(2)	0.7492(2)	0.00552(9)
		o,1	-0.00111(10)	0.00106(3)	0.0018(2)	
		o,2	0.00011(6)	-0.00041(2)	-0.00017(12)	
		o,3	-0.00154(8)	0.00046(3)	-0.01128(14)	
		o,4	0.00000(13)	-0.00028(4)	0.0047(3)	
Te3	0.1682(8)		0.0817(4)	0.54812(10)	0.7526(8)	0.0056(4)
		o,1	-0.0013(5)	-0.00001(17)	-0.0011(13)	
		o,2	-0.001(3)	0.0001(8)	0.006(6)	
I1	0.8318(8)		0.34767(14)	0.75	0.7591(4)	0.0218(3)
		o,1	0.02889(15)	0	0.0932(3)	
		o,2	-0.01800(15)	0	-0.0089(4)	
		o,3	0.0001(2)	0	-0.0335(4)	
		o,4	0.00596(17)	0	-0.0221(4)	
		o,5	0.0008(3)	0	0.0010(5)	
		o,6	-0.0026(2)	0	-0.0113(5)	
I2	0.8318(8)		-0.17524(15)	0.75	0.7370(4)	0.0254(3)
		o,1	-0.03392(15)	0	-0.0879(3)	
		o,2	-0.00962(16)	0	0.0148(4)	
		o,3	-0.00434(19)	0	-0.0074(5)	
		o,4	-0.0032(2)	0	0.0410(5)	
		o,5	-0.0020(2)	0	-0.0104(6)	
		o,6	-0.0011(3)	0	-0.0055(5)	
I3	0.1682(8)		0.1052(2)	0.67498(7)	0.7481(5)	0.0151(3)
		o,1	-0.0031(8)	-0.0001(2)	0.0282(15)	

	o,2	-0.004(4)	0.0007(12)	-0.004(7)

Table S7: ADP harmonic parameters for incommensurate WTe_2I.

Atom	Wave	U11	U22	U33	U12	U13	U23
W1		0.00241(9)	0.00714(9)	0.00482(17)	-0.00014(6)	-0.00143(14)	0.00020(12)
	s,1	-0.00019(12)	0.00021(13)	-0.0004(2)	0.00008(11)	0.00026(12)	-0.00021(13)
	c,1	0.00005(12)	-0.00017(14)	0.00099(17)	-0.00011(11)	-0.00007(13)	-0.00023(13)
Te1		0.00502(12)	0.00856(13)	0.00596(13)	-0.00101(10)	-0.0012(2)	-0.0002(2)
	s,1	0.0010(2)	0.0013(2)	0.0005(2)	-0.00105(18)	-0.00049(16)	0.00068(17)
	c,1	0.0012(2)	0.0029(2)	0.0015(2)	-0.00243(17)	0.00108(17)	-0.00133(17)
Te2		0.00326(14)	0.00726(16)	0.00603(15)	0.00004(13)	-0.0015(3)	-0.0002(3)
	o,1	-0.00010(18)	-0.0005(2)	0.0018(2)	0.00021(17)	0.00013(15)	0.00003(19)
	o,2	-0.00001(16)	0.00011(18)	-0.00068(18)	0.00009(14)	-0.00018(13)	-0.00017(14)
Te3		0.0031(4)	0.0086(6)	0.0050(9)	-0.0011(5)	-0.0010(5)	0.0001(6)
I1		0.0176(4)	0.0156(3)	0.0323(6)	0	-0.0053(4)	0
	o,1	0.0024(4)	-0.0014(4)	0.0101(6)	0	-0.0048(4)	0
	o,2	0.0025(5)	-0.0015(4)	-0.0115(7)	0	0.0078(5)	0
I2		0.0183(4)	0.0158(3)	0.0419(7)	0	-0.0045(4)	0
	o,1	0.0024(4)	-0.0014(4)	0.0123(7)	0	-0.0090(4)	0
	o,2	-0.0010(5)	0.0016(4)	0.0149(6)	0	-0.0041(5)	0
I3		0.0174(6)	0.0089(5)	0.0191(7)	-0.0002(4)	-0.0017(5)	0.0005(5)

Table S8: List of used orthogonalized functions for incommensurate WTe_2I.

Te2	o,1	-	-0.309	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	1.616																		
	o,2	-	0.051	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-0.091	-	-	-	-	-	-	-	-	1.315									
	o,3	-	-0.095	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	0.171	-	-	-	-	-	-	-	-	-0.098	-	-	-	-	-	-	-	1.38	
	o,4	-	-0.448	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	0.853	-	-	-	-	-	-	-	-	-0.097	-	-	-	-	-	-	-	0.168	1.708
Te3	o,1	-	-	-	-	-	-	-	-	-	-	-0.518	-	-	-	-	-	-	-	-	3.414																		
	o,2	-	-	-	-	-	-	-	-	-	-	-2.531	-	-	-	-	-	-	-	-	3.806	-	-	-	-	-	-	-	3.49										
I1	o,1	-	-0.169	-	-	-	-	-	-	-	-	1.408																											
	o,2	-	0.263	-	-	-	-	-	-	-	-	-0.297	-	-	-	-	-	-	-	1.509																			
	o,3	-	-0.439	-	-	-	-	-	-	-	-	0.542	-	-	-	-	-	-	-	-0.646	1.705																		
	o,4	-	0.128	-	-	-	-	-	-	-	-	-0.095	-	-	-	-	-	-	-	0.237	-0.179	1.383																	
	o,5	-	-0.583	-	-	-	-	-	-	-	-	0.652	-	-	-	-	-	-	-	-0.916	0.947	-0.332	1.745																
	o,6	-	-0.361	-	-	-	-	-	-	-	-	0.51	-	-	-	-	-	-	-	-0.481	0.642	0.04	0.348	1.523															
I2	o,1	-	-0.25	-	-	-	-	-	-	-	1.518																												
	o,2	-	-0.188	-	-	-	-	-	-	-	0.291	1.401																											
	o,3	-	0.381	-	-	-	-	-	-	-	-0.603	-0.415	1.627																										
	o,4	-	-0.253	-	-	-	-	-	-	-	0.448	0.197	-0.323	1.449																									
	o,5	-	-0.034	-	-	-	-	-	-	-	-0.005	0.133	-0.15	-0.163	1.439																								
	o,6	-	0.685	-	-	-	-	-	-	-	-1.13	-0.678	1.033	-0.552	-0.046	1.848																							

Table S9: List of distances for incommensurate WTe_2I.

	average / Å	min / Å	max / Å
W1-W1^{i}	2.870(11)	2.781(16)	3.097(16)
W1-W1^{ii}	2.846(11)	2.830(14)	2.862(14)
W1-Te1	2.720(3)	2.684(3)	2.755(3)
W1-Te1^{i}	2.706(8)	2.555(12)	2.856(12)
W1-Te1^{ii}	2.702(8)	2.543(12)	2.851(12)
W1-Te2^{iii}	2.820(7)	2.749(9)	2.905(9)
W1-Te2	2.819(7)	2.739(9)	2.889(9)
W1-Te2^{iv}	2.845(3)	2.813(3)	2.877(3)
W1-Te3^{iii}	2.76(4)	2.73(7)	2.78(7)
W1-Te3	2.73(4)	2.45(7)	2.78(7)
W1-Te3^{iv}	2.74(3)	2.73(6)	2.74(6)
Te3-I3	2.77(3)	2.76(6)	2.79(6)
I1-I1^{iii}	3.415(6)	2.769(8)	4.018(8)
I1-I1^{v}	3.405(6)	2.769(8)	4.018(8)
I1-I2	3.341(6)	2.688(8)	3.933(8)
I1-I2^{vi}	3.189(6)	2.887(8)	3.702(8)
I1-I2^{vii}	3.341(6)	2.688(8)	3.933(8)
I1-I2^{viii}	3.189(6)	2.887(8)	3.702(8)
I1-I3^{iii}	4.084(9)	4.011(15)	4.255(15)
I1-I3^{v}	4.297(9)	4.140(13)	4.407(13)
I1-I3^{ix}	4.084(9)	4.011(15)	4.255(15)
I1-I3^{x}	4.297(9)	4.140(13)	4.407(13)
I2-I2^{iii}	3.419(7)	2.765(9)	4.028(9)
I2-I2^{v}	3.416(7)	2.765(9)	4.029(9)
I2-I2^{ix}	3.419(7)	2.765(9)	4.028(9)
I2-I2^{vii}	0	0	0
I2-I2^{x}	3.416(7)	2.765(9)	4.029(9)
I2-I3^{v}	4.123(8)	4.064(14)	4.250(14)
I2-I3^{x}	4.123(8)	4.064(14)	4.250(14)
I3-I3^{iii}	3.659(15)	3.659(15)	3.659(15)
I3-I3^{v}	3.658(15)	3.658(15)	3.658(15)
I3-I3^{vii}	3.272(11)	3.24(2)	3.29(2)

(i) -x+1,-y+1,-z
(ii) -x+1,-y+1,-z+1
(iii) x,y,z-1
(iv) -x,-y+1,-z+1
(v) x,y,z+1
(vi) x+1,y,z
(vii) x,-y+3/2,z
(viii) x+1,-y+3/2,z
(ix) x,-y+3/2,z-1
(x) x,-y+3/2,z+1
(xi) x-1,y,z

Table S10: List of angles for incommensurate WTe_2I.

	average / °	min / °	max / °
$W1^{i}$-W1-$W1^{ii}$	74.7(3)	70.4(3)	83.2(3)
$W1^{i}$-W1-Te1	57.78(14)	55.55(17)	59.50(17)
$W1^{i}$-W1-$Te1^{i}$	58.3(2)	53.7(2)	60.5(3)
$W1^{i}$-W1-$Te1^{ii}$	104.93(15)	102.07(12)	110.76(16)
$W1^{i}$-W1-$Te2^{iii}$	93.3(3)	90.1(4)	96.5(4)
$W1^{i}$-W1-Te2	140.27(13)	137.64(16)	143.27(12)
$W1^{i}$-W1-$Te2^{iv}$	136.1(4)	127.6(5)	142.3(5)
$W1^{i}$-W1-$Te3^{iii}$	82.2(14)	81.4(14)	89.2(14)
$W1^{i}$-W1-Te3	145.6(13)	145.2(14)	146.3(13)
$W1^{i}$-W1-$Te3^{iv}$	139.1(15)	138.6(15)	140.2(15)
$W1^{ii}$-W1-Te1	58.04(14)	54.70(18)	61.91(19)
$W1^{ii}$-W1-$Te1^{i}$	104.74(15)	100.93(13)	110.0(2)
$W1^{ii}$-W1-$Te1^{ii}$	58.6(2)	56.8(3)	59.9(3)
$W1^{ii}$-W1-$Te2^{iii}$	140.51(12)	137.11(13)	144.01(11)
$W1^{ii}$-W1-Te2	92.9(3)	90.2(4)	94.1(3)
$W1^{ii}$-W1-$Te2^{iv}$	137.0(4)	133.2(6)	141.6(5)
$W1^{ii}$-W1-$Te3^{iii}$	145.8(12)	145.2(12)	146.6(13)
$W1^{ii}$-W1-Te3	87.4(14)	86.4(14)	93.9(16)
$W1^{ii}$-W1-$Te3^{iv}$	138.3(15)	138.0(15)	138.7(15)
Te1-W1-$Te1^{i}$	116.1(3)	109.3(4)	119.9(3)
Te1-W1-$Te1^{ii}$	116.6(3)	111.1(4)	121.3(3)
Te1-W1-$Te2^{iii}$	83.74(15)	81.31(14)	86.70(13)
Te1-W1-Te2	83.82(14)	81.73(17)	86.06(14)
Te1-W1-$Te2^{iv}$	155.34(14)	152.2(3)	159.93(11)
Te1-W1-$Te3^{iii}$	85.2(12)	83.5(12)	87.7(13)
Te1-W1-Te3	87.0(13)	85.8(13)	91.8(14)
Te1-W1-$Te3^{iv}$	151.2(13)	149.5(13)	152.0(13)
$Te1^{i}$-W1-$Te1^{ii}$	79.86(7)	77.14(7)	84.58(9)
$Te1^{i}$-W1-$Te2^{iii}$	99.9(3)	95.4(4)	104.4(5)
$Te1^{i}$-W1-Te2	158.24(13)	156.7(3)	160.69(10)
$Te1^{i}$-W1-$Te2^{iv}$	81.23(16)	79.4(2)	84.66(17)
$Te1^{i}$-W1-$Te3^{iii}$	85.8(14)	84.0(14)	88.1(14)
$Te1^{i}$-W1-Te3	153.9(13)	153.6(14)	154.3(12)
$Te1^{i}$-W1-$Te3^{iv}$	85.3(14)	84.7(14)	86.3(14)
$Te1^{ii}$-W1-$Te2^{iii}$	158.39(13)	156.05(10)	159.76(11)
$Te1^{ii}$-W1-Te2	100.1(3)	96.8(4)	103.8(5)
$Te1^{ii}$-W1-$Te2^{iv}$	81.39(16)	78.55(14)	85.19(17)
$Te1^{ii}$-W1-$Te3^{iii}$	154.5(12)	154.2(12)	154.9(12)
$Te1^{ii}$-W1-Te3	86.4(14)	84.5(14)	98.7(16)
$Te1^{ii}$-W1-$Te3^{iv}$	85.2(14)	84.6(14)	86.1(14)
$Te2^{iii}$-W1-Te2	75.02(8)	72.66(7)	77.19(8)
$Te2^{iii}$-W1-$Te2^{iv}$	78.53(13)	76.69(13)	80.30(15)
$Te2^{iii}$-W1-Te3	80.7(14)	79.8(14)	81.2(13)
$Te2^{iii}$-W1-$Te3^{iv}$	71.7(14)	71.4(14)	72.2(14)
Te2-W1-$Te2^{iv}$	78.43(13)	76.87(16)	79.87(15)
Te2-W1-$Te3^{iii}$	79.0(14)	78.4(14)	80.0(14)
Te2-W1-$Te3^{iv}$	71.8(14)	71.1(14)	72.2(14)
$Te2^{iv}$-W1-$Te3^{iii}$	71.1(12)	70.7(12)	72.2(12)
$Te2^{iv}$-W1-Te3	71.9(13)	70.7(12)	74.8(14)
$Te3^{iii}$-W1-Te3	82.8(16)	82.8(16)	82.8(16)
W1-Te1-$W1^{i}$	63.9(2)	61.8(3)	69.3(3)
W1-Te1-$W1^{ii}$	63.3(2)	61.3(3)	65.4(3)
$W1^{i}$-Te1-$W1^{ii}$	79.8(3)	75.3(3)	89.7(3)
W1-Te2-$W1^{v}$	73.8(3)	71.3(3)	75.8(2)
W1-Te2-$W1^{iv}$	102.09(16)	99.7(2)	105.4(2)
$W1^{v}$-Te2-$W1^{iv}$	102.19(16)	99.1(2)	105.36(19)
W1-Te3-$W1^{v}$	89.9(10)	81.8(5)	90.6(17)

W1-Te3-W1^{iv}	110.9(11)	110.1(17)	114.4(5)
W1-Te3-I3	113.4(11)	112(2)	119.1(5)
W1^{v}-Te3-W1^{iv}	111.2(11)	110.1(7)	111.6(9)
W1^{v}-Te3-I3	114.2(11)	112.3(5)	115.4(7)
W1^{iv}-Te3-I3	114.7(10)	113.6(4)	115.3(19)
I1^{iii}-I1-I1^{v}	176.1(2)	171.3(2)	180
I1^{iii}-I1-I2	89.3(2)	76.22(19)	107.0(2)
I1^{iii}-I1-I2^{vi}	89.7(2)	82.1(2)	97.28(17)
I1^{iii}-I1-I2^{vii}	89.3(2)	76.22(19)	107.0(2)
I1^{iii}-I1-I2^{viii}	89.7(2)	82.1(2)	97.28(17)
I1^{iii}-I1-I3^{v}	154.94(10)	152.26(10)	156.47(8)
I1^{iii}-I1-I3^{x}	154.94(10)	152.26(10)	156.47(8)
I1^{v}-I1-I2	91.0(2)	81.1(2)	100.33(17)
I1^{v}-I1-I2^{vi}	94.6(2)	77.28(18)	99.9(2)
I1^{v}-I1-I2^{vii}	91.0(2)	81.1(2)	100.33(17)
I1^{v}-I1-I2^{viii}	94.6(2)	77.28(18)	99.9(2)
I1^{v}-I1-I3^{iii}	149.64(11)	148.82(13)	151.36(8)
I1^{v}-I1-I3^{ix}	149.64(11)	148.82(13)	151.36(8)
I2-I1-I2^{vi}	167.5(2)	155.8(2)	180
I2-I1-I2^{vii}	0	0	0
I2-I1-I2^{viii}	167.5(2)	155.8(2)	180
I2-I1-I3^{iii}	75.05(15)	72.67(16)	76.11(14)
I2-I1-I3^{v}	66.88(13)	65.76(11)	69.54(16)
I2-I1-I3^{ix}	75.05(15)	72.67(16)	76.11(14)
I2-I1-I3^{x}	66.88(13)	65.76(11)	69.54(16)
I2^{vi}-I1-I2^{vii}	167.5(2)	155.8(2)	180
I2^{vi}-I1-I2^{viii}	0	0	0
I2^{vi}-I1-I3^{iii}	102.09(16)	101.80(18)	102.33(15)
I2^{vi}-I1-I3^{v}	95.29(14)	91.83(14)	102.89(12)
I2^{vi}-I1-I3^{ix}	102.09(16)	101.80(18)	102.33(15)
I2^{vi}-I1-I3^{x}	95.29(14)	91.83(14)	102.89(12)
I2^{vii}-I1-I2^{viii}	167.5(2)	155.8(2)	180
I2^{vii}-I1-I3^{iii}	75.05(15)	72.67(16)	76.11(14)
I2^{vii}-I1-I3^{v}	66.88(13)	65.76(11)	69.54(16)
I2^{vii}-I1-I3^{ix}	75.05(15)	72.67(16)	76.11(14)
I2^{vii}-I1-I3^{x}	66.88(13)	65.76(11)	69.54(16)
I2^{viii}-I1-I3^{iii}	102.09(16)	101.80(18)	102.33(15)
I2^{viii}-I1-I3^{v}	95.29(14)	91.83(14)	102.89(12)
I2^{viii}-I1-I3^{ix}	102.09(16)	101.80(18)	102.33(15)
I2^{viii}-I1-I3^{x}	95.29(14)	91.83(14)	102.89(12)
I3^{iii}-I1-I3^{ix}	47.28(14)	44.9(2)	48.29(11)
I3^{v}-I1-I3^{x}	44.80(13)	43.19(11)	46.3(2)
I1^{xi}-I2-I1	168.9(2)	157.3(3)	180
I1^{xi}-I2-I2^{iii}	94.48(18)	77.86(17)	99.7(2)
I1^{xi}-I2-I2^{v}	89.74(19)	82.2(2)	97.1(2)
I1^{xi}-I2-I2^{ix}	94.48(18)	77.86(17)	99.7(2)
I1^{xi}-I2-I2^{vii}	0	0	0
I1^{xi}-I2-I2^{x}	89.74(19)	82.2(2)	97.1(2)
I1^{xi}-I2-I3^{v}	105.61(14)	104.61(18)	106.13(11)
I1^{xi}-I2-I3^{x}	105.61(14)	104.61(18)	106.13(11)
I1-I2-I2^{iii}	90.67(18)	82.37(19)	99.6(2)
I1-I2-I2^{v}	88.91(19)	76.01(17)	105.7(2)
I1-I2-I2^{ix}	90.67(18)	82.37(19)	99.6(2)
I1-I2-I2^{vii}	0	0	0
I1-I2-I2^{x}	88.91(19)	76.01(17)	105.7(2)
I1-I2-I3^{v}	73.38(13)	71.73(14)	74.28(12)
I1-I2-I3^{x}	73.38(13)	71.73(14)	74.28(12)
I2^{iii}-I2-I2^{v}	175.9(2)	171.3(3)	179.53(17)
I2^{iii}-I2-I2^{ix}	0	0	0
I2^{iii}-I2-I2^{vii}	0	0	0

$I2^{iii}$-I2-$I2^{x}$	175.9(2)	171.3(3)	179.53(17)
$I2^{iii}$-I2-$I3^{v}$	148.13(10)	147.38(11)	149.85(12)
$I2^{iii}$-I2-$I3^{x}$	148.13(10)	147.38(11)	149.85(12)
$I2^{v}$-I2-$I2^{ix}$	175.9(2)	171.3(3)	179.53(16)
$I2^{v}$-I2-$I2^{vii}$	0	0	0
$I2^{v}$-I2-$I2^{x}$	0	0	0
$I2^{ix}$-I2-$I2^{vii}$	0	0	0
$I2^{ix}$-I2-$I2^{x}$	175.9(2)	171.3(3)	179.53(17)
$I2^{ix}$-I2-$I3^{v}$	148.13(10)	147.38(11)	149.85(12)
$I2^{ix}$-I2-$I3^{x}$	148.13(10)	147.38(11)	149.85(12)
$I2^{vii}$-I2-$I2^{x}$	0	0	0
$I2^{vii}$-I2-$I3^{v}$	0	0	0
$I2^{vii}$-I2-$I3^{x}$	0	0	0
$I3^{v}$-I2-$I3^{x}$	46.79(13)	44.87(12)	47.60(14)
Te3-I3-$I1^{iii}$	113.7(8)	112.1(4)	114.3(14)
Te3-I3-$I1^{v}$	114.6(8)	113.1(7)	115.4(4)
Te3-I3-$I2^{iii}$	112.4(8)	110.8(4)	113.0(13)
Te3-I3-$I2^{ix}$	112.4(8)	110.8(4)	113.0(13)
Te3-I3-$I3^{iii}$	87.8(5)	87.8(5)	87.8(5)
Te3-I3-$I3^{v}$	88.2(5)	88.2(5)	88.2(5)
Te3-I3-$I3^{vii}$	176.6(8)	176.4(12)	176.9(5)
$I1^{iii}$-I3-$I1^{v}$	119.6(2)	118.4(3)	120.96(17)
$I1^{iii}$-I3-$I2^{iii}$	39.78(14)	38.23(17)	42.02(13)
$I1^{iii}$-I3-$I2^{ix}$	39.78(14)	38.23(17)	42.02(13)
$I1^{iii}$-I3-$I3^{v}$	152.4(2)	152.4(2)	152.4(2)
$I1^{iii}$-I3-$I3^{vii}$	67.62(17)	66.9(2)	68.42(15)
$I1^{v}$-I3-$I2^{iii}$	132.7(2)	132.17(16)	133.8(3)
$I1^{v}$-I3-$I2^{ix}$	132.7(2)	132.17(16)	133.8(3)
$I1^{v}$-I3-$I3^{iii}$	146.8(4)	146.8(4)	146.8(4)
$I1^{v}$-I3-$I3^{vii}$	66.38(17)	65.86(13)	67.6(3)
$I2^{iii}$-I3-$I2^{ix}$	0	0	0
$I2^{iii}$-I3-$I3^{v}$	144.9(2)	144.9(2)	144.9(2)
$I2^{iii}$-I3-$I3^{vii}$	66.62(16)	66.20(18)	67.60(15)
$I2^{ix}$-I3-$I3^{v}$	144.9(2)	144.9(2)	144.9(2)
$I2^{ix}$-I3-$I3^{vii}$	66.62(16)	66.20(18)	67.60(15)
$I3^{iii}$-I3-$I3^{vii}$	89.9(4)	89.9(4)	89.9(4)
$I3^{v}$-I3-$I3^{vii}$	90.0(3)	90.0(3)	90.0(3)

(i) -x+1,-y+1,-z
(ii) -x+1,-y+1,-z+1
(iii) x,y,z-1
(iv) -x,-y+1,-z+1
(v) x,y,z+1
(vi) x+1,y,z
(vii) x,-y+3/2,z
(viii) x+1,-y+3/2,z
(ix) x,-y+3/2,z-1
(x) x,-y+3/2,z+1
(xi) x-1,y,z

Crystallographic details for commensurate WTe_2I

Table S 11: Occupational waves for commensurate WTe_2I.

Atom	Wave/Parameter	Occ
Te2	delta	0.8318
	x40	0.3211(4)
Te3	delta	0.1682
	x40	0.8231(4)
I1	delta	0.8318
	x40	0.4567(5)
I2	delta	0.8318
	x40	0.1933
I3	delta	0.1682
	x40	0.8366(5)

Table S12: Positional parameters for commensurate WTe_2I.

Atom	Occ	Wave	x	y	z	Ueq/Uiso
W1	1		0.32164(6)	0.495299(18)	0.2518(2)	0.00718(10)
		s,1	-0.00066(16)	0.00147(4)	-0.0298(10)	
		c,1	0.00256(13)	-0.00162(3)	-0.0094(4)	
		s,2	-0.00350(11)	0.00013(3)	-0.0044(6)	
		c,2	-0.00019(14)	0.00012(4)	0.0026(4)	
		s,3	0	0	-0.0949(15)	
		c,3	0.4355	1	0	
Te1	1		0.57916(10)	0.59501(3)	0.2561(3)	0.00847(15)
		s,1	-0.0039(3)	0.00054(8)	0.0279(3)	
		c,1	-0.00876(16)	-0.00040(5)	-0.0007(5)	
		s,2	-0.0009(2)	-0.00033(5)	0.0108(3)	
		c,2	0.00613(17)	-0.00235(5)	-0.0041(3)	
Te2	0.8318		0.07018(16)	0.56910(4)	0.7592(4)	0.00718(18)
		o,1	-0.0008(2)	0.00093(6)	-0.0008(6)	
		o,2	0.0002(3)	0.00012(7)	0.0029(4)	
		o,3	0.0011(4)	-0.00061(11)	-0.0175(8)	
		o,4	-0.0007(3)	0.00003(8)	-0.0030(7)	
Te3	0.1682		0.0811(4)	0.54884(10)	0.7465(8)	0.0077(4)
I1	0.8318		0.3527(6)	0.75	0.7423(14)	0.0627(11)
		o,1	0.0010(9)	0	0.0720(8)	
		o,2	-0.0266(7)	0	0.0347(12)	
		o,3	-0.0065(7)	0	-0.0358(10)	
		o,4	0.0058(11)	0	-0.0214(14)	
I2	0.8318		-0.1823(6)	0.75	0.7503(15)	0.0660(12)
		o,1	-0.0280(8)	0	0.0009(12)	
		o,2	-0.0161(8)	0	0.0755(9)	
		o,3	-0.0021(8)	0	0.0387(11)	
		o,4	0.0110(11)	0	0.0226(18)	
I3	0.1682		0.1055(4)	0.67488(9)	0.7537(9)	0.0168(5)

Table S13: ADP harmonic parameters for commensurate WTe_2I.

Atom	Wave	U11	U22	U33	U12	U13	U23
W1		0.00523(16)	0.01106(18)	0.00526(17)	-0.00038(13)	0.0000(4)	0.0020(2)
	s,1	0.0003(4)	0.0005(4)	-0.0008(3)	0.0009(3)	-0.0001(3)	0.0002(2)
	c,1	0.0002(3)	0.0000(3)	0.0004(3)	0.0002(3)	-0.0004(3)	0.0005(3)
Te1		0.0080(3)	0.0118(3)	0.0056(3)	-0.0009(2)	-0.0037(5)	0.0036(4)
Te2		0.0053(3)	0.0125(3)	0.0037(4)	-0.0006(2)	0.0026(5)	0.0027(4)
	o,1	0.0004(3)	-0.0016(4)	-0.0009(4)	0.0005(3)	0.0006(4)	-0.0009(4)
	o,2	0.0007(5)	-0.0007(5)	0.0002(5)	0.0006(4)	0.0001(2)	-0.0001(3)
Te3		0.0058(8)	0.0144(9)	0.0028(7)	0.0000(8)	0.0027(9)	-0.0003(11)
I1		0.102(2)	0.0259(9)	0.060(2)	0	0.018(2)	0
	o,1	0.005(3)	-0.0021(13)	0.0039(18)	0	-0.0057(15)	0
	o,2	-0.018(3)	0.0008(11)	-0.0075(17)	0	0.001(2)	0
I2		0.106(3)	0.0257(9)	0.067(2)	0	0.009(2)	0
	o,1	0.031(3)	-0.0012(12)	0.018(2)	0	-0.002(2)	0
	o,2	0.008(2)	0.0039(12)	0.0100(18)	0	0.0008(16)	0
I3		0.0182(9)	0.0128(8)	0.0194(9)	-0.0005(7)	-0.0014(11)	-0.0004(10)

Table S14: List of used orthogonalized functions for commensurate WTe_2I.

Te2	o,1	-	-0.269	-	-	-	-	-	-	-	-	-	-	-	-	-	1.548														
	o,2	-	0.16	-	-	-	-	-	-	-	-	-	-	-	-	-	-0.261	-	-	-	-	-	-	1.373							
	o,3	-	-0.32	-	-	-	-	-	-	-	-	-	-	-	-	-	0.53	-	-	-	-	-	-	-0.314	-	-	-	-	-	1.553	
	o,4	-	-0.327	-	-	-	-	-	-	-	-	-	-	-	-	-	0.589	-	-	-	-	-	-	-0.223	-	-	-	-	-	0.367	1.518
I1	o,1	-	-0.069	-	-	-	-	-	-	1.326																					
	o,2	-	0.305	-	-	-	-	-	-	-0.149	-	-	-	-	-	1.603															
	o,3	-	-0.197	-	-	-	-	-	-	0.168	-	-	-	-	-	-0.345	1.437														
	o,4	-	0.413	-	-	-	-	-	-	-0.181	-	-	-	-	-	0.772	-0.308	1.64													
I2	o,1	-	-0.284	-	-	-	-	-	1.573																						
	o,2	-	-0.131	-	-	-	-	-	0.223	1.351																					
	o,3	-	0.257	-	-	-	-	-	-0.44	-0.231	1.488																				
	o,4	-	-0.379	-	-	-	-	-	0.695	0.213	-0.356	1.584																			

Table S15: List of distances for commensurate WTe_2I.

	average / Å	min / Å	max / Å
W1-W1^{i}	2.843(6)	2.825(7)	2.862(7)
W1-W1^{ii}	2.859(6)	2.775(9)	3.080(9)
W1-Te1	2.722(3)	2.689(3)	2.746(3)
W1-Te1^{i}	2.715(5)	2.649(6)	2.794(6)
W1-Te1^{ii}	2.696(5)	2.623(7)	2.761(7)
W1-Te2^{iii}	2.802(6)	2.744(8)	2.863(8)
W1-Te2	2.837(5)	2.787(7)	2.905(7)
W1-Te2^{iv}	2.839(4)	2.814(6)	2.860(6)
W1-Te3^{iii}	2.755(5)	2.755(5)	2.755(5)
W1-Te3	2.766(7)	2.766(7)	2.766(7)
W1-Te3^{iv}	2.739(3)	2.739(3)	2.739(3)
Te3-I3	2.762(3)	2.762(3)	2.762(3)
I1-I1^{iii}	3.416(11)	2.900(12)	3.915(12)
I1-I1^{v}	3.416(11)	2.900(12)	3.915(12)
I1-I2	3.374(14)	2.966(18)	4.015(18)
I1-I2^{vi}	3.143(14)	3.051(17)	3.223(17)
I1-I3^{v}	4.164(8)	4.164(8)	4.164(8)
I1-I3^{vii}	4.164(8)	4.164(8)	4.164(8)
I2-I2^{iii}	3.443(13)	2.967(16)	4.002(16)
I2-I2^{v}	3.443(13)	2.967(16)	4.002(16)
I2-I3^{iii}	4.148(11)	4.148(11)	4.148(11)
I2-I3^{viii}	4.148(11)	4.148(11)	4.148(11)
I3-I3^{ix}	3.287(3)	3.287(3)	3.287(3)

(i) -x+1,-y+1,-z
(ii) -x+1,-y+1,-z+1
(iii) x,y,z-1
(iv) -x,-y+1,-z+1
(v) x,y,z+1
(vi) x+1,y,z
(vii) x,-y+3/2,z+1
(viii) x,-y+3/2,z-1
(ix) x,-y+3/2,z
(x) x-1,y,z

Table S16: List of angles for commensurate WTe_2I.

	average / °	min / °	max / °
W1^{i}-W1-W1^{ii}	74.97(16)	71.72(19)	82.50(17)
W1^{i}-W1-Te1	58.38(10)	57.09(11)	60.83(11)
W1^{i}-W1-Te1^{i}	58.59(12)	57.18(14)	59.34(15)
W1^{i}-W1-Te1^{ii}	104.87(11)	102.29(11)	109.22(11)
W1^{i}-W1-Te2^{iii}	93.0(2)	91.9(2)	93.50(19)
W1^{i}-W1-Te2	140.47(16)	137.74(16)	142.44(15)
W1^{i}-W1-Te2^{iv}	136.3(3)	133.8(3)	139.1(3)
W1^{i}-W1-Te3^{iii}	87.1(2)	87.1(2)	87.1(2)
W1^{i}-W1-Te3	145.68(10)	145.68(10)	145.68(10)
W1^{i}-W1-Te3^{iv}	138.87(18)	138.87(18)	138.87(18)
W1^{ii}-W1-Te1	57.67(10)	56.70(12)	58.57(10)
W1^{ii}-W1-Te1^{i}	105.25(11)	102.55(10)	109.73(11)
W1^{ii}-W1-Te1^{ii}	58.63(12)	54.50(15)	61.06(13)
W1^{ii}-W1-Te2^{iii}	140.04(16)	138.02(16)	142.81(15)
W1^{ii}-W1-Te2	92.9(2)	91.6(2)	94.6(2)
W1^{ii}-W1-Te2^{iv}	136.6(3)	129.4(3)	141.9(3)
W1^{ii}-W1-Te3^{iii}	145.00(12)	145.00(12)	145.00(12)
W1^{ii}-W1-Te3	82.1(2)	82.1(2)	82.1(2)

W1^{ii}-W1-Te3^{iv}	138.71(19)	138.71(19)	138.71(19)
Te1-W1-Te1^{i}	116.87(16)	114.04(17)	119.9(2)
Te1-W1-Te1^{ii}	116.29(17)	111.2(2)	119.63(17)
Te1-W1-Te2^{iii}	83.75(17)	81.88(17)	85.62(16)
Te1-W1-Te2	83.27(17)	81.75(17)	85.50(16)
Te1-W1-Te2^{iv}	155.39(17)	153.53(17)	157.29(16)
Te1-W1-Te3^{iii}	86.47(12)	86.47(12)	86.47(12)
Te1-W1-Te3	85.13(15)	85.13(15)	85.13(15)
Te1-W1-Te3^{iv}	150.85(9)	150.85(9)	150.85(9)
Te1^{i}-W1-Te1^{ii}	79.83(9)	77.81(9)	83.73(9)
Te1^{i}-W1-Te2^{iii}	100.4(2)	97.8(2)	103.4(3)
Te1^{i}-W1-Te2	158.47(17)	157.59(17)	159.61(17)
Te1^{i}-W1-Te2^{iv}	80.83(18)	78.93(18)	83.49(19)
Te1^{i}-W1-Te3^{iii}	85.48(18)	85.48(18)	85.48(18)
Te1^{i}-W1-Te3	154.93(12)	154.93(12)	154.93(12)
Te1^{i}-W1-Te3^{iv}	85.84(11)	85.84(11)	85.84(11)
Te1^{ii}-W1-Te2^{iii}	158.18(18)	156.56(16)	160.50(18)
Te1^{ii}-W1-Te2	99.9(2)	96.6(2)	103.3(3)
Te1^{ii}-W1-Te2^{iv}	81.40(18)	80.4(2)	83.30(18)
Te1^{ii}-W1-Te3^{iii}	153.84(12)	153.84(12)	153.84(12)
Te1^{ii}-W1-Te3	85.9(2)	85.9(2)	85.9(2)
Te1^{ii}-W1-Te3^{iv}	84.74(10)	84.74(10)	84.74(10)
Te2^{iii}-W1-Te2	75.03(19)	73.37(17)	77.4(2)
Te2^{iii}-W1-Te2^{iv}	78.28(18)	77.24(17)	79.01(17)
Te2^{iii}-W1-Te3	78.46(15)	78.46(15)	78.46(15)
Te2^{iii}-W1-Te3^{iv}	71.84(13)	71.84(13)	71.84(13)
Te2-W1-Te2^{iv}	78.91(18)	77.6(2)	80.1(2)
Te2-W1-Te3^{iii}	80.69(8)	80.69(8)	80.69(8)
Te2-W1-Te3^{iv}	71.95(13)	71.95(13)	71.95(13)
Te2^{iv}-W1-Te3^{iii}	71.85(15)	71.85(15)	71.85(15)
Te2^{iv}-W1-Te3	72.28(16)	72.28(16)	72.28(16)
W1-Te1-W1^{i}	63.04(13)	62.00(16)	64.18(11)
W1-Te1-W1^{ii}	63.70(13)	61.85(13)	68.81(17)
W1^{i}-Te1-W1^{ii}	79.82(17)	76.3(2)	89.14(18)
W1-Te2-W1^{v}	73.77(18)	71.83(16)	75.17(19)
W1-Te2-W1^{iv}	101.63(16)	99.85(10)	103.8(2)
W1^{v}-Te2-W1^{iv}	102.28(16)	100.6(2)	104.6(2)
W1-Te3-W1^{v}	89.8(2)	89.8(2)	89.8(2)
W1-Te3-W1^{iv}	111.06(14)	111.06(14)	111.06(14)
W1-Te3-I3	114.59(12)	114.59(12)	114.59(12)
W1^{v}-Te3-W1^{iv}	110.62(14)	110.62(14)	110.62(14)
W1^{v}-Te3-I3	113.31(12)	113.31(12)	113.31(12)
W1^{iv}-Te3-I3	114.85(10)	114.85(10)	114.85(10)
I1^{iii}-I1-I1^{v}	176.2(4)	170.9(4)	179.9(5)
I1^{iii}-I1-I2	90.7(4)	87.0(4)	96.3(4)
I1^{iii}-I1-I2^{vi}	92.1(4)	83.7(4)	98.3(4)
I1^{iii}-I1-I3^{v}	149.9(2)	149.9(2)	149.9(2)
I1^{iii}-I1-I3^{vii}	149.9(2)	149.9(2)	149.9(2)
I1^{v}-I1-I2	89.7(4)	81.3(3)	98.6(4)
I1^{v}-I1-I2^{vi}	91.9(4)	83.5(4)	96.2(4)
I2-I1-I2^{vi}	169.3(4)	165.3(5)	171.8(4)
I2-I1-I3^{v}	72.03(19)	72.03(19)	72.03(19)
I2-I1-I3^{vii}	72.03(19)	72.03(19)	72.03(19)
I2^{vi}-I1-I3^{v}	100.5(2)	100.5(2)	100.5(2)
I2^{vi}-I1-I3^{vii}	100.5(2)	100.5(2)	100.5(2)
I3^{v}-I1-I3^{vii}	46.49(9)	46.49(9)	46.49(9)
I1^{x}-I2-I1	170.3(4)	166.8(3)	175.2(5)
I1^{x}-I2-I2^{iii}	91.0(4)	82.6(3)	95.9(3)
I1^{x}-I2-I2^{v}	91.7(4)	84.3(4)	95.7(4)
I1^{x}-I2-I3^{iii}	105.3(3)	105.3(3)	105.3(3)
I1^{x}-I2-I3^{viii}	105.3(3)	105.3(3)	105.3(3)
I1-I2-I2^{iii}	89.3(4)	80.4(4)	97.3(3)
I1-I2-I2^{v}	90.2(4)	86.9(4)	96.9(4)

I1-I2-I3^{iii}	70.3(3)	70.3(3)	70.3(3)
I1-I2-I3^{viii}	70.3(3)	70.3(3)	70.3(3)
I2^{iii}-I2-I2^{v}	174.9(5)	168.3(6)	178.7(6)
I2^{v}-I2-I3^{iii}	148.1(2)	148.1(2)	148.1(2)
I2^{v}-I2-I3^{viii}	148.1(2)	148.1(2)	148.1(2)
I3^{iii}-I2-I3^{viii}	46.69(14)	46.69(14)	46.69(14)
Te3-I3-I1^{iii}	113.92(12)	113.92(12)	113.92(12)
Te3-I3-I2^{v}	112.40(13)	112.40(13)	112.40(13)
Te3-I3-I3^{ix}	176.75(11)	176.75(11)	176.75(11)
I1^{iii}-I3-I2^{v}	133.28(11)	133.28(11)	133.28(11)
I1^{iii}-I3-I3^{ix}	66.75(8)	66.75(8)	66.75(8)
I2^{v}-I3-I3^{ix}	66.65(10)	66.65(10)	66.65(10)

(i) -x+1,-y+1,-z
(ii) -x+1,-y+1,-z+1
(iii) x,y,z-1
(iv) -x,-y+1,-z+1
(v) x,y,z+1
(vi) x+1,y,z
(vii) x,-y+3/2,z+1
(viii) x,-y+3/2,z-1
(ix) x,-y+3/2,z
(x) x-1,y,z

Crystallographic details for $WTe_2Br_{0.5}$

Table S17: Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å^2) for $WTe_2Br_{0.5}$.

	x	y	z	Uiso*/Ueq
W1	−0.00516 (15)	0.25	−0.1785 (3)	0.0527 (15)
Te1	−0.07421 (12)	0.25	−0.5896 (5)	0.042 (2)
Te2	0.12012 (14)	0.25	0.0912 (5)	0.039 (2)
Br1	−0.2500	0.25	−0.6083 (13)	0.115 (7)

Table S18: for $WTe_2Br_{0.5}$.

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
W1	0.0192 (14)	0.0821 (16)	0.0568 (14)	0	−0.0072 (17)	0
Te1	0.020 (3)	0.048 (3)	0.0574 (18)	0	0.013 (2)	0
Te2	0.047 (3)	0.044 (3)	0.0274 (17)	0	−0.010 (3)	0
Br1	0.145 (9)	0.036 (5)	0.163 (7)	0	0	0

Table S19: Atomic displacement parameters (Å^2) for $WTe_2Br_{0.5}$.

W1—W1^{i}	3.6773 (1)	Te1—Te2^{vi}	3.735 (4)
W1—W1^{ii}	3.6773 (1)	Te1—Te2^{iii}	3.718 (4)
W1—W1^{iii}	2.909 (2)	Te1—Te2^{vii}	3.735 (4)
W1—W1^{iv}	2.909 (2)	Te1—Te2^{iv}	3.718 (4)
W1—Te1	2.835 (4)	Te1—Br1	2.946 (2)
W1—Te1^{v}	3.884 (4)	Te2—W1	2.699 (4)
W1—Te1^{vi}	2.698 (3)	Te2—W1^{iii}	2.718 (3)
W1—Te1^{vii}	2.698 (3)	Te2—W1^{iv}	2.718 (3)
W1—Te2	2.699 (4)	Te2—Te1^{v}	3.825 (4)
W1—Te2^{iii}	2.718 (3)	Te2—Te1^{vi}	3.735 (4)
W1—Te2^{iv}	2.718 (3)	Te2—Te1^{iii}	3.718 (4)
Te1—W1^{viii}	3.884 (4)	Te2—Te1^{vii}	3.735 (4)
Te1—W1	2.835 (4)	Te2—Te1^{iv}	3.718 (4)
Te1—W1^{vi}	2.698 (3)	Te2—Te2^{i}	3.6773 (1)
Te1—W1^{vii}	2.698 (3)	Te2—Te2^{ii}	3.6773 (1)
Te1—Te1^{i}	3.6773 (1)	Br1—Te1	2.946 (2)
Te1—Te1^{ii}	3.6773 (1)	Br1—Te1^{ix}	2.946 (2)
Te1—Te1^{vi}	3.291 (3)	Br1—Br1^{i}	3.6773 (1)
Te1—Te1^{vii}	3.291 (3)	Br1—Br1^{ii}	3.6773 (1)
Te1—Te2^{viii}	3.825 (4)		

Symmetry codes: (i) *x*, *y*−1, *z*; (ii) *x*, *y*+1, *z*; (iii) −*x*, *y*−1/2, −*z*; (iv) −*x*, *y*+1/2, −*z*; (v) *x*, *y*, *z*+1; (vi) −*x*, *y*−1/2, −*z*−1; (vii) −*x*, *y*+1/2, −*z*−1; (viii) *x*, *y*, *z*−1; (ix) −*x*−1/2, −*y*+1/2, *z*.Table S20: for $WTe_2Br_{0.5}$.

W1^{i}—W1—W1^{ii}	180	W1^{vii}—Te1—Br1	118.07 (13)
W1^{i}—W1—W1^{iii}	50.80 (6)	Te1^{i}—Te1—Te1^{ii}	180
W1^{i}—W1—W1^{iv}	129.20 (6)	Te1^{i}—Te1—Te1^{vi}	56.03 (7)
W1^{i}—W1—Te1	90.00 (10)	Te1^{i}—Te1—Te1^{vii}	123.97 (7)
W1^{i}—W1—Te1^{v}	90.00 (8)	Te1^{i}—Te1—	90.00 (8)
W1^{i}—W1—Te1^{vi}	47.04 (7)	Te1^{i}—Te1—Te2^{vi}	60.51 (9)
W1^{i}—W1—Te1^{vii}	132.96 (7)	Te1^{i}—Te1—Te2^{iii}	60.36 (9)
W1^{i}—W1—Te2	90.00 (10)	Te1^{i}—Te1—Te2^{vii}	119.49 (9)
W1^{i}—W1—Te2^{iii}	47.43 (7)	Te1^{i}—Te1—Te2^{iv}	119.64 (9)
W1^{i}—W1—Te2^{iv}	132.57 (7)	Te1^{i}—Te1—Br1	90.00 (5)
W1^{ii}—W1—W1^{iii}	129.20 (6)	Te1^{ii}—Te1—Te1^{vi}	123.97 (7)

W1^{ii}—W1—W1^{iv}	50.80 (6)
W1^{ii}—W1—Te1	90.00 (10)
W1^{ii}—W1—Te1^{v}	90.00 (8)
W1^{ii}—W1—Te1^{vi}	132.96 (7)
W1^{ii}—W1—Te1^{vii}	47.04 (7)
W1^{ii}—W1—Te2	90.00 (10)
W1^{ii}—W1—Te2^{iii}	132.57 (7)
W1^{ii}—W1—Te2^{iv}	47.43 (7)
W1^{iii}—W1—W1^{iv}	78.40 (6)
W1^{iii}—W1—Te1	136.86 (16)
W1^{iii}—W1—Te1^{vi}	87.61 (13)
W1^{iii}—W1—Te1^{vii}	145.05 (13)
W1^{iii}—W1—Te2	57.84 (10)
W1^{iii}—W1—Te2^{iii}	57.20 (10)
W1^{iii}—W1—Te2^{iv}	108.26 (10)
W1^{iv}—W1—Te1	136.86 (16)
W1^{iv}—W1—Te1^{vi}	145.05 (13)
W1^{iv}—W1—Te1^{vii}	87.61 (13)
W1^{iv}—W1—Te2	57.84 (10)
W1^{iv}—W1—Te2^{iii}	108.26 (10)
W1^{iv}—W1—Te2^{iv}	57.20 (10)
Te1—W1—Te1^{v}	138.61 (18)
Te1—W1—Te1^{vi}	72.95 (12)
Te1—W1—Te1^{vii}	72.95 (12)
Te1—W1—Te2	153.1 (2)
Te1—W1—Te2^{iii}	84.02 (14)
Te1—W1—Te2^{iv}	84.02 (14)
Te1^{v}—W1—Te1^{vi}	131.55 (16)
Te1^{v}—W1—Te1^{vii}	131.55 (16)
Te1^{v}—W1—Te2	68.33 (12)
Te1^{v}—W1—Te2^{iii}	66.18 (11)
Te1^{v}—W1—Te2^{iv}	66.18 (11)
Te1^{vi}—W1—	85.92 (8)
Te1^{vi}—W1—Te2	87.57 (15)
Te1^{vi}—W1—Te2^{iii}	89.85 (13)
Te1^{vi}—W1—Te2^{iv}	156.82 (13)
Te1^{vii}—W1—Te2	87.57 (15)
Te1^{vii}—W1—Te2^{iii}	156.82 (13)
Te1^{vii}—W1—	89.85 (13)
Te2—W1—Te2^{iii}	115.04 (15)
Te2—W1—Te2^{iv}	115.04 (15)
Te2^{iii}—W1—Te2^{iv}	85.13 (8)
W1^{viii}—Te1—W1	138.61 (13)
W1^{viii}—Te1—W1^{vi}	48.45 (9)
W1^{viii}—Te1—	48.45 (9)
W1^{viii}—Te1—Te1^{i}	90.00 (8)
W1^{viii}—Te1—Te1^{ii}	90.00 (8)
W1^{viii}—Te1—	95.88 (11)
W1^{viii}—Te1—	95.88 (11)
W1^{viii}—Te1—	150.16 (13)
W1^{viii}—Te1—	150.16 (13)
W1^{viii}—Te1—Br1	105.03 (18)
W1—Te1—W1^{vi}	107.05 (13)
W1—Te1—W1^{vii}	107.05 (13)
W1—Te1—Te1^{i}	90.00 (10)
W1—Te1—Te1^{ii}	90.00 (10)
W1—Te1—Te1^{vi}	51.61 (10)
W1—Te1—Te1^{vii}	51.61 (10)
W1—Te1—Te2^{viii}	97.63 (14)
W1—Te1—Te2^{vi}	148.89 (16)
W1—Te1—Te2^{iii}	46.65 (10)
W1—Te1—Te2^{vii}	148.89 (16)
W1—Te1—Te2^{iv}	46.65 (10)
Te1^{ii}—Te1—	56.03 (7)
Te1^{ii}—Te1—	90.00 (8)
Te1^{ii}—Te1—Te2^{vi}	119.49 (9)
Te1^{ii}—Te1—Te2^{iii}	119.64 (9)
Te1^{ii}—Te1—	60.51 (9)
Te1^{ii}—Te1—Te2^{iv}	60.36 (9)
Te1^{ii}—Te1—Br1	90.00 (5)
Te1^{vi}—Te1—	67.93 (7)
Te1^{vi}—Te1—	62.46 (10)
Te1^{vi}—Te1—	99.81 (13)
Te1^{vi}—Te1—	65.82 (10)
Te1^{vi}—Te1—	136.09 (13)
Te1^{vi}—Te1—	98.22 (10)
Te1^{vi}—Te1—Br1	140.20 (11)
Te1^{vii}—Te1—	62.46 (10)
Te1^{vii}—Te1—	136.09 (13)
Te1^{vii}—Te1—	98.22 (10)
Te1^{vii}—Te1—	99.81 (13)
Te1^{vii}—Te1—	65.82 (10)
Te1^{vii}—Te1—Br1	140.20 (11)
Te2^{viii}—Te1—	74.38 (10)
Te2^{viii}—Te1—	128.28 (14)
Te2^{viii}—Te1—	74.38 (10)
Te2^{viii}—Te1—	128.28 (14)
Te2^{viii}—Te1—Br1	146.01 (13)
Te2^{vi}—Te1—	115.33 (15)
Te2^{vi}—Te1—	58.99 (9)
Te2^{vi}—Te1—	156.19 (15)
Te2^{vi}—Te1—Br1	76.14 (16)
Te2^{iii}—Te1—	156.19 (15)
Te2^{iii}—Te1—	59.28 (9)
Te2^{iii}—Te1—Br1	80.04 (17)
Te2^{vii}—Te1—	115.33 (15)
Te2^{vii}—Te1—Br1	76.14 (16)
Te2^{iv}—Te1—Br1	80.04 (17)
W1—Te2—W1^{iii}	64.96 (11)
W1—Te2—W1^{iv}	64.96 (11)
W1—Te2—Te1^{v}	70.69 (12)
W1—Te2—Te1^{vi}	46.20 (11)
W1—Te2—Te1^{iii}	111.74 (15)
W1—Te2—Te1^{vii}	46.20 (11)
W1—Te2—Te1^{iv}	111.74 (15)
W1—Te2—Te2^{i}	90.00 (10)
W1—Te2—Te2^{ii}	90.00 (10)
W1^{iii}—Te2—W1^{iv}	85.13 (8)
W1^{iii}—Te2—Te1^{vi}	72.07 (12)
W1^{iii}—Te2—Te1^{iii}	49.33 (10)
W1^{iii}—Te2—Te1^{vii}	110.99 (12)
W1^{iii}—Te2—Te1^{iv}	91.00 (10)
W1^{iii}—Te2—Te2^{i}	47.43 (7)
W1^{iii}—Te2—Te2^{ii}	132.57 (7)
W1^{iv}—Te2—Te1^{vi}	110.99 (12)
W1^{iv}—Te2—Te1^{iii}	91.00 (10)
W1^{iv}—Te2—	72.07 (12)
W1^{iv}—Te2—Te1^{iv}	49.33 (10)
W1^{iv}—Te2—Te2^{i}	132.57 (7)
W1^{iv}—Te2—Te2^{ii}	47.43 (7)
Te1^{v}—Te2—Te1^{vi}	105.62 (13)
Te1^{v}—Te2—Te1^{iii}	51.72 (9)
Te1^{v}—Te2—	105.62 (13)
Te1^{v}—Te2—Te1^{iv}	51.72 (9)
Te1^{v}—Te2—Te2^{i}	90.00 (8)
Te1^{v}—Te2—Te2^{ii}	90.00 (8)

W1—Te1—Br1	116.36 (19)	Te1^{vi}—Te2—	115.33 (15)
W1^{vi}—Te1—W1^{vii}	85.92 (8)	Te1^{vi}—Te2—	58.99 (9)
W1^{vi}—Te1—Te1^{i}	47.04 (7)	Te1^{vi}—Te2—	156.19 (15)
W1^{vi}—Te1—Te1^{ii}	132.96 (7)	Te1^{vi}—Te2—Te2^{i}	60.51 (9)
W1^{vi}—Te1—Te1^{vi}	55.45 (10)	Te1^{vi}—Te2—Te2^{ii}	119.49 (9)
W1^{vi}—Te1—	101.20 (10)	Te1^{iii}—Te2—	156.19 (15)
W1^{vi}—Te1—	45.29 (9)	Te1^{iii}—Te2—	59.28 (9)
W1^{vi}—Te1—Te2^{vi}	46.22 (10)	Te1^{iii}—Te2—Te2^{i}	60.36 (9)
W1^{vi}—Te1—Te2^{iii}	102.81 (14)	Te1^{iii}—Te2—Te2^{ii}	119.64 (9)
W1^{vi}—Te1—	88.81 (10)	Te1^{vii}—Te2—	115.33 (15)
W1^{vi}—Te1—Te2^{iv}	153.61 (14)	Te1^{vii}—Te2—Te2^{i}	119.49 (9)
W1^{vi}—Te1—Br1	118.07 (13)	Te1^{vii}—Te2—	60.51 (9)
W1^{vii}—Te1—Te1^{i}	132.96 (7)	Te1^{iv}—Te2—Te2^{i}	119.64 (9)
W1^{vii}—Te1—Te1^{ii}	47.04 (7)	Te1^{iv}—Te2—Te2^{ii}	60.36 (9)
W1^{vii}—Te1—	101.20 (10)	Te2^{i}—Te2—Te2^{ii}	180
W1^{vii}—Te1—	55.45 (10)	Te1—Br1—Te1^{ix}	175.42 (13)
W1^{vii}—Te1—	45.29 (9)	Te1—Br1—Br1^{i}	90.00 (5)
W1^{vii}—Te1—	88.81 (10)	Te1—Br1—Br1^{ii}	90.00 (5)
W1^{vii}—Te1—Te2^{iii}	153.61 (14)	Te1^{ix}—Br1—Br1^{i}	90.00 (5)
W1^{vii}—Te1—	46.22 (10)	Te1^{ix}—Br1—Br1^{ii}	90.00 (5)
W1^{vii}—Te1—	102.81 (14)	Br1^{i}—Br1—Br1^{ii}	180

Symmetry codes: (i) *x*, *y*−1, *z*; (ii) *x*, *y*+1, *z*; (iii) −*x*, *y*−1/2, −*z*; (iv) −*x*, *y*+1/2, −*z*; (v) *x*, *y*, *z*+1; (vi) −*x*, *y*−1/2, −*z*−1; (vii) −*x*, *y*+1/2, −*z*−1; (viii) *x*, *y*, *z*−1; (ix) −*x*−1/2, −*y*+1/2, *z*.

Crystallographic details for $WTe_2Br_{1.25}$

Table S 21: Fractional Atomic Coordinates (×10^4) and Equivalent Isotropic Displacement Parameters (Å^2×10^3) for **$WTe_2Br_{1.25}$**. U_{eq} is defined as 1/3 of the trace of the orthogonalised U_{ij}.

Atom	x	y	z	U_{eq}
W4	5000	3794(2)	723(8)	55(2)
W8	5000	3803(2)	5768(8)	57(2)
W6	1607(5)	3809.8(15)	5719(5)	56(2)
W3	3417(5)	3849.9(16)	2475(5)	58(2)
W2	1886(4)	3782.2(15)	703(5)	57(2)
W5	0	3832(2)	7490(7)	55(2)
W7	3155(5)	3850.8(15)	7480(5)	58(2)
W1	0	3858(2)	2403(8)	64(3)
Te1	0	3357(3)	1159(9)	53(3)
Te3	3411(6)	3323(2)	1265(6)	52(2)
Te13	0	4055(3)	9515(10)	55(3)
Te12	5000	3538(3)	3811(9)	57(3)
Te15	3329(6)	4157(2)	-525(7)	55(2)
Te14	1712(6)	3461(2)	8708(7)	61(3)
Te10	1651(6)	3557(2)	3727(7)	60(3)
Te8	5000	4294(3)	7073(10)	55(3)
Te6	1594(7)	4313.7(17)	7032(7)	52(2)
Te16	5000	3555(3)	8679(10)	60(3)
Te9	0	4186(3)	4440(11)	57(3)
Te11	3342(6)	4177.7(19)	4490(7)	55(2)
Te5	0	3347(3)	6167(10)	59(3)
Te7	3283(7)	3357(2)	6187(7)	58(2)
Te4	5000	4313(3)	1945(12)	63(3)
Te2	1726(7)	4291(3)	1916(8)	71(3)
Br5	5000	2961(5)	3756(16)	63(5)
Br6	5000	2969(5)	8534(18)	64(5)
Br3	1794(15)	2597(4)	6973(16)	78(4)
Br4	1674(12)	2984(4)	3571(14)	71(4)
Br7	0	4636(6)	9607(19)	71(6)
Br8	3170(20)	5000	10520(20)	74(6)
Br1	5000	2249(6)	3950(20)	74(6)
Br9	3160(20)	5000	8530(20)	75(6)
Br10	0	5000	5910(60)	190(40)
Br2	3175(12)	2438(5)	5615(18)	86(5)
Br12	2920(40)	5000	6020(80)	290(50)
Br13	3020(60)	5000	2760(100)	350(80)
Br11	0	5000	3080(70)	240(60)

Table S22: Anisotropic Displacement Parameters (×10[4]) for **$WTe_2Br_{1.25}$**. The anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2} \times U_{11} + ... + 2hka^* \times b^* \times U_{12}]$

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
W4	31(3)	80(5)	55(5)	7(4)	0	0
W8	37(4)	79(5)	53(5)	-3(4)	0	0
W6	34(3)	77(4)	55(4)	-5(3)	1(3)	-1(2)
W3	32(3)	91(4)	51(3)	0(3)	-1(3)	0(2)
W2	31(3)	81(4)	60(4)	5(3)	-1(3)	0(2)
W5	35(4)	76(5)	55(5)	0(4)	0	0
W7	42(3)	80(4)	52(4)	1(3)	-2(3)	0(2)
W1	69(6)	70(5)	55(6)	1(4)	0	0
Te1	26(4)	76(7)	55(7)	-5(5)	0	0
Te3	31(3)	81(5)	45(4)	-2(3)	1(3)	-1(3)
Te13	23(4)	95(8)	49(6)	4(6)	0	0
Te12	24(4)	109(9)	37(6)	-5(6)	0	0
Te15	33(3)	85(5)	46(4)	0(4)	1(3)	2(3)
Te14	28(3)	104(6)	49(5)	-4(5)	2(3)	-1(3)
Te10	25(3)	100(6)	55(5)	-7(4)	1(3)	-2(3)
Te8	35(5)	73(7)	57(7)	-3(5)	0	0
Te6	43(4)	55(4)	59(5)	-5(3)	-2(4)	-1(3)
Te16	33(5)	93(8)	56(7)	-1(6)	0	0
Te9	36(5)	77(7)	58(7)	0(6)	0	0
Te11	32(3)	76(5)	57(4)	-2(4)	0(3)	0(3)
Te5	29(5)	95(9)	52(7)	-1(6)	0	0
Te7	31(3)	84(5)	58(5)	4(4)	1(3)	0(3)
Te4	24(4)	91(8)	74(8)	5(7)	0	0
Te2	20(3)	126(8)	66(6)	-2(5)	-4(3)	3(4)
Br5	20(6)	118(15)	51(11)	3(10)	0	0
Br6	60(10)	65(11)	67(13)	-8(9)	0	0
Br3	57(8)	84(9)	92(11)	-2(8)	21(8)	4(7)
Br4	41(6)	87(9)	86(11)	8(8)	1(7)	1(6)
Br7	29(7)	124(18)	58(12)	-3(11)	0	0
Br8	64(11)	65(11)	94(16)	0	10(12)	0
Br1	41(9)	102(15)	78(14)	0(12)	0	0
Br9	54(10)	92(14)	79(15)	0	13(10)	0
Br10	370(130)	60(20)	150(60)	0	0	0
Br2	36(6)	118(13)	104(13)	27(11)	9(8)	2(6)
Br12	60(20)	450(130)	370(110)	0	110(40)	0
Br13	190(50)	64(18)	800(200)	0	-300(90)	0
Br11	500(200)	50(20)	170(70)	0	0	0

Table S23: Bond Lengths in Å for $\mathbf{WTe_2Br_{1.25}}$.

Atom	Atom	Length/Å
W4	W3	2.789(9)
W4	W3[1]	2.789(9)
W4	Te3	2.725(11)
W4	Te3[1]	2.725(11)
W4	Te15	2.843(11)
W4	Te15[1]	2.843(11)
W4	Te16[2]	2.778(16)
W4	Te4	2.716(17)
W8	W7[1]	2.925(9)
W8	W7	2.925(9)
W8	Te12	2.723(15)
W8	Te8	2.680(15)
W8	Te11	2.883(11)
W8	Te11[1]	2.883(11)
W8	Te7	2.701(11)
W8	Te7[1]	2.701(11)
W6	W5	2.815(9)
W6	W7	2.772(9)
W6	Te10	2.741(11)
W6	Te6	2.730(10)
W6	Te9	2.852(12)
W6	Te11	2.883(11)
W6	Te5	2.682(13)
W6	Te7	2.706(10)
W3	W2	2.781(8)
W3	Te3	2.736(11)
W3	Te12	2.735(12)
W3	Te10	2.758(10)
W3	Te11	2.910(11)
W3	Te4	2.692(13)
W3	Te2	2.706(12)
W2	W1	2.955(9)
W2	Te1	2.775(11)
W2	Te3	2.653(10)
W2	Te13[2]	2.763(11)
W2	Te15	2.713(10)
W2	Te14[2]	2.879(12)
W2	Te2	2.676(13)
W5	Te13	2.731(16)
W5	Te14[3]	2.866(11)
W5	Te14	2.866(11)
W5	Te6	2.738(10)
W5	Te6[3]	2.738(10)
W5	Te5	2.672(16)
W7	Te15[4]	2.849(11)
W7	Te14	2.750(11)
W7	Te8	2.782(11)
W7	Te6	2.653(10)
W7	Te16	2.783(11)
W7	Te7	2.685(12)
W1	Te1	2.668(15)
W1	Te10	2.748(12)
W1	Te10[3]	2.748(12)
W1	Te9	2.933(17)
W1	Te2[3]	2.685(12)
W1	Te2	2.685(12)
Te13	Br7	2.50(3)
Te12	Br5	2.48(3)
Te10	Br4	2.473(19)
Te16	Br6	2.53(2)
Br3	Br2	2.36(2)
Br8	Br9	2.51(3)

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[1]1-x,+y,+z; [2]+x,+y,-1+z; [3]-x,+y,+z; [4]+x,+y,1+z

Table S 24: Bond Angles in ° for $\mathbf{WTe_2Br_{1.25}}$.

Atom	Atom	Atom	Angle/°
W3[1]	W4	W3	74.2(3)
W3[1]	W4	Te15	140.2(4)
W3	W4	Te15[1]	140.2(4)
W3[1]	W4	Te15[1]	90.9(2)
W3	W4	Te15	90.9(2)
Te3[1]	W4	W3[1]	59.5(2)
Te3	W4	W3	59.5(2)
Te3	W4	W3[1]	103.8(4)
Te3[1]	W4	W3	103.8(4)
Te3[1]	W4	Te3	76.6(4)
Te3[1]	W4	Te15	159.3(5)
Te3	W4	Te15	99.3(2)
Te3	W4	Te15[1]	159.3(5)
Te3[1]	W4	Te15[1]	99.3(2)
Te3	W4	Te16[2]	87.6(4)
Te3[1]	W4	Te16[2]	87.6(4)
Te15[1]	W4	Te15	77.3(4)
Te16[2]	W4	W3[1]	140.3(2)
Te16[2]	W4	W3	140.3(2)
Te16[2]	W4	Te15	71.8(4)
Te16[2]	W4	Te15[1]	71.8(4)
Te4	W4	W3	58.5(3)
Te4	W4	W3[1]	58.5(3)
Te4	W4	Te3[1]	118.0(4)
Te4	W4	Te3	118.0(4)
Te4	W4	Te15	82.1(4)
Te4	W4	Te15[1]	82.1(4)
Te4	W4	Te16[2]	146.3(6)
W7	W8	W7[1]	84.1(3)
Te12	W8	W7[1]	134.5(2)
Te12	W8	W7	134.5(2)
Te12	W8	Te11	74.1(4)
Te12	W8	Te11[1]	74.1(4)
Te8	W8	W7[1]	59.3(3)
Te8	W8	W7	59.3(3)
Te8	W8	Te12	152.7(6)
Te8	W8	Te11[1]	84.4(4)
Te8	W8	Te11	84.4(4)

Atom	Atom	Atom	Angle/°
Te8	W8	Te7	116.1(4)
Te8	W8	Te7[1]	116.1(4)
Te11[1]	W8	W7[1]	88.0(2)
Te11	W8	W7	88.0(2)
Te11[1]	W8	W7	141.6(4)
Te11	W8	W7[1]	141.6(4)
Te11	W8	Te11[1]	75.3(4)
Te7	W8	W7[1]	111.0(4)
Te7	W8	W7	56.8(3)
Te7[1]	W8	W7	111.0(4)
Te7[1]	W8	W7[1]	56.8(3)
Te7[1]	W8	Te12	83.1(4)
Te7	W8	Te12	83.1(4)
Te7	W8	Te11	95.4(3)
Te7	W8	Te11[1]	156.9(4)
Te7[1]	W8	Te11[1]	95.5(3)
Te7[1]	W8	Te11	156.9(4)
Te7	W8	Te7[1]	84.9(5)
W5	W6	Te9	93.9(3)
W5	W6	Te11	142.8(3)
W7	W6	W5	73.7(2)
W7	W6	Te9	140.7(4)
W7	W6	Te11	91.0(3)
Te10	W6	W5	138.9(3)
Te10	W6	W7	138.7(3)
Te10	W6	Te9	73.5(4)
Te10	W6	Te11	73.3(3)
Te6	W6	W5	59.2(3)
Te6	W6	W7	57.7(2)
Te6	W6	Te10	150.8(4)
Te6	W6	Te9	83.7(3)
Te6	W6	Te11	83.9(3)
Te9	W6	Te11	76.5(3)
Te5	W6	W5	58.1(3)
Te5	W6	W7	104.8(3)
Te5	W6	Te10	84.8(4)
Te5	W6	Te6	117.3(4)
Te5	W6	Te9	99.2(3)
Te5	W6	Te11	158.1(4)
Te5	W6	Te7	80.7(3)
Te7	W6	W5	104.5(3)
Te7	W6	W7	58.7(3)
Te7	W6	Te10	84.4(3)
Te7	W6	Te6	116.3(3)
Te7	W6	Te9	157.8(4)
Te7	W6	Te11	95.3(3)
W4	W3	Te11	138.8(3)
W2	W3	W4	72.8(2)
W2	W3	Te11	137.6(3)
Te3	W3	W4	59.1(3)
Te3	W3	W2	57.5(2)
Te3	W3	Te10	86.5(3)
Te3	W3	Te11	152.9(4)
Te12	W3	W4	94.4(3)
Te12	W3	W2	143.5(4)
Te12	W3	Te3	86.5(4)
Te12	W3	Te10	80.8(3)
Te12	W3	Te11	73.5(3)
Te10	W3	W4	145.6(4)
Te10	W3	W2	90.9(3)
Te10	W3	Te11	72.6(3)
Te4	W3	W4	59.4(4)

Atom	Atom	Atom	Angle/°
Te4	W3	W2	104.0(4)
Te4	W3	Te3	118.5(4)
Te4	W3	Te12	97.6(4)
Te4	W3	Te10	154.9(5)
Te4	W3	Te11	82.9(4)
Te4	W3	Te2	80.3(3)
Te2	W3	W4	104.7(3)
Te2	W3	W2	58.4(3)
Te2	W3	Te3	115.7(4)
Te2	W3	Te12	156.0(4)
Te2	W3	Te10	91.1(3)
Te2	W3	Te11	82.5(3)
W3	W2	W1	78.5(2)
W3	W2	Te14[2]	142.4(3)
Te1	W2	W3	108.9(3)
Te1	W2	W1	55.4(3)
Te1	W2	Te14[2]	79.6(3)
Te3	W2	W3	60.4(3)
Te3	W2	W1	107.5(3)
Te3	W2	Te1	83.9(3)
Te3	W2	Te13[2]	154.7(4)
Te3	W2	Te15	104.6(3)
Te3	W2	Te14[2]	85.2(3)
Te3	W2	Te2	119.7(4)
Te13[2]	W2	W3	144.7(4)
Te13[2]	W2	W1	81.7(3)
Te13[2]	W2	Te1	82.5(3)
Te13[2]	W2	Te14[2]	71.5(4)
Te15	W2	W3	93.9(3)
Te15	W2	W1	137.1(4)
Te15	W2	Te1	156.8(4)
Te15	W2	Te13[2]	81.2(3)
Te15	W2	Te14[2]	79.7(3)
Te14[2]	W2	W1	130.2(3)
Te2	W2	W3	59.4(3)
Te2	W2	W1	56.7(3)
Te2	W2	Te1	112.0(4)
Te2	W2	Te13[2]	85.3(4)
Te2	W2	Te15	82.9(3)
Te2	W2	Te14[2]	152.7(4)
W6[3]	W5	W6	74.6(3)
W6	W5	Te14[3]	142.4(4)
W6[3]	W5	Te14[3]	91.3(2)
W6	W5	Te14	91.3(2)
W6[3]	W5	Te14	142.4(4)
Te13	W5	W6[3]	139.1(2)
Te13	W5	W6	139.1(2)
Te13	W5	Te14	72.1(4)
Te13	W5	Te14[3]	72.1(4)
Te13	W5	Te6	86.1(4)
Te13	W5	Te6[3]	86.1(4)
Te14[3]	W5	Te14	78.8(4)
Te6[3]	W5	W6	103.4(4)
Te6	W5	W6	58.9(3)
Te6[3]	W5	W6[3]	58.9(3)
Te6	W5	W6[3]	103.4(4)
Te6[3]	W5	Te14[3]	98.2(3)
Te6	W5	Te14[3]	158.0(5)
Te6[3]	W5	Te14	158.0(5)
Te6	W5	Te14	98.2(3)
Te6	W5	Te6[3]	76.4(4)
Te5	W5	W6	58.4(3)

Atom	Atom	Atom	Angle/°
Te5	W5	W6^{3}	58.4(3)
Te5	W5	Te13	149.2(6)
Te5	W5	Te14^{3}	84.3(4)
Te5	W5	Te14	84.3(4)
Te5	W5	Te6^{3}	117.3(4)
Te5	W5	Te6	117.3(4)
W6	W7	W8	78.5(2)
W6	W7	Te15^{4}	141.0(3)
W6	W7	Te8	108.2(3)
W6	W7	Te16	145.6(4)
Te15^{4}	W7	W8	130.0(3)
Te14	W7	W8	138.3(4)
Te14	W7	W6	94.7(3)
Te14	W7	Te15^{4}	79.6(3)
Te14	W7	Te8	156.2(4)
Te14	W7	Te16	78.9(3)
Te8	W7	W8	55.9(3)
Te8	W7	Te15^{4}	78.5(3)
Te8	W7	Te16	85.3(3)
Te6	W7	W8	108.3(3)
Te6	W7	W6	60.4(2)
Te6	W7	Te15^{4}	83.2(3)
Te6	W7	Te14	103.3(3)
Te6	W7	Te8	83.5(3)
Te6	W7	Te16	154.0(4)
Te6	W7	Te7	119.8(3)
Te16	W7	W8	84.2(3)
Te16	W7	Te15^{4}	71.6(3)
Te7	W7	W8	57.4(3)
Te7	W7	W6	59.4(2)
Te7	W7	Te15^{4}	154.3(4)
Te7	W7	Te14	83.6(3)
Te7	W7	Te8	113.3(4)
Te7	W7	Te16	86.2(4)
W2^{3}	W1	W2	85.4(3)
Te1	W1	W2^{3}	58.9(3)
Te1	W1	W2	58.9(3)
Te1	W1	Te10	88.7(4)
Te1	W1	Te10^{3}	88.7(4)
Te1	W1	Te9	154.8(6)
Te1	W1	Te2^{3}	115.2(4)
Te1	W1	Te2	115.2(4)
Te10	W1	W2^{3}	145.4(4)
Te10	W1	W2	87.6(2)
Te10^{3}	W1	W2	145.4(4)
Te10^{3}	W1	W2^{3}	87.6(2)
Te10^{3}	W1	Te10	79.3(4)
Te10^{3}	W1	Te9	72.1(3)
Te10	W1	Te9	72.1(3)
Te9	W1	W2	133.6(2)
Te9	W1	W2^{3}	133.6(2)
Te2^{3}	W1	W2^{3}	56.4(3)
Te2	W1	W2^{3}	111.9(4)
Te2	W1	W2	56.4(3)
Te2^{3}	W1	W2	111.9(4)
Te2^{3}	W1	Te10^{3}	91.8(3)
Te2	W1	Te10^{3}	154.5(5)
Te2	W1	Te10	91.8(3)
Te2^{3}	W1	Te10	154.5(5)
Te2	W1	Te9	82.4(4)
Te2^{3}	W1	Te9	82.4(4)
Te2	W1	Te2^{3}	86.1(5)

Atom	Atom	Atom	Angle/°
W2	Te1	W2^{3}	92.4(4)
W1	Te1	W2	65.7(3)
W1	Te1	W2^{3}	65.7(3)
W4	Te3	W3	61.4(3)
W2	Te3	W4	75.9(3)
W2	Te3	W3	62.1(3)
W2^{4}	Te13	W2^{5}	92.9(4)
W5	Te13	W2^{5}	111.1(4)
W5	Te13	W2^{4}	111.1(4)
Br7	Te13	W2^{5}	113.5(5)
Br7	Te13	W2^{4}	113.5(5)
Br7	Te13	W5	113.2(7)
W8	Te12	W3	110.7(5)
W8	Te12	W3^{1}	110.7(5)
W3	Te12	W3^{1}	75.9(4)
Br5	Te12	W8	116.4(7)
Br5	Te12	W3^{1}	118.3(5)
Br5	Te12	W3	118.3(5)
W4	Te15	W7^{2}	106.0(4)
W2	Te15	W4	73.0(3)
W2	Te15	W7^{2}	101.1(3)
W5	Te14	W2^{4}	104.1(4)
W7	Te14	W2^{4}	99.5(3)
W7	Te14	W5	73.3(3)
W6	Te10	W3	110.9(3)
W6	Te10	W1	111.1(4)
W1	Te10	W3	82.5(3)
Br4	Te10	W6	118.0(6)
Br4	Te10	W3	113.8(5)
Br4	Te10	W1	115.3(5)
W8	Te8	W7^{1}	64.7(3)
W8	Te8	W7	64.7(3)
W7^{1}	Te8	W7	89.5(4)
W6	Te6	W5	62.0(3)
W7	Te6	W6	62.0(2)
W7	Te6	W5	76.9(3)
W4^{4}	Te16	W7^{1}	109.7(4)
W4^{4}	Te16	W7	109.7(4)
W7	Te16	W7^{1}	89.5(5)
Br6	Te16	W4^{4}	115.8(7)
Br6	Te16	W7	114.6(5)
Br6	Te16	W7^{1}	114.6(5)
W6	Te9	W6^{3}	73.5(4)
W6	Te9	W1	102.9(4)
W6^{3}	Te9	W1	102.9(4)
W8	Te11	W3	101.6(3)
W6	Te11	W8	77.4(3)
W6	Te11	W3	102.8(3)
W6^{3}	Te5	W6	79.0(5)
W5	Te5	W6^{3}	63.4(4)
W5	Te5	W6	63.4(4)
W8	Te7	W6	83.6(3)
W7	Te7	W8	65.8(3)
W7	Te7	W6	61.9(3)
W3	Te4	W4	62.1(3)
W3^{1}	Te4	W4	62.1(3)
W3^{1}	Te4	W3	77.3(5)
W2	Te2	W3	62.2(3)
W2	Te2	W1	66.9(3)
W1	Te2	W3	84.7(4)

^{1}1-x,+y,+z; ^{2}+x,+y,-1+z; ^{3}-x,+y,+z; ^{4}+x,+y,1+z; ^{5}-x,+y,1+z