Status Primary QM: Prototyping (P) Pressure/Temperature: Ambient Chemical Formula: Ni0.513 Te
Weight %: Ni19.09 Te80.91 Atomic %: Ni33.91 Te66.09 Compound Name: Nickel Tellurium

Radiation: CuKá1 : 1.5406 d-Spacing: Calculated Intensity: Calculated I/Ic: 10.75

Reference: "THE NICKEL-TELLURIUM SYSTEM". Shchukarev S.A., Apurina M.S. Russ. J. Inorg. Chem. (Engl. Transl.) 5, 1167 (1960). Calculated from LPF using POWD-12++.

SYS: Hexagonal SPGR: P-3m1 (164) AuthCellVol: 67.27 Z: 2
Author's Cell [AuthCell-a: 3.844 AuthCell-c: 5.257 AuthCellVol: 67...] Dcalc: 7.786
Dstruc: 7.77 SS/FOM: F 30.0 = 129(0.006; 34.0) Reference: Ibid.

Space Group: P-3m1 (164) Z: 2 Molecular Weight: 157.71
Crystal Cell [XtlCell-a: 3.844 XtlCell-b: 3.844 XtlCell-c: 5.257 XtlCell.: 90 XtlCell.: 90
XtlCell.: 120 XtlCellVol: 67...] Crystal Data Axial Ratio [c/a: 1.3676]
Reduced Cell [RedCell-a: 3.844 RedCell-b: 3.844 RedCell-c: 5.257 RedCell.: 90 RedCell.: 90
RedCell.: 120 RedCellVol: 67...]

Atomic Coordinates:

Atom	Num	Wyckoff	Symmetry	x	y	z	SOF	ITF	AET
Te	1	2d	3m.	0.33333	0.66666	0.25	1.0		6-b
Ni	2	1b	-3m.	0.0	0.0	0.5	0.013		6-a
Ni	3	1a	-3m.	0.0	0.0	0.0	1.0		6-a

SG Symmetry Operators:

Seq	Operator	Seq	Operator	Seq	Operator	Seq	Operator	Seq	Operator	Seq	Operator
1	x,y,z	3	-y,x-y,z	5	-x+y,-x,z	7	-y,-x,z	9	x,x-y,z	11	-x+y,y,z
2	-x,-y,-z	4	y,-x+y,-z	6	x-y,x,-z	8	y,x,-z	10	-x,-x+y,-z	12	x-y,-y,-z

Pearson: hP3.03 LPF Prototype Structure: Cr0.88 S,hP4,164
Subfile(s): Inorganic, LPF Pattern, Metals & Alloys, Primary Pattern Entry Date: 01/05/2005
Last Modification Date: 01/27/2006

Database Comments: LPF Collection Code: 304964. Sample Preparation: STARTING MATERIALS:Te,Ni. Compound Preparation: powder metallurgical technique. Sample annealed at 1173 K for 6 d in evacuated quartz tube. Unit Cell Data Source: Powder Diffraction.

04-001-7260 (Fixed Slit Intensity) - Cu K1 1.54056Å

2	d(Å)	I	h	k	l	2	d(Å)	I	h	k	l	2	d(Å)	I	h	k	l
16.8512	5.257	68	0	0	1	75.4986	1.2582	6	2	1	0	113.0795	0.9233	2	3	1	0
26.7572	3.329	73	1	0	0	78.0218	1.2237	87m	1	2	1	113.2488	0.9224	1	1	1	5
31.7902	2.8125	999	0	1	1	78.0218	1.2237	m	0	1	4	115.778	0.9094	30m	1	2	4
34.0812	2.6285	99	0	0	2	79.3278	1.2068	41	0	2	3	115.778	0.9094	m	3	1	1
43.8483	2.063	239	0	1	2	85.4875	1.1349	38	1	2	2	117.1671	0.9026	13	2	2	2
47.2527	1.922	259	1	1	0	87.9164	1.1097	26	3	0	0	120.1213	0.8889	14	0	2	5
50.5197	1.8051	13	1	1	1	90.47	1.0849	46m	1	1	4	123.0714	0.8762	2	0	0	6
52.1545	1.7523	2	0	0	3	90.47	1.0849	m	0	3	1	124.3215	0.8711	15	1	3	2
55.1319	1.6645	8	2	0	0	94.2135	1.0514	1	0	0	5	130.5857	0.8479	23m	0	3	4
58.0773	1.5869	133	0	2	1	96.6205	1.0315	3	0	2	4	130.5857	0.8479	m	0	1	6
59.534	1.5515	187m	1	1	2	97.8107	1.0221	56	1	2	3	132.1764	0.8426	1	2	2	3
59.534	1.5515	m	0	1	3	100.3998	1.0026	19	0	1	5	135.4828	0.8323	1	4	0	0
66.4236	1.4063	50	0	2	2	106.5548	0.961	15	2	2	0	139.1337	0.822	12	0	4	1
71.7581	1.3143	18	0	0	4	109.1455	0.9453	1	2	2	1	141.1391	0.8168	24	1	3	3
73.0048	1.2949	3	1	1	3	110.497	0.9375	1	0	3	3	145.39	0.8068	24	1	2	5