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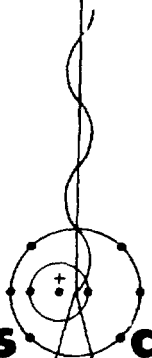
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# Calculated X-Ray Powder Diffraction Patterns of Plutonium

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CALCULATED X-RAY POWDER  
DIFFRACTION PATTERNS OF PLUTONIUM

by

R. B. Roof

ABSTRACT

The X-ray powder diffraction patterns of the six phases of plutonium were calculated for  $\text{Cu K}\alpha_1$  ( $\lambda = 1.540598 \text{ \AA}$ .) The results listed are  $2\theta$ ,  $\sin^2\theta$ ,  $d$  values, integrated intensities, and diffraction indices  $hkl$ .

INTRODUCTION

The metal plutonium is known to exist in six phases. To aid plutonium metallurgists in unravelling complex x-ray diffraction patterns that occur as a result of mechanically and/or thermally induced transformations, it is felt advisable to have diffraction patterns of the individual phases available.

The interplanar spacings and intensities and other relevant information were calculated by use of the ANFC subroutine of the LASL Crystal Structure Code written by A. C. Larson. Space group and atomic position set identification, except where otherwise noted, follows the presentation given in the International Tables for X-ray Crystallography, Vol. I, published for the International Union of Crystallography by the Kynoch Press, Birmingham, England. In the calculations, the atomic scattering factors were corrected for the effects of anomalous dispersion. The scattering factors and anomalous dispersion terms utilized are those given in Vol. IV of the International Tables for X-ray Crystallography. In the absence of any literature values, an isotropic thermal parameter was arbitrarily selected, and applied, so that the calculated pattern may more properly approach one that an investigator would see under the normal conditions of room temperature. A (+) sign following a listed diffraction index is to be interpreted as meaning that there are additional reflections having the same interplanar spacing, but they are not listed in an effort to conserve space.

The references cited are, in the author's subjective opinion, the best with regard to total crystallographic information. Their perusal may lead to others that might be of interest to a particular investigator.

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## Material:

alpha Plutonium

## Structure:

Monoclinic,  $P2_1/m$ , (#11),  $Z = 16$ 

## Atom Positions:

2 Pu in (e)	.345	.250	.162
2 Pu in (e)	.767	.250	.168
2 Pu in (e)	.128	.250	.340
2 Pu in (e)	.657	.250	.457
2 Pu in (e)	.025	.250	.618
2 Pu in (e)	.473	.250	.653
2 Pu in (e)	.328	.250	.926
2 Pu in (e)	.869	.250	.894

## Lattice Constants:

$$a = 6.183 \pm 1 \text{ \AA} \quad c = 10.963 \pm 1$$

$$b = 4.822 \pm 1 \quad \beta = 101.79 \pm 1^\circ$$

## Volume:

$$319.96 \text{ \AA}^3$$

## Density:

$$(\text{calculated})({}^{239}\text{Pu}) \quad 19.846 \text{ g/cm}^3$$

## Thermal Parameters:

Isotropic: plutonium  $B = 0.20$ 

## Scattering Factors:

 $\text{Pu}^0$ , corrected for anomalous dispersion.

## X-ray wavelength for calculated pattern:

1.540598  $\text{\AA}$ . Integrated Intensities

## References:

W.H. Zachariasen and F.H. Ellinger, Acta Cryst. 16, 777-783 (1963).

TWO THETA	SIN $\theta$ THETA	D SPACING	INT.	H	K	L
8.23	.0852	10.7317	.6	0	0	1
14.62	.0162	6.0526	.1	1	0	0
15.25	.0176	5.8037	.1	1	0	-1
16.51	.0206	5.3659	.0	0	0	2
18.23	.0251	4.8638	.2	1	0	1
19.73	.0293	4.4971	.5	1	0	-2
20.17	.0307	4.3988	1.0	0	1	-1
23.57	.0417	3.7718	.3	1	1	0
23.97	.0431	3.7089	1.2	1	1	-1
24.29	.0443	3.6610	.3	1	0	2
24.80	.0461	3.5866	1.9	0	1	2
24.87	.0464	3.5772	.5	0	0	3
26.00	.0506	3.4248	.9	1	1	1
26.20	.0514	3.3987	.0	1	0	-3
27.09	.0549	3.2888	1.1	1	1	-2
28.95	.0625	3.0818	2.2	2	0	-1
29.49	.0648	3.0263	.7	2	0	0
30.67	.0698	2.9158	11.3	1	1	2
30.79	.0705	2.9018	2.3	2	0	-2
31.10	.0719	2.8738	18.7	0	1	-3
31.52	.0738	2.8362	5.5	1	0	3
32.20	.0769	2.7788	43.3	1	1	-3
32.31	.0774	2.7687	21.6	2	0	1
33.37	.0824	2.6829	32.6	0	0	4
33.63	.0837	2.6626	.1	1	0	-4
34.51	.0880	2.5968	4.6	2	1	-1
34.67	.0888	2.5855	47.6	2	0	-3
34.98	.0903	2.5633	3.8	2	1	0

TWO THETA	SIN $\theta$ THETA	D SPACING	INT.	H	K	L
36.10	.0968	2.4863	3.9	2	1	-2
36.73	.0993	2.4447	3.7	1	1	3
36.93	.1003	2.4319	.4	2	0	2
37.26	.1021	2.4110	90.0	0	2	0
37.43	.1029	2.4010	100.0	2	1	1
38.23	.1072	2.3524	.0	0	2	-1
38.36	.1080	2.3445	35.3	0	1	-4
38.60	.1092	2.3308	24.4	1	1	-4
39.39	.1136	2.2858	4.9	1	0	4
39.52	.1143	2.2786	12.7	2	1	-3
40.07	.1174	2.2486	2.6	2	0	-4
40.23	.1183	2.2398	.0	1	2	0
40.48	.1197	2.2265	.0	1	2	-1
41.01	.1227	2.1992	.0	0	2	-2
41.56	.1258	2.1714	6.1	2	1	2
41.64	.1263	2.1672	2.7	1	0	-5
41.78	.1272	2.1602	.1	1	2	1
42.06	.1288	2.1463	.3	0	0	5
42.51	.1314	2.1249	.2	1	2	-2
42.87	.1336	2.1078	.5	2	0	3
43.79	.1391	2.0655	4.8	1	1	4
43.90	.1397	2.0607	1.2	3	0	-1
44.42	.1429	2.0379	.0	2	1	-4
44.60	.1440	2.0308	12.1	3	0	-2
44.80	.1458	2.0175	1.1	3	0	0
44.98	.1463	2.0136	.1	1	2	2
45.32	.1484	1.9993	.2	0	2	3
45.87	.1519	1.9767	.0	1	1	-5

TWO SINSO THETA SPACING INT. H K L			TWO SINSO THETA SPACING INT. H K L			TWO SINSO THETA SPACING INT. H K L							
48.12	.1530	1.9665	.0	1	2	-3	53.50	.2026	1.7113	9.7	2	1	4
48.26	.1523	1.9600	.9	0	1	-5	53.01	.2000	1.7022	.5	1	1	-6
48.57	.1503	1.9087	2.6	2	0	-5	53.91	.2055	1.6994	.9	2	0	-6
48.93	.1505	1.9306	2.2	3	0	-3	54.00	.2009	1.6852	.2	3	1	-8
47.01	.1591	1.9313	1.3	2	1	3	54.69	.2110	1.6770	3.0	0	1	-6
47.49	.1621	1.9131	1.2	3	0	1	55.15	.2103	1.6600	.3	3	1	2
47.73	.1637	1.9001	3.7	1	0	5	55.34	.2156	1.6500	3.7	1	2	4
47.86	.1606	1.8909	1.1	2	2	-1	55.75	.2106	1.6476	.0	3	0	-5
47.97	.1652	1.8909	1.0	3	1	-1	55.07	.2194	1.6400	2.0	2	2	-4
48.22	.1669	1.8857	.4	2	2	0	56.51	.2201	1.6273	.1	1	0	6
48.62	.1695	1.8710	6.2	3	1	-2	56.73	.2257	1.6213	1.7	3	0	3
48.90	.1713	1.8612	4.5	3	1	0	57.10	.2204	1.6110	2.1	1	2	-5
49.09	.1725	1.8500	1.3	2	2	-2	57.00	.2309	1.6031	.4	0	2	-5
49.59	.1750	1.8370	3.2	1	2	3	57.05	.2310	1.6020	2.3	2	1	-6
49.77	.1771	1.8305	6.0	2	0	4	57.97	.2300	1.5896	.1	0	3	-1
50.10	.1793	1.8193	.0	1	0	-6	58.00	.2356	1.5869	.4	2	2	3
50.13	.1795	1.8102	12.7	2	2	1	58.91	.2010	1.5665	1.0	3	2	-1
50.07	.1810	1.8067	3.0	2	1	-5	59.00	.2025	1.5602	.6	1	0	-7
50.72	.1834	1.7986	.2	3	0	-4	59.22	.2001	1.5591	2.1	3	1	-5
50.61	.1841	1.7955	.5	3	1	-3	59.05	.2059	1.5535	.0	1	3	0
50.00	.1805	1.7933	19.9	0	2	4	59.00	.2061	1.5529	10.2	3	2	-2
51.02	.1855	1.7806	2.1	0	0	6	59.64	.2073	1.5490	.1	1	3	-1
51.06	.1850	1.7872	.0	1	2	-0	59.72	.2079	1.5473	.9	3	2	0
51.34	.1876	1.7782	.2	3	1	1	59.92	.2090	1.5425	.1	4	0	-1
51.51	.1800	1.7729	.1	3	0	2	59.95	.2096	1.5419	1.3	1	1	6
51.56	.1892	1.7710	.7	1	1	5	59.99	.2099	1.5400	.1	4	0	-2
51.01	.1900	1.7633	30.5	2	2	-3	60.04	.2503	1.5397	.2	0	3	-2
53.07	.2020	1.7122	.3	2	2	2							

TWO SINSO THETA SPACING INT. H K L			TWO SINSO THETA SPACING INT. H K L			TWO SINSO THETA SPACING INT. H K L							
60.17	.2513	1.5367	.2	3	1	3	61.20	.2592	1.5131	.6	4	0	0
60.32	.2525	1.5331	1.0	0	0	7	61.00	.2606	1.5089	2.0	3	2	-3
60.63	.2500	1.5262	.1	1	3	1	61.01	.2607	1.5006	.3	4	0	-3
60.05	.2560	1.5211	0.4	2	1	5	61.04	.2601	1.4990	1.7	3	0	-6
61.10	.2503	1.5155	2.3	2	2	-5	61.06	.2602	1.4906	1.1	3	2	1
61.19	.2590	1.5136	.1	1	3	-2	61.96	.2550	1.4964	.7	2	0	-7
62.06	.2637	1.4903	3.3	1	3	5	62.06	.2637	1.4903	3.3	1	3	5
62.36	.2600	1.4879	6.0	1	1	-7	62.36	.2600	1.4879	6.0	1	1	-7
63.00	.2730	1.4743	.2	3	0	4	63.00	.2730	1.4743	.2	3	0	4
63.12	.2739	1.4717	1.0	1	3	2	63.12	.2739	1.4717	1.0	1	3	2
63.24	.2709	1.4692	7.0	4	1	-1	63.24	.2709	1.4692	7.0	4	1	-1
63.31	.2730	1.4670	11.7	4	1	-2	63.31	.2730	1.4670	11.7	4	1	-2
63.39	.2760	1.4661	2.5	0	3	-3	63.39	.2760	1.4661	2.5	0	3	-3
63.60	.2700	1.4610	13.0	0	1	7	63.60	.2700	1.4610	13.0	0	1	7
63.79	.2792	1.4579	6.9	2	2	4	63.79	.2792	1.4579	6.9	2	2	4
64.03	.2810	1.4530	6.0	1	3	-3	64.03	.2810	1.4530	6.0	1	3	-3
64.07	.2813	1.4522	.7	1	2	-6	64.07	.2813	1.4522	.7	1	2	-6
64.13	.2819	1.4509	.2	4	0	-4	64.13	.2819	1.4509	.2	4	0	-4
64.09	.2807	1.4437	1.0	4	1	0	64.09	.2807	1.4437	1.0	4	1	0
64.59	.2855	1.4017	.1	3	2	-0	64.59	.2855	1.4017	.1	3	2	-0
64.69	.2862	1.4030	.2	4	1	-3	64.69	.2862	1.4030	.2	4	1	-3
64.06	.2876	1.4035	2.0	0	2	6	64.06	.2876	1.4035	2.0	0	2	6

TMO THETA	SIN80 THETA	0 SPACING	INT.	H	K	L	TMO THETA	SIN80 THETA	0 SPACING	INT.	H	K	L	TMO THETA	SIN80 THETA	0 SPACING	INT.	H	K	L
65.11	.2896	1.8315	15.7	3	1	-6	70.71	.3388	1.3313	1.0	2	0	-8	76.18	.3886	1.2487	.1	4	1	-6
65.23	.2905	1.8292	.7	2	1	-7	70.75	.3351	1.3306	6.7	4	1	2	76.27	.3813	1.2478	.5	4	2	1
65.27	.2909	1.8283	.1	3	2	2	71.19	.3388	1.3234	.5	4	1	-5	76.58	.3839	1.2432	.3	4	2	-4
65.48	.2921	1.8251	.7	2	3	-1	71.53	.3416	1.3188	.8	1	1	-8	76.81	.3859	1.2408	1.2	3	0	-8
65.73	.2945	1.8195	.6	2	3	0	71.73	.3432	1.3188	1.0	1	3	4	77.08	.3882	1.2363	.2	5	0	-2
65.77	.2948	1.8188	.3	1	0	7	71.89	.3486	1.3122	.7	1	2	-7	77.46	.3914	1.2312	2.3	5	0	-1
65.88	.2951	1.8181	.2	2	0	6	71.98	.3458	1.3188	1.0	3	1	-7	77.58	.3918	1.2306	.1	3	3	1
66.24	.2985	1.8098	5.1	3	1	4	72.19	.3478	1.3076	.8	2	3	-4	77.68	.3933	1.2282	.2	1	3	5
66.44	.3001	1.8068	.6	2	3	-2	72.58	.3503	1.3014	1.5	4	0	3	77.88	.3958	1.2256	.6	2	1	7
66.85	.3034	1.7984	.6	1	3	3	72.72	.3515	1.2994	.1	4	2	-1	77.91	.3953	1.2252	.2	5	0	-3
67.02	.3048	1.7953	.4	4	1	1	72.78	.3528	1.2984	.1	4	2	-2	78.18	.3969	1.2228	.3	1	2	7
67.30	.3071	1.7901	17.9	2	3	1	73.09	.3585	1.2937	1.1	0	2	7	78.13	.3971	1.2223	.3	2	2	6
67.34	.3074	1.7894	1.1	4	1	-4	73.15	.3558	1.2928	.1	4	0	-6	78.28	.3984	1.2203	.1	3	0	6
67.36	.3075	1.7898	.9	2	2	-6	73.17	.3553	1.2928	1.5	0	1	8	78.45	.3999	1.2181	.8	1	0	-9
67.62	.3096	1.7843	.5	4	0	2	73.26	.3568	1.2918	.8	1	3	-5	78.62	.4013	1.2168	1.8	1	1	8
67.93	.3121	1.7788	6.6	0	3	4	73.56	.3585	1.2866	.2	0	3	-5	79.04	.4049	1.2105	.4	5	0	8
68.07	.3133	1.7762	8.6	4	0	-5	73.78	.3603	1.2833	.1	2	1	-8	79.25	.4068	1.2078	3.1	2	3	4
68.42	.3161	1.7702	.8	1	0	-8	73.89	.3612	1.2816	.6	4	2	0	79.29	.4071	1.2073	.2	4	0	-7
68.71	.3184	1.7651	2.5	2	3	-3	74.07	.3628	1.2789	.3	4	2	-3	79.43	.4083	1.2055	10.1	8	4	8
68.88	.3198	1.7621	.6	3	0	-7	74.12	.3632	1.2781	.3	2	3	3	79.51	.4085	1.2046	.2	1	3	-6
68.94	.3203	1.7611	.8	1	1	7	74.47	.3661	1.2738	2.0	3	2	-6	79.80	.4114	1.2009	.9	3	1	-4
68.97	.3206	1.7605	.8	2	1	6	74.58	.3671	1.2714	.8	2	2	-7	79.83	.4117	1.2005	.7	4	2	2
69.65	.3261	1.7488	.2	1	2	6	74.86	.3694	1.2674	.5	3	3	-1	79.94	.4127	1.1991	.1	5	0	-4
69.86	.3278	1.7454	1.8	3	2	3	74.87	.3695	1.2672	.4	2	0	7	79.99	.4131	1.1985	.1	3	3	-4
70.09	.3297	1.7415	.1	0	0	8	75.36	.3737	1.2602	1.7	3	3	-2	80.03	.4135	1.1980	.8	8	4	1
70.12	.3308	1.7409	1.3	2	3	2	75.53	.3751	1.2578	.3	3	2	4	80.06	.4137	1.1976	.1	5	1	-2
70.19	.3306	1.7398	1.1	3	0	5	75.58	.3754	1.2571	1.3	3	3	0	80.28	.4149	1.1959	.1	2	0	-9
70.49	.3338	1.7369	.2	2	2	5	75.62	.3758	1.2566	1.1	1	0	8	80.23	.4151	1.1955	1.1	0	3	-6

TMO THETA	SINQ THETA	D SPACING	INT.	H	K	L
80.26	.4154	1.1952	.0	4	2	5
80.44	.4169	1.1930	2.5	5	1	-1
80.48	.4173	1.1924	.0	0	0	9
80.58	.4181	1.1912	1.0	1	2	-8
80.61	.4185	1.1900	.1	3	3	2
80.89	.4208	1.1874	.1	5	1	-3
81.01	.4219	1.1859	.8	3	2	-7
81.25	.4240	1.1830	.0	3	1	6
81.32	.4245	1.1823	.0	1	4	0
81.42	.4254	1.1810	.2	1	1	9
81.48	.4259	1.1803	.0	1	4	-1
81.59	.4268	1.1790	.5	4	1	4
81.81	.4287	1.1764	1.2	5	0	1
81.83	.4289	1.1762	.0	0	4	-2
82.00	.4304	1.1741	.0	5	1	0
82.16	.4318	1.1722	.2	9	2	-0
82.25	.4326	1.1712	2.2	4	1	-7+
82.34	.4334	1.1701	.0	1	4	1
82.55	.4351	1.1677	.0	2	3	-6
82.75	.4369	1.1654	1.4	2	2	-0
82.84	.4376	1.1644	.0	1	4	-2
82.90	.4382	1.1636	.1	5	1	-4
83.15	.4404	1.1607	10.9	5	0	-5+
83.44	.4424	1.1575	.5	0	1	9
84.06	.4483	1.1505	.0	3	3	-5
84.50	.4524	1.1452	2.0	4	2	3
84.56	.4526	1.1450	.0	1	4	2
84.69	.4537	1.1436	.5	1	3	6

TMO THETA	SINQ THETA	D SPACING	INT.	H	K	L
84.75	.4542	1.1429	7.5	2	0	8+
84.80	.4547	1.1424	.0	0	4	-3
84.88	.4554	1.1415	.1	3	3	3
85.00	.4571	1.1393	.2	4	2	-6
85.37	.4597	1.1362	.0	1	4	-3
85.48	.4606	1.1350	3.3	2	3	5
85.68	.4623	1.1329	2.1	3	0	-9
85.71	.4626	1.1325	3.4	4	0	5
85.74	.4629	1.1322	.0	5	0	2
86.09	.4659	1.1285	.1	5	1	-5
86.23	.4671	1.1271	.0	1	0	9
86.49	.4694	1.1243	.7	4	0	-0
86.65	.4708	1.1227	.2	2	4	-1
86.74	.4716	1.1217	.6	2	2	7
86.81	.4722	1.1210	2.0	1	3	-7
86.92	.4731	1.1199	.1	2	4	0
87.32	.4766	1.1158	.0	3	0	7
87.46	.4779	1.1143	.9	1	2	0
87.53	.4784	1.1137	.2	5	0	-6
87.57	.4788	1.1133	.3	2	4	-2
87.60	.4790	1.1129	3.0	4	3	-1
87.66	.4796	1.1123	5.0	4	3	-2
87.68	.4798	1.1121	.1	2	1	8
87.94	.4821	1.1094	6.6	1	4	3+
88.36	.4857	1.1053	2.6	2	4	1
88.60	.4878	1.1029	2.0	3	1	-9
88.62	.4880	1.1027	.2	3	2	-0

TMO THETA	SINQ THETA	D SPACING	INT.	H	K	L
88.64	.4881	1.1025	.9	4	1	5
88.67	.4880	1.1022	3.0	5	1	2
88.72	.4888	1.1017	.4	4	4	3
88.89	.4903	1.1001	.1	5	2	-2
88.90	.4904	1.1000	.1	4	3	-3
88.94	.4907	1.0996	4.3	0	4	-4
89.08	.4920	1.0982	.0	1	4	-4
89.16	.4926	1.0975	.3	1	1	9
89.25	.4935	1.0965	3.3	5	2	-1
89.28	.4937	1.0963	7.0	3	3	-6
89.32	.4941	1.0959	2.7	1	0	-10
89.39	.4946	1.0952	.3	2	3	-7
89.42	.4949	1.0949	.4	4	1	-8
89.66	.4971	1.0926	6.0	2	4	-3
89.70	.4974	1.0922	.3	5	2	-3
90.06	.5005	1.0880	.1	3	2	6
90.23	.5020	1.0872	.0	1	2	-9
90.25	.5021	1.0870	.2	3	1	7
90.31	.5027	1.0865	2.4	3	3	4
90.39	.5034	1.0857	.1	4	2	4
90.45	.5039	1.0851	.6	5	1	-6
90.61	.5053	1.0836	.2	2	0	-10
90.80	.5070	1.0818	.7	5	2	0
90.80	.5073	1.0815	.1	5	0	3
90.99	.5086	1.0801	.1	2	4	2
91.02	.5089	1.0798	.2	4	3	1
91.05	.5092	1.0795	.2	4	2	-7
91.32	.5115	1.0770	.5	4	3	-6

TWO SINSO D				TWO SINSO D				TWO SINSO D			
THETA	SPACING	INT.	H K L	THETA	SPACING	INT.	H K L	THETA	SPACING	INT.	H K L
91.69	.5100	1.0736	.1 5 2 -4	96.47	.5563	1.0327	10.4 2 2 0	99.75	.5047	1.0074	.1 4 3 -6
91.74	.5152	1.0732	.0 0 0 10	96.77	.5509	1.0304	.2 6 0 -2	99.03	.5053	1.0060	2.4 5 0 -0+
91.95	.5170	1.0713	.2 2 2 -0	96.02	.5594	1.0299	.9 0 3 0	100.00	.5075	1.0069	.5 5 1 4+
92.22	.5194	1.0600	.0 0 2 9	96.06	.5597	1.0296	.7 4 1 6	100.11	.5070	1.0007	.0 6 1 -3
92.25	.5196	1.0606	1.1 1 1 -10	96.92	.5602	1.0291	.3 3 3 5	100.44	.5006	1.0023	.2 3 1 0
92.51	.5219	1.0663	.9 1 4 4	97.13	.5620	1.0275	.0 5 0 4	100.53	.5914	1.0017	1.1 6 1 -1
92.00	.5205	1.0637	.0 1 3 7	97.15	.5623	1.0273	.1 6 0 -3	100.57	.5917	1.0014	.1 3 4 -4
92.04	.5207	1.0634	.0 2 3 6	97.00	.5644	1.0254	3.5 3 2 -0+	100.01	.5930	.9996	.0 0 0 4-6
92.04	.5207	1.0624	.5 2 4 -4	97.42	.5646	1.0252	.7 2 4 -5	100.07	.5943	.9992	.0 1 1 10
93.06	.5267	1.0614	.2 5 0 -7	97.43	.5647	1.0251	5.6 4 2 5	101.09	.5961	.9977	4.7 1 2 -10
93.53	.5300	1.0573	3.5 5 2 1+	97.46	.5649	1.0240	.0 5 2 2	101.20	.5971	.9969	.0 3 4 2
93.76	.5320	1.0553	.6 5 1 3	97.40	.5651	1.0247	.2 3 0 0	101.37	.5905	.9957	.0 1 0 -11
93.92	.5302	1.0539	.0 4 0 6	97.57	.5659	1.0240	.0 6 0 -1	101.44	.5992	.9951	.4 2 3 7
93.97	.5306	1.0535	.6 1 4 -5	97.60	.5669	1.0231	.7 3 4 -3	101.53	.5999	.9945	.0 6 0 -5
94.26	.5371	1.0511	.1 0 4 5	97.77	.5676	1.0224	.0 4 1 -9	101.71	.6015	.9932	.5 6 1 -0
94.51	.5393	1.0489	3.5 4 3 2	97.90	.5687	1.0214	.0 1 0 10	102.10	.6055	.9900	.9 1 3 0
94.67	.5407	1.0475	.0 0 1 10	97.95	.5692	1.0210	.0 1 2 9	102.25	.6061	.9895	.1 2 0 -11
94.00	.5419	1.0460	.1 2 4 3	98.10	.5704	1.0199	.4 3 4 1	102.40	.6070	.9880	.4 2 2 -10
94.03	.5421	1.0462	.4 4 0 -9	98.22	.5715	1.0189	1.2 4 2 -4	102.55	.6006	.9874	.1 6 1 0
94.07	.5425	1.0458	11.9 5 2 -5	98.20	.5720	1.0185	1.1 1 4 5	102.64	.6094	.9860	.1 5 2 3
94.03	.5430	1.0454	.2 4 3 -5	98.57	.5745	1.0163	1.7 3 1 -10	102.79	.6107	.9857	.1 6 0 1
95.25	.5457	1.0427	.4 1 3 -0	98.61	.5740	1.0160	.0 2 1 9	102.01	.6109	.9856	1.0 5 1 -0
95.51	.5400	1.0405	.3 3 4 -1	98.70	.5759	1.0150	.1 6 0 -4	103.15	.6130	.9832	.0 2 4 -6
95.62	.5400	1.0396	.0 3 0 -10	99.06	.5707	1.0126	.0 3 2 7	103.37	.6156	.9810	.0 3 3 -0
95.66	.5493	1.0393	.1 2 0 9	99.21	.5000	1.0115	.3 4 3 3	103.03	.6161	.9813	.2 4 0 7
95.60	.5495	1.0391	.0 3 3 -7	99.26	.5005	1.0110	.3 5 2 -6	103.57	.6173	.9804	1.4 0 2 -10
96.00	.5522	1.0366	3.2 5 1 -7+	99.57	.5031	1.0000	1.3 6 0 0	103.64	.6179	.9800	.1 5 3 -2
96.21	.5501	1.0300	.3 3 4 0	99.72	.5004	1.0076	.3 6 1 -2	104.02	.6211	.9774	1.7 5 3 -1

TWO SINSO D				TWO SINSO D				TWO SINSO D			
THETA	SPACING	INT.	H K L	THETA	SPACING	INT.	H K L	THETA	SPACING	INT.	H K L
104.29	.6234	.9756	1, 1 0 0 11	107.52	.6506	.9550	.2 4 1-10	110.28	.6733	.9368	.5 2 0-7
104.37	.6281	.9751	.8 1 1-11	107.56	.6508	.9588	.3 1 4-7	110.37	.6748	.9383	.0 6 1 2
104.47	.6250	.9748	.2 5 3-3+	107.59	.6511	.9587	.1 3 2-10	110.86	.6788	.9355	.2 6 2-4
104.53	.6254	.9748	.1 6 1-3	107.62	.6514	.9588	.3 2 2 9	110.95	.6788	.9350	.0 6 0-7
104.70	.6269	.9729	.0 3 4-5	107.77	.6526	.9535	.0 5 1 5	111.07	.6798	.9343	3, 1 5 1-9
104.72	.6271	.9728	1, 0 5 0 5	107.96	.6542	.9528	1, 3 1 5 9+	111.12	.6802	.9340	.0 2 1 10
104.85	.6281	.9719	.0 3 3 6	108.02	.6547	.9528	.0 2 0 10	111.18	.6807	.9337	.1 1 0 11
104.93	.6288	.9714	.4 5 2-7	108.13	.6556	.9518	.0 1 5-1	111.26	.6813	.9332	.2 3 4 4
105.02	.6296	.9708	.1 1 3-9	108.38	.6577	.9488	.1 4 4-1	111.38	.6822	.9326	.5 1 5 2
105.19	.6318	.9697	.4 4 3 4	108.45	.6582	.9495	.0 4 4-2	111.58	.6839	.9314	.1 2 3 8
105.26	.6316	.9693	.2 2 1-11	108.47	.6584	.9493	.9 5 3 1	111.63	.6843	.9312	.9 0 5 3
105.35	.6328	.9687	.1 1 4 6	108.49	.6586	.9492	.1 0 5 2	111.74	.6852	.9306	2, 5 6 2 0
105.55	.6348	.9678	.8 3 4 3	108.63	.6597	.9488	.0 6 1-6	112.01	.6874	.9291	.0 5 2-6
105.57	.6342	.9673	.0 6 0-6	108.75	.6608	.9476	.6 0 4 7	112.03	.6875	.9290	.3 4 4 1
105.62	.6344	.9678	.0 5 3 0	108.78	.6618	.9475	.4 6 2-2	112.25	.6893	.9278	2, 2 1 5-3+
105.80	.6362	.9658	.0 6 1 1	109.03	.6631	.9468	.0 1 5 1	112.35	.6902	.9272	.2 4 4-8
105.82	.6363	.9657	.1 4 2 6	109.13	.6639	.9452	.7 3 0 9	112.50	.6928	.9268	1, 7 3 3-9
105.87	.6368	.9653	.5 4 3-7	109.16	.6641	.9452	.1 5 2 4	112.62	.6923	.9258	.8 4 3 5
106.17	.6392	.9635	.1 2 4 5	109.19	.6644	.9451	.3 6 2-3	112.65	.6925	.9256	2, 9 5 3 2
106.46	.6417	.9616	.7 4 1 7	109.53	.6672	.9431	.4 3 2 8	113.16	.6967	.9229	.3 6 0 3
106.59	.6424	.9611	.1 5 3-4	109.55	.6673	.9430	.0 1 5-2	113.18	.6968	.9228	.3 1 3 9
106.63	.6431	.9605	.0 0 5 1	109.57	.6675	.9429	.3 4 4 0	113.47	.6991	.9213	.4 4 3-8
106.76	.6442	.9598	.7 4 2-9	109.62	.6679	.9425	.0 6 2-1	113.63	.7005	.9204	.3 2 5-1
106.81	.6446	.9594	2, 5 2 3-9	109.76	.6698	.9418	.2 4 4-3	113.65	.7006	.9203	.0 1 2-11
106.98	.6468	.9584	.0 3 0-11	109.89	.6701	.9410	.1 5 3-5	113.83	.7028	.9198	.0 6 2-5
107.10	.6478	.9577	.3 0 3 9	109.98	.6708	.9405	.0 1 2 10	113.88	.7024	.9191	.1 5 0 6
107.28	.6485	.9565	.1 6 0 2	110.06	.6715	.9408	.0 3 1-11	113.92	.7028	.9189	.2 2 5 0
107.33	.6489	.9562	1, 4 0 1 11	110.16	.6724	.9394	1, 1 3 4-6	113.96	.7031	.9187	.2 1 4 7



TWO SINGO D				TWO SINGO D				TWO SINGO D												
TWO THETA	SINGO THETA	SPACING	INT.	H	K	L	TWO THETA	SINGO THETA	SPACING	INT.	H	K	L	TWO THETA	SINGO THETA	SPACING	INT.	H	K	L
114.00	.7030	.9185	.2	2	4	6	118.20	.7363	.8977	.0	6	2	6	122.33	.7674	.8793	.0	8	1-12	
114.11	.7043	.9179	.0	6	1	7	118.29	.7370	.8973	.5	5	3	3	122.73	.7703	.8777	.0	2	6	11
114.35	.7062	.9166	.0	1	1	11	118.43	.7380	.8966	.1	0	4	8	122.89	.7715	.8770	1.6	2	5	3+
114.37	.7063	.9166	.2	3	3	7	118.46	.7383	.8965	.6	2	5	2	122.92	.7718	.8768	.0	4	3	9
114.59	.7081	.9154	.7	5	3	6+	118.53	.7388	.8962	1.4	1	1-12+		123.05	.7727	.8763	.4	7	0	-1
114.63	.7083	.9152	.3	4	0	6+	118.93	.7419	.8943	.5	0	12		123.09	.7730	.8761	.0	3	0	10
115.05	.7117	.9131	.3	1	5	3	119.03	.7426	.8939	.4	2	1-12		123.74	.7777	.8735	.3	3	5	-1
115.18	.7137	.9124	.2	6	2	1	119.09	.7431	.8936	1.0	2	4	8	123.75	.7778	.8730	.5	2	4	7
115.25	.7133	.9121	.0	1	0-12		119.19	.7438	.8932	.4	4	1-11		123.87	.7787	.8729	1.8	3	3-10	
115.52	.7150	.9107	7.7	2	5	1	119.32	.7449	.8925	.0	0	3	10	123.89	.7788	.8729	.0	3	1-12	
115.73	.7171	.9096	.0	2	0-12		119.74	.7481	.8906	.0	3	2-11		123.91	.7790	.8728	.0	2	3	9
115.84	.7179	.9091	.5	4	0	2	120.08	.7506	.8891	.3	6	2	2	124.15	.7806	.8710	1.5	6	1	0
115.88	.7182	.9089	.6	4	2	7+	120.28	.7515	.8886	.5	1	5	0	124.17	.7808	.8717	.1	6	2	7
116.16	.7204	.9075	2.9	0	5	4	120.44	.7533	.8875	.1	3	0-12		124.33	.7828	.8711	1.1	3	5	-2
116.31	.7216	.9068	2.0	4	4	5+	120.68	.7551	.8864	.2	6	0	4	124.43	.7827	.8707	.3	1	2	11
116.38	.7222	.9064	1.2	6	1	3	120.71	.7553	.8863	.0	2	5	4	124.50	.7830	.8701	.0	3	5	0
116.50	.7237	.9055	1.0	1	3-10		120.84	.7563	.8857	2.0	5	2	9+	124.62	.7841	.8699	.0	1	4	8
116.66	.7244	.9051	.7	1	4	8	120.89	.7567	.8855	.0	2	2	10	125.05	.7872	.8682	.0	7	1	-3
116.80	.7255	.9044	2.3	0	2-11		121.15	.7586	.8844	1.7	4	4	3	125.10	.7875	.8680	.7	7	1	-2
116.97	.7267	.9036	1.1	2	5	3	121.20	.7590	.8842	.5	5	1-10		125.17	.7880	.8677	.3	5	0	7
117.02	.7271	.9034	.3	4	2-10		121.22	.7592	.8841	.6	6	1	8	125.25	.7886	.8674	.3	6	3	-2
117.12	.7279	.9029	1.3	5	1	6	121.55	.7616	.8826	.0	7	0	3	125.69	.7917	.8657	.2	5	3	4
117.15	.7281	.9027	.6	3	4	7	121.60	.7620	.8824	.6	7	0	-2	125.71	.7918	.8657	.2	7	0	-5
117.28	.7291	.9021	2.0	5	2	5	121.78	.7633	.8817	.2	4	4	6	125.72	.7919	.8656	.0	6	3	-3
117.80	.7335	.8994	.1	5	0-10		121.86	.7639	.8813	.7	4	3	6	125.97	.7937	.8607	.1	7	0	8
117.86	.7336	.8993	.0	6	0	8	121.91	.7643	.8811	.1	1	5	-5	126.05	.7942	.8643	.9	3	4	8+
117.89	.7339	.8992	.2	4	1	8	122.14	.7660	.8801	1.5	3	2	9	126.12	.7948	.8640	.3	3	3	0
118.03	.7350	.8985	1.6	2	3-10		122.25	.7668	.8797	.1	0	5	5	126.23	.7955	.8636	1.2	6	3	-1

TWO THETA	SIN <sup>2</sup> THETA	D SPACING	INT.	H	K	L	TWO THETA	SIN <sup>2</sup> THETA	D SPACING	INT.	H	K	L	TWO THETA	SIN <sup>2</sup> THETA	D SPACING	INT.	H	K	L	
126.28	.7958	.8635	.0	2	1	11	130.07	.8219	.8497	.0	4	0	12	134.02	.8531	.8340	1.9	0	3	11	
126.37	.7965	.8631	.2	5	4	-2+	130.14	.8224	.8494	.7	7	0	-6	135.19	.8547	.8332	.3	4	3	10	
126.45	.7971	.8628	7.7	7	1	-8	130.24	.8230	.8491	.1	5	0	-11	135.29	.8554	.8329	.1	3	2	-12	
126.61	.7982	.8622	2.0	7	1	-1	130.27	.8232	.8489	.2	2	4	-9	135.49	.8566	.8323	.8	3	5	-5	
126.64	.7988	.8621	.2	1	3	16+	130.31	.8234	.8489	.9	6	5	-6	135.52	.8567	.8322	.0	5	3	5	
126.69	.7987	.8619	.0	6	2	3+	130.37	.8239	.8486	.3	6	0	5	135.59	.8572	.8320	.6	6	2	4	
126.83	.7997	.8614	3.3	5	4	-1	130.48	.8244	.8484	1.7	6	1	-9	136.39	.8628	.8296	.5	1	5	6	
126.88	.8001	.8612	.0	3	5	1	130.53	.8249	.8481	.3	7	0	1	136.48	.8626	.8290	13.5	2	4	0	
127.11	.8016	.8603	.1	1	5	5	130.64	.8256	.8478	.0	0	4	9	136.58	.8632	.8291	.0	7	0	-7	
127.20	.8029	.8597	.6	1	0	12	130.81	.8268	.8472	.1	3	5	2	136.67	.8637	.8288	.1	7	2	-3+	
127.39	.8036	.8593	.3	5	4	-3	131.03	.8282	.8464	1.0	1	3	-11	136.69	.8639	.8288	.2	6	3	-6+	
127.51	.8045	.8588	.3	5	2	6	131.06	.8284	.8463	2.1	1	1	12	136.73	.8641	.8287	1.6	7	2	-2	
127.68	.8056	.8582	.6	6	3	-4	131.28	.8296	.8457	.1	6	3	-5	137.14	.8665	.8275	.9	7	0	2	
127.84	.8067	.8576	.1	3	4	6	132.15	.8356	.8427	.3	5	2	-10	137.54	.8689	.8264	3.7	2	5	5	
128.06	.8082	.8568	.0	1	4	-9	132.18	.8357	.8426	.3	6	2	-8+	137.83	.8706	.8256	4.0	3	4	-9+	
128.26	.8096	.8561	.1	4	4	4	132.28	.8364	.8423	0.1	4	1	9	137.88	.8709	.8254	15.9	3	0	-13+	
128.38	.8104	.8557	.1	4	2	8	132.38	.8371	.8419	2.1	5	4	1	137.93	.8712	.8253	.0	5	4	2	
128.40	.8109	.8554	1.4	4	0	9	132.59	.8384	.8413	.4	1	0	-13	138.14	.8728	.8247	.0	2	2	11	
128.72	.8128	.8544	.2	6	3	0	132.89	.8403	.8403	.0	6	3	1	138.36	.8736	.8241	3.7	7	2	-4	
128.79	.8132	.8542	.7	5	4	0	133.38	.8434	.8387	.8	2	5	-6	138.47	.8743	.8238	.2	6	0	-10	
128.84	.8136	.8540	.1	5	1	7	133.47	.8440	.8385	1.2	0	2	-12	138.55	.8748	.8236	1.0	7	2	-1	
129.05	.8158	.8533	4.5	5	3	-8+	133.76	.8458	.8376	1.0	4	3	7	138.61	.8750	.8235	.0	3	2	10	
129.11	.8154	.8531	.2	1	2	-12+	134.01	.8474	.8368	.5	4	1	-12	139.05	.8758	.8233	.1	1	4	9	
129.38	.8172	.8521	.2	1	5	-6+	134.09	.8479	.8366	.7	7	1	-6	139.78	.8757	.8232	.0	3	3	-11	
129.67	.8192	.8511	2.8	2	2	-12+	134.19	.8485	.8362	1.1	5	1	-11	139.87	.8777	.8222	1.7	4	4	-8	
129.85	.8204	.8505	.8	4	2	-11	134.22	.8487	.8361	14.6	5	4	-5	139.14	.8782	.8220	.0	6	3	2	
129.94	.8210	.8501	.1	5	4	-4	134.33	.8498	.8358	.3	6	1	5	139.55	.8805	.8209	3.4	1	5	-7	
130.00	.8214	.8499	.1	3	5	-4	134.58	.8505	.8353	.0	7	1	1								

TWO THETA	SINSD THETA	D SPACING	INT.	H	K	L	TWO THETA	SINSD THETA	D SPACING	INT.	H	K	L	TWO THETA	SINSD THETA	D SPACING	INT.	H	K	L
140.16	.8859	.8193	3.2	5	3	9+	145.28	.9118	.8071	3.5	3	5	4	150.63	.9357	.7963	.5	4	0	13
140.23	.8843	.8191	.0	2	3	10	145.68	.9129	.8062	4.0	4	2	9	150.76	.9363	.7961	.0	1	6	-1
140.34	.8849	.8189	.0	3	4	7	145.82	.9136	.8059	.7	2	4	-10	151.17	.9380	.7953	.3	4	3	0
140.66	.8867	.8188	.5	5	4	-6	145.86	.9143	.8056	6.0	7	0	0	151.47	.9393	.7948	.0	0	6	2
140.78	.8874	.8177	3.7	4	5	-1	146.22	.9156	.8050	.2	5	4	3	151.61	.9399	.7946	1.5	7	1	-8
140.87	.8879	.8175	6.3	4	5	-2	146.56	.9172	.8043	.3	4	5	1	151.75	.9404	.7943	1.2	1	2	-13+
141.03	.8887	.8171	.5	7	1	-7	146.70	.9179	.8040	.1	3	1	11	152.26	.9425	.7934	.2	4	4	6
141.28	.8901	.8165	.7	5	2	7	146.81	.9184	.8038	5.1	7	0	3	152.37	.9430	.7933	.6	1	3	-12
141.34	.8904	.8163	7.5	0	5	7	146.86	.9187	.8037	12.0	0	6	0	152.57	.9438	.7929	.0	1	6	1
141.64	.8921	.8156	2.1	7	1	2	147.11	.9198	.8032	.8	4	5	-4	152.61	.9439	.7928	.0	7	1	3
141.70	.8924	.8154	.0	3	0	11	147.52	.9218	.8023	2.8	2	1	12	153.32	.9468	.7917	.9	2	3	-12
141.92	.8936	.8149	.0	3	3	9	147.75	.9228	.8019	1.7	5	0	-12	153.54	.9478	.7913	7.3	0	5	2
141.98	.8939	.8147	.5	7	2	-5	147.89	.9235	.8016	2.5	0	4	-10	153.63	.9480	.7912	.0	4	3	-11+
142.32	.8957	.8139	.3	7	2	0	147.93	.9237	.8015	.1	4	0	10	153.73	.9484	.7910	12.7	5	1	-12
142.41	.8962	.8137	2.7	0	1	13+	147.96	.9238	.8014	.0	0	6	-1	153.95	.9492	.7906	.0	4	1	10
142.45	.8964	.8136	.1	3	1	-13	147.98	.9239	.8014	.1	4	2	-12	154.26	.9500	.7901	1.7	4	4	-9
142.59	.8971	.8133	.6	4	5	0	148.09	.9244	.8012	2.2	7	2	-6	154.49	.9513	.7898	.5	4	5	-5
142.88	.8987	.8126	.1	4	5	-3	148.23	.9251	.8009	.2	5	2	-11	155.24	.9540	.7886	.9	1	5	-8
143.10	.8998	.8120	1.4	6	1	-10	148.42	.9260	.8005	.0	6	2	5	156.15	.9573	.7873	.1	3	4	-10
143.30	.9009	.8116	.0	6	2	-9	148.58	.9263	.8003	2.1	6	3	3	156.28	.9576	.7872	.7	2	4	9
143.52	.9020	.8111	9.7	3	5	-6	148.65	.9270	.8000	1.0	7	2	1	156.29	.9578	.7871	1.8	3	5	-7
143.59	.9024	.8109	7.6	1	4	-10	148.98	.9285	.7994	8.5	6	1	6	156.96	.9601	.7861	.0	6	0	-11
143.70	.9030	.8106	.6	2	5	-7+	149.78	.9321	.7979	2.4	5	3	6	157.28	.9689	.7850	.0	1	1	13
144.09	.9050	.8097	1.7	1	2	12	149.94	.9328	.7976	.0	1	5	7	157.30	.9613	.7857	.7	4	1	-13
144.77	.9084	.8082	.1	6	3	-7	150.01	.9330	.7975	.0	2	5	6	157.81	.9630	.7850	.0	1	6	2
144.99	.9095	.8077	1.0	5	1	8	150.43	.9340	.7967	.0	1	6	0	157.87	.9632	.7849	1.3	5	3	-10
145.15	.9103	.8073	6.8	1	3	11	150.47	.9350	.7966	.0	5	4	-7	157.92	.9633	.7848	1.4	6	3	-8
							150.56	.9354	.7964	.5	1	0	13	158.45	.9651	.7841	.1	0	6	-3

TWO THETA	SINSD THETA	D SPACING	INT.	H	K	L	TWO THETA	SINSD THETA	D SPACING	INT.	H	K	L
158.82	.9653	.7840	.0	7	2	07	169.30	.9913	.7737	15.8	7	3	03 +
159.10	.9672	.7832	1.2	6	4	02	169.53	.9917	.7735	3.7	7	3	02
159.38	.9677	.7830	2.3	4	5	00	169.96	.9923	.7733	2.7	6	0	7
159.57	.9685	.7827	4.0	3	5	5 +	170.03	.9925	.7732	3.1	1	6	3
160.07	.9701	.7821	.5	1	6	03 +	170.41	.9930	.7730	.4	4	5	06
160.16	.9703	.7820	.2	5	0	4	170.68	.9934	.7729	1.0	0	0	03
160.25	.9706	.7819	.8	6	4	03	170.86	.9936	.7728	.1	5	4	00
160.50	.9716	.7815	.1	0	3	12	171.05	.9940	.7728	6.7	3	2	11
161.00	.9726	.7810	1.7	2	5	08 +	172.38	.9956	.7720	.6	2	1	14
161.07	.9730	.7809	35.9	3	2	13	172.63	.9961	.7716	18.1	2	6	1
161.23	.9734	.7808	1.2	3	4	00							
161.35	.9737	.7806	3.3	1	0	14							
161.50	.9742	.7804	2.7	6	4	01							
162.10	.9750	.7790	.7	7	0	09							
162.33	.9764	.7796	1.0	6	2	10							
162.57	.9770	.7793	.0	1	4	10							
164.00	.9806	.7779	1.1	7	0	4							
164.22	.9812	.7777	.6	2	6	01							
165.00	.9830	.7769	.0	3	3	12							
165.23	.9835	.7767	.2	2	6	0							
165.50	.9842	.7764	1.0	6	4	04							
165.83	.9848	.7762	5.4	6	3	4							
166.23	.9856	.7759	.4	6	1	11							
166.84	.9861	.7757	2.7	5	2	0							
167.50	.9883	.7748	1.2	4	5	3							
168.04	.9892	.7745	1.0	2	6	02							
168.66	.9902	.7741	1.1	5	0	9							

Material:

beta Plutonium

Structure:

Monoclinic,  $I2/m$ , ( ),  $Z = 34$

Atom Positions:

2 Pu in	.000	.000	.000
4 Pu in	.146	.000	.387
4 Pu in	.337	.000	.082
4 Pu in	.434	.000	.672
4 Pu in	.500	.220	.000
8 Pu in	.145	.268	.108
8 Pu in	.167	.150	.753

Lattice Constants:

$a = 9.284 \pm 2 \text{ \AA}$      $c = 7.859 \pm 2$   
 $b = 10.463 \pm 2$      $\beta = 92.13 \pm 2^\circ$

Volume:

$762.88 \text{ \AA}^3$

Density:

(calculated) ( $^{239}\text{Pu}$ )  $17.688 \text{ g/cm}^3$

Thermal Parameters:

Isotropic: plutonium  $B = 0.50$

Scattering Factors:

$\text{Pu}^0$ , corrected for anomalous dispersion.

X-ray wavelength for calculated pattern:

$1.540598 \text{ \AA}$ . Integrated Intensities

References:

W.H. Zachariasen and F.H. Ellinger, Acta Cryst. 16, 369-375 (1963).

Space Group  $I2/m$  is not a standard representation in the International Tables for X-ray Crystallography.

Its use is justified by the near orthogonality of  $\beta = 92.13^\circ$ .

Conversion to space group  $C2/m$ , (#12), results in lattice constants of

$a = 11.939 \text{ \AA}$      $c = 9.284$   
 $b = 10.463$      $\beta = 138.87^\circ$

with atom positions

2 Pu in (a)	.000	.000	.000
4 Pu in (i)	.387	.000	.241
4 Pu in (i)	.082	.000	.745
4 Pu in (i)	.672	.000	.238
4 Pu in (h)	.000	.220	.500
8 Pu in (j)	.108	.268	.963
8 Pu in (j)	.753	.150	.586

The listed indices hkl are for space group  $I2/m$ .

2 $\theta$ THETA	SIN $^2$ THETA	D SPACING	INT.	H	K	L
12.74	.0123	6.9417	.2	1	1	0
14.89	.0150	6.2818	.8	0	1	1
14.49	.0159	6.1872	.4	1	0	-1
15.88	.0171	5.8873	.3	1	0	1
16.93	.0217	5.2313	.7	0	2	0
19.12	.0276	4.6388	.8	2	0	0
22.36	.0376	3.9731	.3	1	2	-1
22.63	.0385	3.9268	.8	0	0	2
22.72	.0388	3.9186	.2	1	2	1
23.48	.0414	3.7856	.1	2	1	-1
24.17	.0438	3.6796	2.1	2	1	1
25.35	.0493	3.4788	.7	2	2	0
25.73	.0496	3.4593	.1	1	1	-2
26.36	.0528	3.3778	.8	1	1	2
27.38	.0557	3.2646	.7	1	3	0
27.97	.0584	3.1875	.8	0	3	1
28.88	.0602	3.1485	.1	0	2	2
29.22	.0636	3.0536	3.9	2	0	-2
30.11	.0675	2.9657	3.8	3	1	0
30.34	.0685	2.9437	11.5	2	0	2
30.65	.0698	2.9146	.2	3	0	-1
31.46	.0735	2.8417	.1	3	0	1
33.85	.0848	2.6458	16.8	2	3	-1
33.97	.0853	2.6372	188.0	2	2	-2
34.25	.0867	2.6158	32.1	0	4	0
34.35	.0872	2.6088	41.4	2	3	1
34.95	.0902	2.5654	25.6	2	2	2
35.22	.0915	2.5462	37.7	3	2	-1

TWO SINSO D				TWO SINSO D				TWO SINSO D			
THETA	SPACING	INT.	H K L	THETA	SPACING	INT.	H K L	THETA	SPACING	INT.	H K L
35.25	.0917	2.5443	13.0 1 0 0 3	46.15	.1536	1.9653	3.6 4 0 2	52.70	.1970	1.7350	1.1 4 0 0
35.31	.0920	2.5396	15.7 0 1 0 3	46.20	.1539	1.9634	.0 0 0 4	52.70	.1975	1.7331	.2 3 5 0
35.50	.0929	2.5267	31.9 1 3 0 2	46.22	.1541	1.9624	1.7 3 0 3	52.80	.1983	1.7297	2.3 2 2 0
35.94	.0952	2.4971	90.0 3 2 1	46.40	.1552	1.9553	.1 2 4 2	53.22	.2006	1.7190	.0 5 2 0
35.96	.0953	2.4954	66.5 1 0 3 1	46.62	.1566	1.9467	.0 3 4 0	54.00	.2067	1.6944	4.9 5 2 1
37.31	.1023	2.4002	15.9 3 1 0 2	47.05	.1593	1.9299	.7 2 3 0	54.15	.2072	1.6923	.0 1 3 0
37.37	.1026	2.4045	23.6 1 4 0 1	47.19	.1602	1.9285	.2 3 4 1	54.27	.2080	1.6889	.6 2 2 4
37.60	.1030	2.3900	19.3 1 4 1	47.75	.1630	1.9032	1.0 1 1 0	54.89	.2096	1.6827	.4 4 1 3
38.66	.1096	2.3270	6.0 3 1 2	47.91	.1609	1.8972	.2 3 2 0	54.50	.2102	1.6802	.1 5 1 0
38.79	.1103	2.3194	9.0 4 0 0	48.03	.1656	1.8920	.3 4 2 2	54.69	.2110	1.6760	3.0 1 6 0
38.89	.1108	2.3139	10.1 3 3 0	48.13	.1663	1.8890	1.7 4 3 0	54.83	.2120	1.6729	.2 1 3 4
39.35	.1133	2.2601	2.4 1 2 0 3	48.17	.1666	1.8874	3.7 2 3 3	54.86	.2122	1.6720	1.0 1 6 1
39.52	.1143	2.2705	5.4 2 4 0	48.50	.1687	1.8757	1.0 1 1 4	55.13	.2181	1.6647	1.0 3 1 0
39.82	.1159	2.2622	7.0 2 1 0 3	48.87	.1711	1.8621	.5 4 3 1	56.10	.2211	1.6301	.0 5 3 0
40.00	.1170	2.2523	6.4 1 2 3	48.93	.1715	1.8601	1.7 2 5 0	56.23	.2221	1.6340	0.6 0 5 3
41.05	.1229	2.1971	10.0 4 1 0 1	49.29	.1739	1.8471	.0 2 5 1	56.26	.2223	1.6330	2.9 5 1 2
41.10	.1232	2.1945	.6 2 1 3	49.50	.1753	1.8398	4.7 4 2 2	56.32	.2227	1.6323	.1 2 6 0
41.44	.1252	2.1770	21.6 0 3 0 2	49.55	.1756	1.8382	1.3 0 2 4	57.13	.2287	1.6109	.2 3 1 4
41.89	.1270	2.1551	2.0 4 1 1	49.57	.1758	1.8374	.0 3 2 3	57.30	.2299	1.6065	.4 3 4 0
42.60	.1320	2.1203	.0 4 2 0	49.71	.1767	1.8327	1.6 2 0 0	57.41	.2307	1.6039	.5 4 4 0
43.17	.1350	2.0937	3.0 0 3 0 3	49.87	.1770	1.8270	.9 5 1 0	57.60	.2324	1.5979	.2 3 5 0
44.34	.1424	2.0413	5.1 1 5 0	49.97	.1784	1.8230	.0 1 4 0 3	57.81	.2336	1.5937	2.2 0 6 2
44.47	.1432	2.0357	.6 3 0 0 3	50.05	.1789	1.8210	3.7 5 0 0 1	58.45	.2384	1.5776	1.1 4 3 0 3
44.59	.1439	2.0304	1.2 4 0 0 2	50.16	.1797	1.8173	.5 1 5 0 2	58.62	.2397	1.5735	.1 3 5 2
44.70	.1451	2.0221	.0 0 5 0 1	50.51	.1820	1.8055	0.2 1 4 3 4	58.71	.2403	1.5712	.0 4 4 2
44.87	.1457	2.0182	.1 3 3 0 2	50.95	.1850	1.7910	.0 5 0 1	58.75	.2406	1.5703	9.0 0 4 4
45.63	.1504	1.9866	1.2 2 4 0 2	51.15	.1863	1.7805	.2 2 0 0	58.77	.2408	1.5690	1.5 3 4 3
46.04	.1529	1.9697	2.0 3 3 2	52.42	.1950	1.7402	5.0 4 1 0 3 4	59.25	.2404	1.5582	.9 1 0 0 5

TMO SINSO THETA SPACING			TMO SINSO THETA SPACING			TMO SINSO THETA SPACING					
INT.	H	K L	INT.	H	K L	INT.	H	K L			
59.46	.2659	1.5533	.1	0	1 -5	63.12	.2739	1.4718	1.1	4	0 4
59.47	.2460	1.5530	.3	2	5 -3	63.26	.2752	1.4698	.1	0	7 -1
59.76	.2482	1.5403	10.6	6	0 0	63.41	.2762	1.4637	1.5	4	2 -4
59.90	.2498	1.5411	8.4	5	0 -3	63.62	.2794	1.4573	.0	6	0 -2
60.06	.2504	1.5393	.9	1	0 5	63.84	.2796	1.4569	3.7	2	1 5
60.39	.2529	1.5317	10.2	4	3 3 +	64.76	.2868	1.4384	3.3	1	6 -3
60.43	.2533	1.5306	4.0	2	5 3	65.06	.2893	1.4322	1.0	0	3 5
60.47	.2535	1.5298	1.0	5	3 -2	65.13	.2897	1.4312	.6	5	2 3
60.60	.2545	1.5268	6.2	4	0 -8	65.22	.2904	1.4298	.7	1	6 3
60.99	.2575	1.5100	6.2	3	3 -4	65.60	.2935	1.4219	.0	3	0 -5
61.93	.2578	1.5170	.5	4	5 1	65.66	.2939	1.4209	.9	1	5 -4 +
61.15	.2588	1.5143	7.4	2	6 -2	65.87	.2956	1.4168	3.6	4	2 4
61.26	.2596	1.5119	1.4	6	1 -1	66.26	.2987	1.4093	.1	1	5 4
61.75	.2634	1.5018	4.0	2	4 -4	66.56	.3011	1.4039	3.2	6	2 -2
61.78	.2636	1.5003	10.0	2	6 2	66.62	.3016	1.4027	.7	2	7 -1
61.96	.2650	1.4954	4.5	3	6 -1	66.79	.3029	1.3995	.3	6	3 -1
62.05	.2657	1.4945	17.0	5	0 -1 +	66.92	.3040	1.3971	.0	2	7 1
62.10	.2661	1.4934	17.1	1	2 -5	67.10	.3054	1.3938	.4	4	6 0
62.20	.2668	1.4912	.6	6	1 1	67.40	.3078	1.3883	.0	5	5 0
62.28	.2674	1.4895	2.4	2	1 -5	67.64	.3097	1.3841	2.4	1	7 -2
62.35	.2680	1.4880	7.4	5	0 3	67.69	.3102	1.3830	.5	6	3 1
62.43	.2686	1.4863	12.1	3	6 1	67.77	.3108	1.3817	.0	2	3 -5
62.59	.2699	1.4828	1.2	6	2 0	67.87	.3116	1.3799	.1	3	0 5
62.81	.2715	1.4783	2.9	5	2 -3	67.93	.3122	1.3787	.0	1	7 2
62.83	.2717	1.4778	6.4	5	4 1	68.30	.3151	1.3722	.4	3	2 -5
62.87	.2720	1.4770	16.9	3	3 4 +	68.36	.3156	1.3712	.2	6	2 2
62.93	.2725	1.4757	3.3	1	7 0	68.85	.3196	1.3626	.0	5	1 -4
63.01	.2731	1.4741	3.2	2	4 4	69.26	.3229	1.3556	.0	2	3 5

TMO THETA	SINSO THETA	D SPACING	INT.	H	K L
69.83	.3251	1.3509	.5	4	5 -3
69.83	.3276	1.3458	1.6	3	7 0
70.03	.3293	1.3424	.0	6	1 -3
70.26	.3311	1.3387	1.1	1	4 -5
70.53	.3333	1.3342	2.5	3	2 5
70.72	.3349	1.3311	1.2	6	4 0
70.92	.3366	1.3276	.9	5	4 -3
70.99	.3377	1.3266	.6	1	4 5
71.13	.3383	1.3244	.1	3	6 -3
71.22	.3391	1.3229	1.4	4	6 -2
71.29	.3396	1.3217	.1	4	5 3
71.37	.3403	1.3205	.5	5	5 -2
71.49	.3413	1.3186	13.0	4	4 -4
71.72	.3432	1.3149	2.2	7	0 -1 +
71.80	.3438	1.3137	1.9	5	1 4
71.83	.3441	1.3131	1.5	4	1 -5 +
72.10	.3463	1.3089	.8	0	0 6
72.17	.3469	1.3079	5.2	0	0 0
72.39	.3487	1.3048	.0	4	6 2
72.43	.3490	1.3038	.6	0	6 -4
72.45	.3492	1.3035	.0	3	6 3
72.67	.3511	1.3001	.2	6	1 3
72.74	.3516	1.2990	.1	7	0 1
72.80	.3522	1.2980	.0	0	7 3
72.83	.3524	1.2976	2.6	5	5 2
73.11	.3547	1.2933	1.7	5	4 3
73.14	.3550	1.2928	.0	1	1 -6
73.59	.3587	1.2861	.1	3	5 4

TWO SINES D				TWO SINES D				TWO SINES D						
THETA	SIN	THETA	SPACING	THETA	SIN	THETA	SPACING	THETA	SIN	THETA	SPACING	H	K	L
			TNT.				TNT.				TNT.			
73.81	.3606	1.2027	3.1 0 0 0	76.96	.3672	1.2300	.9 5 1 4	82.34	.4333	1.1702	4.0 7 2 3			
74.01	.3623	1.2100	1.0 1 1 6	76.99	.3675	1.2375	.9 4 3 5 +	82.36	.4335	1.1699	.1 7 3 2			
74.04	.3625	1.2794	7.2 3 7 2	77.05	.3679	1.2368	3.5 4 7 1	82.77	.4371	1.1651	1.0 7 0 3			
74.07	.3628	1.2789	.5 1 8 1	77.09	.3683	1.2361	1.6 2 2 0 6	82.87	.4379	1.1648	1.2 5 7 0			
74.09	.3629	1.2766	.5 5 3 0 4	77.25	.3697	1.2340	1.3 6 5 1	82.91	.4383	.1635	2.5 6 2 4 +			
74.22	.3640	1.2767	.0 1 8 1	77.31	.3692	1.2332	.8 7 1 2	82.94	.4385	1.1632	1.5 1 8 3			
74.32	.3649	1.2753	.4 7 2 1	77.81	.3694	1.2265	.1 6 3 3	83.05	.4395	1.1619	2.0 1 6 5			
74.47	.3661	1.2731	3.3 6 4 2	78.10	.3699	1.2227	.2 6 5 1	83.25	.4412	1.1597	.1 8 0 0			
74.53	.3666	1.2722	1.4 2 0 6	78.17	.3675	1.2217	.0 2 5 5	83.35	.4421	1.1505	5.7 4 0 6 +			
74.69	.3688	1.2698	.3 0 2 6	78.20	.3677	1.2214	1.0 5 0 5	83.49	.4433	1.1569	.6 6 6 0			
74.73	.3683	1.2692	.1 4 1 5	78.27	.3683	1.2205	.9 3 4 5 +	83.68	.4450	1.1548	.1 5 6 3			
74.90	.3697	1.2668	2.2 3 7 2	78.80	.4028	1.2136	1.5 2 2 6 +	83.75	.4455	1.1500	4.1 1 6 5			
75.14	.3714	1.2633	1.0 2 6 4	79.12	.4056	1.2095	.1 1 3 6	83.79	.4459	1.1535	2.1 1 9 0			
75.24	.3726	1.2619	.7 6 3 3	79.54	.4092	1.2041	.2 6 2 0 4	83.83	.4463	1.1531	.3 3 3 6			
75.31	.3732	1.2609	.0 7 1 2	79.59	.4096	1.2035	1.0 2 5 5	84.11	.4486	1.1508	.0 0 9 1			
75.32	.3733	1.2607	2.0 7 2 1	79.69	.4105	1.2022	.3 2 8 2	84.22	.4497	1.1487	1.2 4 6 4 +			
75.41	.3741	1.2595	.4 5 6 1	79.82	.4117	1.2006	2.2 7 0 3 +	84.42	.4514	1.1465	.1 8 1 1			
75.46	.3745	1.2588	.0 2 8 0	80.25	.4154	1.1952	.5 2 8 2	84.65	.4534	1.1440	.4 2 4 6			
75.64	.3760	1.2562	1.0 0 5 5	80.40	.4166	1.1935	1.5 7 3 2 +	84.86	.4552	1.1417	1.3 4 7 3			
75.65	.3761	1.2560	2.0 2 7 3	80.41	.4167	1.1932	.3 3 8 1	85.09	.4572	1.1392	1.3 4 8 0			
76.13	.3801	1.2494	.1 5 6 1 +	80.72	.4194	1.1895	.1 5 2 5	85.27	.4588	1.1373	2.9 7 2 3			
76.19	.3806	1.2495	6.0 6 4 2	80.84	.4204	1.1891	.6 3 8 1	85.34	.4594	1.1365	.5 6 5 3			
76.25	.3812	1.2477	4.0 2 0 6	81.25	.4240	1.1830	1.0 1 7 0 4	85.54	.4611	1.1344	.6 8 1 1			
76.29	.3815	1.2472	.0 2 6 4	81.34	.4247	1.1828	.0 3 1 6	85.74	.4629	1.1322	.9 8 2 0			
76.48	.3831	1.2406	.3 4 7 1	81.72	.4280	1.1775	1.1 5 0 5	85.77	.4631	1.1319	1.8 5 6 3			
76.51	.3834	1.2401	1.8 2 7 3	81.82	.4288	1.1763	.2 1 7 4	85.85	.4638	1.1311	1.2 4 2 6			
76.75	.3854	1.2409	.0 0 0 2	81.94	.4299	1.1766	.3 7 4 1	86.32	.4679	1.1261	1.4 2 4 6			
76.89	.3866	1.2389	1.3 7 3 0	82.30	.4330	1.1706	.0 8 4 6							



TWO THETA	SINSD THETA	D SPACING	INT.	H	K	L
86.34	.4688	1.1259	.7	3	3	6
86.45	.4698	1.1248	1.8	4	6	4
86.53	.4697	1.1239	.5	4	7	3
86.56	.4700	1.1236	1.2	8	8	=2
86.60	.4704	1.1232	.8	5	7	=2
86.69	.4712	1.1222	1.8	4	8	6
86.94	.4733	1.1197	.8	7	5	8
87.00	.4739	1.1198	.1	5	5	4
87.02	.4748	1.1188	.2	1	8	=7
87.04	.4742	1.1186	1.8	4	5	=5+
87.08	.4745	1.1182	.1	6	6	=2
87.14	.4750	1.1177	1.8	2	9	=1
87.24	.4759	1.1166	.3	6	1	=5
87.34	.4768	1.1155	.2	8	1	=7
87.41	.4774	1.1148	.1	2	9	1
87.73	.4802	1.1116	.1	7	1	=4
87.84	.4812	1.1185	.2	6	5	3
87.99	.4825	1.1098	.2	5	7	2+
88.07	.4832	1.1082	.1	1	9	=2
88.22	.4844	1.1067	.1	5	4	=5
88.29	.4851	1.1060	.2	1	5	=6
88.35	.4856	1.1054	.3	1	7	2
88.69	.4886	1.1020	.4	3	6	=5
88.72	.4888	1.1018	.8	3	7	4
88.74	.4890	1.1015	.9	6	6	2
88.78	.4894	1.1011	1.8	8	8	2
88.86	.4901	1.1004	.3	3	8	=3

TWO THETA	SINSD THETA	D SPACING	INT.	H	K	L
88.95	.4908	1.0995	.8	4	8	=2
89.05	.4917	1.0986	2.7	8	2	=2
89.12	.4924	1.0978	.9	1	5	6
89.18	.4928	1.0973	.1	4	2	6
89.40	.4948	1.0951	.8	8	3	=1
89.51	.4957	1.0941	.4	1	2	=7
89.53	.4959	1.0939	1.2	2	1	=7
89.81	.4984	1.0911	.8	7	4	=3+
90.06	.5005	1.0888	.8	4	8	2
90.09	.5008	1.0885	.6	8	8	4
90.11	.5010	1.0883	.1	3	8	3
90.12	.5011	1.0882	.8	3	9	8
90.38	.5033	1.0858	1.6	7	5	=2+
90.48	.5042	1.0848	1.3	1	2	7
90.51	.5044	1.0846	.7	8	3	1
90.60	.5059	1.0838	.8	5	1	=6
90.70	.5061	1.0828	1.8	8	7	5
90.77	.5068	1.0821	1.7	3	6	5
91.27	.5118	1.0775	1.3	8	2	2
91.40	.5123	1.0763	.4	6	1	5
91.47	.5129	1.0756	.8	2	1	7
91.61	.5141	1.0743	.8	7	1	4
91.68	.5147	1.0737	.8	5	4	5
92.14	.5187	1.0696	.1	8	1	=3
92.21	.5193	1.0689	.8	6	3	=5
92.26	.5197	1.0685	.8	6	7	=1
92.31	.5202	1.0680	1.8	8	3	7+

TWO THETA	SINSD THETA	D SPACING	INT.	H	K	L
92.38	.5207	1.0675	.9	3	8	=7
92.70	.5235	1.0646	.4	2	8	=4+
92.73	.5238	1.0643	.1	7	4	3
92.94	.5256	1.0625	2.9	8	9	3
92.96	.5258	1.0623	1.8	5	8	=1
93.10	.5270	1.0611	.5	6	7	1
93.17	.5276	1.0605	2.9	2	7	=5
93.20	.5279	1.0602	.9	8	4	8
93.30	.5288	1.0593	.9	4	4	=6
93.65	.5319	1.0562	.7	5	8	1
93.78	.5330	1.0551	.2	3	5	=6
93.81	.5332	1.0549	.1	2	8	4
94.12	.5359	1.0522	.2	3	9	=2
94.39	.5383	1.0499	2.8	7	6	=1
94.50	.5393	1.0490	.7	2	3	=7
94.56	.5397	1.0485	1.6	2	7	5
94.76	.5415	1.0468	.2	8	6	=6
94.82	.5420	1.0463	.1	8	10	8
94.85	.5422	1.0461	.4	5	1	6
94.86	.5424	1.0459	.8	3	2	=7
94.95	.5432	1.0452	.1	3	9	2
95.30	.5461	1.0423	.1	3	8	7
95.37	.5468	1.0417	.1	7	6	1
95.48	.5477	1.0408	.1	8	1	3
95.66	.5493	1.0393	1.2	5	3	=6
95.69	.5496	1.0391	.1	2	9	=3
96.29	.5508	1.0342	1.3	3	5	6
96.39	.5556	1.0334	.8	6	3	5

TMO THETA	SINQ THETA	D SPACING	INT.	H	K	L	TMO THETA	SINQ THETA	D SPACING	INT.	H	K	L	TMO THETA	SINQ THETA	D SPACING	INT.	H	K	L
96.46	.5562	1.0328	.9	2	3	7	99.70	.5842	1.0078	1.3	9	2	-1	102.87	.6114	.9852	.1	5	9	0
96.49	.5565	1.0326	2.0	4	9	-1	99.86	.5856	1.0066	2.0	5	3	6	102.91	.6117	.9849	.0	6	6	4
96.51	.5567	1.0324	.2	0	4	-2	100.30	.5894	1.0033	1.4	6	7	-3	102.93	.6119	.9848	.5	3	10	-1
96.52	.5568	1.0323	3.6	2	9	3	100.58	.5911	1.0019	.3	8	3	3+	103.08	.6132	.9837	1.4	9	1	2
96.56	.5571	1.0320	.7	7	0	-5	100.52	.5913	1.0018	.2	1	8	-5	103.12	.6135	.9834	2.2	0	3	7
96.60	.5574	1.0317	.6	7	3	4	100.1	.5914	1.0017	.0	9	1	-2	103.24	.6145	.9827	.0	8	0	4
96.65	.5579	1.0313	1.2	0	4	6+	100.78	.5928	1.0004	.9	5	6	-5	103.28	.6149	.9823	3.0	5	8	3
96.70	.5591	1.0302	1.2	1	10	1	100.88	.5944	.9991	1.5	6	2	-6	103.32	.6152	.9821	.1	1	7	-6
96.98	.5608	1.0287	2.7	1	4	-7	100.96	.5951	.9986	2.8	6	0	0+	103.35	.6155	.9819	1.9	3	10	1
97.05	.5610	1.0281	1.1	4	9	1	101.15	.5967	.9972	1.0	5	0	-3	103.38	.6157	.9817	1.6	0	0	8
97.10	.5618	1.0277	2.4	2	6	-6	101.22	.5973	.9967	.5	1	0	5	103.45	.6163	.9812	1.2	6	0	6
97.13	.5620	1.0275	1.0	0	3	-3	101.24	.5974	.9966	.3	1	9	-4+	103.90	.6208	.9777	.1	4	0	4
97.19	.5626	1.0270	.4	9	0	-1	101.88	.5995	.9949	.0	7	0	5	104.02	.6212	.9774	1.5	7	2	5
97.33	.5630	1.0259	.1	9	1	0	101.70	.6014	.9933	2.6	4	0	-4	104.17	.6224	.9764	.0	1	7	6
97.88	.5678	1.0222	.3	3	2	7	101.88	.6023	.9926	.0	1	9	4	104.19	.6225	.9763	.0	5	0	-7
97.96	.5692	1.0210	4.2	1	4	7	101.93	.6034	.9917	4.6	7	7	0	104.25	.6231	.9758	1.2	5	6	5+
98.00	.5694	1.0207	.7	2	10	0	102.00	.6040	.9912	4.0	5	7	4	104.59	.6260	.9736	1.3	2	5	-7
98.07	.5702	1.0201	.4	4	1	-7	102.01	.6041	.9911	.4	4	1	7	104.63	.6263	.9734	.1	6	8	-2
98.36	.5727	1.0179	.8	6	0	-6	102.04	.6043	.9909	.8	4	7	-5	104.89	.6285	.9716	.3	4	7	5
98.45	.5735	1.0172	.7	9	9	1	102.20	.6056	.9898	2.6	2	10	-2	104.91	.6286	.9715	1.7	9	0	-3+
98.71	.5757	1.0152	.1	0	0	-0	102.24	.6060	.9895	.7	6	5	-5	105.33	.6322	.9688	.1	7	6	3
98.75	.5761	1.0149	.2	8	4	2	102.33	.6068	.9889	4.7	7	6	-3	105.41	.6328	.9683	.0	1	1	8+
98.78	.5763	1.0147	.0	2	6	6	102.34	.6069	.9888	.0	0	5	7	105.47	.6334	.9679	.1	7	7	-2
98.87	.5788	1.0125	4.0	7	2	-5	102.38	.6072	.9886	2.9	9	3	0	105.50	.6336	.9677	.2	2	0	-8+
99.10	.5797	1.0117	.1	5	7	-0	102.41	.6074	.9883	1.6	3	4	-7	105.63	.6340	.9668	.4	9	3	-2
99.26	.5805	1.0110	1.3	0	10	2	102.74	.6103	.9861	.0	7	5	-4	105.78	.6368	.9659	.2	5	5	-6
99.38	.5815	1.0102	.0	8	5	-1	102.77	.6105	.9859	.9	2	10	2	105.80	.6362	.9658	1.4	0	2	4
99.52	.5827	1.0091	1.0	6	6	-0	102.85	.6112	.9853	.0	6	7	3	105.82	.6363	.9657	1.0	8	6	0

THO SINSO D			THO SINSO D			THO SINSO D		
THETA	SPACING	INT.	THETA	SPACING	INT.	THETA	SPACING	INT.
M	K	L	M	K	L	M	K	L
105.93	.6372	.9658	109.03	.6631	.9060	112.06	.6942	.9205
105.95	.6374	.9649	109.16	.6641	.9052	113.03	.6956	.9236
106.02	.6380	.9648	109.26	.6649	.9047	113.07	.6959	.9238
106.30	.6404	.9626	109.28	.6651	.9045	113.09	.6961	.9233
106.36	.6404	.9623	109.32	.6655	.9043	113.29	.6977	.9222
106.54	.6423	.9611	109.42	.6663	.9037	113.37	.6980	.9218
106.61	.6429	.9607	109.45	.6665	.9035	113.39	.6985	.9217
106.64	.6432	.9605	109.71	.6686	.9020	113.52	.6996	.9210
106.71	.6430	.9600	109.70	.6692	.9017	113.58	.7000	.9207
106.76	.6442	.9598	110.16	.6723	.9394	113.61	.7002	.9205
107.15	.6474	.9573	110.44	.6746	.9378	113.63	.7005	.9204
107.18	.6477	.9571	110.64	.6762	.9367	113.71	.7011	.9200
107.31	.6487	.9564	110.81	.6776	.9357	113.73	.7012	.9199
107.37	.6493	.9560	110.83	.6778	.9356	113.80	.7020	.9191
107.49	.6503	.9552	111.00	.6793	.9344	113.96	.7030	.9187
107.73	.6523	.9537	111.07	.6830	.9321	114.36	.7063	.9166
107.81	.6530	.9533	111.65	.6845	.9311	114.41	.7066	.9164
108.09	.6553	.9516	111.70	.6849	.9308	114.52	.7074	.9158
108.17	.6559	.9511	111.74	.6852	.9306	114.74	.7093	.9146
108.25	.6565	.9507	111.83	.6859	.9301	114.89	.7105	.9139
108.48	.6585	.9492	111.86	.6862	.9299	114.97	.7110	.9135
108.59	.6594	.9486	111.91	.6866	.9296	115.00	.7113	.9133
108.68	.6602	.9480	112.25	.6894	.9278	115.03	.7116	.9132
108.82	.6613	.9472	112.34	.6901	.9273	115.09	.7120	.9129
108.94	.6623	.9466	112.56	.6918	.9261	115.23	.7132	.9121
108.96	.6625	.9464	112.73	.6932	.9252	115.28	.7135	.9119
108.99	.6627	.9462	112.82	.6939	.9247	115.46	.7150	.9110
109.01	.6629	.9461						

TWO THETA	SIN <sup>2</sup> THETA	D SPACING	INT.	H	K	L	TWO THETA	SIN <sup>2</sup> THETA	D SPACING	INT.	H	K	L	TWO THETA	SIN <sup>2</sup> THETA	D SPACING	INT.	H	K	L	
115.51	.7153	.9108	1.6	9	4	3	119.29	.7046	.8927	.7	5	0	5	123.10	.7730	.8761	.0	2	7	7	
115.56	.7157	.9105	1.1	10	0	2	119.39	.7456	.8922	.0	4	0	8	123.14	.7733	.8759	.8	4	11	1	
115.57	.7158	.9104	.0	3	6	7	119.74	.7480	.8906	.6	9	4	3	123.18	.7736	.8758	.0	2	11	3	
115.83	.7179	.9091	.1	3	11	0	120.05	.7594	.8892	.3	6	1	7	123.26	.7742	.8754	.0	7	7	4	
115.93	.7187	.9086	.2	2	10	4	120.22	.7516	.8885	2.2	5	4	7	123.35	.7749	.8751	.1	5	8	5	
116.14	.7203	.9076	.1	2	4	0	120.38	.7522	.8881	1.1	7	6	5	123.52	.7761	.8744	.6	10	4	0	
116.22	.7209	.9072	1.8	5	10	1	120.36	.7527	.8879	.4	3	11	2	123.62	.7768	.8740	.4	7	9	0	
116.26	.7212	.9070	.1	8	7	1	120.42	.7532	.8876	.9	5	9	4	123.70	.7774	.8737	.1	5	9	4	
116.29	.7215	.9069	1.0	9	5	2	120.51	.7538	.8872	.5	10	3	1	123.74	.7777	.8735	.4	4	9	5	
117.08	.7270	.9030	1.4	5	10	1	120.62	.7547	.8867	.8	8	3	5	123.80	.7782	.8732	.1	4	11	1	
117.14	.7281	.9028	1.2	2	8	6	120.81	.7561	.8859	.8	2	7	7	123.89	.7788	.8728	.2	8	7	3	
117.17	.7283	.9026	1.7	4	2	0	121.02	.7577	.8849	1.8	9	6	1	123.99	.7795	.8725	.8	7	0	7	
117.92	.7341	.8998	.4	4	5	7	121.11	.7583	.8846	1.0	7	3	6	124.08	.7801	.8721	.3	8	2	6	
117.96	.7345	.8998	.0	6	8	4	121.13	.7585	.8805	1.5	8	0	6	124.12	.7805	.8719	1.4	0	12	0	
118.18	.7361	.8978	.1	6	7	5	121.33	.7600	.8836	.1	3	11	2	124.15	.7807	.8718	.9	1	0	9	
118.29	.7370	.8973	.8	0	7	7	121.55	.7616	.8826	.2	10	2	2	124.46	.7829	.8706	.8	9	3	4	
118.35	.7378	.8970	.0	10	2	2	121.72	.7629	.8819	.9	6	9	3	124.61	.7840	.8704	.0	7	8	3	
118.59	.7393	.8959	2.0	9	3	4	121.76	.7632	.8817	.0	10	1	3	124.70	.7847	.8696	.3	0	1	9	4
118.62	.7395	.8957	.5	9	1	4	121.80	.7635	.8816	.2	6	8	4	124.94	.7864	.8686	3.8	1	10	5	
118.69	.7397	.8957	.7	2	4	8	122.15	.7661	.8801	.8	5	7	6	125.18	.7881	.8677	.0	8	8	0	
118.68	.7400	.8955	.0	10	0	2	122.19	.7664	.8799	.1	2	11	3	125.26	.7886	.8674	.8	1	9	6	
118.73	.7403	.8952	.1	7	7	4	122.28	.7670	.8795	1.6	4	2	0	125.31	.7890	.8672	1.0	4	8	6	
118.82	.7410	.8948	.1	3	3	8	122.39	.7678	.8791	3.9	6	6	6	125.40	.7902	.8666	.1	6	10	0	
118.85	.7413	.8947	.3	3	6	7	122.49	.7686	.8786	.6	9	6	1	125.67	.7916	.8658	.4	1	0	9	
118.91	.7417	.8944	.6	10	3	1	122.58	.7692	.8783	.3	5	1	8	125.71	.7919	.8656	.4	5	10	3	
119.08	.7424	.8940	.0	0	11	3	122.80	.7709	.8773	.5	8	6	4	125.79	.7924	.8653	.0	1	10	3	
119.07	.7429	.8937	.2	6	3	7	122.91	.7716	.8769	.7	9	0	5	125.87	.7930	.8650	1.4	0	5	5	
119.11	.7433	.8935	.7	9	5	2	123.01	.7724	.8765	.2	6	7	5								

TWO THETA	SINSD THETA	D SPACING	INT.	H	K	L	TWO THETA	SINSD THETA	D SPACING	INT.	H	K	L	TWO THETA	SINSD THETA	D SPACING	INT.	H	K	L
125.92	.7933	.8648	.2	9	2	5+	129.33	.8169	.8523	.2	8	8	2	132.38	.8365	.8422	1.2	3	9	6
125.98	.7938	.8646	1.0	6	3	7	129.40	.8177	.8519	.3	5	6	7+	132.39	.8371	.8419	.0	11	8	1
126.00	.7942	.8644	.6	7	3	6	129.50	.8180	.8517	1.2	4	8	6	132.57	.8383	.8413	2.0	8	2	6
126.10	.7946	.8641	3.2	7	6	5	129.64	.8190	.8512	.2	8	12	2+	132.66	.8388	.8418	.2	7	8	7
126.28	.7959	.8638	.7	1	9	6	129.65	.8191	.8511	1.3	10	0	0	132.77	.8396	.8407	.0	11	1	0
126.36	.7964	.8632	.2	1	12	1	129.93	.8209	.8502	.2	1	8	7	132.93	.8405	.8402	1.8	10	5	1
126.38	.7965	.8631	3.5	4	10	4	130.00	.8214	.8499	4.3	6	10	2	132.96	.8408	.8401	.1	10	2	4
126.53	.7976	.8625	.1	1	12	1	130.26	.8231	.8490	.6	2	1	9	133.07	.8414	.8398	2.9	8	5	5
126.69	.7987	.8619	.0	3	5	0	130.35	.8237	.8487	.7	9	6	3+	133.30	.8429	.8390	2.9	10	3	3
126.80	.7995	.8615	.0	10	1	3	130.39	.8240	.8486	.1	9	7	0	133.49	.8441	.8384	1.3	2	12	2
127.00	.8012	.8606	.0	7	2	7	130.53	.8249	.8481	.4	3	0	9	133.58	.8447	.8381	2.1	2	3	9
127.06	.8013	.8605	.4	2	1	9	130.70	.8260	.8475	.2	9	5	4	133.64	.8450	.8380	.3	7	5	6
127.15	.8019	.8602	.3	4	9	5	130.71	.8261	.8475	.0	9	0	5	133.66	.8452	.8379	.4	8	4	6
127.21	.8024	.8600	.0	1	2	9+	130.79	.8267	.8472	.6	10	4	2	133.70	.8454	.8378	.0	8	11	3
127.82	.8066	.8577	.8	10	3	3	130.96	.8278	.8467	.7	3	5	8	133.89	.8466	.8372	3.0	3	2	9
127.85	.8068	.8576	.0	7	9	2	131.00	.8280	.8465	.0	8	3	9	134.08	.8478	.8366	.1	9	2	5
128.01	.8079	.8570	3.1	8	7	3	131.02	.8282	.8464	.0	5	11	0	134.12	.8481	.8365	1.9	2	6	8
128.03	.8081	.8569	.1	2	12	0	131.06	.8284	.8463	.9	10	5	1	134.26	.8490	.8360	.4	2	12	2
128.26	.8096	.8561	.6	8	6	4	131.10	.8287	.8462	.3	2	6	0	134.48	.8493	.8353	1.6	3	12	1+
128.32	.8100	.8559	.0	5	10	3	131.21	.8294	.8458	1.8	1	8	7	134.68	.8516	.8347	2.4	9	7	2
128.44	.8108	.8555	.0	8	6	0	131.24	.8296	.8457	.1	6	5	7	135.01	.8536	.8337	1.4	3	10	5
128.52	.8114	.8551	.3	6	6	6	131.35	.8303	.8453	.0	4	7	7	135.07	.8540	.8336	1.9	3	12	1
128.70	.8126	.8545	.3	5	3	0	131.62	.8321	.8445	.4	4	0	0	135.47	.8564	.8324	3.1	9	6	3+
128.79	.8133	.8542	.0	1	2	9	132.04	.8348	.8431	2.7	6	0	8	135.66	.8576	.8318	.5	3	0	9
128.94	.8142	.8537	.0	1	11	4	132.14	.8355	.8427	.3	3	10	4	135.77	.8583	.8315	5.0	3	9	6+
129.19	.8159	.8528	.0	4	10	4	132.21	.8359	.8425	1.6	6	10	2	135.85	.8588	.8312	2.1	11	2	1
129.28	.8166	.8524	.3	0	0	6	132.26	.8362	.8423	.0	8	0	2	136.05	.8600	.8306	2.7	4	11	3+
														136.14	.8605	.8300	1.4	7	2	7+

TMO THETA	SINSO THETA	D SPACING	TMT.	H	K	L	TMO THETA	SINSO THETA	D SPACING	TMT.	H	K	L	TMO THETA	SINSO THETA	D SPACING	TMT.	H	K	L
136.22	.8610	.8301	.7	5	3	8	141.51	.8913	.8159	.8	11	1	2	146.56	.9173	.8003	1.1	6	11	1
136.76	.8642	.8286	.8	4	7	7	141.80	.8929	.8152	9.1	6	0	8 +	146.69	.9179	.8008	.3	2	11	-5
136.81	.8645	.8285	3.7	3	11	-4	141.82	.8930	.8151	.7	3	8	7	147.05	.9196	.8033	2.0	6	8	-6
136.84	.8647	.8284	.5	11	1	-2	141.87	.8933	.8150	.1	10	5	-3	147.21	.9203	.8029	.3	9	8	1
137.09	.8662	.8276	1.2	7	0	7	141.93	.8937	.8148	4.0	7	10	1	147.31	.9208	.8027	.1	9	3	-6
137.14	.8665	.8275	.4	2	3	9	142.13	.8947	.8144	.1	8	9	1	147.46	.9215	.8020	.3	6	4	-8
137.29	.8674	.8271	1.6	1	4	-9 +	142.44	.8963	.8136	2.1	0	11	-5	147.65	.9224	.8020	.8	11	2	-3
137.33	.8676	.8270	.8	3	8	-7	143.00	.8993	.8123	.8	5	5	-8	147.70	.9226	.8019	.3	8	8	-4
137.66	.8696	.8260	.2	9	5	4	143.27	.9007	.8116	2.5	11	0	-3	147.76	.9229	.8018	.4	1	13	0
138.09	.8721	.8249	3.6	11	2	1 +	143.46	.9017	.8112	1.7	4	6	-8	147.79	.9231	.8018	1.9	8	7	-5
138.19	.8727	.8246	1.3	5	11	2	143.76	.9033	.8105	.1	0	4	6	147.82	.9232	.8017	.1	2	10	6
138.27	.8732	.8244	.5	4	1	-9	143.90	.9040	.8102	.8	7	8	-5	147.92	.9237	.8015	.4	3	12	-3
138.30	.8733	.8243	2.3	9	7	2	144.10	.9050	.8097	1.6	10	1	-5	147.95	.9238	.8014	2.9	11	4	-1
138.73	.8758	.8231	.9	1	12	3	144.25	.9058	.8094	7.8	10	4	-4	148.05	.9243	.8012	1.6	7	7	-6 +
139.02	.8774	.8223	1.3	9	1	-6	144.70	.9081	.8083	.8	11	3	-2	148.09	.9244	.8012	.8	4	12	-2
139.17	.8783	.8219	.3	1	4	9	144.81	.9086	.8081	1.6	2	10	-6	148.21	.9250	.8009	.3	7	1	-8
139.30	.8791	.8216	6.6	3	11	4	144.97	.9094	.8077	2.1	9	8	-1	148.33	.9256	.8007	1.7	7	4	7 +
139.34	.8793	.8215	2.8	3	2	9	144.99	.9095	.8077	1.6	6	9	-5	148.75	.9275	.7999	1.8	8	3	-7
139.55	.8805	.8209	.8	6	5	7	145.00	.9100	.8075	.1	6	11	-1	149.05	.9288	.7993	1.2	3	7	-8
139.98	.8829	.8198	.5	11	3	0	145.17	.9104	.8073	.8	0	9	-7	149.21	.9295	.7990	2.2	2	9	-7 +
140.05	.8833	.8196	3.5	1	7	-8	145.26	.9109	.8071	.7	10	6	-2	149.31	.9300	.7988	.2	2	11	5
140.19	.8841	.8192	.8	8	1	-7	145.42	.9117	.8068	1.2	3	4	-9	149.64	.9314	.7982	3.7	2	5	-9
140.26	.8845	.8191	.5	10	6	0	145.66	.9129	.8062	.8	9	4	5	150.25	.9341	.7970	.1	0	12	2
140.35	.8850	.8188	.1	8	9	-1	145.85	.9138	.8058	.8	7	9	-4	150.32	.9344	.7969	.9	0	12	-0
140.39	.8852	.8187	.8	7	10	-1	146.02	.9146	.8055	.1	6	2	8	150.36	.9346	.7968	.8	3	12	3
140.96	.8883	.8173	2.0	0	10	-6	146.05	.9147	.8054	.8	0	5	-9	150.39	.9347	.7967	2.9	11	3	2
141.11	.8892	.8169	.8	10	2	4	146.41	.9165	.8046	1.6	4	3	-9	150.48	.9351	.7966	.8	10	6	2
141.41	.8908	.8162	1.4	4	12	0	146.46	.9167	.8045	.9	4	1	9							



## Material:

 $\gamma$  Plutonium

## Structure:

Orthorhombic, Fddd, (#70), Z = 8

Origin at  $\bar{T}$ .

## Atom Positions:

8 Pu in (a) .125 .125 .125

## Lattice Constants:

a =  $3.1587 \pm 4 \text{ \AA}$ .  
 b =  $5.7682 \pm 4$   
 c =  $10.162 \pm 2$

## Volume:

 $185.15 \text{ \AA}^3$ 

## Density:

(calculated)( $^{239}\text{Pu}$ ) 17.148 g/cm<sup>3</sup>

## Thermal Parameters:

Isotropic: plutonium B = 0.50

## Scattering Factors:

Pu<sup>0</sup>, corrected for anomalous dispersion.

## X-ray wavelength for calculated pattern:

1.540598  $\text{\AA}$ . Integrated Intensities

## References:

W.H. Zachariasen and F.H. Ellinger,  
Acta Cryst. B, 431-433 (1955).

TWO THETA	SIN <sup>2</sup> THETA	D SPACING	D	INT.	H	K	L
33.50	.0831	2.6729	100.0	1 1 1			
35.30	.0919	2.5405	43.0	0 0 4			
35.77	.0943	2.5002	83.0	0 2 2			
42.10	.1290	2.1445	53.0	1 1 3			
56.00	.2210	1.6307	22.2	1 1 5			
56.73	.2257	1.6213	21.4	1 3 1			
61.03	.2609	1.5002	16.7	2 0 2			
62.83	.2717	1.4770	15.6	1 3 3			
63.66	.2782	1.4605	14.9	0 2 6			
64.50	.2853	1.4421	7.1	0 4 0			
67.57	.3092	1.3052	12.4	2 2 0			
70.39	.3322	1.3365	.0	2 2 2			
73.60	.3589	1.2859	9.6	1 1 7			
74.17	.3636	1.2774	9.4	1 3 5			
74.66	.3677	1.2703	4.6	0 0 8			
75.79	.3773	1.2541	8.0	0 4 4			
78.60	.4012	1.2162	16.0	2 2 0			
83.65	.4447	1.1551	6.0	2 0 6			
90.17	.5015	1.0077	5.0	1 3 7			
91.27	.5111	1.0775	5.7	1 5 1			
91.00	.5161	1.0723	.0	2 2 6			
94.00	.5427	1.0456	5.3	1 1 9			
95.30	.5462	1.0423	10.6	2 4 2			
96.55	.5570	1.0321	5.2	1 5 3			
96.76	.5580	1.0300	5.2	3 1 1			
102.10	.6040	.9905	4.9	3 1 3			
103.32	.6152	.9821	.0	2 4 0			
106.97	.6459	.9500	4.0	0 2 10			

TWO THETA	SIN <sup>2</sup> THETA	D SPACING	D	INT.	H	K	L
107.33	.6400	.9562	4.0	1 5 5			
107.83	.6531	.9532	4.0	0 4 0			
109.27	.6650	.9446	4.0	0 6 2			
110.73	.6770	.9362	9.6	2 2 0			
111.76	.6850	.9300	4.0	1 3 9			
113.17	.6967	.9229	4.0	3 1 5			
113.76	.7015	.9197	4.0	3 3 1			
117.00	.7301	.9015	9.0	2 4 6			
119.66	.7475	.8910	5.0	3 3 3			
123.03	.7726	.8764	5.2	1 1 11			
125.01	.7869	.8680	5.3	1 5 7			
120.60	.8125	.8546	5.5	2 0 10			
130.91	.8270	.8460	2.9	0 0 12			
132.01	.8346	.8432	5.0	3 1 7			
132.75	.8390	.8400	5.0	3 3 5			
134.24	.8489	.8361	6.1	0 6 6			
139.44	.8799	.8212	6.7	2 6 0			
140.14	.8830	.8190	.0	2 2 10			
141.00	.8910	.8161	.0	2 4 0			
143.60	.9029	.8107	.0	2 6 2			
146.15	.9152	.8052	7.9	1 3 11			
151.02	.9391	.7940	9.3	1 7 1			
154.56	.9515	.7897	5.2	4 0 0			
160.30	.9707	.7810	13.4	1 5 9			
107.67	.9710	.7810	27.3	2 6 4			
162.66	.9773	.7792	15.2	3 3 7			
165.94	.9850	.7761	10.7	1 7 3			
166.02	.9860	.7754	20.0	3 5 1			



## Material:

delta Plutonium

## Structure:

Cubic,  $Fm\bar{3}m$ , (#225),  $Z = 4$ 

## Atom Positions:

4 Pu in (a) .000 .000 .000

## Lattice Constants:

 $a = 4.6371 \pm 4 \text{ \AA}$ .

## Volume:

99.71  $\text{\AA}^3$ 

## Density:

(calculated)( $^{239}\text{Pu}$ ) 15.921  $\text{g/cm}^3$ 

## Thermal Parameters:

Isotropic: plutonium  $B = 0.75$ 

## Scattering factors:

 $\text{Pu}^0$ , corrected for anomalous dispersion.

## X-ray wavelength for calculated pattern:

1.540598  $\text{\AA}$ . Integrated Intensities

## References:

F.H. Ellinger, J. of Metals, 1256-1259, October (1956).

2 $\theta$ THETA	SIN $^2$ THETA	D SPACING	INT.	H	K	L
33.40	.0020	2.6772	100.0	1	1	1
38.81	.1100	2.3186	49.6	0	0	2
56.85	.2200	1.6395	32.3	0	2	2
66.86	.3035	1.3981	36.5	1	1	3
78.26	.3311	1.3386	10.4	2	2	2
83.28	.4415	1.1593	4.8	0	0	4
92.79	.5243	1.0638	15.0	1	3	3
95.96	.5519	1.0369	14.2	0	2	4
108.94	.6623	.9465	12.7	2	2	4
119.35	.7451	.8920	17.3	1	1	5 +
140.00	.8830	.8197	8.6	0	4	4
150.69	.9650	.7830	61.6	1	3	5
170.69	.9930	.7729	87.0	2	4	4 +

## Material:

delta-prime Plutonium

## Structure:

Tetragonal,  $I4/mmm$ , (#139),  $Z = 2$ 

## Atom Positions:

2 Pu in (a) .000 .000 .000

## Lattice Constants:

$$a = 3.339 \pm 3 \text{ \AA}$$

$$c = 4.446 \pm 7$$

## Volume:

$$49.568 \text{ \AA}^3$$

## Density:

$$(\text{calculated})({}^{239}\text{Pu}) \quad 16.013 \text{ g/cm}^3$$

## Thermal Parameters:

Isotropic: plutonium  $B = 0.75$ 

## Scattering Factors:

 $\text{Pu}^0$ , corrected for anomalous dispersion.

## X-ray wavelength for calculated pattern:

1.540598  $\text{\AA}$ . Integrated Intensities

## References:

 F.H. Ellinger, J. of Metals,  
 1256-1259, October (1956).

TWO THETA	SIN <sup>2</sup> THETA	D SPACING	INT.	H	K	L
33.54	.0832	2.6699	100.0	0	1	1
38.08	.1064	2.3610	35.2	1	1	0
40.55	.1201	2.2230	14.7	0	0	2
54.95	.2129	1.6695	11.6	0	2	0
56.84	.2265	1.6185	20.8	1	1	2
65.90	.2961	1.4155	25.7	1	2	1
69.31	.3234	1.3546	10.9	0	1	3
70.08	.3330	1.3350	10.4	0	2	2
81.06	.4258	1.1805	3.4	2	2	0
87.74	.4803	1.1115	1.4	0	0	4
91.03	.5090	1.0797	5.2	0	3	1
93.69	.5322	1.0559	5.0	1	3	0
94.16	.5363	1.0519	9.9	1	2	3
95.26	.5458	1.0426	4.0	2	2	2
99.99	.5867	1.0056	4.5	1	1	4
107.73	.6523	.9530	8.5	1	3	2
112.73	.6932	.9252	4.2	0	2	4
116.35	.7219	.9066	8.6	2	3	1
119.89	.7492	.8900	4.4	0	3	3
127.40	.8037	.8593	4.7	0	1	5
134.67	.8515	.8347	2.6	0	4	0
144.30	.9061	.8092	6.4	2	2	4
150.41	.9300	.7967	15.1	1	4	1
156.30	.9500	.7870	4.7	3	3	0
157.53	.9620	.7853	19.6	2	3	3
160.60	.9716	.7815	11.3	0	4	2

## Material:

epsilon Plutonium

## Structure:

Cubic,  $I\bar{m}3m$ , (#229),  $Z = 2$ 

## Atom Positions:

2 Pu in (a) .000 .000 .000

## Lattice Constants:

 $a = 3.6361 \pm 4 \text{ \AA}$ 

## Volume:

48.07  $\text{\AA}^3$ 

## Density:

(calculated)( $^{239}\text{Pu}$ ) 16.512  $\text{g/cm}^3$ 

## Thermal Parameters:

Isotropic: plutonium  $B = 1.00$ 

## Scattering Factors:

 $\text{Pu}^0$ , corrected for anomalous dispersion.

## X-ray wavelength for calculated pattern:

1.540598  $\text{\AA}$ . Integrated Intensities

## References:

F.H. Ellinger, J. of Metals, 1256-1259, October (1956).

TWO THETA	SIN $\theta$	D SPACING	INT.	H	K	L
34.87	.8898	2.5711	180.0	0	1	1
50.10	.7795	1.8181	16.9	0	0	2
62.52	.6693	1.4884	32.6	1	1	2
73.62	.5590	1.2856	9.5	0	2	2
84.12	.4488	1.1498	12.9	0	1	3
94.42	.3386	1.0097	3.3	2	2	2
104.97	.2283	.9718	17.2	1	2	3
115.86	.1181	.9098	2.1	0	0	4
126.88	.0078	.8570	13.5	1	1	4+
142.67	.8976	.8131	11.5	0	2	4
167.88	.9873	.7752	31.1	2	3	3