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The Crystal Structures and Powder Diffraction Patterns of the Uranium Tellurides: A Critical Review

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Abstract

A critical review of all of the reported structures and powder diffraction patterns in the uranium telluride system has been undertaken.

1. Structures that are correct:

- Cubic - UTe : no experimental pattern exists. Retain calculated 15-865.
- Cubic - U_3Te_4 : retain the poor quality 12-610 but adopt the pattern calculated here.
- Cubic U_2Te_3 : no experimental pattern exists. Adopt pattern calculated here.
- Orthorhombic UTe_2 : Adopt the new pattern of Boehme et al.
- Monoclinic αUTe_3 : Adopt the new pattern of Boehme et al.
- Orthorhombic βUTe_3 : Adopt pattern calculated here.
- Orthorhombic UTe_5 : Adopt the new pattern of Boehme et al.

2. Structures in need of refinement:

- Orthorhombic U_2Te_3 : Adopt pattern calculated here over 34-807.
- Hexagonal U_7Te_{12} : Adopt pattern calculated here but retain 24-1368.

- Orthorhombic $\text{UTe}_{1.78}$: Adopt pattern calculated here and retain our modified 21-1404 reported for U_4Te_7 .
- Orthorhombic $\text{UTe}_{2.5}$: Adopt pattern calculated here.
- Orthorhombic $\text{UTe}_{3.4}$: Accept recent pattern of Boehme et al.

3. Phases for which no structures or reliable patterns exist:

- Orthorhombic U_3Te_4 : no published pattern.
- Tetragonal U_3Te_5 : three patterns 21-1407, 34-766 and 34-896 exist but all are of very poor quality.

4. Phases which probably do not exist:

- Tetragonal $\text{UTe}_{1.78}$
- Tetragonal UTe_2
- Cubic UTe_2
- U_3Te_7 (21-1402)
- U_3Te_8 (21-1406)

1 Introduction

The many allowed oxidation states of the actinide metals make the phase diagrams of their Chalcogenide compounds among the most complex known. Researchers have long been plagued with what appeared to be mixtures of an endless series of phases in these systems. Many of the phases have been poorly characterized using powder diffraction patterns which were either nonexistent, incorrect or incomplete. To assess this problem, we have undertaken a critical review of all of the reported structures and powder diffraction patterns in the most complicated of the systems, the uranium tellurides. The phase diagram for this system continues to change with the newest phase reported as recently as 1989[22]. Figure 1 shows the currently understood phase diagram[9] as updated by this study and illustrates the number of phases which have been described. An extremely valuable structural survey of this system is contained in the thermodynamic summary of F. Grønvold, J. Drowart and E. F. Westrum[13]. We will not repeat all of the references given there, but will concentrate on those most pertinent to our goal of establishing a set of consistent powder diffraction standards and confirming the various proposed structural models.

The paper will be divided into sections treating every reported phase in the U-Te system, including reports which we conclude to be erroneous.

Figure 1: Phase diagram for the tellurium uranium system.

2 Reported Phases in the U-Te System

The principal tool in evaluating the proposed structural models and establishing powder diffraction standards will be the calculated powder diffraction pattern as computed using POWD10[26]. Calculation of the powder diffraction pattern simultaneously evaluates the structural model and the experimental powder diffraction pattern. Only the two most recent structural reports in this system have refined thermal motion parameters for the U and Te atoms[22, 21]. In both studies an isotropic B of $1.0 \text{ \AA}^2$ represents the motion of the uranium well. The tellurium has an average B of about $1.3 \text{ \AA}^2$ in the UTe_5 structure with one particularly anomalous value[21]. In the $\beta\text{-UTe}_3$ structure, the three Te atoms each have a value of B near $.5 \text{ \AA}^2$ [22].

With only two structure determinations available for which B's have been determined, it is difficult to choose representative values to be used in the computations. We have assumed that the βUTe_3 values of $1.0 \text{ \AA}^2$ for uranium and $0.5 \text{ \AA}^2$ for Te are the most representative and have used these values in all our computations except for the UTe_5 and $\beta\text{-UTe}_3$ structures where the published values are used. Anomalous dispersion corrections were applied to all atoms in the computations. A second essential tool in this investigation was the Crystal Data data base as published by the International Centre for Diffraction Data[30]. This, along with the NBS*LATTICE program of Himes and Mighell[19], proved invaluable in assessing isostructural models based on unit cell information.

Table 1 gives the metric information for the cells of the various U-Te phases. In addition, the computed values for the density, linear absorption coefficient for Cu K_α radiation, and the computed value for the reference Intensity Ratio I/I_c are given. Table 3 gives the structural parameters used to obtain the calculated powder diffraction patterns. The occupancy values are as required by program POWD10, namely they are the fraction of the maximum occupancy allowed for the space group. They are followed by the Wykoff site notation .

Phase	Space Group	a (Å)	b (Å)	c (Å)	α	β	γ	Z
UTe[10]	Fm3m	6.160						4
U ₃ Te ₄ [18]	I43d	9.442[12]						3
U ₂ Te ₃ [18]	I43d	9.390[12]						3
U ₂ Te ₃ [1]	Pnma	12.32[34]	4.45	11.83				4
U ₇ Te ₁₂ [4]	P6 ₃ /m	12.309		4.242				1
UTe _{1.78} [16]	Immm	4.162[3]	6.124	13.958				4
UTe ₂ [16]	Immm	4.16170	6.1276	13.9650				4
α UTe ₃ [29]	P2 ₁ /m	6.090[3]	4.226	10.302		98		12
β UTe ₃ [22]	Cmcm	4.338	24.743	4.338				4
UTe ₅ [21]	Pnma	17.9150	10.4070	4.2200				4

Table 1: Space group and unit cells for the U-Te phases.

Phase	ρ_{obs}	ρ_{cal}	μ	I/I_c
UTe	10.37[8]	10.371	2053	21.142
U ₃ Te ₄ – <i>cubic</i>	9.46[17]	9.660	1997	15.70
U ₂ Te ₃ – <i>cubic</i>	9.02[17]	9.184	1933	14.36
U ₂ Te ₃ – <i>orthorhombic</i>		8.794	1851	5.04
U ₇ Te ₁₂		9.54	2048	17.70
UTe _{1.78}		9.68	1875	9.22
UTe ₂		9.20	2021	9.87
α UTe ₃		7.85	1826	9.78
β UTe ₃		8.86	2059	6.57
UTe ₅		7.39	1826	3.97

Table 2: Physical constants for the U-Te phases.

Phase	Atom	x	y	z	Occupancy
UTe[10]	U	0.000000	0.000000	0.000000	.0208(100% 4a)
Cubic	TE	0.500000	0.500000	0.500000	.0208 (100% 4b)
U ₃ Te ₄ [18]	U	0.375000	0.000000	0.250000	0.25 (100% 12a)
Cubic	Te	0.083330	0.083330	0.083330	0.3333 (100% 16c)
U ₂ Te ₃ [18]	U	0.375000	0.000000	0.250000	0.2222 (88.9% 12a)
Cubic	Te	0.083330	0.083330	0.083330	0.3333 (100% 16c)
U ₂ Te ₃ [1]	U1	0.029300	0.250000	0.326100	.50 (100% 4c)
Orthorhombic	U2	0.149500	0.750000	0.036000	.50 (100% 4c)
	Te1	0.049700	0.250000	0.876900	.50 (100% 4c)
	Te2	0.125100	0.750000	0.438600	.50 (100% 4c)
	Te3	0.207900	0.250000	0.191700	.50 (100% 4c)
U ₇ Te ₁₂ [4]	U1	0.000000	0.000000	0.250000	.0833 (17% 2a)
Hexagonal	U2	0.150000	0.280000	0.250000	.5000 (100% 6h)
	Te1	0.510000	0.380000	0.250000	.5000 (100% 6h)
	Te2	0.240000	0.000000	0.250000	.5000 (100% 6h)
UTe _{1.78} [16]	U	0.000000	0.000000	0.134800	.25 (100% 4i)
Orthorhombic	TE1	0.300000	0.000000	0.297700	.2225 (89% 4j)
	TE2	0.000000	0.251000	0.500000	.2225 (89% 4h)

Table 3: Atom locations and site occupancy.

UTe ₂ [16] Orthorhombic	U	0.000000	0.000000	0.134800	.25 (100% 4i)
	Te1	0.500000	0.000000	0.297700	.25 (100% 4j)
	Te2	0.000000	0.251000	0.500000	.25 (100% 4h)
α UTe ₃ [29] Monoclinic	U	0.373230	0.250000	0.156020	.50 (100% 2e)
	Te1	0.799100	0.250000	0.063200	.50 (100% 2e)
	Te2	0.704200	0.250000	0.667900	.50 (100% 2e)
	Te3	0.279900	0.250000	0.659100	.50 (100% 2e)
β UTe ₃ [22] Orthorhombic	U	0.000000	0.833100	0.250000	.25 (100% 4c)
	Te1	0.000000	0.072000	0.250000	.25 (100% 4c)
	Te2	0.000000	0.427700	0.250000	.25 (100% 4c)
	Te3	0.000000	0.703900	0.250000	.25 (100% 4c)
UTe ₅ [21] Orthorhombic	U	0.407930	0.250000	0.386100	.5 (100% 4c)
	Te1	0.163840	0.565200	0.387900	.5 (100% 8d)
	Te2	0.040800	0.250000	0.621100	.5 (100% 4c)
	Te3	0.739900	0.250000	0.354000	.5 (100% 4c)
	Te4	0.000000	0.000000	0.000000	.5 (100% 4c)

Table 3: (continued). Atom locations and site occupancy.

3 UTe

This phase was first reported by Ferro[10] to be a cubic NaCl structure. It has since been reported by many authors but surprisingly, no one has ever published a powder pattern for this phase. The average lattice parameter from the many reports is about 6.160 Å. A calculated powder pattern done at NBS exists in the Powder Diffraction File (PDF) as pattern number 15-856. Calculating the structure as an NaCl type with space group Fm3m and $a = 6.160$ Å gives the expected good agreement with the NBS calculated pattern PDF 15-856 as shown in Table 4.

d	I^{rel}	Calculated	d	I^{rel}	PDF 15-856
		hkl			hkl
3.556	13	1 1 1	3.56	18	1 1 1
3.080	100	2 0 0	3.08	100	2 0 0
2.178	68	2 2 0	2.18	70	2 2 0
1.8573	5	3 1 1	1.858	8	3 1 1
1.7782	23	2 2 2	1.779	25	2 2 2
1.5400	10	4 0 0	1.541	10	4 0 0
1.4132	2	3 3 1	1.414	4	3 3 1
1.3774	25	4 2 0	1.378	25	4 2 0
1.2574	18	4 2 2	1.258	20	4 2 2
1.1855	1	5 1 1	1.186	2	5 1 1
1.0889	5	4 4 0	1.089	6	4 4 0
1.0412	1	5 3 1	1.042	2	5 3 1
1.0267	11	6 0 0+	1.027	14	6 0 0
0.9740	8	6 2 0	0.974	10	6 2 0
0.9394	<1	5 3 3	0.940	2	5 3 3
0.9287	7	6 2 2	0.929	10	6 2 2
0.8891	2	4 4 4	0.890	4	4 4 4
0.8626	1	7 1 1+	0.863	2	7 1 1
0.8542	7	6 4 0	0.855	10	6 4 0
0.8232	13	6 4 2	0.824	18	6 4 2
0.8020	1	7 3 1+	0.802	4	7 3 1

Table 4: Calculated (left) and the NBS calculated (right) PDF pattern (15-856) for UTe.

4 U_3Te_4 ($\text{UTe}_{1.333}$)

4.1 U_3Te_4 -Cubic

Ferro[10] described U_3Te_4 and proposed a cubic structure, isostructural with Th_3P_4 . There is a solid solution region covering the range $\text{UTe}_{1.333}$ to $\text{UTe}_{1.5}$ in the phase diagram. The cubic cell stretches from 9.442[12] Å on the U rich side to 9.390[12] Å on the Te rich side. Most authors (see [13]) report the lattice parameter closer to 9.410 Å or the 9.40 Å originally reported by Ferro and available as PDF pattern 12-610. We have calculated the end members using the Th_3P_4 structure as determined by Meisel[18]. Since we calculated the end members of this series, the d' 's in our patterns are shifted from the PDF values, as shown in Table 5. The agreement of our calculated intensities with the data of Ferro, indicates that the overall structure model chosen, is correct. However, the calculated density of 9.660 g/cm³ is somewhat larger than the 9.46 g/cm³ reported by Matson, Moody and Himes[17]. This indicates that the samples that most researchers have reported as U_3Te_4 were probably uranium deficient. The U and Te atomic positions are given in Table 3. These sites are fully occupied in the ideal U_3Te_4 stoichiometry.

d	I^{rel}	Calculated hkl	d	I^{rel}	PDF 12-610 hkl
3.855	28	2 1 1	3.804	30	2 1 1
3.338	2	2 2 0			
2.986	100	3 1 0	2.945	100	3 1 0
2.523	77	3 2 1	2.500	80	3 2 1
2.111	23	4 2 0	2.091	50	4 2 0
2.013	15	3 3 2	1.995	40	3 3 2
1.9273	12	4 2 2	1.9080	40	4 2 2
1.8517	12	4 3 1	1.8350	50	5 1 0
1.7239	6	5 2 1	1.7120	10	5 2 1
			1.6720	10	4 4 0
1.6193	2	5 3 0			
1.5317	25	5 3 2+	1.5190	80	6 1 1
1.4929	8	6 2 0	1.4820	40	6 2 0
1.4569	13	5 4 1	1.4460	50	5 4 1
1.3922	5	6 3 1	1.3790	30	6 3 1
1.3628	5	4 4 4	1.3530	40	4 4 4
1.3353	3	5 4 3+	1.3230	20	7 1 0
1.3094	4	6 4 0	1.2980	30	6 4 0
1.2849	12	7 2 1+	1.2760	90	7 2 1
1.2617	4	6 4 2	1.2540	40	6 4 2
1.1991	2	6 5 1	1.1890	30	6 5 1
1.1803	1	8 0 0	1.1720	5	8 0 0

Table 5: Calculated (left) and the observed (12-610) powder pattern for cubic U_3Te_4 .

Calculated			PDF 12-610		
d	I ^{rel}	hkl	d	I ^{rel}	hkl
1.1622	1	7 4 1	1.1550	5	7 4 1
1.1285	1	6 5 3	1.1220	40	6 5 3
1.1128	3	8 2 2+	1.1150	10	8 2 2
			1.1060	40	6 6 0
1.0976	7	7 4 3+	1.0910	70	7 5 0
1.0691	4	7 5 2	1.0630	50	7 5 2
1.0556	1	8 4 0	1.0500	20	8 4 0
1.0302	3	8 4 2	1.0250	60	8 4 2
1.0182	11	9 2 1+	1.0130	100	9 2 1
0.9953	6	8 5 1+	.99000	100	8 5 1
0.9739	2	7 6 3+			
0.9637	2	8 4 4			
0.9538	2	8 5 3+			
0.9349	4	7 7 2+			
0.9171	3	9 5 0+			
0.9003	2	7 6 5			
0.8843	1	8 7 1			
0.8767	4	8 6 4+			
0.8692	2	10 3 3+			
0.8619	2	10 4 2			
0.8548	4	8 7 3+			

Table 5: (continued). Calculated (left) and the observed (12-610) powder pattern for cubic U₃Te₄.

d	I ^{rel}	Calculated		d	I ^{rel}	PDF 12-610
		hkl				hkl
0.8412	1	9 6 3+				
0.8346	2	8 8 0				
0.8281	1	9 7 0+				
0.8157	7	10 5 3+				
0.8096	3	10 6 0+				
0.8038	2	11 4 1+				
0.7924	1	9 6 5				
0.7868	2	8 8 4+				
0.7814	3	9 7 4+				

Table 5: (continued). Calculated (left) and the observed (12-610) powder pattern for cubic U₃Te₄.

4.2 U_3Te_4 -Orthorhombic

There is also an orthorhombic phase with the stoichiometry U_3Te_4 [34]. This is a defect material which has the stibnite (Sb_2S_3) structure. The stoichiometric material, with all lattice sites filled has the formula U_2Te_3 and is discussed in detail below. The lattice parameters for the orthorhombic U_3Te_4 phase have been determined and are give in Table 7. No powder pattern has ever been published for this phase. However, since our assessment of the reported lattice parameters (Table 7) shows that they do not vary much across the solid solution range and since a small uranium deficiency will not greatly effect the intensities, the powder patterns for this series should not vary much.

The stibnite structure (orthorhombic U_3Te_4), shown in Table 3 has two independent uranium atoms and three independent telluriums. Even though it may be reasonable to assume that the uranium sublattice is more likely to have vacancies, there is no way of establishing which uranium site or sites receives the vacancies without a Rietveld refinement of a good powder pattern. Until such a pattern and refined model is available, there is no justification for the calculation of any patterns on this side of the solid solution.

5 U_2Te_3 ($\text{UTe}_{1.5}$)

5.1 U_2Te_3 -Cubic

This phase represents the other side of the solid solution range from $\text{UTe}_{1.333}$ to ($\text{UTe}_{1.5}$). L. K. Matson et al.[17] have measured the density of this Th_3P_4 structure type on both sides of the solid solution range to be 9.46 g/cm^3 on the high uranium side (U_3Te_4) and 9.02 g/cm^3 on the high tellurium side (U_2Te_3). They report the lattice parameter for each of these phases to be equal at $9.397 \text{ \AA}$. We choose to use $9.390 \text{ \AA}$ [12] which is close to the value reported by most other authors for this phase see [13].

No powder pattern for the U_2Te_3 cubic defect phase has ever been published. To simulate this pattern we assumed that the vacancies go to the single uranium site in the lattice. In the 3:4 stoichiometry, all sites are completely filled. The 2:3 stoichiometry is most easily achieved by leaving the Te sites filled and placing 88.8% of a uranium atom on each site. Any other model will require placing vacancies on both the Te and U sites. Zachariasen[35] also proposed the uranium defect model, however, Carter[7] suggests that some degree of cation vacancy pairing should occur. Since this will not effect the powder pattern (assuming no superlattice exists), we ignore this possibility in our model. The uranium vacancy model produces a calculated density of 9.184 g/cm^3 . This is reasonably close to the value of 9.02 g/cm^3 reported by Matson, Moody and Himes[17]. The calculated pattern shown in Table 6 is compared to the only available pattern in this

system—namely the other side of the solid solution, U_3Te_4 [10].

d	I^{rel}	Calculated hkl	d	I^{rel}	PDF 12-610 hkl
3.833	21	2 1 1	3.804	30	2 1 1
3.320	1	2 2 0			
2.969	100	3 1 0	2.945	100	3 1 0
2.510	79	3 2 1	2.500	80	3 2 1
2.100	20	4 2 0	2.091	50	4 2 0
2.002	13	3 3 2	1.995	40	3 3 2
1.9167	13	4 2 2	1.9080	40	4 2 2
1.8415	11	4 3 1	1.8350	50	5 1 0
1.7144	5	5 2 1	1.7120	10	5 2 1
			1.6720	10	4 4 0
1.6104	3	5 3 0			
1.5233	24	5 3 2	1.5190	80	6 1 1
1.4847	8	6 2 0	1.4820	40	6 2 0
1.4489	13	5 4 1	1.4460	50	5 4 1
1.3845	5	6 3 1	1.3790	30	6 3 1
1.3553	5	4 4 4	1.3530	40	4 4 4
1.3280	4	5 4 3	1.3230	20	7 1 0
1.3022	3	6 4 0	1.2980	30	6 4 0
1.2778	11	7 2 1	1.2760	90	7 2 1
1.2548	4	6 4 2	1.2540	40	6 4 2
1.1925	2	6 5 1	1.1890	30	6 5 1
			1.1720	5	8 0 0

Table 6: Calculated pattern for cubic U_2Te_3 (left) and the observed (12-610) pattern for U_3Te_4 .

Calculated			PDF 12-610		
d	I^{rel}	hkl	d	I^{rel}	hkl
1.1558	1	7 4 1	1.1550	5	7 4 1
1.1223	1	6 5 3	1.1220	40	6 5 3
1.1066	3	8 2 2	1.1150	10	8 2 2
			1.1060	40	8 3 2
1.0916	7	7 4 3	1.0910	70	7 5 0
1.0632	4	7 5 2	1.0630	50	7 5 2
1.0498	1	8 4 0	1.0500	20	8 4 0
1.0369	1	9 1 0	1.0250	60	8 4 2
1.0245	3	8 4 2	1.0130	100	9 2 1
1.0125	11	9 2 1	.99000	100	8 5 1
0.9898	6	8 5 1			
0.9685	2	7 6 3			
0.9584	2	8 4 4			
0.9485	2	8 5 3			
0.9298	4	7 7 2			
0.9120	3	9 5 0			
0.8953	2	7 6 5			
0.8795	1	8 7 1			
0.8718	3	8 6 4+			
0.8644	1	10 3 3+			
0.8572	2	10 4 2			
0.8501	4	8 7 3+			

Table 6: (continued). Calculated pattern for cubic U_2Te_3 (left) and the observed (12-610) pattern for U_3Te_4 .

Calculated			PDF 12-610		
d	I^{rel}	hkl	d	I^{rel}	hkl
0.8365	1	9 6 3+			
0.8300	2	8 8 0			
0.8236	1	9 7 0+			
0.8112	7	10 5 3+			
0.8052	3	10 6 0+			
0.7993	2	11 4 1+			
0.7880	1	9 6 5			
0.7825	2	8 8 4+			
0.7771	3	9 7 4+			

Table 6: (continued). Calculated pattern for cubic U_2Te_3 (left) and the observed (12-610) pattern for U_3Te_4 .

5.2 U_2Te_3 -Orthorhombic

Ferro[10] and later Suski et al.[32] report that an orthorhombic phase also covers the same phase region as the cubic U_3Te_4 (i.e. $\text{UTe}_{1.33}$) to U_2Te_3 (i.e. $\text{UTe}_{1.5}$). Suski and Janus[34] showed that the orthorhombic modification is the stable variety while the cubic form is a high temperature metastable modification. Suski[32] in 1976 gave the lattice parameters of the end members of the solid solution as shown in Table 7. In 1980 he and Janus[34] showed that in fact, both end members had the same lattice parameters. The values we have used are from the orthorhombic U_2Te_3 shown in Table 1.

These phases are reported to be isostructural with U_2S_3 and U_2Se_3 by Suski[32]. This has been confirmed by Slovyanskikh et al.[28] who reported U_2Te_3 as isostructural with Sb_2S_3 .

The "ideal" structure for the U_2Te_3 stoichiometry is that of Sb_2S_3 (stibnite). This model fills the two independent uranium sites and the three independent tellurium sites. This structure goes nonstoichiometric (probably on the cation sublattice) to give the orthorhombic form of U_3Te_4 discussed above. Our calculated density for the orthorhombic form of U_2Te_3 is 8.749 g/cm^3 .

A problem here is to establish which axis ($11.86 \text{ \AA}$ and $12.46 \text{ \AA}$) is a and which is the c axis. The isostructural Sb_2S_3 structure has a and c nearly identical, and the related structures Th_2S_3 , U_2S_3 and Np_2S_3 [35] have no clear trend indicating which should be longer. Calculated U-Te distances

Phase	Reference	a (Å)	b (Å)	c (Å)
U ₂ Te ₃	Suski 1980[34]	11.83	4.45	12.31
U ₂ Te ₃	Suski 1976[32]	11.79	4.433	12.34
U ₂ Te ₃	Slovyanskikh 1977[28]	11.71	4.36	12.22
U ₃ Te ₄	Suski 1976[32]	11.86	4.401	12.46
U ₃ Te ₄	Suski 1980[34]	11.83	4.45	12.33

Table 7: Lattice parameters for the orthorhombic U₂Te₃–U₃Te₄ solid solution range.

with the axis in each orientation produce a weak argument: with $a=12.46$ Å and $c=11.86$ Å, the distance from U1 to Te3 is closer to the distance from U1 to Te2. In addition, the powder patterns agree a bit better with the axis chosen this way. This very weak argument leads us to choose the orientation given in Table 1.

We should also note how poorly the current PDF pattern for U₂Te₃ (34-807)[28] and the deleted pattern (21-1408)[27] match each other or the calculated pattern shown in Table 8. For a number of reasons (even with the doubt about the model mentioned above), we prefer to use the calculated pattern as representative of this phase until an experimental pattern becomes available. As soon as an adequate experimental pattern is available we suggest that a Rietveld refinement be carried out to establish more firmly the orientation of the a and c axis and much more importantly, to refine the

x, y and z values of the U and Te atoms. It is clear from Zachariasen's[35] work that these values vary considerably among the isostructural materials. The powder pattern calculated with the a and c axis reversed are not so different that a phase identification would not treat them as identical.

Calculated			PDF 34-807		PDF 21-1408	
d	I ^{rel}	hkl	d	I ^{rel}	d	I ^{rel}
8.533	8	1 0 1				
6.160	18	2 0 0				
5.915	5	0 0 2				
5.464	49	2 0 1				
5.332	2	1 0 2				
4.267	8	2 0 2				
4.165	13	0 1 1				
3.946	2	1 1 1				
3.680	22	3 0 1				
3.756	17	1 0 3			3.74	20
3.607	8	2 1 0				
3.417	71	1 1 2				
3.373	43	3 0 2	3.386	30	3.35	20
3.321	12	2 0 3				
3.080	100	2 1 2	3.058	50		
			2.984	30		
2.951	62	0 1 3	2.967	40	2.96	10
2.870	24	1 1 3				
2.844	4	3 0 3	2.849	80	2.83	10
			2.821	70		
2.732	40	4 0 2			2.72	100
2.688	34	3 1 2				

Table 8: Calculated and PDF patterns (34-807 and 21-1408) for U₂Te₃.

d	I _{rel}	Calculated hkl	PDF 34-807 d	I _{rel}	PDF 21-1408 d	I _{rel}
2.666	14	2 0 4	2.652	100	2.51	40
2.533	16	4 1 0				
2.476	26	4 1 1				
2.427	5	4 0 3				
2.415	10	1 1 4+				
2.397	8	3 1 3+	2.392	30		
2.328	5	4 1 2			2.33	20
2.324	5	1 0 5				
2.287	16	2 1 4	2.301	30		
2.275	14	5 0 2			2.27	10
2.225	45	0 2 0				
2.209	14	2 0 5	2.181	30	2.212	30
2.153	1	1 2 1				
2.131	10	4 1 3+				
2.121	10	5 1 1				
2.112	27	3 1 4				
2.089	22	0 1 5				
2.061	8	2 2 1				
2.050	19	3 0 5+	2.045	40	2.00	20
2.023	3	6 0 1+				
1.9717	4	0 0 6+				
1.9469	5	1 0 6				

Table 8: (continued). Calculated and PDF patterns (34-807 and 21-1408)
for U₂Te₃.

Calculated			PDF 34-807			PDF 21-1408	
d	I ^{rel}	hkl	d	I ^{rel}		d	I ^{rel}
1.9398	4	6 0 2					
1.9301	6	3 2 1					
1.9237	5	4 1 4					
1.9143	5	1 2 3					
1.8915	6	5 1 3					
1.8644	44	6 1 0+				1.87	80
1.8212	10	6 0 3					
1.8036	6	4 2 0					
1.7830	1	4 2 1					
1.7780	1	0 2 4+					
1.7525	1	3 2 3					
1.7420	1	5 1 4					
1.7252	20	4 2 2+					
1.7083	6	2 2 4					
1.6869	3	7 0 2+				1.69	100
1.6743	1	1 0 7					
1.6606	3	4 0 6					
1.6506	1	3 1 6					
1.6402	2	4 2 3					
1.6298	10	2 0 7+					
1.6212	3	7 1 1					
1.6072	6	7 0 3+				1.61	70

Table 8: (continued). Calculated and PDF patterns (34-807 and 21-1408) for U₂Te₃.

d	I ^{rel}	Calculated hkl	PDF 34-807 d	I ^{rel}	PDF 21-1408 d	I ^{rel}
1.5905	7	5 2 2				
1.5799	2	0 1 7			1.58	20
1.5772	2	6 1 4+				
1.5675	7	2 2 5+			1.56	70
1.5558	1	4 1 6				
1.5508	4	6 0 5				
1.5398	3	4 2 4				
1.5304	5	2 1 7				
1.5271	3	8 0 1+			1.52	10
1.5124	4	7 0 4				
1.5077	12	3 2 5+				
1.4968	2	6 2 1				
1.4903	2	8 0 2			1.49	30
1.4787	2	0 0 8				
1.4756	3	0 2 6				
1.4718	2	0 3 1				
1.4644	7	6 1 5+				
1.4621	4	6 2 2				
1.4418	1	5 2 4+			1.45	10
1.4344	2	4 2 5+				
1.4291	5	1 3 2+				
1.4222	1	6 0 6				

Table 8: (continued). Calculated and PDF patterns (34-807 and 21-1408)

for U₂Te₃.

d	I^{rel}	Calculated	PDF 34-807			PDF 21-1408	
		hkl	d	I^{rel}		d	I^{rel}
1.4132	4	8 1 2					
1.4093	10	6 2 3					
1.4058	16	4 1 7					
1.4011	11	2 3 2					
1.3943	5	1 1 8+					
1.3884	5	0 3 3				1.39	10
1.3796	2	1 3 3				1.37	20
1.3682	1	2 1 8					
1.3659	1	8 0 4					
1.3579	4	3 3 2+				1.356	10
1.3547	4	6 1 6					
1.3460	2	7 1 5					
1.3442	2	7 2 2+					
1.3364	2	4 3 0					
1.3336	3	9 0 2					
1.3308	4	4 2 6					
1.3280	5	4 3 1+				1.324	30
1.3148	9	2 2 7+					
1.3058	5	8 1 4+					
1.3029	8	7 2 3+					
1.3004	4	9 1 1					

Table 8: (continued). Calculated and PDF patterns (34-807 and 21-1408) for U_2Te_3 .

d	I^{rel}	Calculated	PDF 34-807	I^{rel}	PDF 21-1408	I^{rel}
		hkl				
1.2962	3	2 3 4				
1.2932	2	9 0 3			1.291	40
1.2775	4	9 1 2			1.278	10
1.2723	4	6 2 5				
1.2679	3	5 0 8				
1.2606	7	0 1 9+				
1.2593	7	7 1 6				
1.2568	6	0 3 5			1.255	10
1.2508	4	7 2 4+				
1.2423	3	9 0 4+			1.244	20
1.2396	4	8 1 5+				
1.2316	3	0 2 8+				
1.2254	2	10 0 1				

Table 8: (continued). Calculated and PDF patterns (34-807 and 21-1408) for U_2Te_3 .

Phase	Reference	a (Å)	b (Å)	c (Å)
U_3Te_5	Slovyanskikh 1977[28]	7.987	8.728	13.046
$\text{U}_3\text{Te}'_5$	Slovyanskikh 1977[28]	7.99	8.738	12.88

Table 9: Lattice parameters for the reported orthorhombic forms of U_3Te_5 .

6 U_3Te_5 ($\text{UTe}_{1.666}$)

Slovyanskikh et al.[27] reported the existence of U_3Te_5 and their powder pattern was abstracted as PDF 21-1407. Again in 1977 Slovyanskikh et al.[28] confirmed the observation, after Suski and Reizner-Netter[31] had expressed doubts about its existence, and identified two types containing a bit less uranium than called for in the formula. The orthorhombic unit cells for the two types were given as shown in Table 9. The powder patterns for these two materials were abstracted as PDF 34-766 and 34-896.

The first report of Slovyanskikh et al.[27] was later corrected by Ellert, Sevast'yanov and Slovyanskikh[9] to actually be U_7Te_{12} . Thus, we have compared the deleted pattern PDF 21-1408 to the calculated one for U_7Te_{12} . The two patterns which remain for U_3Te_5 were determined using a Debye-Scherrer camera and only give the dozen or so most intense lines to a very low degree of accuracy. It is clear that a better standard is needed. However, in the absence of a structural model, no calculated pattern can be produced. In order to use the Crystal Data database to try to find isomorphous structure

types, more precise cell information will be required.

7 U_7Te_{12} ($\text{UTe}_{1.714}$)

Breeze et al.[3] first reported a phase of this stoichiometry and their pattern appears as PDF 24-1368. Breeze and Brett[4] determined the crystal structure of this phase as being isostructural with Th_7S_{12} [35]. Using this model we have calculated the pattern for U_7Te_{12} . We have compared this pattern in Table 10 to that reported by Breeze et al.[3] and to the pattern (PDF 21-1407) reported by Slovyanskikh et al.[27] initially claimed to be U_3Te_5 but later claimed to be U_7Te_{12} [9]. It is interesting to note that even though all of the experimental data was collected with low resolution cameras, the disagreement with the proposed model is worse than it should be. A carefully measured experimental pattern of this phase and a Rietveld analysis will be required before anything more certain can be said about its existence or structure.

d	I^{rel}	Calculated hkl	PDF 24-1368 d	I^{rel}	PDF 21-1407 d	I^{rel}
10.660	100	1 0 0				
6.155	5	1 1 0				
5.330	5	2 0 0				
4.029	9	2 1 0	4.01	50		
3.941	1	1 0 1	3.95	20		
3.553	3	3 0 0				
3.493	1	1 1 1				
3.319	27	2 0 1	3.31	30		
3.077	4	2 2 0	3.08	20		
2.957	23	3 1 0				
2.921	47	2 1 1	2.91	100	2.91	100
2.724	2	3 0 1	2.715	90	2.72	75
			2.658	30		
2.491	2	2 2 1	2.485	50	2.49	35
2.446	9	3 2 0+	2.421	50	2.43	35
2.326	3	1 4 0+	2.326	90	2.31	100
2.257	2	4 0 1	2.256	20		
2.121	10	0 0 2	2.118	50	2.12	50
2.080	3	1 0 2	2.010	40		
2.040	5	1 4 1+				
2.015	1	2 4 0			2.02	25
2.005	1	1 1 2				

Table 10: Calculated and PDF patterns (24-1368 and 21-1407) for U_7Te_{12} .

d	I ^{rel}	Calculated	PDF 24-1368		PDF 21-1407	
		hkl	d	I ^{rel}	d	I ^{rel}
1.9707	1	2 0 2				
1.9146	1	1 5 0				
1.9049	3	5 0 1				
1.8768	2	2 1 2	1.875	30	1.87	15
1.8469	2	3 3 1				
1.8197	5	2 4 1+				
1.7451	8	1 5 1+	1.744	20		
1.7234	8	3 1 2+				
1.7069	2	5 2 0	1.705	30	1.70	35
			1.656	20	1.66	5
1.6197	2	3 4 1	1.619	50	1.61	60
1.6023	4	3 2 2+				
1.5835	12	5 2 1	1.582	60	1.58	75
1.5673	2	1 4 2+	1.566	60	1.56	60
1.5386	1	4 4 0				
1.5228	2	7 0 0	1.520	40	1.52	15
1.5180	2	6 1 1				
1.4607	1	2 4 2	1.460	40	1.46	5
1.4212	1	1 5 2			1.43	15
1.4119	1	1 7 0				
1.3649	5	5 4 0+			1.375	15
1.3397	1	1 7 1			1.338	100

Table 10: (continued). Calculated and PDF patterns (24-1368 and 21-1407) for U₇Te₁₂.

d	I ^{rel}	Calculated hkl	PDF 24-1368 d	I ^{rel}	PDF 21-1407 d	I ^{rel}
1.3342	4	2 1 3				
1.3325	4	8 0 0				
1.3298	4	5 2 2			1.316	35
					1.295	25
1.2450	2	7 2 1+			1.246	5
1.2370	2	7 0 2			1.237	5
1.2309	1	5 5 0				
1.2083	1	1 4 3				
1.1969	1	1 8 1			1.197	35
1.1753	1	1 7 2+				
1.1574	1	2 4 3			1.161	15
1.1541	3	7 3 1				
1.1478	4	5 4 2+			1.149	15
1.1374	1	1 5 3			1.135	5
1.1283	3	8 0 2			1.116	15
1.1217	1	8 2 1			1.102	75
1.0889	3	5 2 3			1.089	100
1.0646	1	5 5 2			1.065	5
1.0605	1	0 0 4			1.058	5
					1.049	25
					1.044	15
					1.036	5

Table 10: (continued). Calculated and PDF patterns (24-1368 and 21-1407) for U₇Te₁₂.

d	<i>I</i> ^{rel}	Calculated hkl	PDF 24-1368 d	<i>I</i> ^{rel}	PDF 21-1407 d	<i>I</i> ^{rel}
1.0338	1	10 0 1			1.032	25
					1.019	100
					1.000	75
0.9982	1	3 1 4			0.998	85
					0.996	25
0.9927	1	7 5 1+			0.991	25
0.9855	2	3 9 0				
0.9842	1	10 1 1			0.983	75
					0.980	15
0.9730	1	3 2 4			0.974	25
0.9579	1	7 2 3				
0.9243	1	11 1 0+				
0.9232	1	6 7 1				
0.9146	1	7 3 3				
0.9031	1	1 11 1				
0.9008	1	5 2 4				
0.8983	1	8 2 3				
0.8937	3	3 9 2+				
0.8703	1	7 0 4				
0.8499	1	5 9 1				
0.8474	2	11 1 2+				
0.8374	2	4 5 4+				

Table 10: (continued). Calculated and PDF patterns (24-1368 and 21-1407) for U₇Te₁₂.

8 $\text{UTe}_{1.78}$

8.1 $\text{UTe}_{1.78}$ —Orthorhombic

The story in this section of the phase diagram gets particularly complicated. All phases reported in this vicinity appear to be defect structures of UTe_2 . Whether any of these phases actually exist at all is problematical. Breeze et al.[3] report an orthorhombic structure which extends from UTe_2 to $\text{UTe}_{1.78}$. There are many confirming reports of this structure with the UTe_2 stoichiometry but only a few reporting uranium deficient compositions[27]. The powder diffraction file has pattern 21-1404 reported as U_4Te_7 (i.e. $\text{UTe}_{1.75}$) from Slovyanskikh et al.[27]. This is the only published pattern in this range of stoichiometry that could be orthorhombic. Our calculated pattern shown in Table 11 is based on the UTe_2 structure[16] and the lattice parameter of Breeze et al.[3] shown in Table 1. The vacancies are placed equally on the two tellurium sites for lack of a better assumption. The PDF pattern 21-1404 has been corrected for some minor errors from the original paper[27].

d	I^{rel}	Calculated hkl	PDF 21-1404 d	I^{rel}
5.608	38	0 1 1	5.62	40
3.988	5	1 0 1		
3.705	8	0 1 3	3.76	50
3.490	2	0 0 4		
3.442	9	1 1 0		
			3.25	10
3.102	100	1 0 3	3.10	100
3.062	19	0 2 0		
2.804	28	0 2 2	2.81	100
			2.75	60
2.540	17	0 1 5	2.55	60
			2.51	10
2.451	44	1 1 4	2.46	40
2.429	57	1 2 1	2.44	40
2.326	8	0 0 6		
2.318	7	1 0 5	2.31	10
2.302	22	0 2 4	2.22	70
2.179	11	1 2 3	2.19	20
2.081	19	2 0 0	2.08	5
2.020	2	0 3 1	2.02	10
1.9510	4	2 1 1		

Table 11: Calculated pattern for $UTe_{1.78}$ (left) and the observed (21-1404) for the claimed U_4Te_7 .

d	I^{rel}	Calculated hkl	PDF 21-1404 d	I^{rel}
1.9274	1	1 1 6	1.93	10
1.8960	13	0 1 7	1.91	80
1.8693	1	0 3 3	1.87	80
1.8484	4	1 2 5		
1.8328	2	1 3 0		
1.8144	2	2 1 3		
1.7727	1	1 3 2		
1.7448	3	0 0 8	1.74	5
1.7211	5	2 2 0	1.72	5
			1.70	70
1.6711	10	2 2 2	1.67	10
1.6478	4	0 3 5	1.65	60
1.6226	10	1 3 4	1.62	60
1.6098	7	2 1 5	1.61	5
1.5563	11	1 1 8	1.56	50
1.5506	13	1 2 7+		
1.5436	12	2 2 4	1.53	5
1.5310	7	0 4 0	1.50	40
1.4494	1	2 3 1		
1.4264	4	0 3 7	1.43	40
1.4015	8	2 1 7	1.40	40
1.3907	1	2 3 3		

Table 11: (continued). Calculated pattern for $UTe_{1.78}$ (left) and the observed (21-1404) for the claimed U_4Te_7 .

d	I^{rel}	Calculated hkl	PDF 21-1404 d	I^{rel}
1.3729	12	1 4 3	1.372	100
1.3370	2	2 0 8		
1.3295	6	3 0 3	1.324	20
1.3129	3	1 2 9	1.316	10
1.2935	5	1 1 10	1.295	70
1.2918	4	2 3 5		
1.2789	2	0 4 6+	1.281	30
1.2701	1	0 2 10		
1.2637	5	1 3 8		
1.2615	6	3 1 4	1.262	30
1.2585	8	3 2 1		
1.2425	2	0 1 11	1.246	30
1.2332	5	2 4 0	1.231	30
1.2195	2	3 2 3		
1.2138	3	1 0 11	1.211	20
			1.197	10
1.1766	4	2 3 7	1.176	50
1.1508	2	0 4 8+	1.150	10
			1.142	50
			1.128	10
1.1216	1	0 5 5	1.121	10
1.1135	3	1 5 4	1.113	80

Table 11: (continued). Calculated pattern for $UTe_{1.78}$ (left) and the observed (21-1404) for the claimed U_4Te_7 .

d	I^{rel}	Calculated hkl	PDF 21-1404 d	I^{rel}
1.1104	3	1 3 10		
1.0900	4	3 3 4+		
1.0874	4	0 2 12	1.087	80
1.0841	2	2 2 10		
1.0777	1	0 3 11	1.077	10
1.0692	3	3 1 8		
1.0668	4	2 1 11+	1.066	50
			1.059	20
1.0436	2	0 5 7	1.044	30
1.0405	2	4 0 0+	1.032	70
1.0099	1	0 6 2	1.020	5
1.0071	2	2 4 8	1.011	5
1.0038	4	3 4 3	1.0??	60
0.9970	1	0 0 14	0.999	80
0.9888	3	1 6 1	0.988	30
0.9873	2	2 5 5		
0.9852	1	4 2 0	0.981	20
0.9797	2	3 2 9+	0.979	10
0.9755	2	4 2 2	0.975	30
0.9746	2	1 5 8		
0.9715	2	3 1 10		

Table 11: (continued). Calculated pattern for $U\text{Te}_{1.78}$ (left) and the observed (21-1404) for the claimed $U_4\text{Te}_7$.

d	I^{rel}	Calculated hkl	PDF 21-1404 d	I^{rel}
0.9695	1	1 6 3		
0.9637	4	2 2 12+		
0.9587	2	3 3 8		
0.9570	2	2 3 11		
0.9511	3	1 4 11		
0.9498	1	4 0 6		
0.9481	3	4 2 4		
0.9363	1	3 0 11		
0.9341	1	1 6 5		
0.9329	2	2 5 7		
0.9164	1	2 6 0		
0.9122	2	4 1 7		
0.9103	1	3 5 2		
0.9086	2	2 6 2+		
0.8991	3	2 0 14+		
0.8936	1	4 0 8		
0.8880	2	3 5 4+		
0.8863	4	2 6 4+		
0.8813	1	0 5 11		
0.8798	1	4 3 5		
0.8724	1	0 0 16		

Table 11: (continued). Calculated pattern for $UTe_{1.78}$ (left) and the observed (21-1404) for the claimed U_4Te_7 .

d	I^{rel}	Calculated hkl	PDF 21-1404 d	I^{rel}
0.8706	5	1 2 15		
0.8606	3	4 4 0+		
0.8462	1	2 4 12		
0.8406	2	4 3 7		
0.8355	2	0 4 14+		
0.8315	1	1 7 4		
0.8207	2	3 6 1		
0.8194	2	5 0 3		
0.8169	1	3 3 12		
0.8125	2	3 5 8		
0.8115	1	2 5 11		
0.8096	1	3 6 3		
0.8071	1	4 4 6		
0.8055	1	1 0 17		
0.8051	1	2 7 1+		
0.8045	1	2 0 16		
0.8035	1	1 7 6		
0.8027	2	5 1 4+		
0.8019	2	5 2 1		
0.8011	2	0 7 7		
0.7988	2	3 4 11		

Table 11: (continued). Calculated pattern for $UTe_{1.78}$ (left) and the observed (21-1404) for the claimed U_4Te_7 .

8.2 UTe_{1.78}-Tetragonal

There are a number of reports of a tetragonal UTe₂ that will be discussed below. Klein-Haneveld and Jellinek[15, 16] reported a tetragonal UTe_{1.77}¹ to be tetragonal with the ThAs₂ structure and a cell of $a = 4.243 \text{ \AA}$ and $c = 8.946 \text{ \AA}$. In their second report they note that this phase can only be stabilized in the presence of germanium. It is probable that this phase was UTeGe. They never again claimed it to be a uranium telluride. Our conclusion is that the reports of tetragonal UTe_{1.77} are so tenuous that a calculated pattern based on a defect ThAs₂ structure is not justified.

9 UTe₂

Three forms of UTe₂ have been claimed to exist: orthorhombic, tetragonal and cubic phases.

9.1 UTe₂-Orthorhombic

Klein-Haneveld and Jellinek[16] first reported and unambiguously established the crystal structure of orthorhombic UTe₂. The results of the structure analysis are given in Tables 1 and 3. This orthorhombic form has since been reported by numerous authors and recently confirmed by Rietveld analysis[2]. The editors of the Powder Diffraction File have deleted

¹This was erroneously initially reported to be UTe_{1.87}[15] and later corrected to be UTe_{1.77}[16].

the very poor pattern (21-1405)[27] in preference to the still rather poor, but better, pattern 24-1370 of Klein-Haneveld and Jellinek[16]. Boehme et al.[2] have produced a high quality pattern in conjunction with the current study. Table 12 shows the calculated pattern along with the current PDF pattern and the new one of Boehme et al.[2].

This powder pattern is a substantial improvement over PDF 24-1370 in that it corrects a number of problems. It is also considerably better than PDF 21-1405 in that a number of major errors have been corrected.

d	I^{rel}	Calculated hkl	Boehme et al.[2] d	I^{rel}	PDF 24-1370 d	I^{rel}
6.982	0	0 0 2			6.98	<1
5.611	28	0 1 1	5.612	30	5.61	<1
3.988	3	1 0 1	3.987	12	3.99	<1
3.707	6	0 1 3	3.708	17	3.71	<1
3.491	1	0 0 4			3.49	<1
3.443	6	1 1 0	3.442	22	3.44	<1
3.103	100	1 0 3	3.104	100	3.10	100
3.088	7	1 1 2			3.09	100
3.064	14	0 2 0	3.066	38	3.06	20
2.806	31	0 2 2	2.807	48	2.806	35
2.541	17	0 1 5	2.542	27	2.541	20
2.451	42	1 1 4	2.452	49	2.451	50
2.430	58	1 2 1	2.430	54	2.430	75
2.328	7	0 0 6	2.327	15	2.327	10
2.319	3	1 0 5			2.319	10
2.303	22	0 2 4	3.304	31	2.303	30
2.180	10	1 2 3	2.180	17	2.180	10
2.081	21	2 0 0	2.081	20	2.081	20
2.021	2	0 3 1			2.021	5
1.9942	0	2 0 2	1.9969	36	1.994	<1
1.9510	3	2 1 1	1.9513	15	1.951	5
1.9282	1	1 1 6	1.9203	24	1.928	<1

Table 12: Calculated and observed patterns (Boehme et al. and 24-1370)
for orthorhombic UTe_2 .

d	I ^{rel}	Calculated hkl	Boehme et al.[2] d	I ^{rel}	PDF 24-1370 d	I ^{rel}
1.8970	12	0 1 7	1.8968	24	1.987	15
1.8704	1	0 3 3	1.8719	14	1.870	2
1.8534	0	0 2 6			1.853	10
1.8491	6	1 2 5	1.8490	16	1.849	10
1.8336	1	1 3 0			1.834	2
1.8145	1	2 1 3			1.814	2
1.7990	<1	1 0 7			1.799	<1
1.7874	<1	2 0 4			1.787	<1
1.7735	1	1 3 2			1.773	2
1.7456	3	0 0 8			1.746	2
1.7214	5	2 2 0			1.721	5
1.6713	12	2 2 2	1.6716	16	1.671	20
1.6487	4	0 3 5	1.6489	16	1.648	5
1.6233	11	1 3 4	1.6237	22	1.623	20
1.6100	7	2 1 5	1.6097	15	1.610	15
1.5569	11	1 1 8	1.5567	21	1.557	50
1.5513	7	1 2 7+	1.5519	19	1.551	50
1.5439	11	2 2 4	1.5435	15	1.544	50
1.5319	7	0 4 0	1.5323	15	1.532	10
1.5167	0	0 2 8			1.517	<1
1.5042	0	0 1 9			1.504	<1
1.4963	0	0 4 2			1.496	<1

Table 12: (continued). Calculated and observed patterns (Boehme et al. and 24-1370) for orthorhombic UTe₂.

d	I^{rel}	Calculated hkl	Boehme et al.[2] d	I^{rel}	PE 24-1370 d	I^{rel}
1.4539	0	1 0 9			1.454	2
1.4498	1	2 3 1			1.450	2
1.4403	<1	1 3 6			1.440	<1
1.4300	<1	1 4 1			1.430	10
1.4272	5	0 3 7	1.4271	11	1.427	10
1.4208	<1	0 4 4			1.403	15
1.4019	8	2 1 7	1.4016	11	1.402	15
1.3965	<1	0 0 10			1.397	15
1.3910	<1	2 3 3			1.391	2
1.3840	0	2 2 6			1.384	<1
1.3804	0	3 0 1			1.380	<1
1.3736	12	1 4 3	1.3740	25	1.374	25
1.3530	<1	3 1 0	1.3545	7	1.353	<1
1.3374	2	2 0 8			1.337	5
1.3295	6	3 0 3	1.3288	8	1.329	10
1.3283	<1	3 1 2			1.328	10
1.3135	3	1 2 9	1.3133	8	1.314	5
1.2941	4	1 1 10			1.294	15
1.2923	4	2 3 5	1.2922	11	1.292	15
1.2796	2	0 4 6+	1.2796	9	1.280	5
1.2782	<1	1 4 5			1.278	5
1.2707	1	0 2 10			1.271	2

Table 12: (continued). Calculated and observed patterns (Boehme et al. and 24-1370) for orthorhombic UTe_2

d	I^{rel}	Calculated hkl	Boehme et al.[2] d	I^{rel}	PDF 24-1370 d	I^{rel}
1.2643	5	1 3 8	1.2643	12	1.264	30
1.2616	4	3 1 4	1.2611	12	1.262	30
1.2586	6	3 2 1	1.2583	10	1.259	30
1.2431	2	0 1 11	1.2429	11	1.243	2
1.2424	<1	3 0 5			1.242	2
1.2336	6	2 4 0	1.2336	14	1.236	10
		2 4 0			1.234	10
1.2257	0	2 2 8	1.2255	2	1.226	<1
1.2208	<1	0 5 1			1.221	10
1.2196	1	3 2 3	1.2193	2	1.220	10
1.2148	0	2 4 2			1.215	10
1.2143	2	1 0 11	1.2139	9	1.214	10
1.1851	<1	0 5 3	1.1854	<1	1.185	<1
1.1770	4	2 3 7	1.1772	9	1.77	10
1.1756	<1	1 5 0			1.1760	10
1.1697	<1	3 1 6			1.170	2
1.1660	0	1 4 7			1.166	2
1.1637	<1	0 0 12			1.164	2
1.1632	<1	2 4 4			1.1630	2
1.1596	1	2 0 10+	1/1593	1	1.160	2
		2 0 10+			1.159	2

Table 12: (continued). Calculated and observed patterns (Boehme et al. and 24-1370) for orthorhombic UTe_2 .

Calculated			Boehme et al.[2]		PDF 24-1370	
d	I ^{rel}	hkl	d	I ^{rel}	d	I ^{rel}
1.1514	2	0 4 8+	1.1514	7		
1.1476	<1	3 3 0				
1.1141	2	1 5 4	1.1141	8		
1.1110	3	1 3 10	1.1085	13		
1.0902	4	3 3 4+				
1.0879	4	0 2 12	1.0878	9		
1.0845	<1	2 2 10				
1.0782	1	0 3 11				
1.0694	3	3 1 8				
1.0672	2	2 1 11+				
1.0624	0	2 3 9				
1.0442	2	0 5 7	1.0450	9		
1.0404	2	4 0 0+	1.0422	7		
1.0342	0	3 0 9				
1.0105	1	0 6 2				
1.0075	2	2 4 8				
1.0041	5	3 4 3				
1.0017	<1	4 1 3				
0.9975	1	0 0 14				
0.9894	3	1 6 1	0.9895	10		
0.9877	2	2 5 5	0.9872	7		
0.9852	<1	4 2 0				

Table 12: (continued). Calculated and observed patterns (Boehme et al. and 24-1370) for orthorhombic UTe₂.

d	I ^{rel}	Calculated hkl	Boehme et al.[2] d	I ^{rel}	PDF 24-1370 d	I ^{rel}
0.9799	2	3 2 9+				
0.9751	2	1 5 8+				
0.9717	2	3 1 10				
0.9701	<1	1 6 3				
0.9641	5	2 2 12	0.9640	8		
0.9629	1	4 1 5				
0.9617	0	0 5 9				
0.9589	2	3 3 8	0.9600	8		
0.9574	2	2 3 11				
0.9516	3	1 4 11				
0.9498	<1	4 0 6				
0.9481	2	4 2 4				
0.9366	1	3 0 11				
0.9347	<1	1 6 5				
0.9333	3	2 5 7				
0.9246	<1	2 4 10				
0.9168	<1	2 6 0	0.9158	7		
0.9122	3	4 1 7				
0.9106	<1	3 5 2				
0.9090	2	2 6 2+				
0.9072	<1	4 2 6				

Table 12: (continued). Calculated and observed patterns (Boehme et al. and 24-1370) for orthorhombic UTe₂.

d	I^{rel}	Calculated hkl	Boehme et al.[2] d	I^{rel}	PDF 24-1370 d	I^{rel}
0.8994	2	1 5 10+	0.8993	8		
0.8937	<1	4 0 8				
0.8882	2	3 5 4+				
0.8867	3	2 6 4+				
0.8817	<1	0 5 11				
0.8799	1	4 3 5				
0.8728	<1	0 0 16				
0.8711	6	1 2 15				
0.8607	3	4 4 0+				
0.8580	0	4 2 8+				
0.8493	<1	3 0 13				
0.8465	<1	2 4 12				
0.8407	3	4 3 7				
0.8357	2	1 6 9+		0.8358	11	
0.8343	<1	4 0 10				
0.8320	2	1 7 4				
0.8210	3	3 6 1				
0.8194	3	5 0 3				

Table 12: (continued). Calculated and observed patterns (Boehme et al. and 24-1370) for orthorhombic UTe_2 .

9.2 UTe₂-Tetragonal

Ferro[10] first reported UTe₂ and indexed it as tetragonal with a cell of $a = 4.006 \text{ \AA}$ and $c = 7.471 \text{ \AA}$. This phase was later shown to be not UTe₂ but UOTe by Klein-Haneveld and Jellinek[14]. Slovyanskikh et al.[27] reported an unindexed powder pattern for UTe₂ and referred to the structure as tetragonal. It is not clear that this reference is not simply a repetition of the Ferro claim. Their powder pattern has been abstracted as PDF 21-1405. Grønvold[13] refer to a report by Pletyushkin[23] claiming a tetragonal form with lattice parameters of $a = 4.016 \text{ \AA}$ and $c = 7.49 \text{ \AA}$. Since these lattice parameters are similar to the original erroneous report on UTeO, this report is also open to question.

Klein Haneveld and Jellinek[15] reported a solid solution range for tetragonal UTe_{2-x} with x varying from 0 to 0.13. They later claimed this phase only to be stable in the presence of a small amount of Ge. However this material is listed in the Crystal Data data base as UTeGe. This material is questionable. The authors did report a crystal structure while thinking this phase was stoichiometric UTe₂. Since then the structure of this material has been determined as UTeGe with a reduced unit cell of $a = 4.11 \text{ \AA}$ and $c = 9.27 \text{ \AA}$. The non-reduced cell reported in later articles has $c = 17.60 \text{ \AA}$.

In summary, each of the reports of tetragonal UTe₂ is open to serious question. There has not been an unambiguous report to date, establishing the existence of this phase.

9.3 UTe₂-Cubic

Recently Pfoertsch and Ruud[24] reported a powder pattern (PDF 35-1483) for a cubic form of UTe₂. They propose a space group of Pa3 for it. This is the same space group for pyrite (FeS₂) type structures and the PDF card states that this material has the pyrite structure. We have attempted to simulate this pattern using the structure of pyrite as determined by Brostigen and Kjekshus[5] with U in the 4(a) site and the Te in 8(c) with x set to .3840 and a = 5.469. This computation and the published pattern are shown in Table 13. It is clear from the poor agreement between the calculated and observed intensities that this material does not have the pyrite structure. Even more noticeable is that the density calculates to 20.03 g/cm³. The indexing on the card is consistent with the reported cell parameter of 5.469 Å.

In order to make the density equal to a more reasonable 10.0 g/cm³ rather than 20 g/cm³ in a cubic cell with edge = 5.469 Å, you must put 2 uranium atoms and 4 tellurium atoms into the Primitive cell. (The hkl's require that the cell be primitive). This can only be done in a cubic cell by putting U at the origin and Te at either 1/4,1/4,1/4 or at 3/4,3/4,3/4. We have computed these models also. In neither case do we get anything remotely resembling the reported pattern.

Since this is the first and only report of a cubic UTe₂ and since no chemical analysis confirmation was carried out, we must doubt the validity of this report. The sample, originally from China[25], has been lost so further

testing is impossible. We must conclude that this sample is not a form of UTe_2 .

d	I^{rel}	Calculated hkl	d	I^{rel}	PDF 35-1483 hkl
3.158	38	1 1 1	3.154	100	1 1 1
2.734	94	2 0 0	2.735	40	2 0 0
2.446	63	2 1 0			
2.233	52	2 1 1	2.230	10	2 1 1
1.9336	49	2 2 0	1.932	50	2 2 0
1.8230	1	2 2 1	1.823	6	2 2 1
1.6490	100	3 1 1	1.6489	45	3 1 1
1.5788	15	2 2 2	1.5783	10	2 2 2
1.5168	18	0 2 3			
1.4617	23	3 2 1+			
			1.3678	6	4 0 0
1.3264	1	4 1 0+			
1.2547	9	3 3 1	1.2554	18	3 3 1
1.2229	12	4 2 0+	1.2236	12	4 2 0
1.1934	9	4 2 1			
1.1660	4	3 3 2			
1.1164	11	4 2 2	1.1168	14	4 2 2

Table 13: Calculated pattern for the postulated pyrite structured UTe_2 (left) and the reported (35-1483) pattern.

10 $\text{UTe}_{2.5}$

Slovyanskikh et al.[27] reported three phases in between UTe_2 and UTe_3 . These are U_3Te_7 ($\text{UTe}_{2.333}$ abstracted as PDF 21-1402), U_2Te_5 ($\text{UTe}_{2.5}$ abstracted as PDF 21-1409) and U_3Te_8 ($\text{UTe}_{2.667}$ abstracted as PDF 21-1406). Grønvold et al.[13] argue that there is only one phase in this region, namely that of U_2Te_5 . They refer to a pattern published in a contract report to the International Atomic Energy Agency[12] that has never been abstracted into the open literature. We therefore have included this pattern in Table 14. This pattern was reported to be taken on a Guinier camera. The d's have been computed from the reported $\sin^2 \theta$ values and the intensities have been left as visual estimates. We should note that in this study the authors simply prepared compositions of various stoichiometries and reported diffraction patterns of the resulting material. It is possible that their patterns are multi-phase.

$\text{UTe}_{2.5}$ was observed in the recent study by Boehme et al.[2] in mixtures containing UTe_2 and UTe_3 . They indexed it as orthorhombic with a unit cell similar to that reported for UTe_5 ; however, a uranium deficient UTe_5 model failed to predict any pattern resembling their observed pattern. No further structural investigation is possible without a better starting model. We conclude that $\text{UTe}_{2.5}$ is a real phase and that the Grønvold et al.[13] pattern shown in table 14 probably was of a mixture containing this phase.

Boehme et al.			Grønvold et al.	
d	I ^{rel}	hkl	d	I ^{rel}
17.024	14	0 0 1		
8.546	18	0 0 2		
5.702	17	0 0 3		
4.280	18	0 0 4		
3.926	5	0 1 4		
3.744	2	0 2 3		
			3.442	vw
3.181	100	1 2 1	3.182	vs
			3.027	m
2.738	9	0 1 6	2.778	m
			2.433	s
2.374	17	1 3 3	2.376	vw
			2.362	w
			2.257	vw
2.230	7	1 3 4		
			2.175	vw
			2.092	s
			1.8625	vw
1.714	30	1 4 6	1.7202	vw
			1.6706	w
1.617	2	2 4 0		
1.519	4	0 3 10	1.5189	m
1.371	3	0 6 7	1.3709	w
			1.3416	w
1.224	6	0 5 11		
1.101	5	0 9 1		

Table 14: Boehme et al. and Grønvold et al. patterns for UTe_{2.5}.

11 UTe_3

11.1 αUTe_3

This phase was first published by Slovyanskikh et al.[27]. Their very poor camera pattern was abstracted and remains in the current PDF as 21-1403. Breeze et al.[3] indexed their pattern as monoclinic (abstracted as PDF 27-929) with the parameters shown in Table 1. In addition they suggested that it might be isomorphous with ZrS_3 . The ZrS_3 type structures were determined by Furuseth et al.[11], however, more recently the more analogous isomorphous structure of USe_3 has been determined by Salem et al.[29]. Our computation is based on the Salem et al. model shown in Tables 1 and 3 and is compared to the two older experimental patterns and the recent one of Boehme et al.[2] in Table 15.

Calculated			Boehme et al.			27-929		21-1403	
d	I ^{rel}	hkl	d	I ^{rel}		d	I ^{rel}	d	I ^{rel}
10.200	44	0 0 1	10.239	59		10.2	50		
6.031	4	1 0 0	6.048	5					
5.540	26	-1 0 1	5.546	8		5.54	20		
5.100	10	0 0 2	5.118	26		5.08	30	5.11	30
4.901	21	1 0 1	4.915	6		4.89	20		
4.192	5	-1 0 2	4.198	3					
		0 1 1	3.902	<1					
3.400	3	0 0 3	3.410	6					
3.256	100	0 1 2	3.258	100		3.25	100	3.25	20
3.008	12	-2 0 1+	3.205	6					
		2 0 0				3.01	30	3.11	100
		-2 0 1	3.017	16					
2.978	3	-1 1 2	2.973	1				2.88	10
2.788	20	2 0 1	2.787	29				2.83	30
2.770	24	-2 0 2+				2.770	50		
2.650	7	0 1 3	2.653	5					
2.550	6	0 0 4	2.556	31		2.545	40	2.57	100
2.529	20	-1 1 3	2.531	4					
2.475	5	-1 0 4	2.479	4				2.48	20
2.451	33	-2 1 1+	2.455	19		2.449	60		
2.430	6	-2 0 3	2.436	6					
2.335	22	1 1 3	2.325	14				2.33	20

Table 15: Calculated pattern for αUTe_3 (left) and the observed (27-929 and 21-1403).

Calculated			Boehme et al.			27-929			21-1403		
d	I ^{rel}	hkl	d	I ^{rel}		d	I ^{rel}		d	I ^{rel}	
2.328	26	2 1 1				2.323	50		2.25	30	
2.317	16	-2 1 2									
2.239	5	1 0 4	2.246	4							
2.184	8	0 1 4	2.187	10		2.181	30		2.19	30	
2.136	6	-1 1 4	2.137	2							
2.115	25	0 2 0+	2.116	3		2.107	50		2.12	10	
2.096	5	-2 0 4	2.111	12					2.07	20	
2.071	2	0 2 1	2.068	2					2.05	20	
		0 0 5	2.045	3							
2.020	6	-1 0 5	2.024	4					2.03	20	
		1 2 0	1.996	11							
1.9759	3	-1 2 1+	1.973	<1							
1.9537	2	0 2 2									
1.9419	3	1 2 1									
1.9222	2	3 0 1									
1.8914	5	2 1 3+	1.894	2		1.887	30				
1.8782	4	-2 1 4	1.880	2							
1.8556	6	1 0 5	1.861	3					1.86	40	
1.8467	3	-3 0 3	1.841	1							
1.8276	4	-3 1 1+	1.820	2					1.82	10	
1.7828	3	-3 1 2+	1.782	1					1.78	10	
1.7500	5	3 1 1	1.753	<1							

Table 15: (continued). Calculated pattern for αUTe_3 (left) and the observed (27-929 and 21-1403).

d	I^{rel}	Calculated hkl	Boehme et al. d	I^{rel}	27-929 d	I^{rel}	21-1403 d	I^{rel}
1.7301	4	-2 2 1+	1.730	1				
		0 0 6+	1.704	9				
1.7000	7	-3 0 4	1.700	4	1.697	30	1.70	100
1.6924	6	-3 1 3						
1.6850	8	2 2 1			1.683	30		
1.6810	10	-2 2 2	1.681	2				
		2 1 4	1.681	2				
1.6337	4	3 0 3						
1.6279	3	0 2 4	1.628	1			1.62	5
1.6080	2	-1 2 4						
1.5954	2	-2 2 3						
1.5767	2	-1 1 6+	1.579	1			1.58	20
1.5432	3	-3 0 5						
1.5377	3	1 2 4	1.540	1				
1.5224	5	-4 0 1+	1.525	2	1.524	30	1.50	10
1.4954	3	2 2 3						
1.4888	5	-2 2 4+	1.484	2			1.48	20
1.4783	4	-2 1 6+					1.47	10
1.4606	4	-1 2 5	1.460	<1				
1.4498	2	-3 1 5	1.450	<1			1.42	10
1.3983	2	3 1 4						
1.3949	5	1 2 5	1.396	1				

Table 15: (continued). Calculated pattern for αUTe_3 (left) and the observed (27-929 and 21-1403).

d	I^{rel}	Calculated hkl	Boehme et al. d	I^{rel}	27-929 d	I^{rel}	21-1403 d	I^{rel}
1.3910	4	-3 2 3						
1.3821	5	4 1 1+	1.384	2			1.380	30
1.3762	5	-4 1 3+	1.376	2				
1.3590	6	0 3 2						
1.3290	2	2 1 6	1.326	2			1.327	30
1.3250	6	0 2 6+						
1.3205	5	-2 1 7	1.323	1				
1.3154	2	1 3 2					1.318	30
1.3063	2	1 1 7	1.309	1			1.307	20
1.3024	2	0 3 3						
1.2929	3	3 2 3	1.294	1				
1.2873	2	-1 3 3	1.282	1			1.285	10
1.2788	3	3 1 5	1.278	1			1.278	30
1.2767	4	-2 3 1+	1.276	1				
1.2593	3	1 3 3+						
1.2566	3	-2 3 2						
1.2467	3	-3 2 5	1.246	1			1.248	10
1.2445	2	-4 1 5					1.241	10
1.2356	4	-4 2 1+						
1.2252	2	-1 3 4						
1.2207	3	0 1 8					1.222	90

Table 15: (continued). Calculated pattern for αUTe_3 (left) and the observed (27-929 and 21-1403).

d	I ^{rel}	Calculated hkl	Boehme et al. d	I ^{rel}	27-929 d	I ^{rel}	21-1403 d	I ^{rel}
1.2133	5	-3 1 7+	1.119	<1			1.116	20
		1 1 9						
1.1697	3	3 1 6+						
1.1135	3	-5 1 4+						
1.0997	3	5 1 2						
1.0575	2	0 4 0	1.023	1			1.052	10
1.0550	3	3 2 6+						
1.0517	3	-5 2 2+						
1.0360	2	5 0 4					1.022	50
		0 0 10						
1.0150	3	4 3 1+						
1.0127	3	-4 3 3+						
1.0098	2	-2 0 10						
0.9916	2	0 1 10+					0.998	20
0.9896	2	2 2 8+					0.993	40
0.9888	2	2 4 1					0.991	30
0.9880	2	-2 4 2						
0.9850	2	-2 2 9						
0.9563	2	4 1 7+						
0.9457	3	0 3 8+						
0.9444	3	-5 2 6+						
0.9422	3	-3 3 7+						

Table 15: (continued). Calculated pattern for αUTe_3 (left) and the observed (27-929 and 21-1403).

11.2 βUTe_3 and $\text{UTe}_{3.4}$

Slovyanskikh et al.[27] reported a crude powder pattern for a material with 77% Te. Later, Breeze et al.[3] reported a phase with the composition $\text{UTe}_{3.38}$ as being tetragonal with cell parameters of $a = 8.703 \text{ \AA}$ and $c = 13.09 \text{ \AA}$ and a powder pattern similar to that of Slovyanskikh et al.[27]. Their powder pattern was abstracted as PDF 24-1369. Suski[32] confirmed this phase reporting lattice parameters of $a = 8.672 \text{ \AA}$ and $c = 13.014 \text{ \AA}$. Recently, Boehme et al.[2] have proven the existence of a $\text{UTe}_{3.4}$ composition and established an improved powder pattern.

Noel and Levet[22] have just published the crystal structure of a phase they call βUTe_3 which has the NdTe_3 structure. Their paper claims to disprove that the $\text{UTe}_{3.38}$ phase exists and asserts that it was probably a mixture of βUTe_3 and free Te. The calculated powder pattern for βUTe_3 shown in Table 16, shows reasonable agreement with the older published patterns and quite a lot of similarity with the higher quality pattern of Boehme et al.[2] for $\text{UTe}_{3.4}$. Note that the cells for the three patterns listed in Table 16 differ, producing different hkl 's. The calculated UTe_3 pattern is based on the Noel and Levet[22] cell given in Table 1. The PDF 24-1369 pattern is for $\text{UTe}_{3.38}$ based on the tetragonal cell of Slovyanskikh et al.[27] with $a = 8.703 \text{ \AA}$ and $c = 13.086 \text{ \AA}$. The orthorhombic pattern for UTe_3 of Boehme et al.[2] was indexed with $a = 6.382 \text{ \AA}$ $b = 6.475 \text{ \AA}$ and $c = 12.408 \text{ \AA}$.

We do not believe the work of Noel and Levet is sufficient to prove that

a cation deficient compound does not exist. In fact, if the UTe_3 compound were the correct phase in the recent accurate diffraction work, then free tellurium should have been observed. The most reasonable explanation of the experimental observations is that the structure of βUTe_3 allows a range of uranium deficiencies covering the range from 3.0 to at least 3.4 Te.

UTe _{3.4}		Boehme et al.[2]		UTe _{3.38}		24-1369		UTe ₃		Calculated
d	I ^{rel}	hkl		d	I ^{rel}	hkl		d	I ^{rel}	hkl
12.426	17	0 0 1						12.379	11	0 2 0
6.484	<1	0 1 0								
6.202	30	0 0 2						6.189	15	0 4 0
				5.19	40	1 0 2				
4.271	<1	1 1 1						4.266	10	0 2 1
4.138	<1	0 0 3						4.126	1	0 6 0
3.470	2	1 0 3								
3.196	9	2 0 0						3.186	33	1 1 1
3.102	100	0 0 4		3.07	100	2 2 0		3.095	42	0 8 0
3.056	18	1 1 3						3.055	10	0 6 1
								2.994	100	1 3 1
2.886	49	1 2 0		2.877	100	1 1 4				
2.835	1	2 0 2								
2.802	<1	0 1 4								
2.791	<1	1 0 4						2.791	16	1 7 0
2.617	43	1 2 2		2.608	100	2 0 4				
2.318	10	0 1 5		2.319	40	3 1 3				
2.177	16	1 1 5		2.172	60	4 0 0		2.174	7	0 10 1
2.125	<1	0 3 1						2.133	3	2 4 0
2.067	10	0 0 6		2.054	40	4 0 2		2.063	4	0 12 0

Table 16: Observed patterns for UTe_{3.4} Boehme et al. and UTe_{3.38} (24-1369), and the calculated pattern for β UTe₃.

UTe _{3.4}		Boehme et al.[2]		UTe _{3.38}		24-1369		UTe ₃		Calculated
d	I ^{rel}	hkl		d	I ^{rel}	hkl		d	I ^{rel}	hkl
2.013	<1	3 0 2						2.017	1	1 11 0
				1.811	30	4 0 4				
1.772	7	0 0 7		1.775	60	4 2 3		1.768	3	0 14 0
1.619	2	0 4 0		1.615	40	5 0 3				
				1.537	50	4 4 0				
1.469	<1	1 1 8		1.495	30	4 4 2		1.465	4	0 16 1
1.378	4	0 0 9		1.375	50	6 2 0		1.380	15	3 5 1
				1.356	40	5 3 4				
1.327	3	1 4 5		1.325	50	6 0 4		1.326	11	11 7 1
1.319	7	1 1 9						1.316	1	0 18 1
1.283	1	4 3 0						1.281	4	1 15 2
1.227	<1	5 1 2								
1.175	<1	1 4 7								
1.162	<1	0 3 9						1.167	2	2 8 3
1.128	2	0 0 11						1.125	2	0 22 0
1.102	<1	3 5 1						1.107	1	1 21 1
1.090	<1	3 2 9						1.092	1	0 22 1
1.034	<1	0 0 12						1.032	1	0 24 0
1.019	<1	2 6 1						1.020	5	1 21 2

Table 16: (Continued). Observed patterns for UTe_{3.4} Boehme et al. and UTe_{3.38} (24-1369), and the calculated pattern for β UTe₃.

12 UTe₅

The highest percentage of tellurium in a uranium telluride has been reported by Slovyanskikh et al.[27] as UTe₅. It has been confirmed by Noel[20] and his powder pattern has been abstracted as PDF 36-1291. In 1985 Noel[21] published the crystal structure of this phase which is of a new type. The crystal structure information is given in Tables 1 and 3. This model was used to compute the powder pattern shown in Table 17. The recently reported experimental pattern of Boehme et al.[2] is included. The new pattern reports a number of weak reflections that calculate but were not previously reported.

Calculated			36-1291		Boehme et al.	
d	I ^{rel}	hkl	d	I ^{rel}	d	I ^{rel}
8.958	12	2 0 0	8.952	5	8.959	13
6.789	100	2 1 0	6.800	40	6.809	40
5.203	18	0 2 0	5.215	10	5.211	22
4.499	1	2 2 0			4.502	1
4.108	3	1 0 1			4.180	1
		4 1 0			4.117	3
3.911	5	0 1 1			3.918	3
3.821	1	1 1 1				
3.584	8	2 1 1			3.591	4
3.446	18	3 0 1	3.447	5	3.451	11
3.272	66	3 1 1	3.269	20	3.275	44
3.235	7	2 3 0				
3.078	69	2 2 1+	3.079	20	3.079	50
2.986	1	6 0 0+				
2.873	75	3 2 1+	2.870	50	2.876	66
2.743	18	4 3 0+	2.743	30	2.747	29
2.680	21	0 3 1+	2.679	5	2.684	14
2.650	22	1 3 1+	2.647	5	2.652	16
2.602	39	0 4 0+				
2.590	73	6 2 0+	2.595	100	2.592	100
2.567	18	2 3 1				
2.498	6	2 4 0	2.498	5	2.503	6
2.445	30	3 3 1+	2.445	15	2.450	23

Table 17: Calculated pattern for UTe₅ (left) and observed, 36-1291 (middle),
Boehme et al. (right).

d	I ^{rel}	Calculated hkl	d	I ^{rel}	Boehme et al. d	I ^{rel}
2.418	14	5 2 1	2.417	5	2.421	10
2.373	24	6 1 1	2.371	10	2.375	19
2.300	5	4 3 1	2.301	2	2.304	3
2.263	6	6 3 0	2.261	5	2.266	5
2.250	3	4 4 0+				
2.198	6	1 4 1+				
2.189	7	8 1 0+	2.187	5	2.191	7
2.150	7	2 4 1	2.151	5	2.154	4
2.146	6	5 3 1				
2.110	1	0 0 2				
2.096	3	1 0 2			2.086	1
2.054	23	1 1 2	2.055	5	2.059	8
2.027	9	2 5 0	2.028	10	2.031	8
2.017	4	7 2 1+				
1.9895	8	3 0 2+	1.985	2	1.989	7
1.9852	10	4 4 1+				
1.9615	5	6 4 0	1.961	5	1.965	7
1.9554	4	0 2 2+				
1.9438	7	1 2 2+	1.943	2	1.946	2
1.8814	15	8 3 0	1.880	30	1.883	14
1.8583	8	3 2 2+	1.855	5	1.853	3
1.8508	7	7 3 1+				

Table 17: (continued). Calculated pattern for UTe₅ (left) and observed, 36-1291 (middle), Boehme et al. (right).

d	I ^{rel}	Calculated hkl	d	I ^{rel}	Boehme et al. d	I ^{rel}
1.8182	9	5 0 2	1.817	2	1.821	2
1.8003	12	9 0 1	1.799	10	1.801	8
1.7937	9	1 3 2+				
1.7817	10	3 5 1	1.782	5	1.786	6
1.7740	7	9 1 1				
1.7655	6	10 1 0	1.763	10	1.767	6
1.7345	8	0 6 0	1.736	20	1.738	9
1.7258	7	3 3 2+				
1.7184	5	8 3 1+				
1.7075	3	6 5 0	1.708	10	1.710	5
1.7029	2	2 6 0				
1.6973	1	8 4 0				
1.6555	3	5 5 1			1.659	1
1.6358	1	6 2 2			1.638	12
1.6287	2	10 1 1				
1.6174	1	4 6 0				
1.6104	5	5 3 2+			1.615	4
1.5979	2	9 3 1+				
1.5918	1	10 3 0+				
1.5828	10	6 5 1			1.585	6
1.5804	9	3 4 2+				
1.5720	2	10 2 1			1.575	2

Table 17: (continued). Calculated pattern for UTe₅ (left) and observed, 36-1291 (middle), Boehme et al. (right).

d	<i>I</i> ^{rel}	Calculated hkl	36-1291 d	<i>I</i> ^{rel}	Boehme et al. d	<i>I</i> ^{rel}
1.5538	6	7 2 2+			1.556	2
1.5493	4	3 6 1+				
1.5194	2	11 0 1			1.520	1
1.5103	5	4 6 1+			1.514	4
1.5035	3	11 1 1+			1.510	2
1.4998	2	6 6 0+				
1.4929	3	12 0 0+			1.494	1
1.4903	3	5 4 2				
1.4805	5	9 4 1				
1.4767	12	1 5 2			1.478	7
1.4738	12	7 3 2+			1.476	6
1.4642	5	5 6 1			1.468	4
1.4585	3	11 2 1				
1.4479	3	9 0 2				
1.4382	2	3 5 2+			1.436	1
1.4339	2	8 5 1				
1.4110	1	4 7 0			1.415	<1
1.4074	1	12 0 1				
1.4022	2	0 7 1+				
1.3949	8	9 2 2+			1.397	3
1.3918	5	11 3 1				
1.3854	1	2 7 1				

Table 17: (continued). Calculated pattern for UTe₅ (left) and observed, 36-1291 (middle), Boehme et al. (right).

d	I ^{rel}	Calculated hkl	36-1291 d	I ^{rel}	Boehme et al. d	I ^{rel}
1.3801	2	7 4 2+				
1.3713	2	12 3 0+			1.371	1
1.3651	4	3 7 1			1.368	2
1.3616	4	9 5 1				
1.3578	8	10 5 0+			1.359	7
1.3540	5	1 2 3				
1.3426	6	2 2 3+			1.345	1
1.3382	4	4 7 1			1.339	1
1.3362	4	9 3 2+			1.334	1
1.3309	2	6 7 0				
1.3241	1	3 2 3				
1.3121	3	11 4 1			1.313	2
1.3074	3	3 6 2+				
1.3042	8	12 3 1+			1.306	12
1.3009	5	0 8 0+			1.304	3
1.2949	1	12 4 0				
1.2925	2	10 5 1				
1.2900	2	2 3 3				
1.2874	2	2 8 0				
1.2837	1	4 6 2				
1.2796	1	14 0 0				
1.2736	3	3 3 3				

Table 17: (continued). Calculated pattern for UTe₅ (left) and observed, 36-1291 (middle), Boehme et al. (right).

d	I^{rel}	Calculated hkl	36-1291 d	I^{rel}	Boehme et al. d	I^{rel}
1.2704	4	13 2 1+			1.271	1
1.2652	5	9 4 2			1.267	2
1.2631	4	6 1 3				
1.2550	3	5 6 2				
1.2516	4	4 3 3+			1.252	1
1.2491	4	9 6 1+				
1.2461	2	10 6 0				
1.2426	1	14 2 0			1.243	1
1.2386	2	8 7 0+				
1.2313	3	2 8 1+			1.216	1

Table 17: (continued). Calculated pattern for UTe_5 (left) and observed, 36-1291 (middle), Boehme et al. (right).

13 Summary and Conclusions

The status of the powder diffraction patterns and structural models for the phases in the uranium tellurium system is:

1. UTe – The cubic structural model is correct. An experimental pattern for this phase is needed. In the interim the calculated 15-865 should be used.
2. U_3Te_4 – The cubic structural model is correct. The calculated pattern represents a considerable improvement over the early Debye-Scherrer pattern with visual intensities and should be adopted as the standard until a modern experimental pattern becomes available. Pattern 12-610 is poor but should be retained until a better one becomes available.
3. U_3Te_4 – The orthorhombic structure of this defect phase needs to be refined in order to establish the locations of the vacancies. No experimental pattern has ever been published.
4. U_2Te_3 (Cubic) – The cubic form has never had a powder pattern published. The reasonable assumptions in our calculated model lead us to recommend the adoption of this pattern as a PDF reference until a proper experimental pattern becomes available.
5. U_2Te_3 (Orthorhombic) – The orthorhombic stibnite structural model is in bad need of refinement against a good powder diffraction pattern, which does not presently exist. The current PDF patterns contain

substantial errors. We recommend the use of our calculated pattern as an improvement over the existing standards; however, this pattern is almost certain to have substantial disagreement with the true powder pattern if one is ever measured. Pattern 34-807 is quite poor but should be retained pending publication of a better one.

6. U_3Te_5 - There is neither a structural model nor a reliable powder diffraction pattern for this phase. A high quality experimental pattern and structure analysis is needed. Patterns 21-1407, 34-766 and 34-896 almost certainly contain substantial errors.
7. U_7Te_{12} - Only poorly measured Debye-Scherrer data is available for this phase. The structural model produces a calculated powder pattern in substantial disagreement with the observed. Both a new experimental pattern and structural refinement are needed here. In the meantime 24-1368 should be retained.
8. $\text{UTe}_{1.78}$ (Orthorhombic) - It is not clear that this Orthorhombic defect UTe_2 structure exists. If it does the calculated powder pattern produced here should be more representative than the PDF pattern reported as U_4Te_7 (21-1404) which we have corrected for some minor errors.
9. $\text{UTe}_{1.78}$ (Tetragonal)- There is no good evidence that the tetragonal phase exists.

10. UTe_2 (Orthorhombic)- The Orthorhombic UTe_2 has a correct crystal structure. Powder pattern 21-1405 contains major errors and should be deleted. Pattern 24-1370 also contains large errors and should be rejected. The calculated pattern is much more representative of this material. The new experimental pattern of Boehme et al. should be used as the reference.
11. UTe_2 (Tetragonal)- The tetragonal reports of UTe_2 do not warrant including this as a real phase.
12. UTe_2 (Cubic)- The recent report of a cubic UTe_2 has substantial problems with the structural model. We recommend that pattern 35-1483 be deleted.
13. $\text{UTe}_{2.5}$ - This is probably the only phase lying between UTe_2 and UTe_3 . There is no structural model to produce a calculated pattern. The published powder pattern (21-1409) contains major errors and should be rejected in favor of the recent pattern by Boehme et al. Patterns 21-1402 and 21-1406 claiming to represent U_3Te_7 and U_3Te_8 should be deleted in that there is no support that these phases exist.
14. αUTe_3 - The proposed crystal structure is correct and the pattern computed here represents a substantial improvement over 21-1403 and 27-929. The recent pattern of Boehme et al. should be used to represent this phase.

15. βUTe_3 – The recent model of Noel is correct and the calculated pattern reported here is the only one available to represent this phase.
16. $\text{UTe}_{3.4}$ – This phase based on the βUTe_3 structure clearly exists and the recent pattern of Boehme et al. should replace 23-1309.
17. UTe_5 – The model of Noel accurately predicts the observed pattern 36-1291 and is therefore correct. The recent pattern of Boehme et al. is most complete and should replace 36-1291.

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